wwPDB X-ray Structure Validation Summary Report (i)

Mar 6, 2026 – 11:39 AM UTC

PDB ID	:	4U55 / pdb_00004u55
Title	:	Crystal structure of Cryptopleurine bound to the yeast 80S ribosome
Authors	:	Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.
Deposited on	:	2014-07-24
Resolution	:	3.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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:

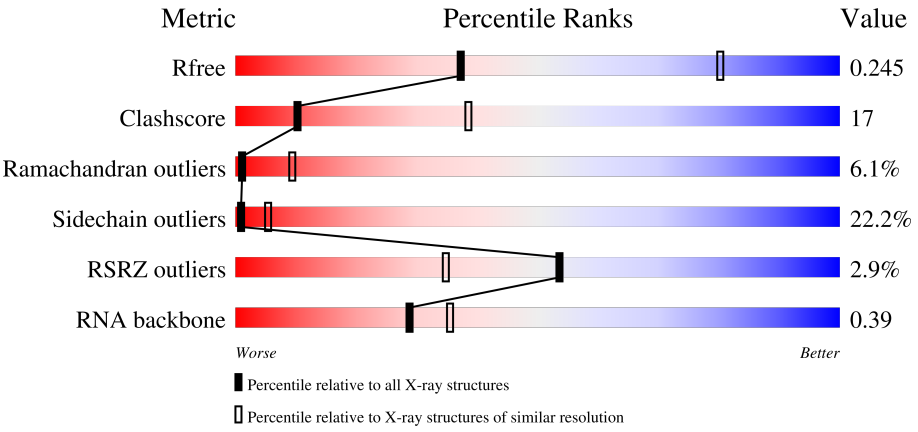
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	1800	3% 35% 45% 17%
1	6	1800	2% 39% 44% 17%
2	S0	251	3% 33% 37% 12% 18%
2	s0	251	4% 31% 35% 14% 18%

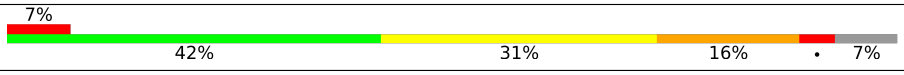
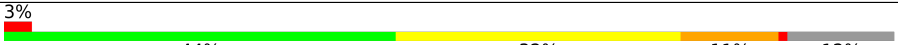
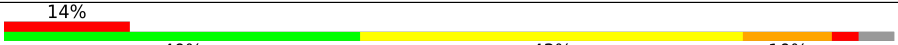
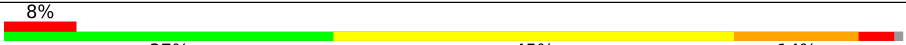
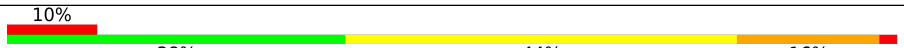
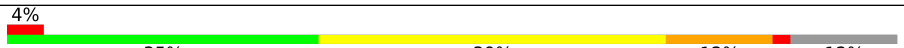
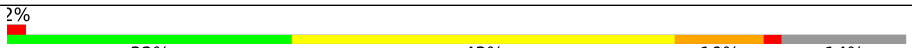
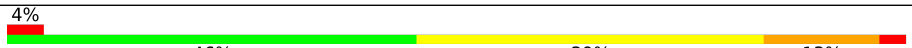
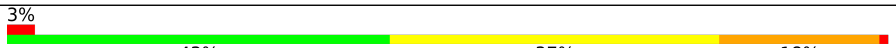
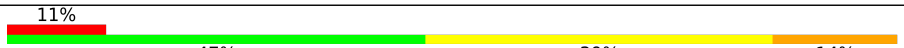
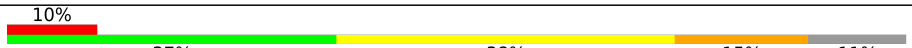
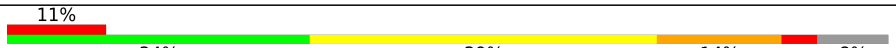
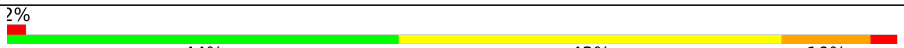
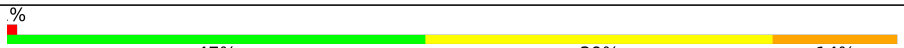
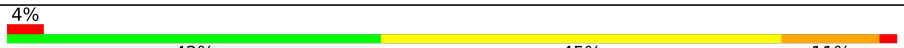
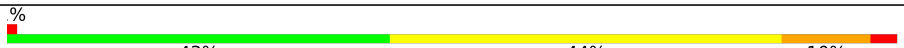
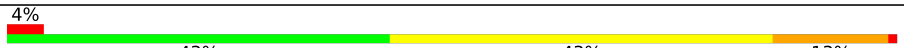
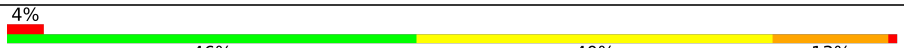
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	S1	254	6% 22% 46% 16% 16%
3	s1	254	3% 37% 37% 10% 15%
4	S2	253	2% 37% 37% 10% 14%
4	s2	253	2% 38% 33% 13% 14%
5	S3	239	5% 49% 31% 11% 7%
5	s3	239	12% 43% 35% 15% 7%
6	S4	260	2% 44% 42% 12%
6	s4	260	2% 48% 36% 14%
7	S5	224	8% 42% 38% 11% 8%
7	s5	224	4% 37% 36% 17% 8%
8	S6	236	13% 47% 41% 8%
8	s6	236	7% 42% 39% 10% 8%
9	S7	189	2% 40% 38% 16%
9	s7	189	3% 48% 36% 14%
10	S8	200	2% 49% 34% 10% 6%
10	s8	200	3% 47% 36% 10% 6%
11	S9	196	8% 44% 33% 15% 6%
11	s9	196	5% 44% 35% 14% 6%
12	C0	105	14% 40% 41% 10% 9%
12	c0	105	16% 33% 41% 16% 9%
13	C1	155	7% 58% 30% 11%
13	c1	155	4% 47% 37% 10% 6%
14	C2	142	4% 39% 38% 9% 13%
14	c2	142	6% 43% 32% 11% 13%
15	C3	150	3% 45% 41% 11%

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	D6	97	10% 37% 40% 12% 10%
28	d6	97	4% 45% 41% 13%
29	D7	81	53% 35% 10%
29	d7	81	51% 35% 14%
30	D8	66	11% 41% 39% 14% 5%
30	d8	66	33% 47% 14% 5%
31	D9	55	4% 45% 38% 13%
31	d9	55	9% 33% 45% 15%
32	E0	60	3% 60% 32% 7%
33	E1	76	8% 30% 34% 20% 9% 7%
33	e1	76	16% 34% 45% 16% 5%
34	SR	318	4% 45% 42% 10%
34	sR	318	5% 51% 43% 6%
35	SM	273	12% 32% 20% 6% 42%
35	sM	273	8% 22% 13% 62%
36	1	3396	40% 41% 11% 7%
36	5	3396	43% 38% 11% 7%
37	3	121	46% 44% 10%
37	7	121	49% 43% 8%
38	4	158	46% 41% 13%
38	8	158	3% 43% 47% 10%
39	L2	253	49% 40% 9%
39	l2	253	43% 43% 12%
40	L3	386	48% 38% 13%
40	l3	386	44% 42% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
41	L4	361	47% 39% 12%
41	l4	361	43% 41% 12%
42	L5	296	46% 42% 11%
42	l5	296	48% 41% 9%
43	L6	175	48% 34% 7% 11%
43	l6	175	48% 34% 7% 10%
44	L7	243	47% 35% 7% 9%
44	l7	243	50% 31% 9% 8%
45	L8	255	47% 34% 11% 9%
45	l8	255	4% 41% 37% 12% 9%
46	L9	191	2% 48% 36% 14%
46	l9	191	39% 39% 20%
47	M0	220	4% 46% 32% 17%
47	m0	220	2% 43% 38% 16%
48	M1	173	45% 40% 10%
48	m1	173	43% 38% 15%
49	M3	198	43% 41% 10%
49	m3	198	40% 46% 11%
50	M4	137	3% 49% 40% 9%
50	m4	137	47% 42% 11%
51	M5	203	52% 34% 14%
51	m5	203	47% 39% 12%
52	M6	198	4% 51% 40% 9%
52	m6	198	2% 51% 36% 12%
53	M7	183	7% 48% 42% 9%

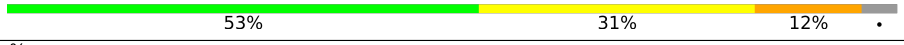
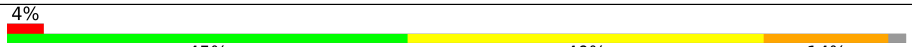
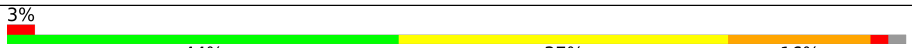
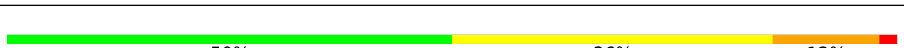
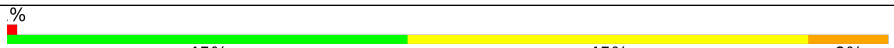
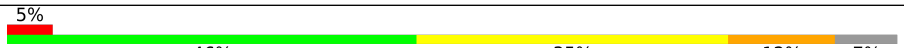
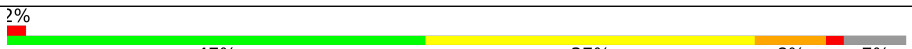
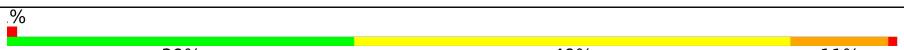
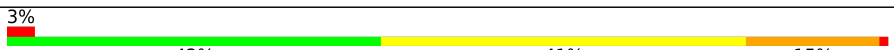
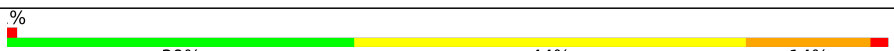
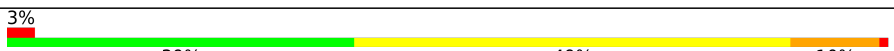
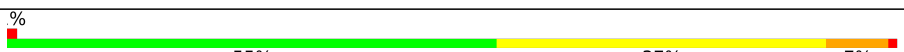
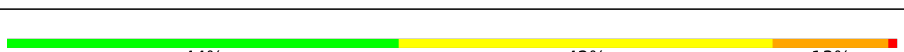
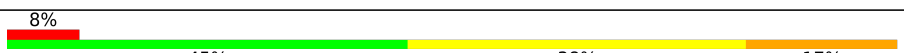
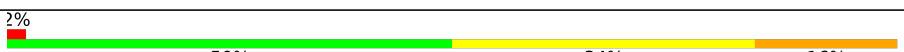
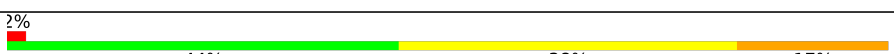
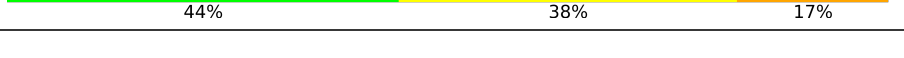
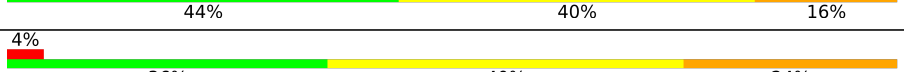
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	m7	183	41% 37% 7% 15%
54	M8	185	52% 37% 10%
54	m8	185	56% 31% 12%
55	M9	188	5% 53% 35% 12%
55	m9	188	2% 55% 35% 10%
56	N0	172	50% 35% 13%
56	n0	172	2% 55% 33% 13%
57	N1	159	59% 28% 13%
57	n1	159	58% 31% 11%
58	N2	120	4% 45% 30% 8% 17%
58	n2	120	2% 33% 35% 12% 18%
59	N3	136	51% 38% 10%
59	n3	136	60% 33% 7%
60	N4	155	6% 41% 19% 37%
60	n4	155	5% 47% 32% 7% 13%
61	N5	141	48% 25% 11% 14%
61	n5	141	35% 38% 10% 15%
62	N6	126	52% 37% 10%
62	n6	126	2% 45% 40% 14%
63	N7	135	45% 36% 18%
63	n7	135	37% 41% 18%
64	N8	148	43% 39% 16%
64	n8	148	45% 35% 19%
65	N9	58	3% 41% 40% 17%
65	n9	58	2% 48% 36% 10% 5%

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
78	q2	105	2% 49% 40% 10%
79	Q3	91	2% 51% 33% 16%
79	q3	91	% 51% 40% 10%
80	e0	62	6% 45% 39% 16%
81	p0	311	% 26% 14% 5% 54%
82	m2	160	81% 12% 6%
83	p1	47	83% 17%
84	p2	46	91% 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	1	3413	-	-	-	X
85	MG	1	3650	-	-	-	X
85	MG	1	3669	-	-	-	X
85	MG	1	3849	-	-	-	X
85	MG	2	1924	-	-	-	X
85	MG	2	1926	-	-	-	X
85	MG	2	1928	-	-	-	X
85	MG	2	1947	-	-	-	X
85	MG	2	1950	-	-	-	X
85	MG	2	1959	-	-	-	X
85	MG	2	1968	-	-	-	X
85	MG	2	1975	-	-	-	X
85	MG	2	2016	-	-	-	X
85	MG	2	2020	-	-	-	X
85	MG	2	2021	-	-	-	X
85	MG	5	3799	-	-	-	X
85	MG	5	3885	-	-	-	X
85	MG	6	1953	-	-	-	X
85	MG	6	2029	-	-	-	X
85	MG	s6	301	-	-	-	X
86	OHX	1	3954	-	-	X	-
86	OHX	1	3968	-	-	X	-
86	OHX	1	3973	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	1	4000	-	-	X	-
86	OHX	1	4025	-	-	X	-
86	OHX	1	4029	-	-	X	-
86	OHX	1	4041	-	-	X	-
86	OHX	1	4042	-	-	X	-
86	OHX	1	4053	-	-	X	-
86	OHX	1	4054	-	-	X	-
86	OHX	1	4079	-	-	X	-
86	OHX	1	4083	-	-	X	-
86	OHX	1	4145	-	-	X	-
86	OHX	1	4149	-	-	X	-
86	OHX	1	4154	-	-	X	-
86	OHX	1	4155	-	-	X	-
86	OHX	1	4162	-	-	X	-
86	OHX	1	4171	-	-	X	-
86	OHX	1	4196	-	-	X	-
86	OHX	2	2031	-	-	X	-
86	OHX	2	2044	-	-	X	-
86	OHX	2	2075	-	-	X	-
86	OHX	2	2089	-	-	X	-
86	OHX	2	2090	-	-	X	-
86	OHX	2	2098	-	-	X	-
86	OHX	2	2131	-	-	X	-
86	OHX	2	2145	-	-	X	-
86	OHX	2	2161	-	-	X	-
86	OHX	5	3944	-	-	X	-
86	OHX	5	3964	-	-	X	-
86	OHX	5	3975	-	-	X	-
86	OHX	5	3980	-	-	X	-
86	OHX	5	4003	-	-	X	-
86	OHX	5	4004	-	-	X	-
86	OHX	5	4013	-	-	X	-
86	OHX	5	4022	-	-	X	-
86	OHX	5	4035	-	-	X	-
86	OHX	5	4037	-	-	X	-
86	OHX	5	4057	-	-	X	-
86	OHX	5	4068	-	-	X	-
86	OHX	5	4083	-	-	X	-
86	OHX	5	4093	-	-	X	-
86	OHX	5	4146	-	-	X	-
86	OHX	5	4191	-	-	X	-
86	OHX	5	4193	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	OHX	5	4200	-	-	X	-
86	OHX	5	4201	-	-	X	-
86	OHX	5	4202	-	-	X	-
86	OHX	5	4205	-	-	X	-
86	OHX	5	4219	-	-	X	-
86	OHX	5	4236	-	-	X	-
86	OHX	5	4240	-	-	X	-
86	OHX	5	4245	-	-	X	-
86	OHX	6	2060	-	-	X	-
86	OHX	6	2121	-	-	X	-
86	OHX	6	2147	-	-	X	-
86	OHX	6	2171	-	-	X	-
86	OHX	7	219	-	-	X	-
86	OHX	7	226	-	-	X	-
86	OHX	8	216	-	-	X	-
86	OHX	8	225	-	-	X	-
86	OHX	8	226	-	-	X	-
86	OHX	O1	201	-	-	X	-
86	OHX	O7	105	-	-	X	-

2 Entry composition (i)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
35	SM	159	Total	C	N	O	0	0	0
			1104	652	221	231			
35	sM	104	Total	C	N	O	0	0	0
			679	402	140	137			

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
81	p0	143	Total	C	N	O	S	0	0	0
			1076	686	192	195	3			

- Molecule 82 is a protein called Unknown protein chain m2.

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

- Molecule 83 is a protein called Unknown protein chain p1.

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

- Molecule 84 is a protein called Unknown protein chain p2.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	2	125	Total 125	Mg 125	0	0
85	S4	1	Total 1	Mg 1	0	0
85	S8	1	Total 1	Mg 1	0	0
85	D0	1	Total 1	Mg 1	0	0
85	D3	1	Total 1	Mg 1	0	0
85	SM	1	Total 1	Mg 1	0	0
85	1	469	Total 469	Mg 469	0	0
85	3	14	Total 14	Mg 14	0	0
85	4	21	Total 21	Mg 21	0	0
85	L2	1	Total 1	Mg 1	0	0
85	L3	3	Total 3	Mg 3	0	0
85	L4	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	L5	2	Total Mg 2 2	0	0
85	L7	3	Total Mg 3 3	0	0
85	L8	1	Total Mg 1 1	0	0
85	M0	3	Total Mg 3 3	0	0
85	M1	1	Total Mg 1 1	0	0
85	M3	3	Total Mg 3 3	0	0
85	M5	1	Total Mg 1 1	0	0
85	M6	1	Total Mg 1 1	0	0
85	M7	5	Total Mg 5 5	0	0
85	M9	1	Total Mg 1 1	0	0
85	N0	1	Total Mg 1 1	0	0
85	N3	2	Total Mg 2 2	0	0
85	N5	1	Total Mg 1 1	0	0
85	N6	2	Total Mg 2 2	0	0
85	N8	5	Total Mg 5 5	0	0
85	O2	1	Total Mg 1 1	0	0
85	O4	1	Total Mg 1 1	0	0
85	O5	1	Total Mg 1 1	0	0
85	O7	3	Total Mg 3 3	0	0
85	Q2	1	Total Mg 1 1	0	0
85	6	148	Total Mg 148 148	0	0

Continued on next page...

Continued from previous page...

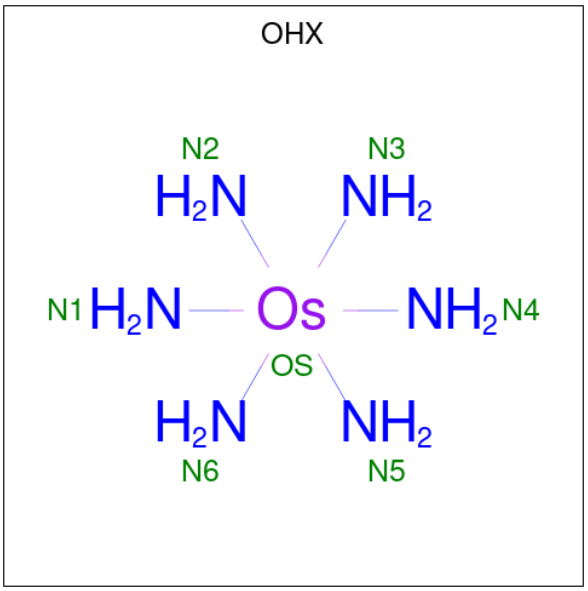
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	s1	1	Total Mg 1 1	0	0
85	s6	1	Total Mg 1 1	0	0
85	s8	2	Total Mg 2 2	0	0
85	c1	1	Total Mg 1 1	0	0
85	c7	1	Total Mg 1 1	0	0
85	c8	1	Total Mg 1 1	0	0
85	c9	1	Total Mg 1 1	0	0
85	d3	1	Total Mg 1 1	0	0
85	d4	1	Total Mg 1 1	0	0
85	d6	1	Total Mg 1 1	0	0
85	sM	2	Total Mg 2 2	0	0
85	5	505	Total Mg 505 505	0	0
85	7	17	Total Mg 17 17	0	0
85	8	14	Total Mg 14 14	0	0
85	l2	1	Total Mg 1 1	0	0
85	l3	1	Total Mg 1 1	0	0
85	l4	1	Total Mg 1 1	0	0
85	l5	2	Total Mg 2 2	0	0
85	l7	1	Total Mg 1 1	0	0
85	l9	1	Total Mg 1 1	0	0
85	m0	1	Total Mg 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	m1	1	Total Mg 1 1	0	0
85	m5	2	Total Mg 2 2	0	0
85	m6	1	Total Mg 1 1	0	0
85	m7	5	Total Mg 5 5	0	0
85	n0	2	Total Mg 2 2	0	0
85	n3	2	Total Mg 2 2	0	0
85	n6	1	Total Mg 1 1	0	0
85	n8	4	Total Mg 4 4	0	0
85	n9	1	Total Mg 1 1	0	0
85	o1	1	Total Mg 1 1	0	0
85	o3	1	Total Mg 1 1	0	0
85	o4	2	Total Mg 2 2	0	0
85	o7	1	Total Mg 1 1	0	0
85	q0	1	Total Mg 1 1	0	0
85	q1	1	Total Mg 1 1	0	0
85	q3	1	Total Mg 1 1	0	0

- Molecule 86 is osmium (III) hexammine (CCD ID: OHX) (formula: $H_{12}N_6Os$).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	2	1	Total 7	N 6	Os 1	0	0
86	S8	1	Total 7	N 6	Os 1	0	0
86	C1	1	Total 7	N 6	Os 1	0	0
86	C3	1	Total 7	N 6	Os 1	0	0
86	C5	1	Total 7	N 6	Os 1	0	0
86	C8	1	Total 7	N 6	Os 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	D9	1	Total 7	N 6	Os 1	0	0
86	SR	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0
86	1	1	Total 7	N 6	Os 1	0	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	L3	1	Total 7	N 6	Os 1	0	0
86	L3	1	Total 7	N 6	Os 1	0	0
86	L3	1	Total 7	N 6	Os 1	0	0
86	L4	1	Total 7	N 6	Os 1	0	0
86	M0	1	Total 7	N 6	Os 1	0	0
86	M5	1	Total 7	N 6	Os 1	0	0
86	M7	1	Total 7	N 6	Os 1	0	0
86	M7	1	Total 7	N 6	Os 1	0	0
86	M8	1	Total 7	N 6	Os 1	0	0
86	M9	1	Total 7	N 6	Os 1	0	0
86	N1	1	Total 7	N 6	Os 1	0	0
86	N9	1	Total 7	N 6	Os 1	0	0
86	O1	1	Total 7	N 6	Os 1	0	0
86	O2	1	Total 7	N 6	Os 1	0	0
86	O3	1	Total 7	N 6	Os 1	0	0
86	O7	1	Total 7	N 6	Os 1	0	0
86	O7	1	Total 7	N 6	Os 1	0	0
86	O9	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0
86	6	1	Total 7	N 6	Os 1	0	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

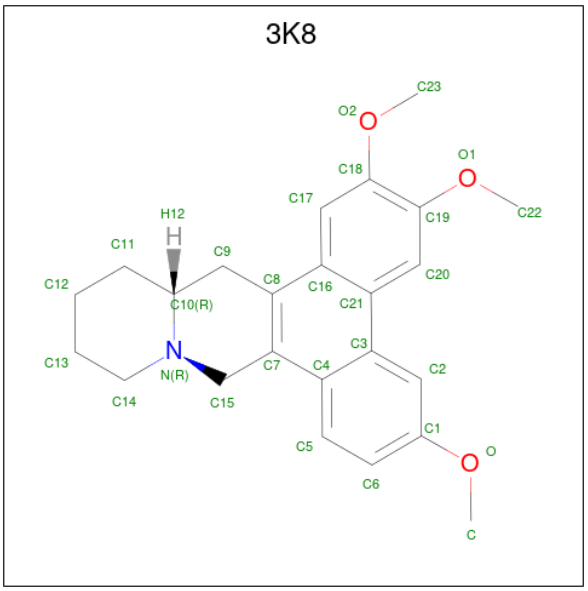
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
86	8	1	Total	N	Os	0	0
			7	6	1		
86	8	1	Total	N	Os	0	0
			7	6	1		
86	l3	1	Total	N	Os	0	0
			7	6	1		
86	l3	1	Total	N	Os	0	0
			7	6	1		
86	l3	1	Total	N	Os	0	0
			7	6	1		
86	l4	1	Total	N	Os	0	0
			7	6	1		
86	l4	1	Total	N	Os	0	0
			7	6	1		
86	l5	1	Total	N	Os	0	0
			7	6	1		
86	l5	1	Total	N	Os	0	0
			7	6	1		
86	l5	1	Total	N	Os	0	0
			7	6	1		
86	l9	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m0	1	Total	N	Os	0	0
			7	6	1		
86	m1	1	Total	N	Os	0	0
			7	6	1		
86	m4	1	Total	N	Os	0	0
			7	6	1		
86	m5	1	Total	N	Os	0	0
			7	6	1		
86	m6	1	Total	N	Os	0	0
			7	6	1		
86	m7	1	Total	N	Os	0	0
			7	6	1		
86	m8	1	Total	N	Os	0	0
			7	6	1		
86	m9	1	Total	N	Os	0	0
			7	6	1		
86	n1	1	Total	N	Os	0	0
			7	6	1		

Continued on next page...

Continued from previous page...

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

- Molecule 87 is (14aR)-2,3,6-trimethoxy-11,12,13,14,14a,15-hexahydro-9H-dibenzo[f,h]pyrido[1,2-b]isoquinoline (CCD ID: 3K8) (formula: $C_{24}H_{27}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
87	2	1	Total C N O 28 24 1 3	0	0
87	6	1	Total C N O 28 24 1 3	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
88	D6	1	Total Zn 1 1	0	0
88	D7	1	Total Zn 1 1	0	0
88	D9	1	Total Zn 1 1	0	0

Continued on next page...

Continued from previous page...

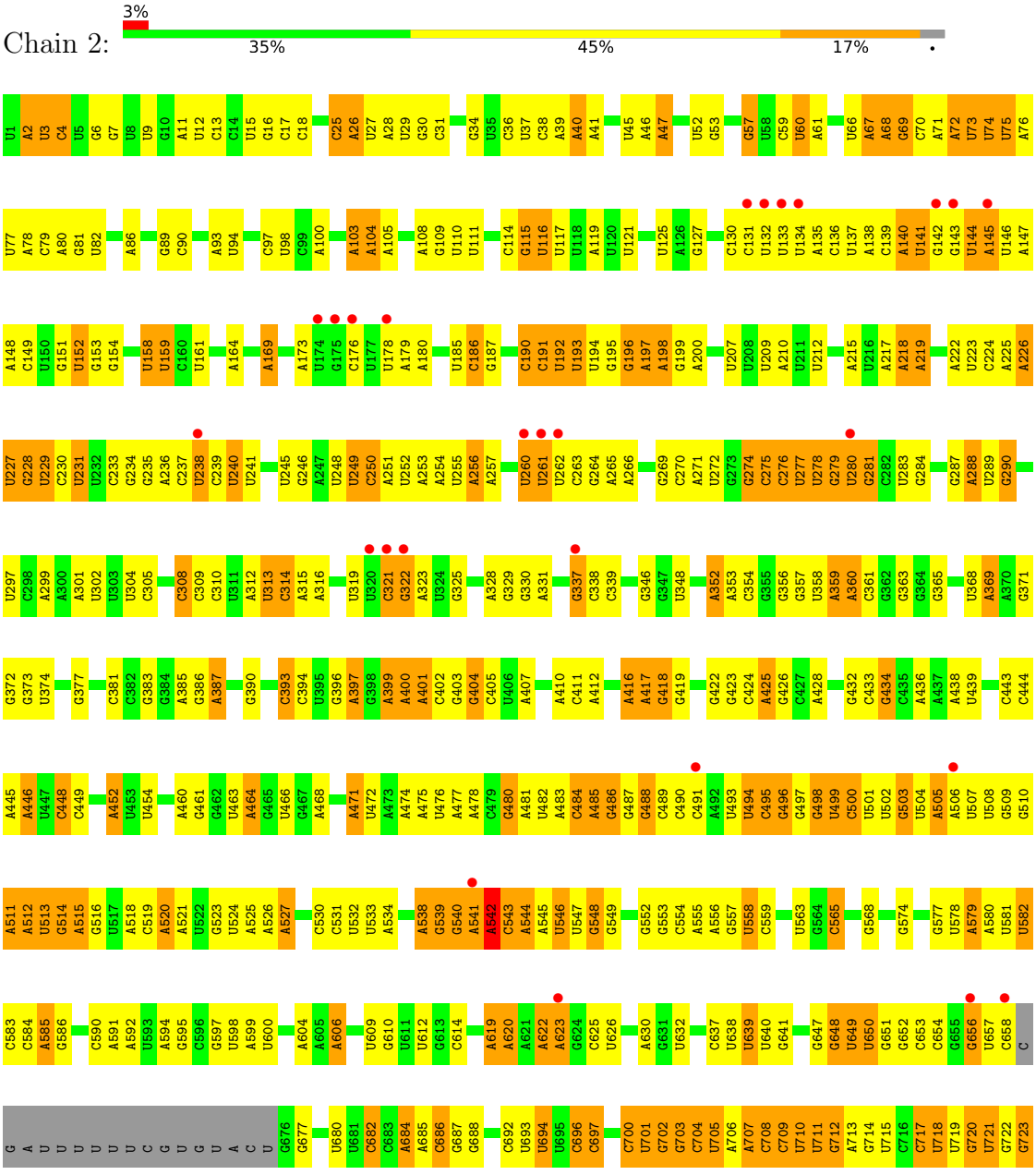
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
88	E1	1	Total Zn 1 1	0	0
88	O7	1	Total Zn 1 1	0	0
88	Q0	1	Total Zn 1 1	0	0
88	Q2	1	Total Zn 1 1	0	0
88	Q3	1	Total Zn 1 1	0	0
88	d6	1	Total Zn 1 1	0	0
88	d7	1	Total Zn 1 1	0	0
88	d9	1	Total Zn 1 1	0	0
88	e1	1	Total Zn 1 1	0	0
88	o7	1	Total Zn 1 1	0	0
88	q0	1	Total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

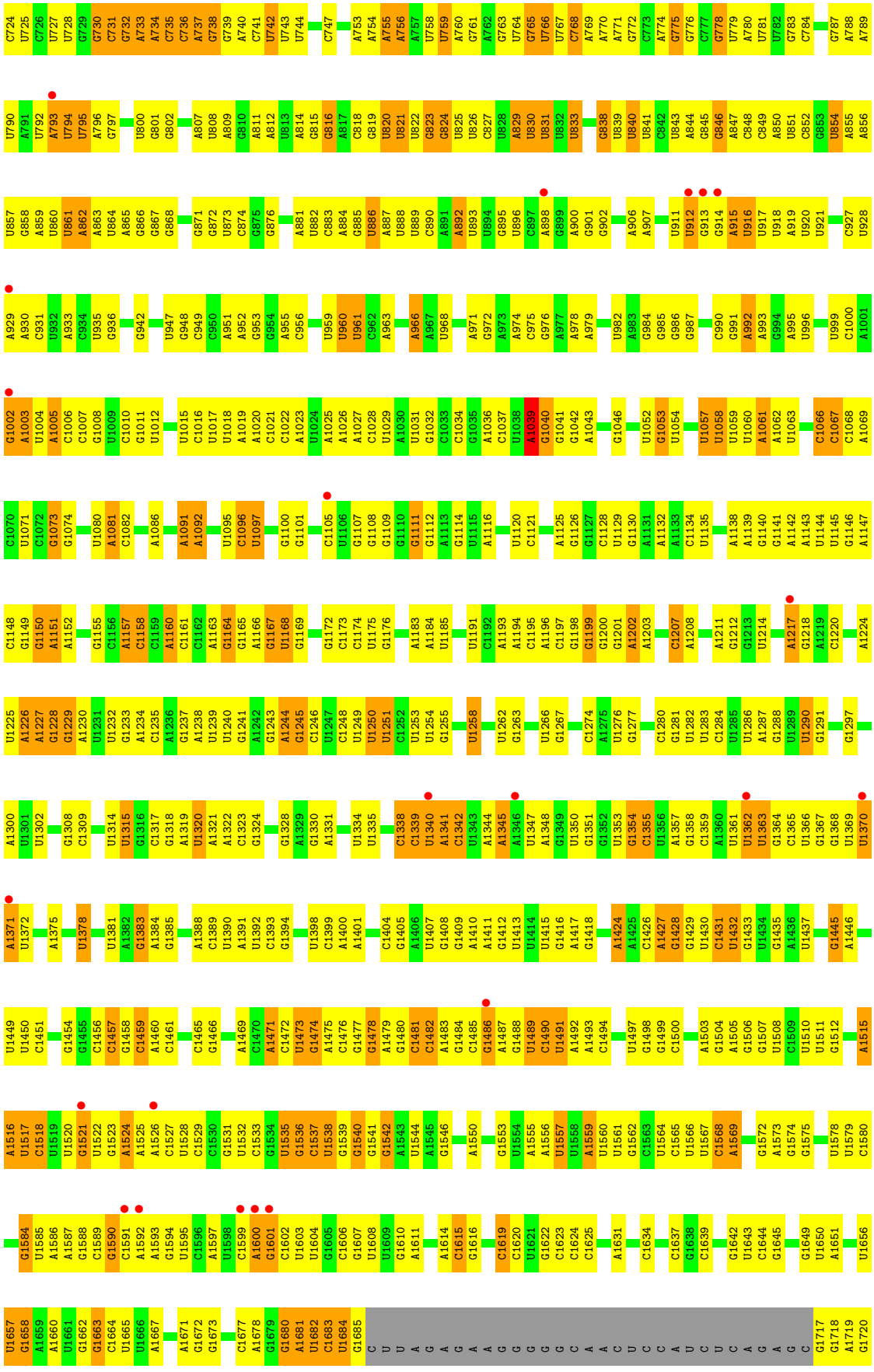
3 Residue-property plots (i)

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

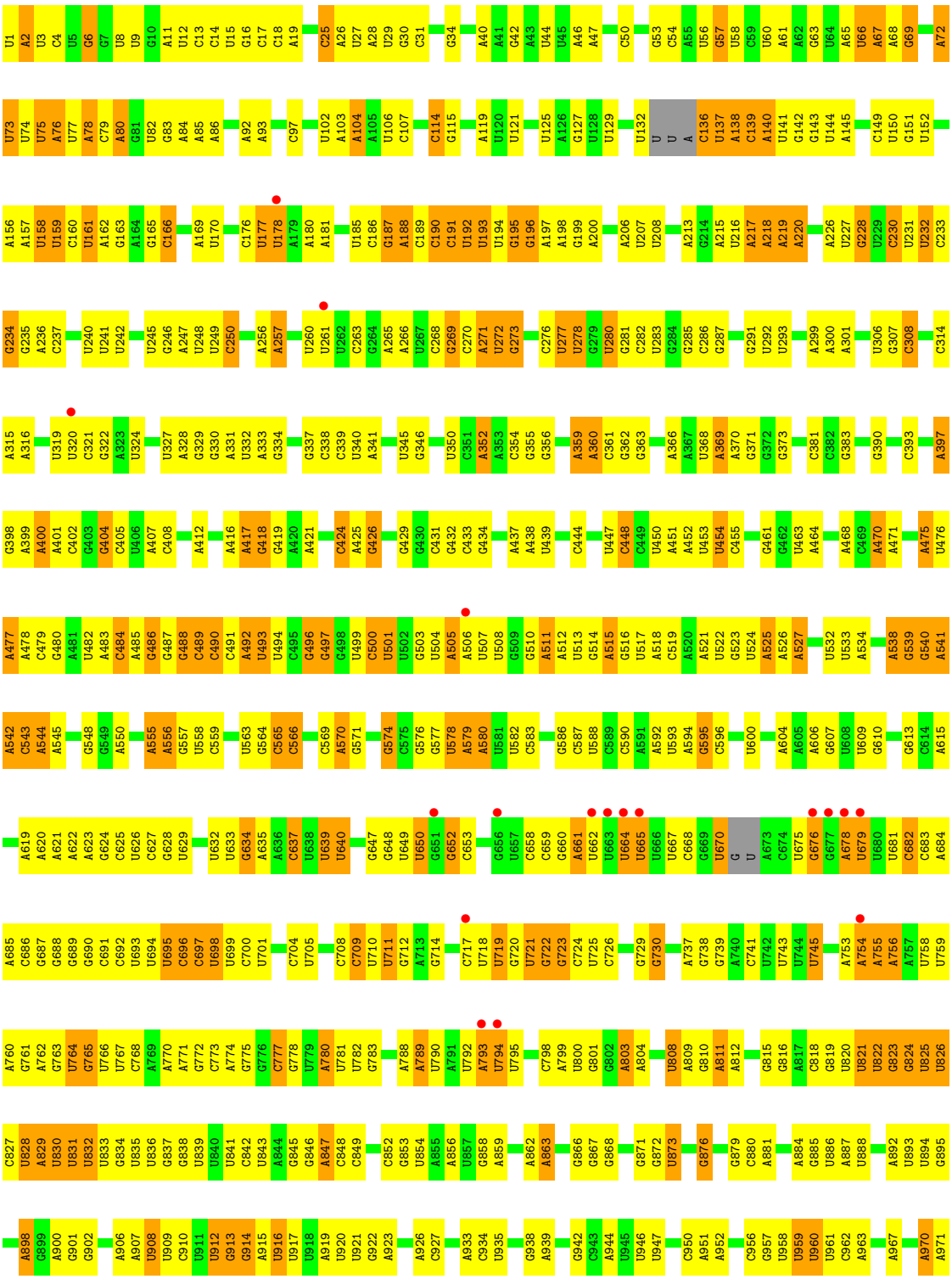
Chain 2:

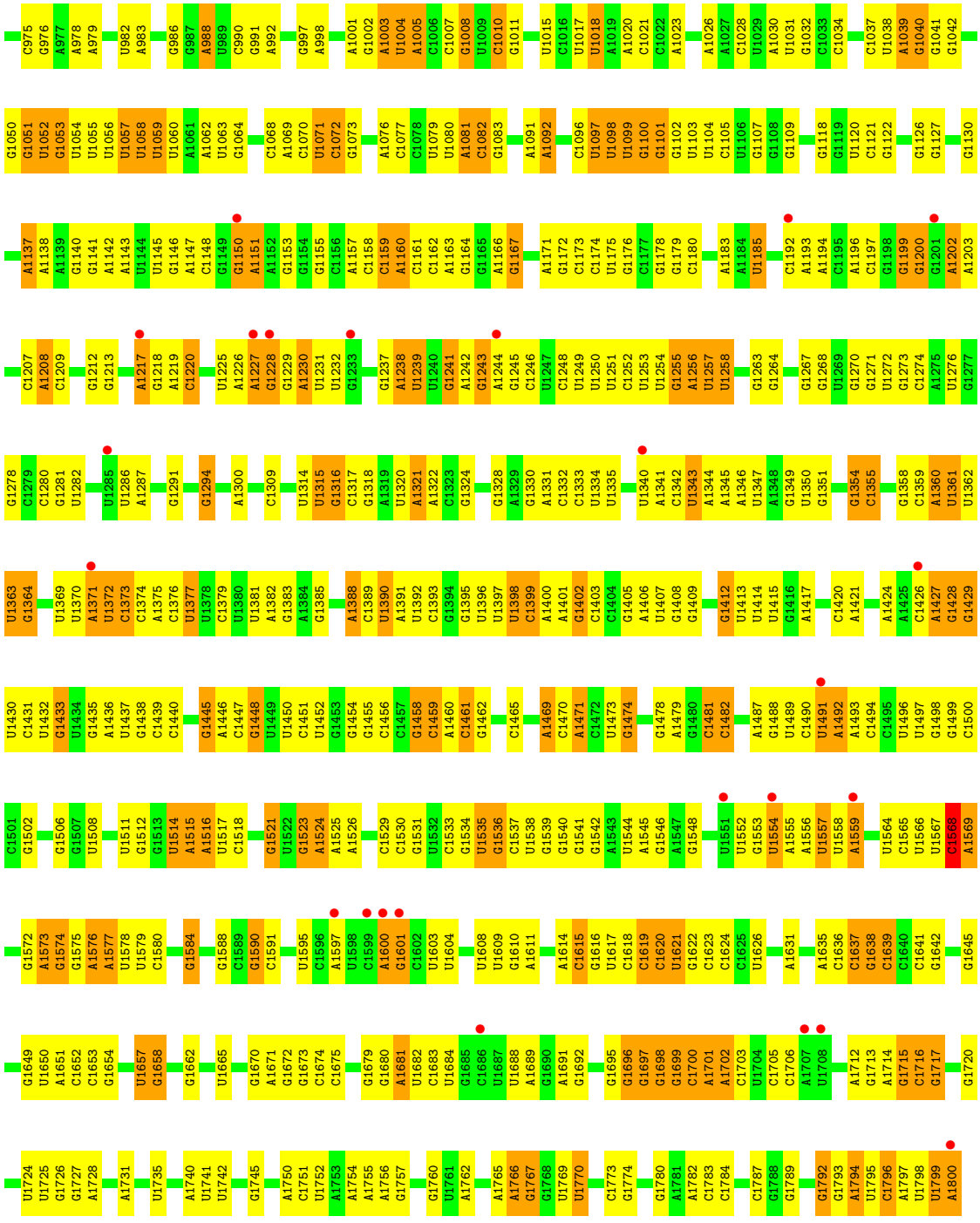




• Molecule 1: 18S ribosomal RNA

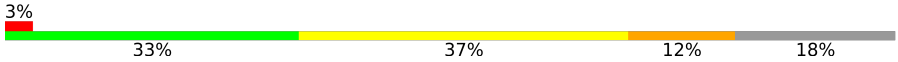
Chain 6:

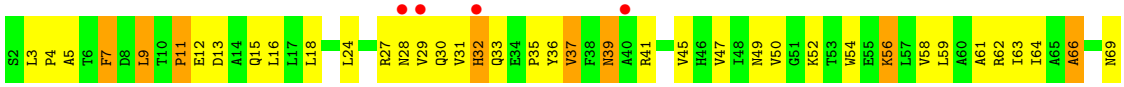


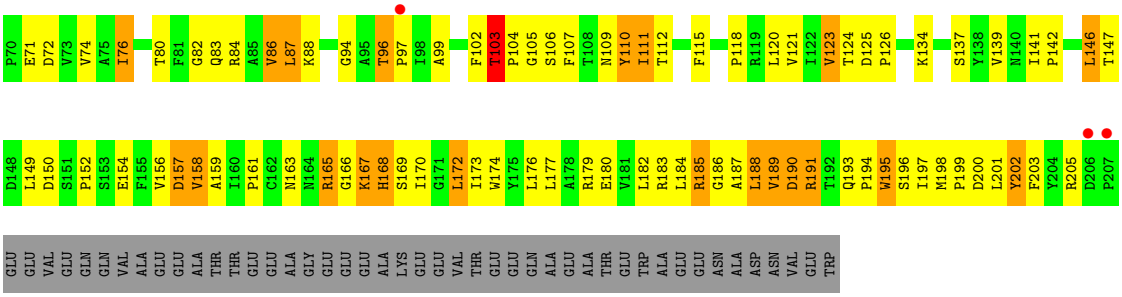


• Molecule 2: 40S ribosomal protein S0-A

Chain S0:

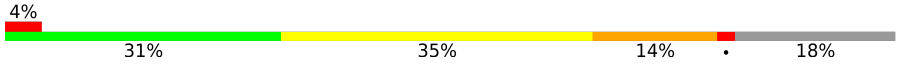


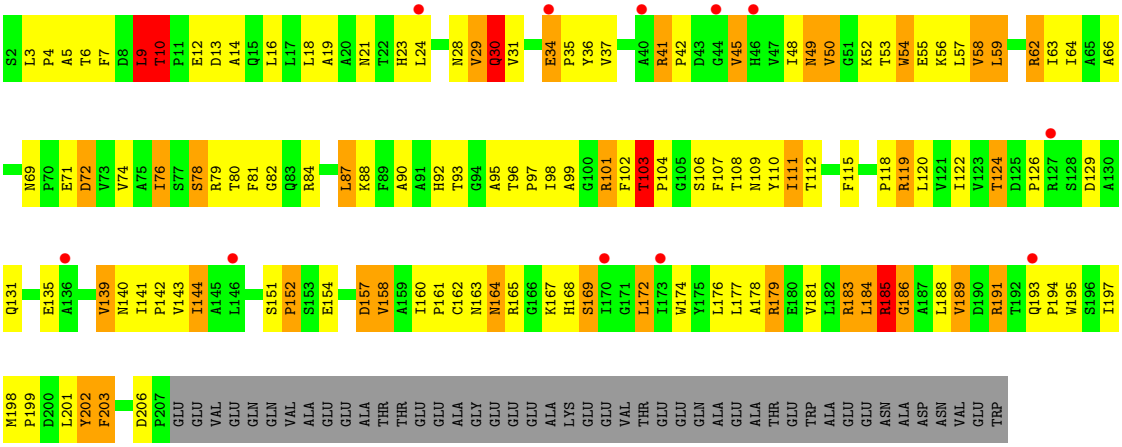




• Molecule 2: 40S ribosomal protein S0-A

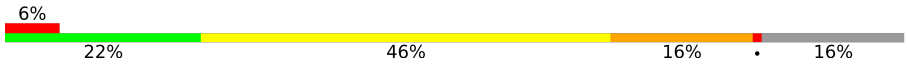
Chain s0:

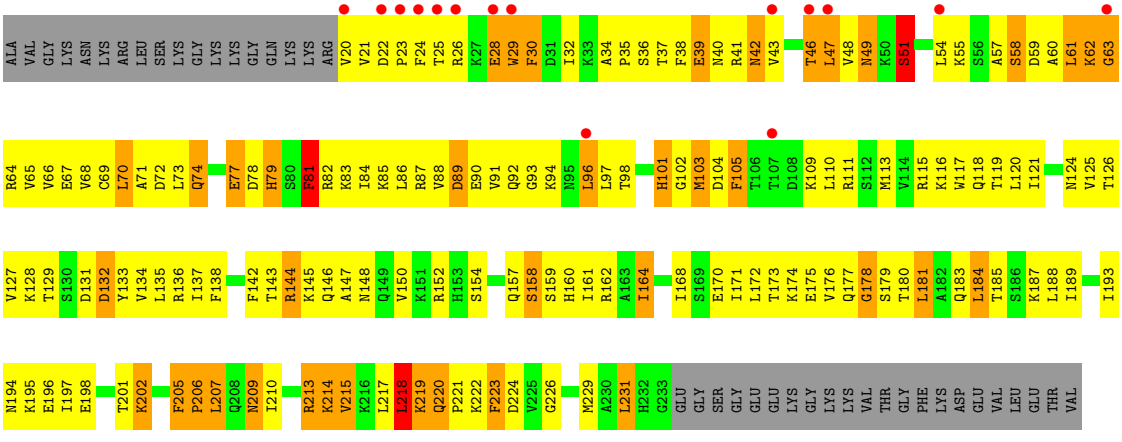




• Molecule 3: 40S ribosomal protein S1-A

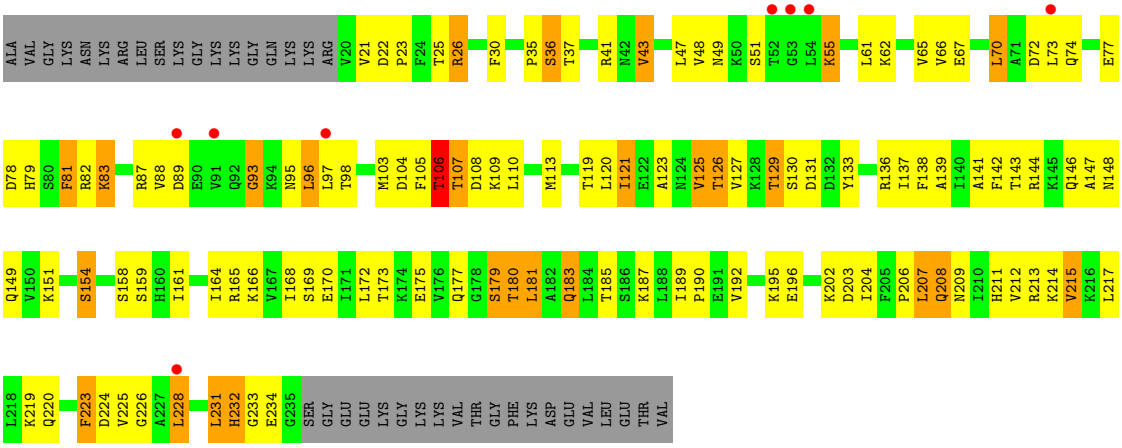
Chain S1:





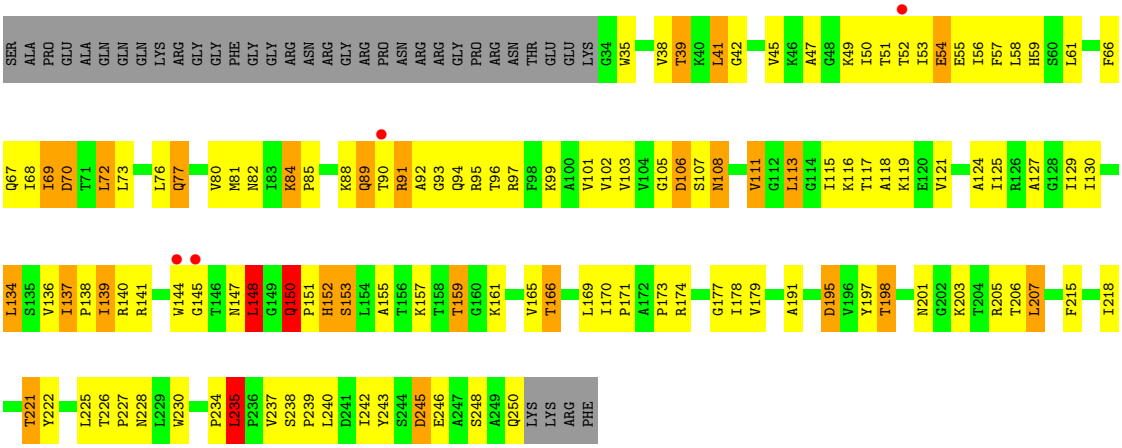
• Molecule 3: 40S ribosomal protein S1-A

Chain s1:



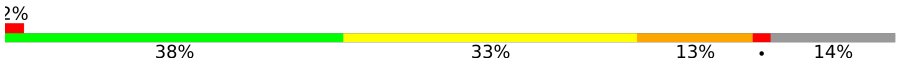
• Molecule 4: 40S ribosomal protein S2

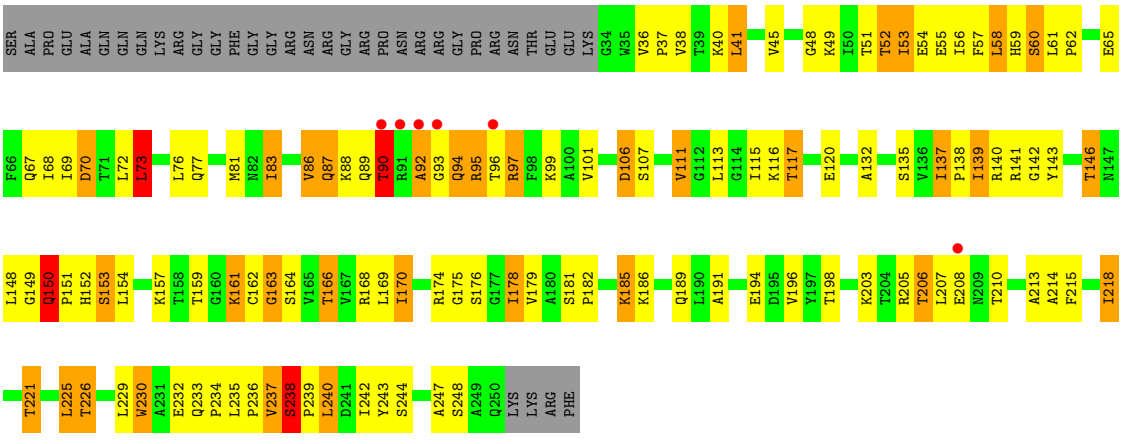
Chain S2:



• Molecule 4: 40S ribosomal protein S2

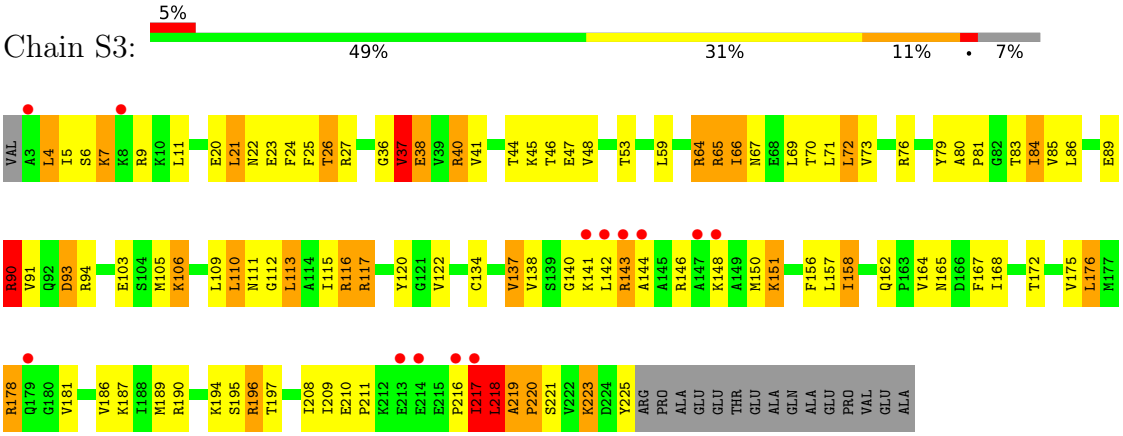
Chain s2:





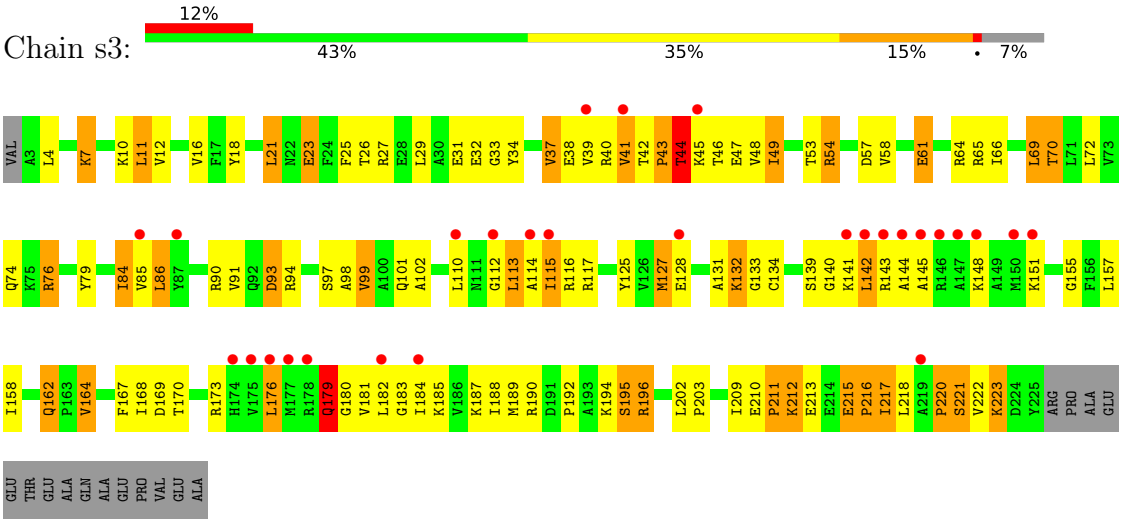
• Molecule 5: 40S ribosomal protein S3

Chain S3:



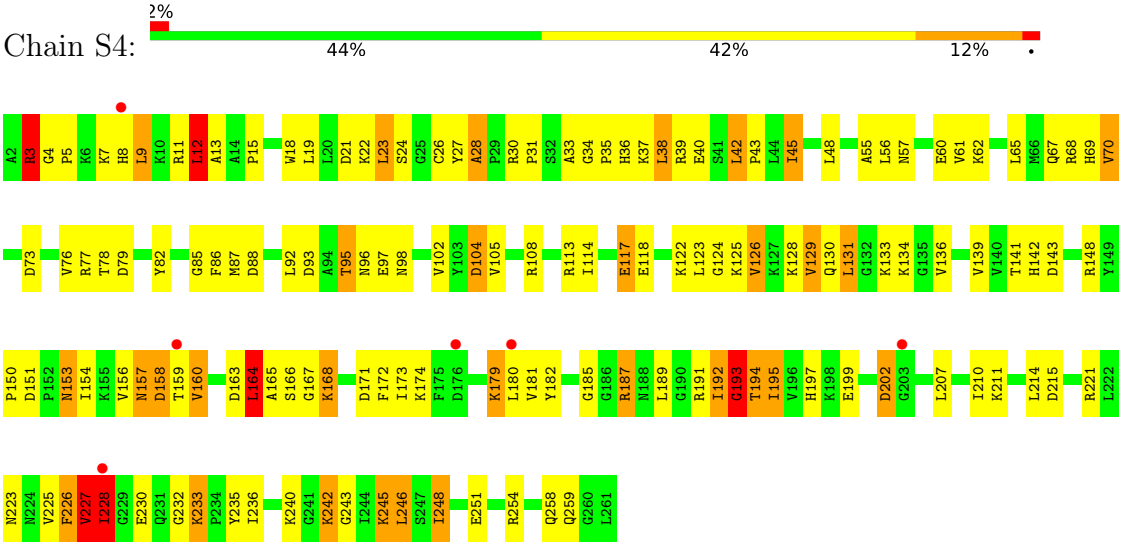
• Molecule 5: 40S ribosomal protein S3

Chain s3:



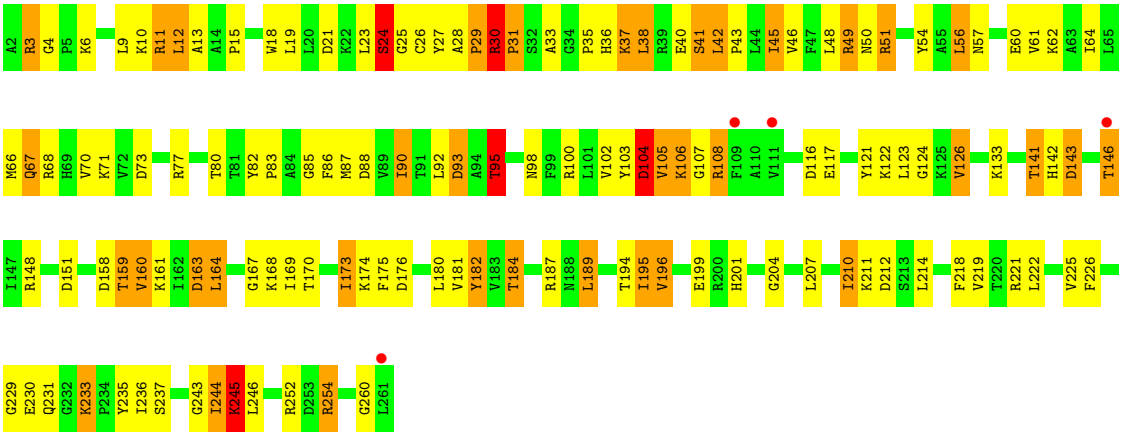
• Molecule 6: 40S ribosomal protein S4-A

Chain S4:

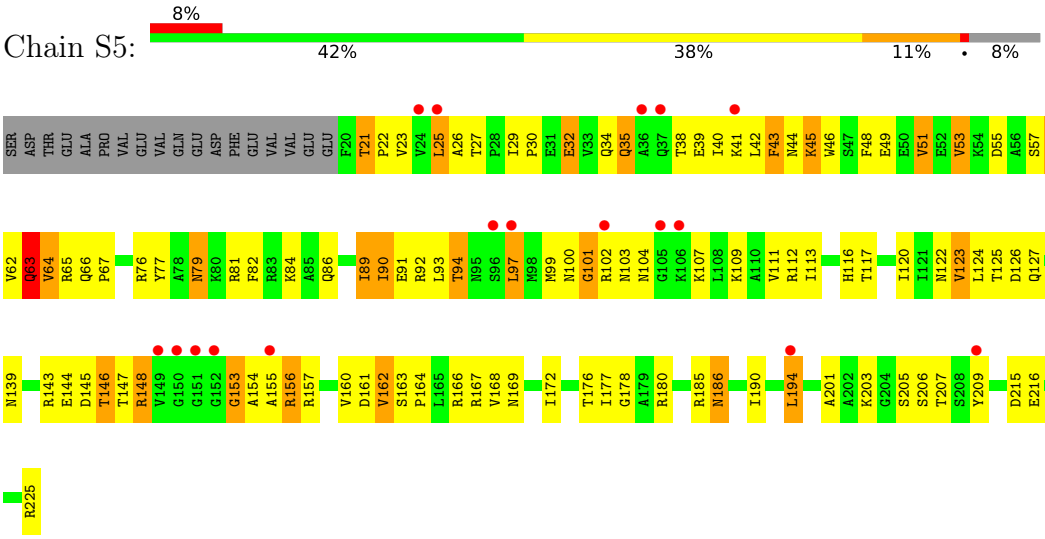


• Molecule 6: 40S ribosomal protein S4-A

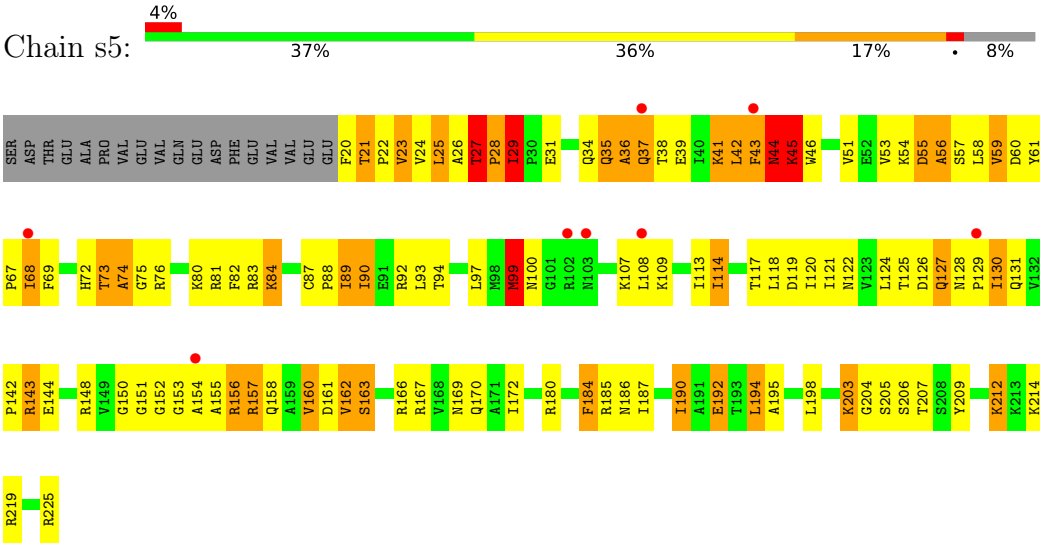
Chain s4:



• Molecule 7: 40S ribosomal protein S5

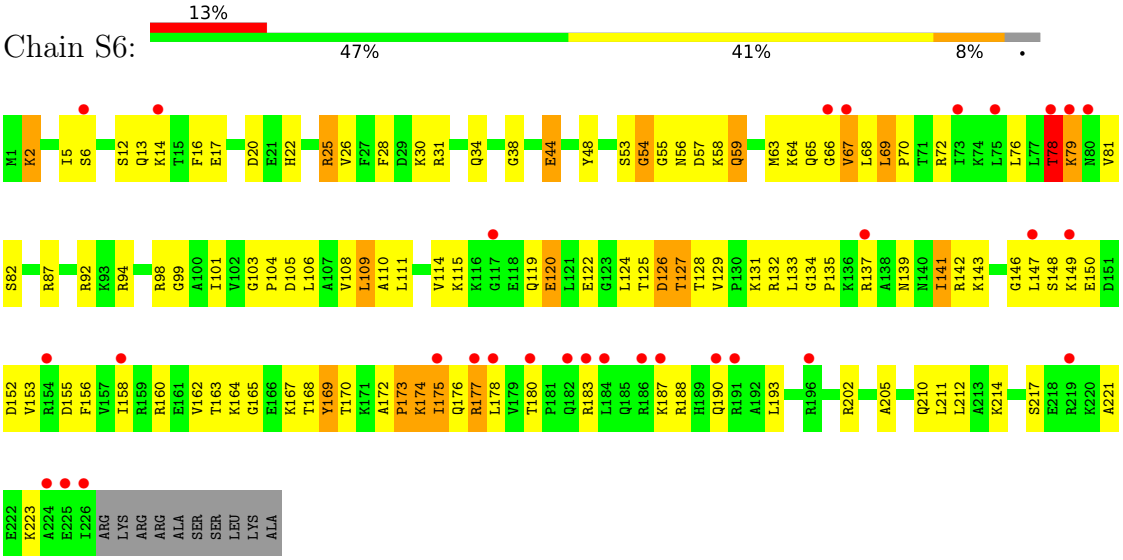


• Molecule 7: 40S ribosomal protein S5



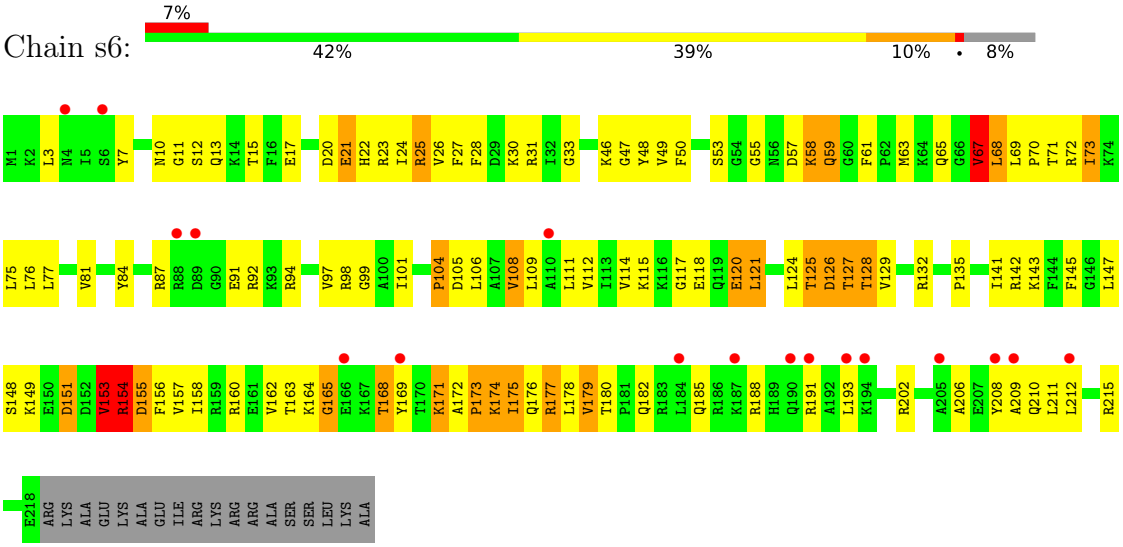
• Molecule 8: 40S ribosomal protein S6-A

Chain S6:



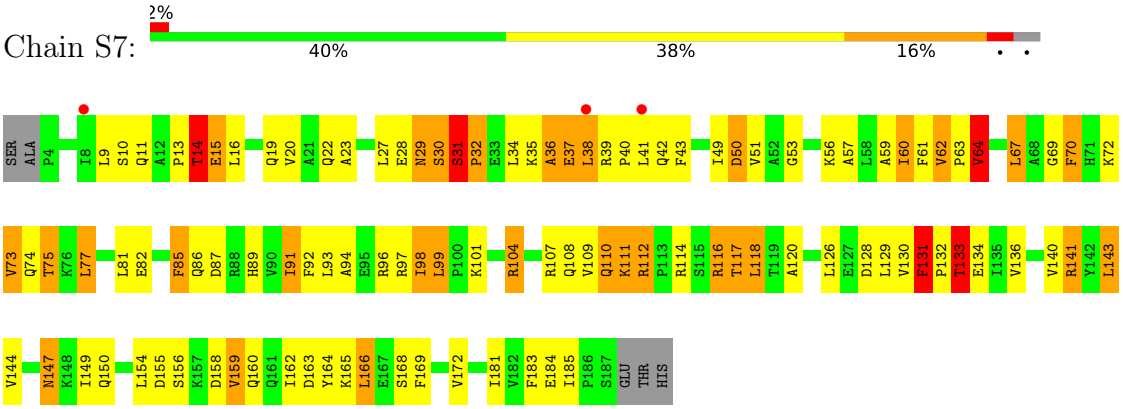
• Molecule 8: 40S ribosomal protein S6-A

Chain s6:



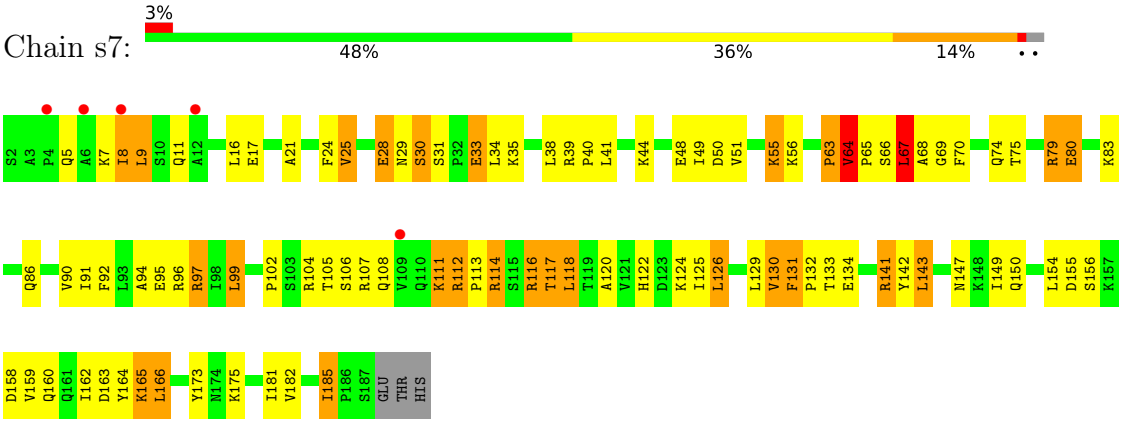
• Molecule 9: 40S ribosomal protein S7-A

Chain S7:



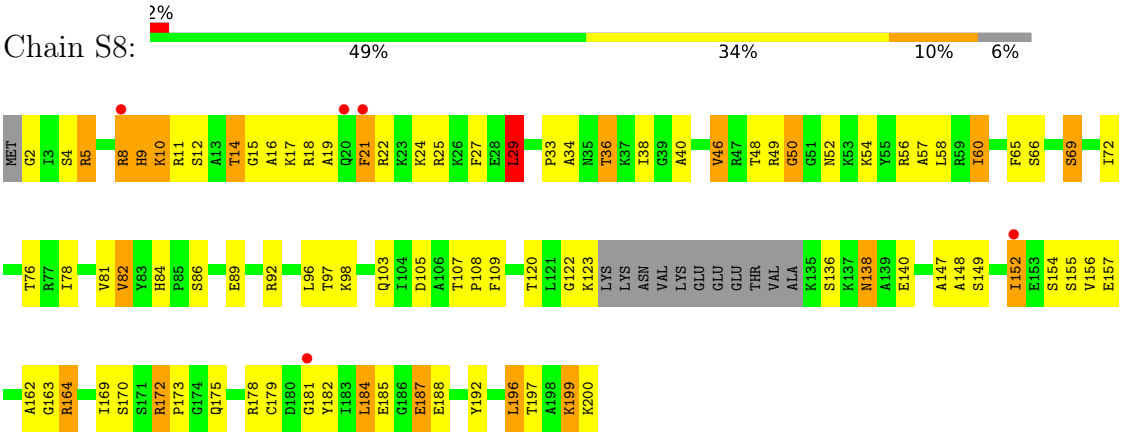
• Molecule 9: 40S ribosomal protein S7-A

Chain s7:



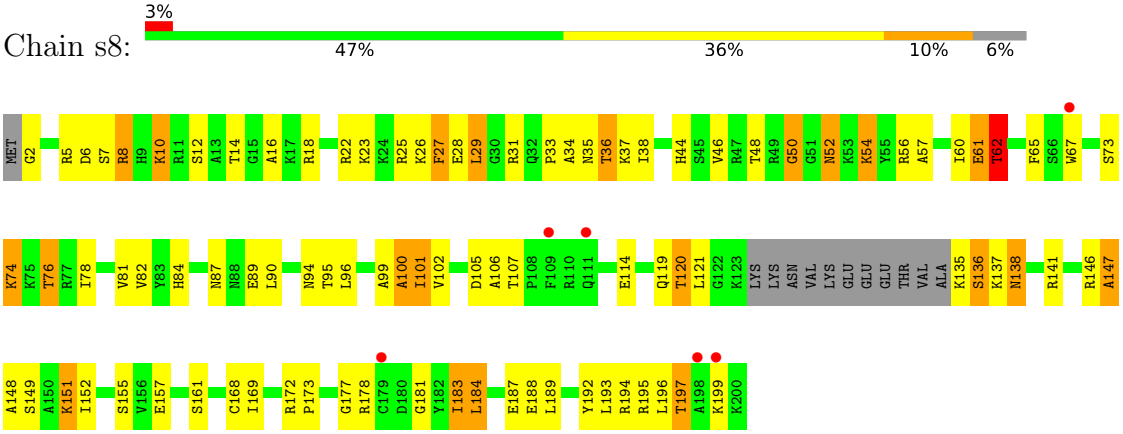
• Molecule 10: 40S ribosomal protein S8-A

Chain S8:



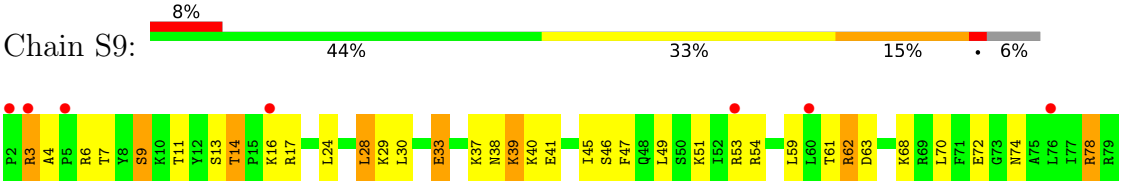
• Molecule 10: 40S ribosomal protein S8-A

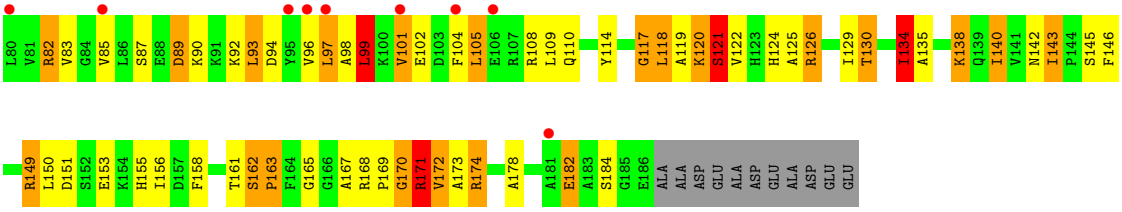
Chain s8:



• Molecule 11: 40S ribosomal protein S9-A

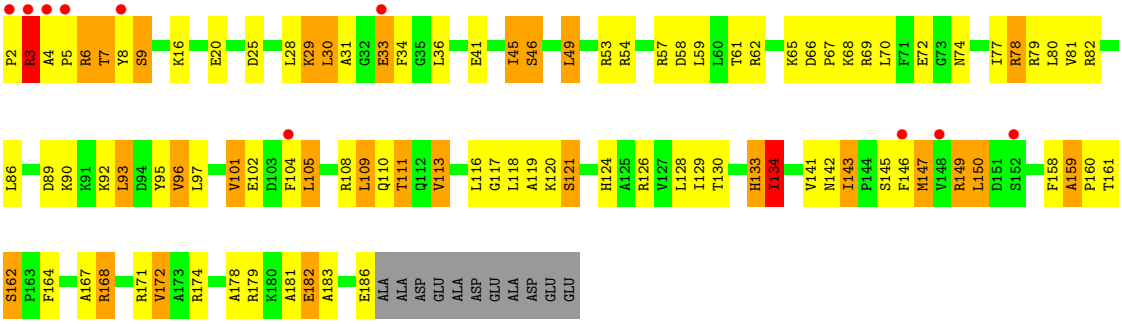
Chain S9:





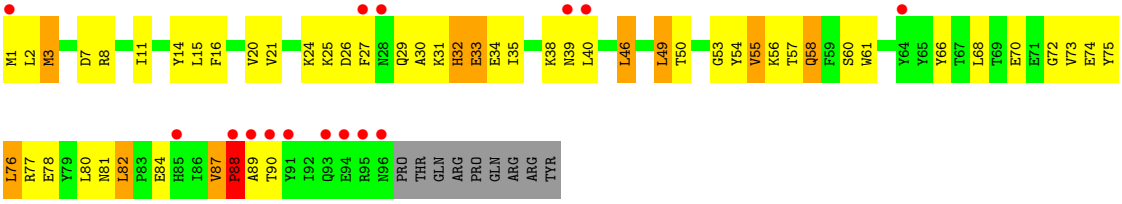
• Molecule 11: 40S ribosomal protein S9-A

Chain s9:



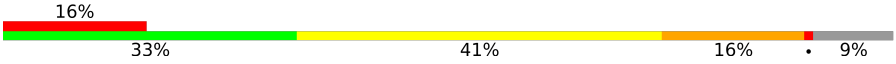
• Molecule 12: 40S ribosomal protein S10-A

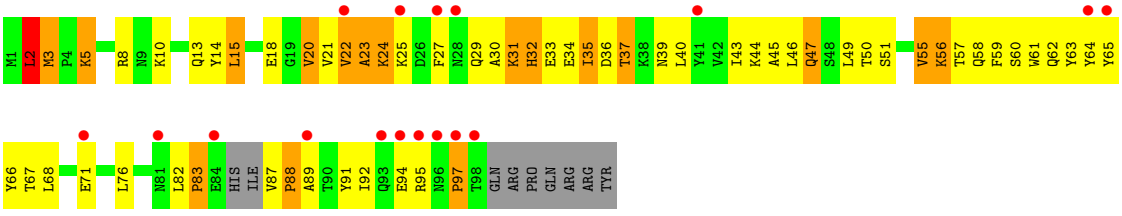
Chain C0:



• Molecule 12: 40S ribosomal protein S10-A

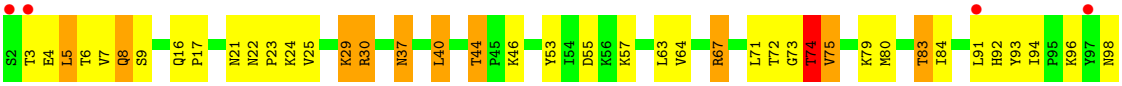
Chain c0:

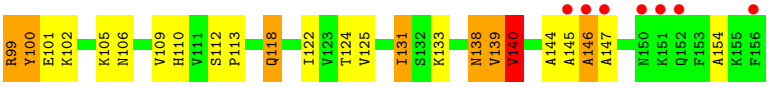




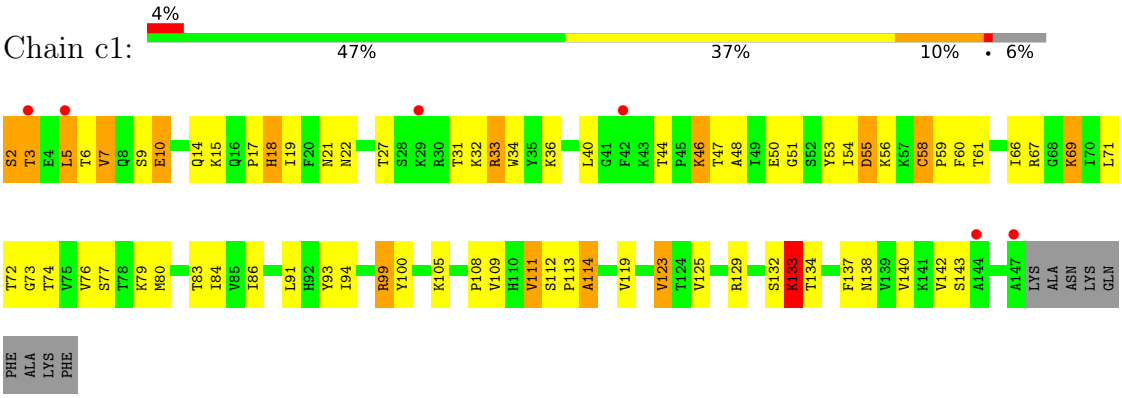
• Molecule 13: 40S ribosomal protein S11-A

Chain C1:

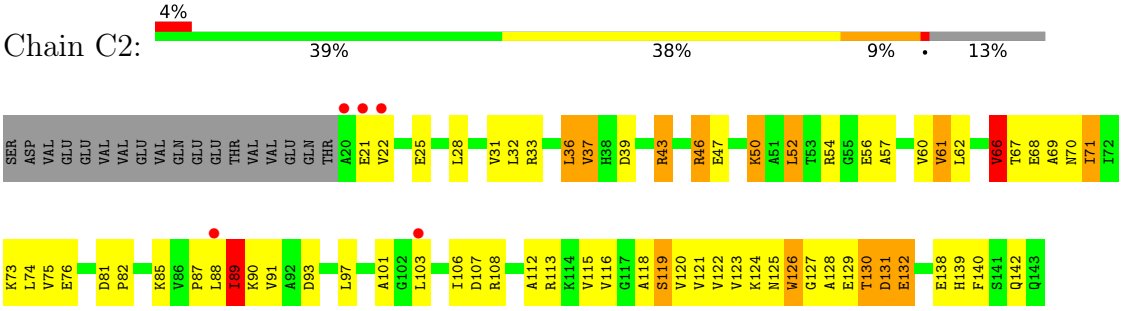




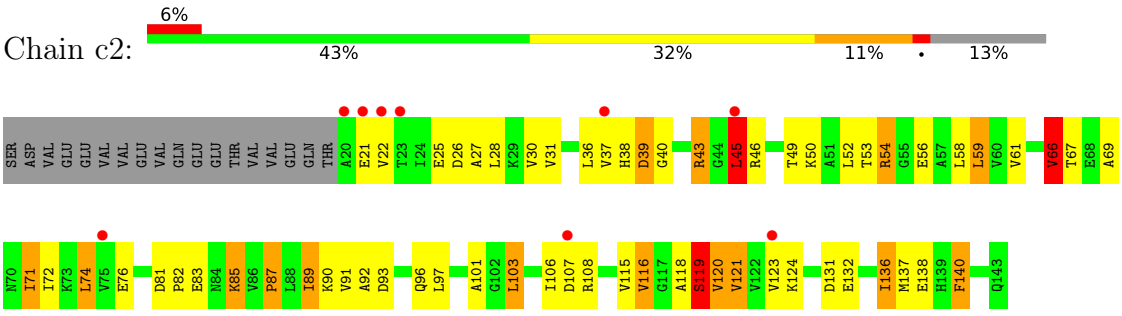
• Molecule 13: 40S ribosomal protein S11-A



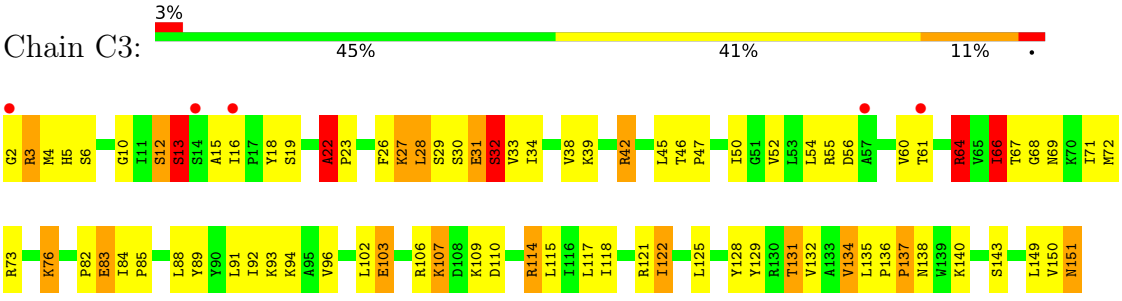
• Molecule 14: 40S ribosomal protein S12



• Molecule 14: 40S ribosomal protein S12

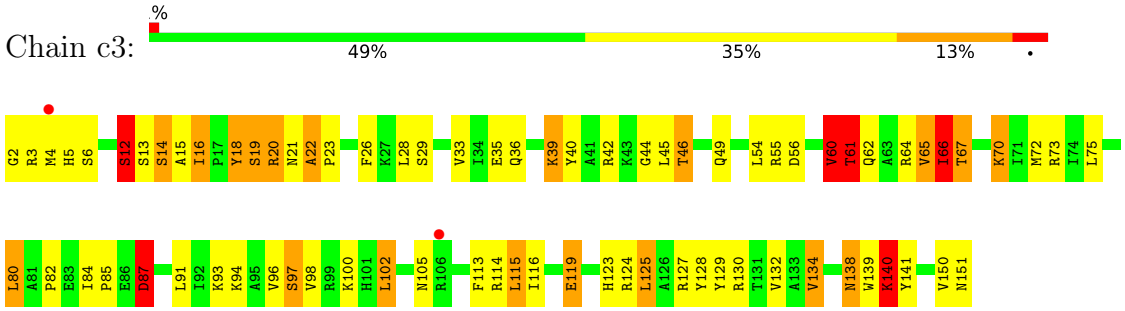


• Molecule 15: 40S ribosomal protein S13



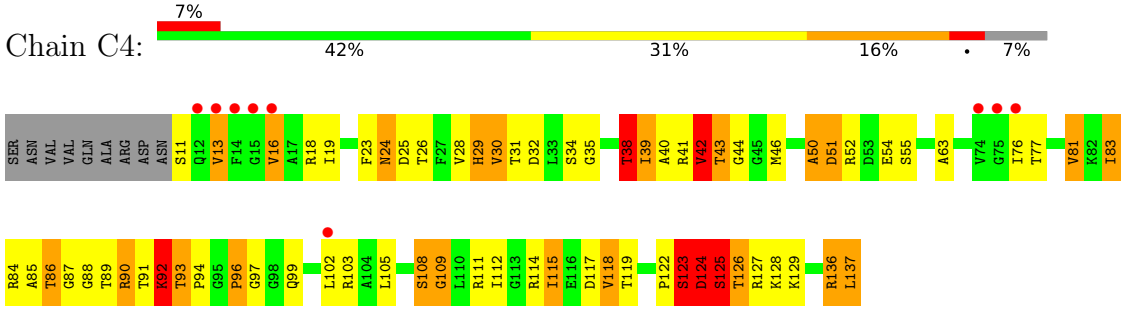
• Molecule 15: 40S ribosomal protein S13

Chain c3:



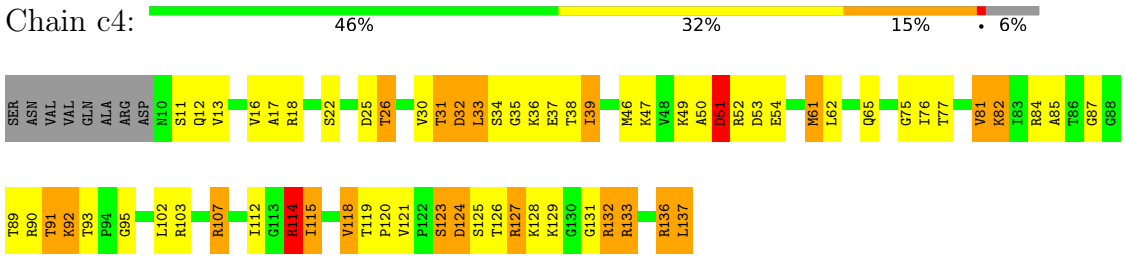
• Molecule 16: 40S ribosomal protein S14-A

Chain C4:



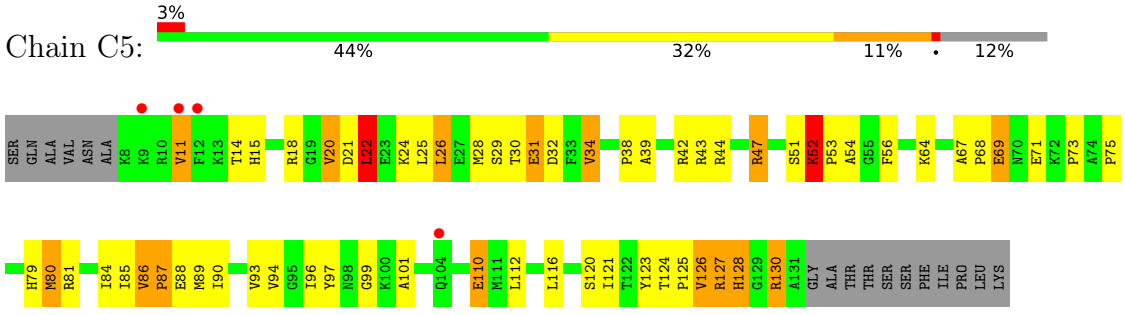
• Molecule 16: 40S ribosomal protein S14-A

Chain c4:



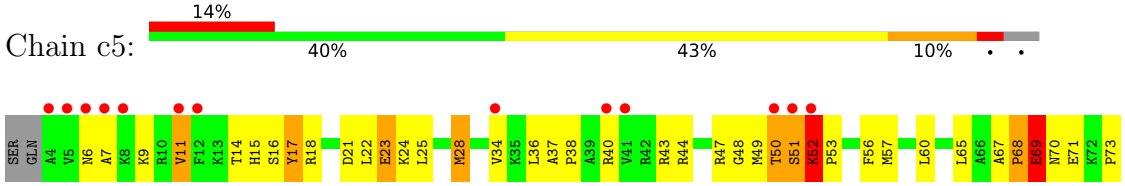
• Molecule 17: 40S ribosomal protein S15

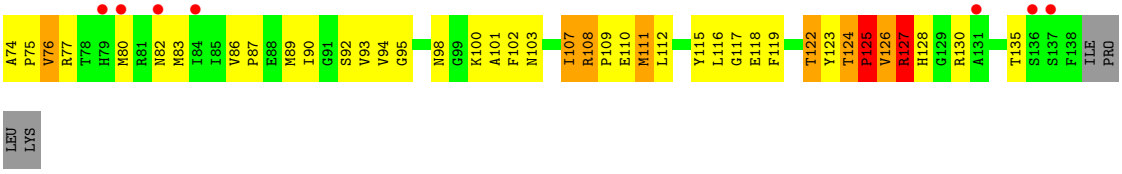
Chain C5:



• Molecule 17: 40S ribosomal protein S15

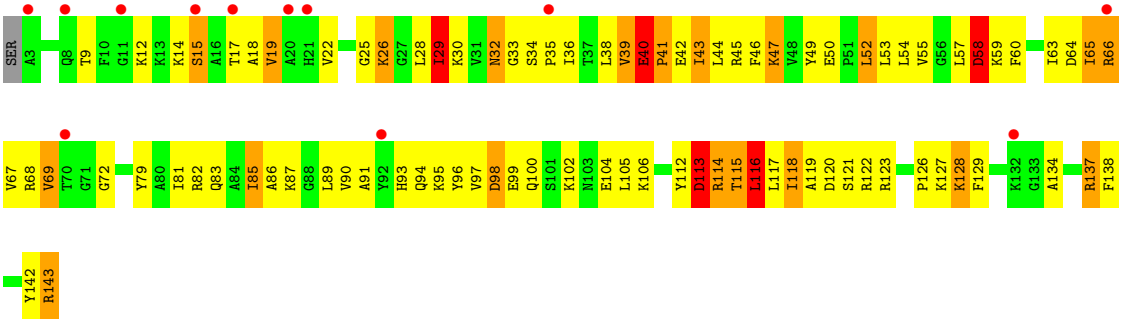
Chain c5:





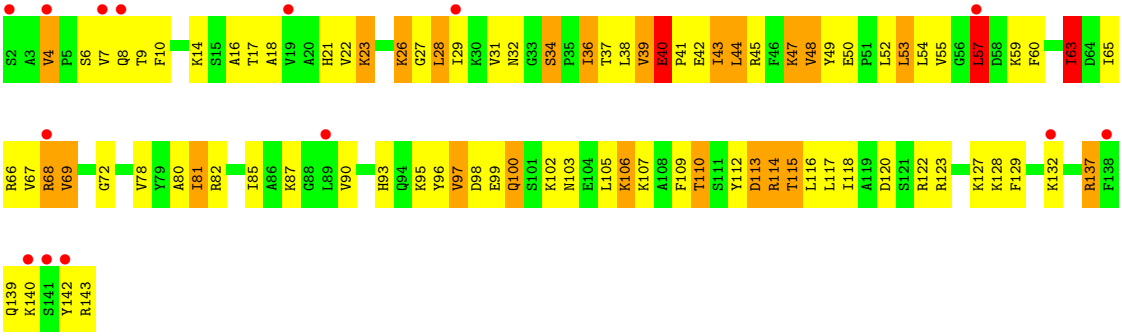
• Molecule 18: 40S ribosomal protein S16-A

Chain C6:



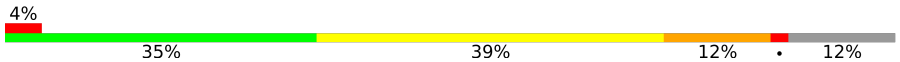
• Molecule 18: 40S ribosomal protein S16-A

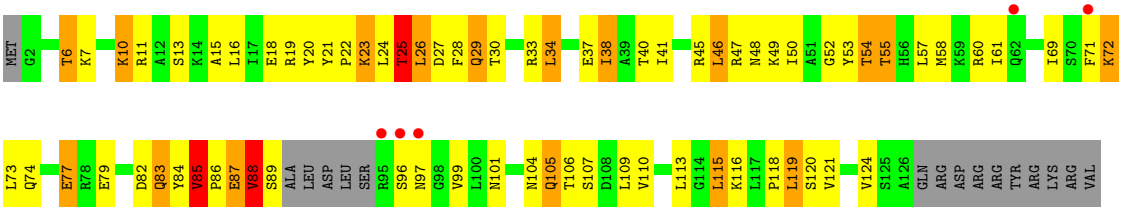
Chain c6:



• Molecule 19: 40S ribosomal protein S17-A

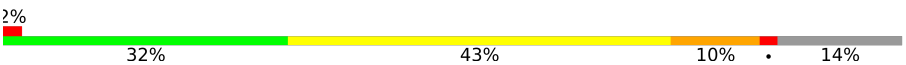
Chain C7:

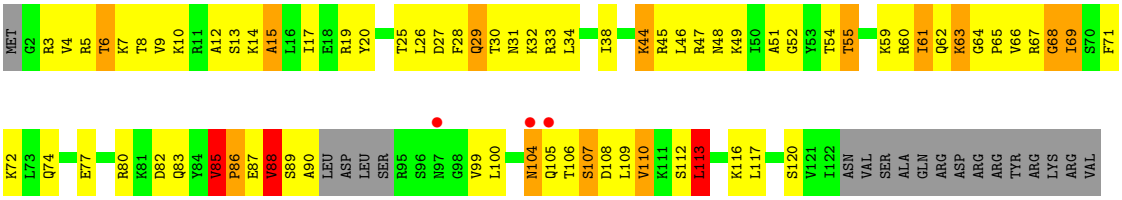




• Molecule 19: 40S ribosomal protein S17-A

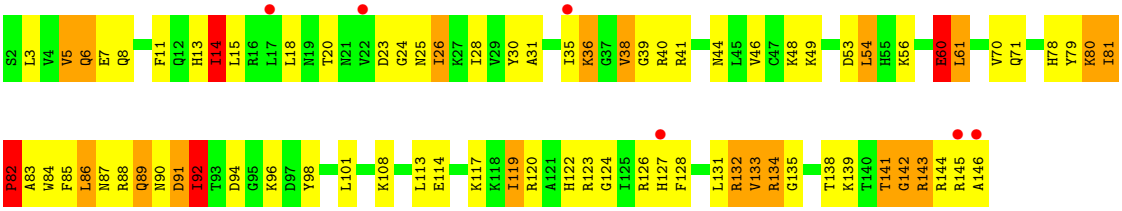
Chain c7:





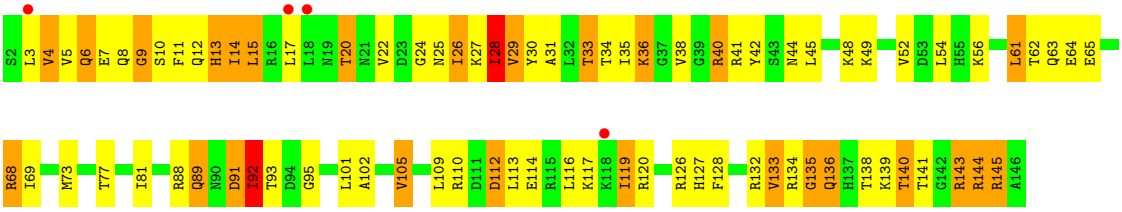
• Molecule 20: 40S ribosomal protein S18-A

Chain C8:



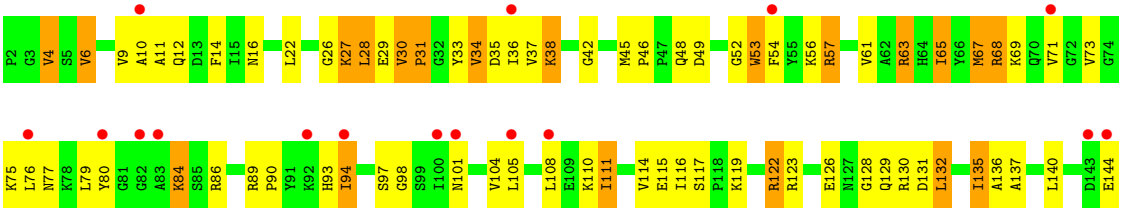
• Molecule 20: 40S ribosomal protein S18-A

Chain c8:



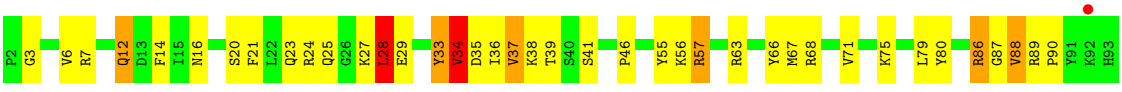
• Molecule 21: 40S ribosomal protein S19-A

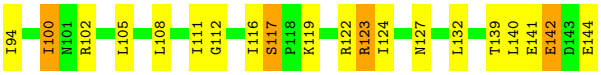
Chain C9:



• Molecule 21: 40S ribosomal protein S19-A

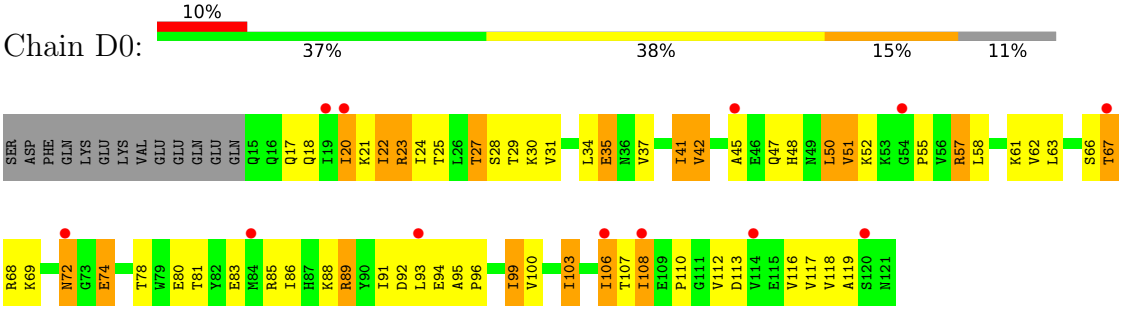
Chain c9:





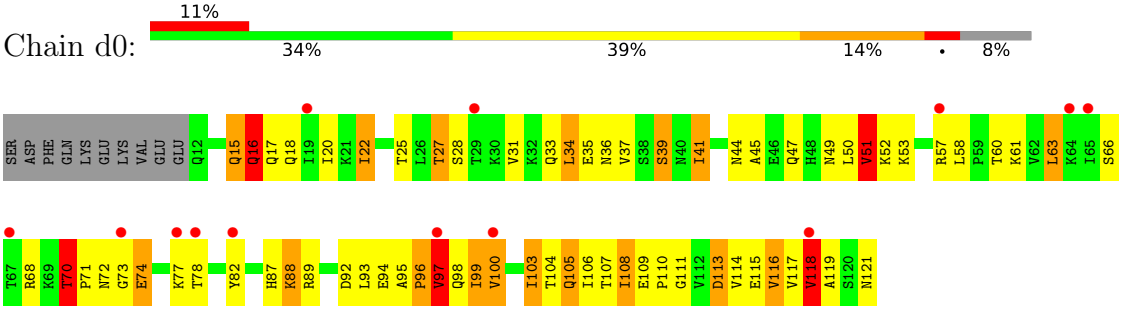
• Molecule 22: 40S ribosomal protein S20

Chain D0:



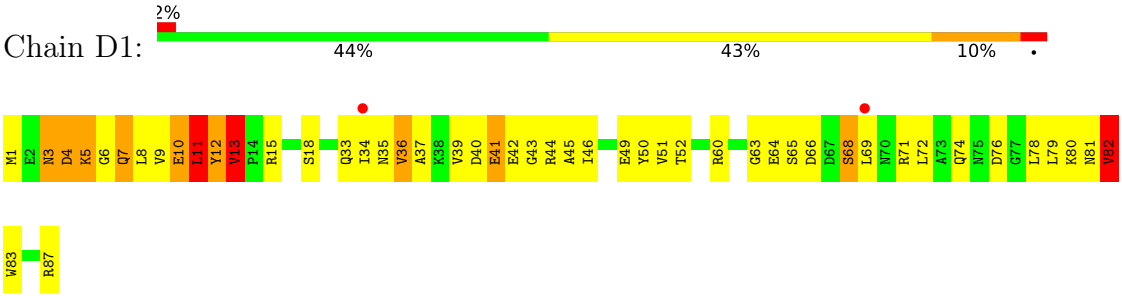
• Molecule 22: 40S ribosomal protein S20

Chain d0:



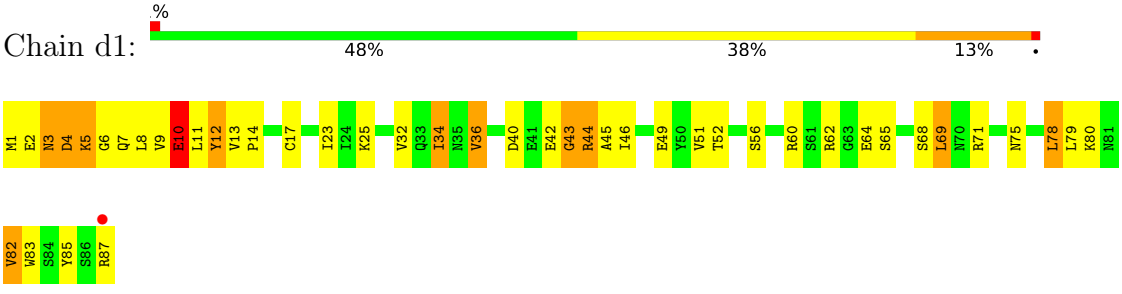
• Molecule 23: 40S ribosomal protein S21-A

Chain D1:



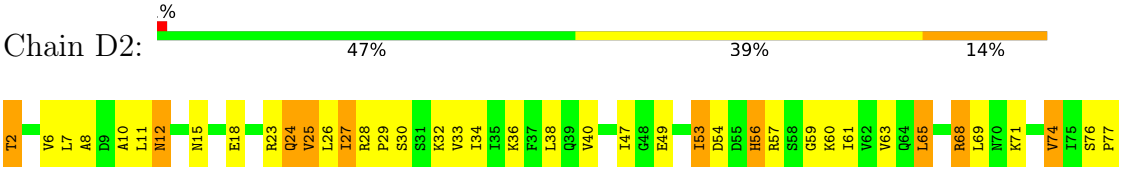
• Molecule 23: 40S ribosomal protein S21-A

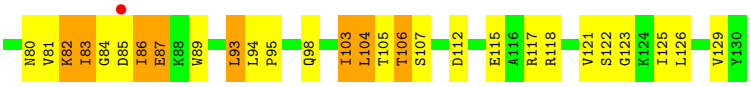
Chain d1:



• Molecule 24: 40S ribosomal protein S22-A

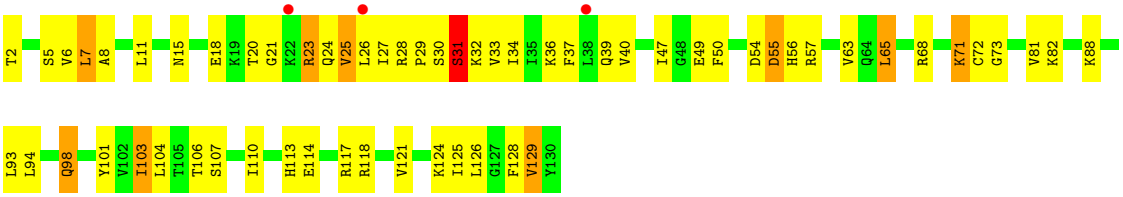
Chain D2:





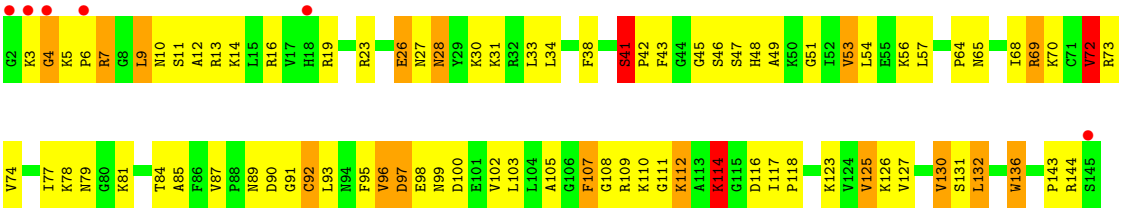
• Molecule 24: 40S ribosomal protein S22-A

Chain d2:



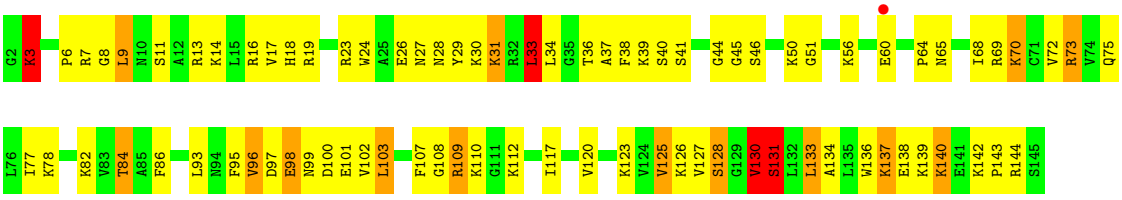
• Molecule 25: 40S ribosomal protein S23-A

Chain D3:



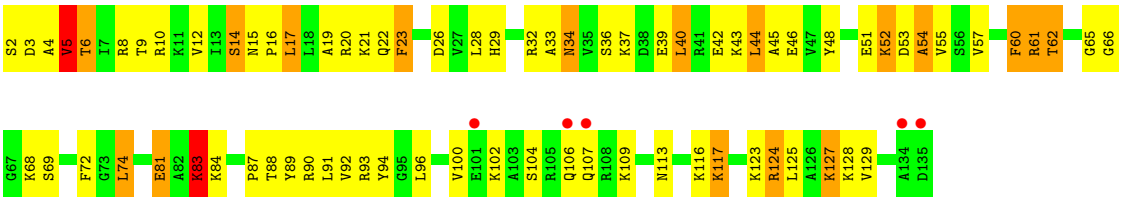
• Molecule 25: 40S ribosomal protein S23-A

Chain d3:



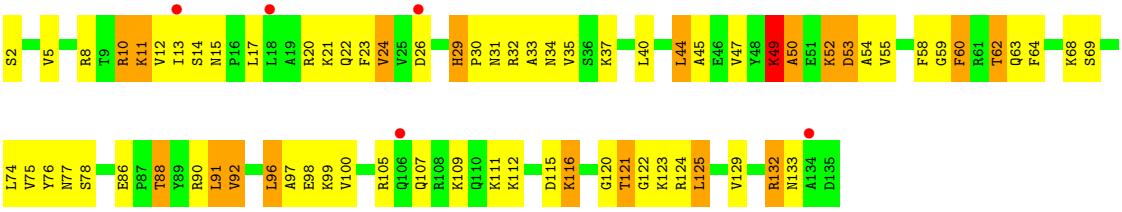
• Molecule 26: 40S ribosomal protein S24-A

Chain D4:



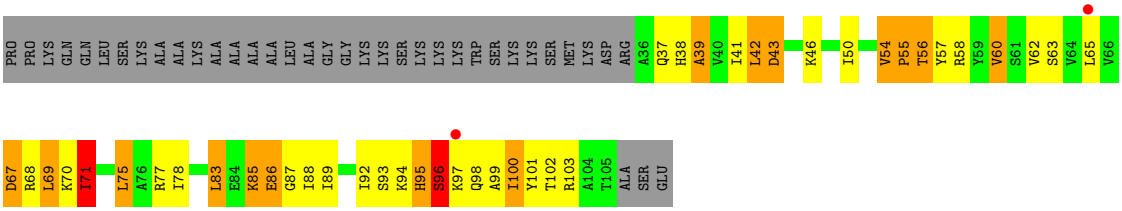
• Molecule 26: 40S ribosomal protein S24-A

Chain d4:



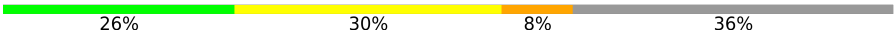
• Molecule 27: 40S ribosomal protein S25-A

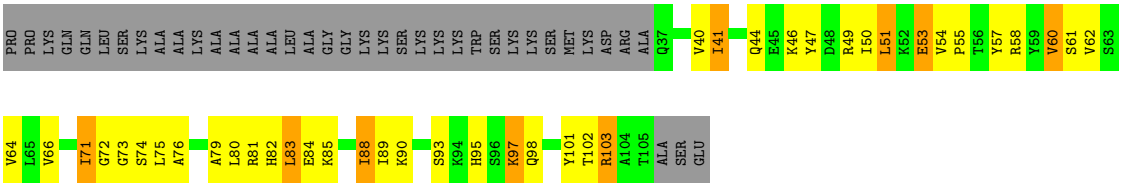
Chain D5:



• Molecule 27: 40S ribosomal protein S25-A

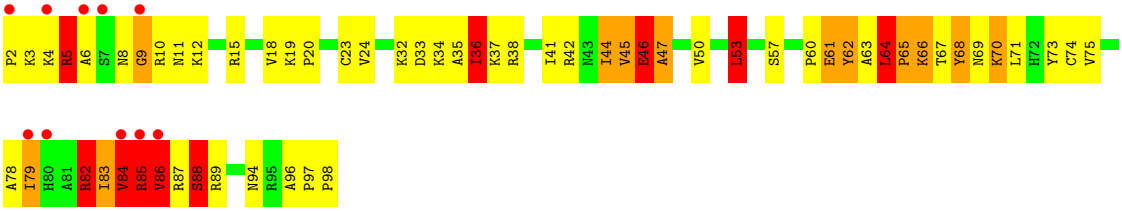
Chain d5:





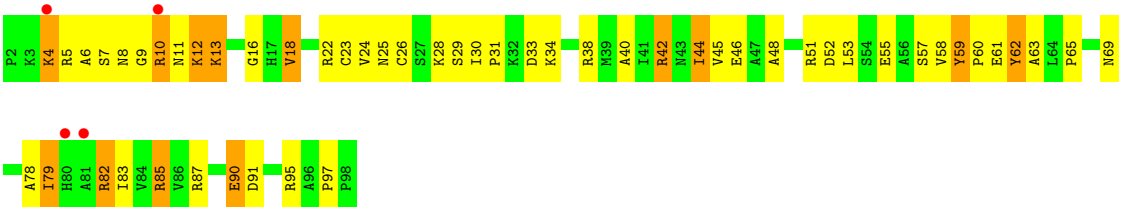
• Molecule 28: 40S ribosomal protein S26-B

Chain D6:



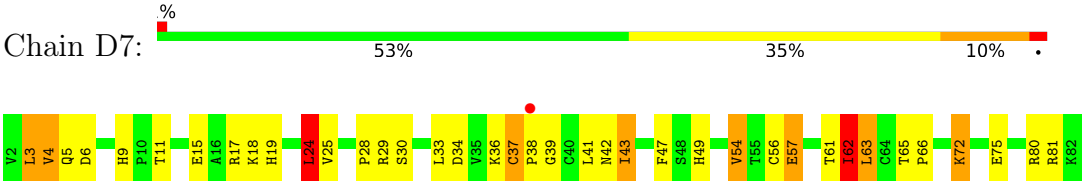
• Molecule 28: 40S ribosomal protein S26-B

Chain d6:



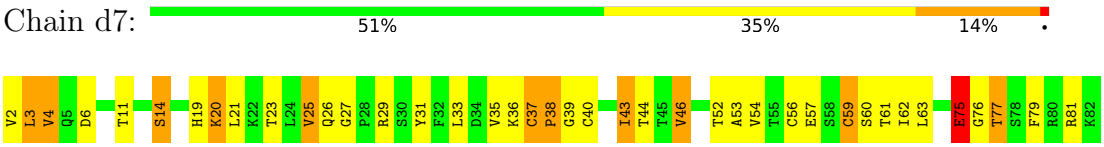
• Molecule 29: 40S ribosomal protein S27-A

Chain D7:



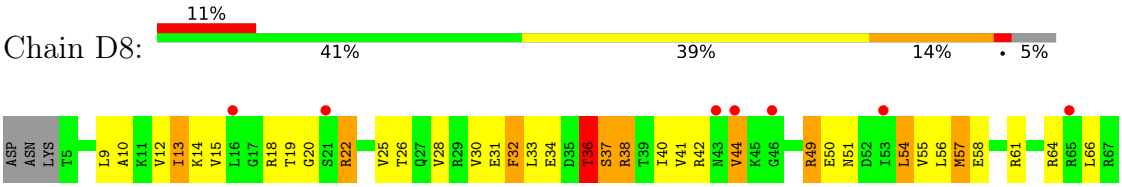
• Molecule 29: 40S ribosomal protein S27-A

Chain d7:



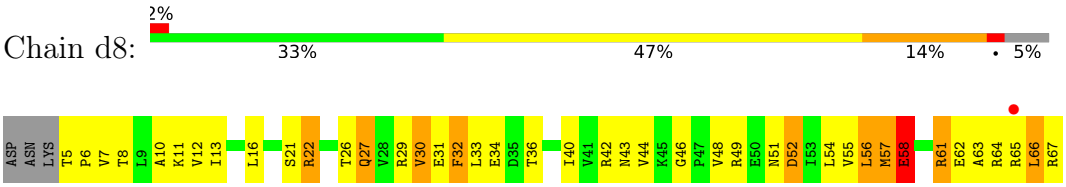
• Molecule 30: 40S ribosomal protein S28-A

Chain D8:



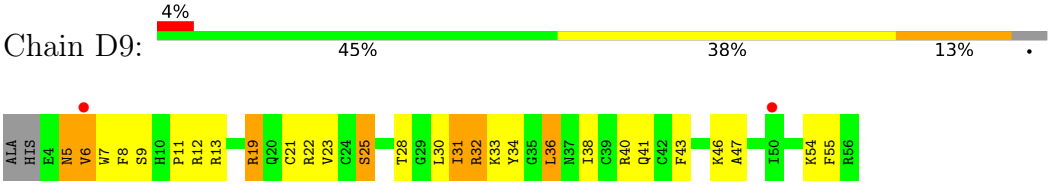
• Molecule 30: 40S ribosomal protein S28-A

Chain d8:



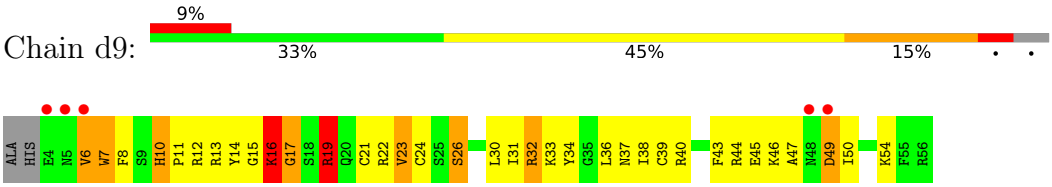
• Molecule 31: 40S ribosomal protein S29-A

Chain D9:



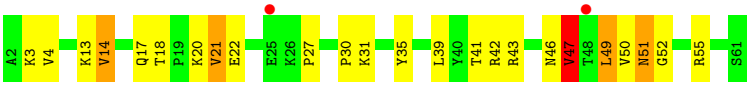
• Molecule 31: 40S ribosomal protein S29-A

Chain d9:

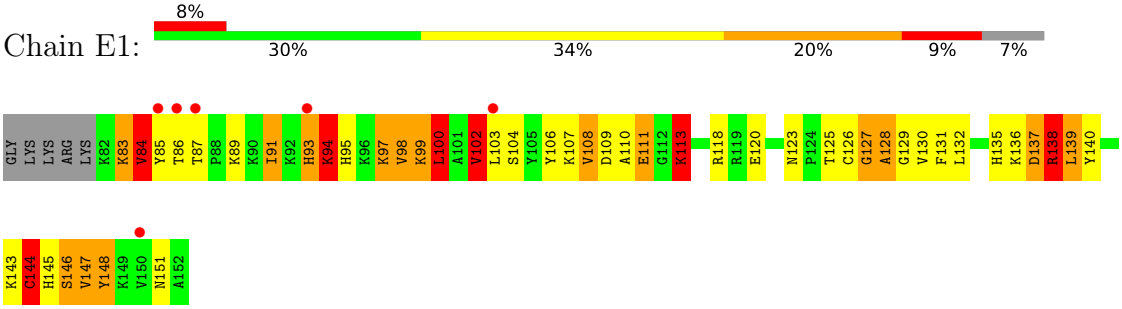


• Molecule 32: 40S ribosomal protein S30-A

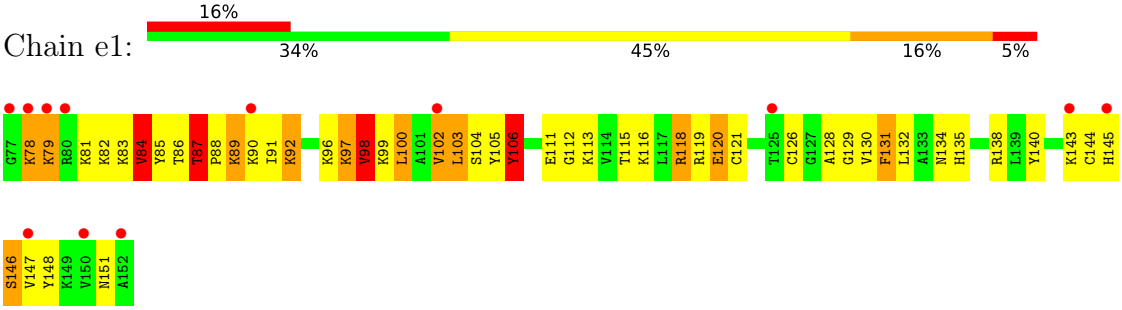
Chain E0:



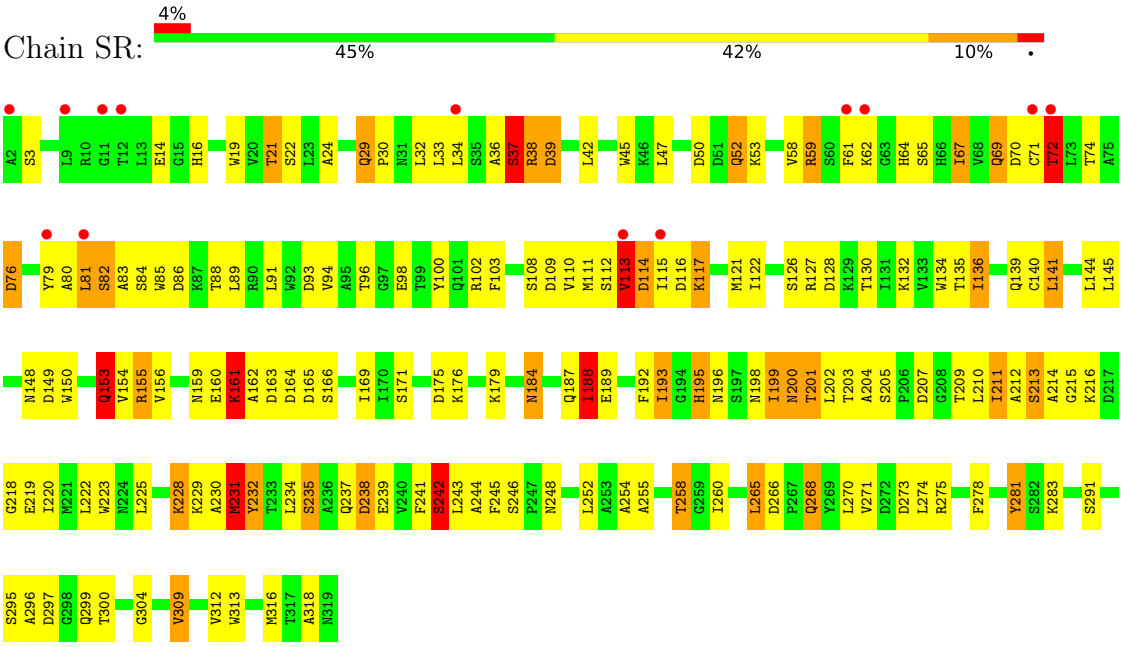
• Molecule 33: Ubiquitin-40S ribosomal protein S31



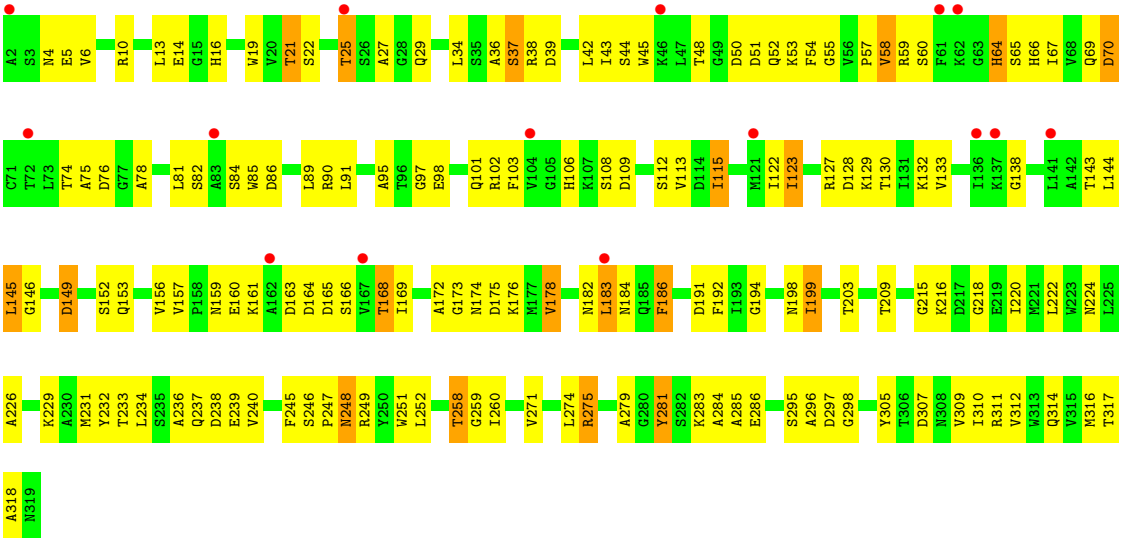
• Molecule 33: Ubiquitin-40S ribosomal protein S31



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

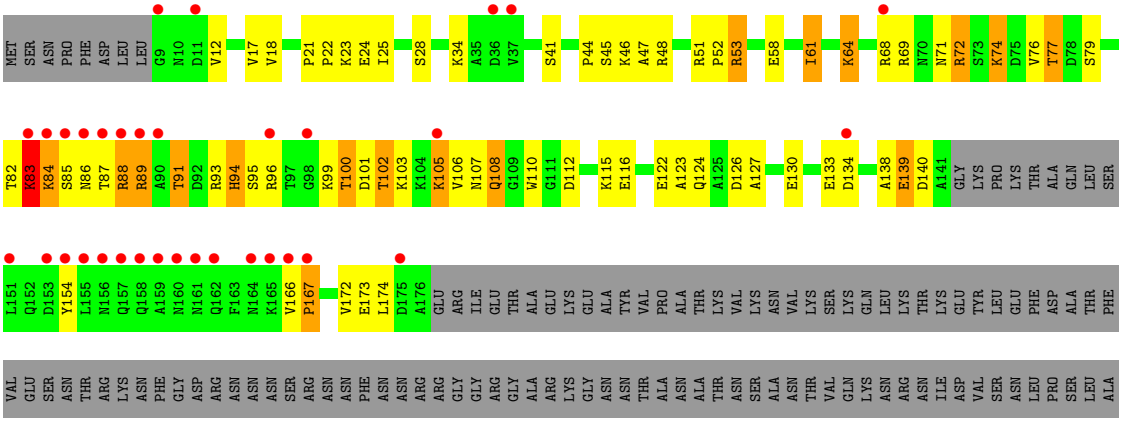


• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein



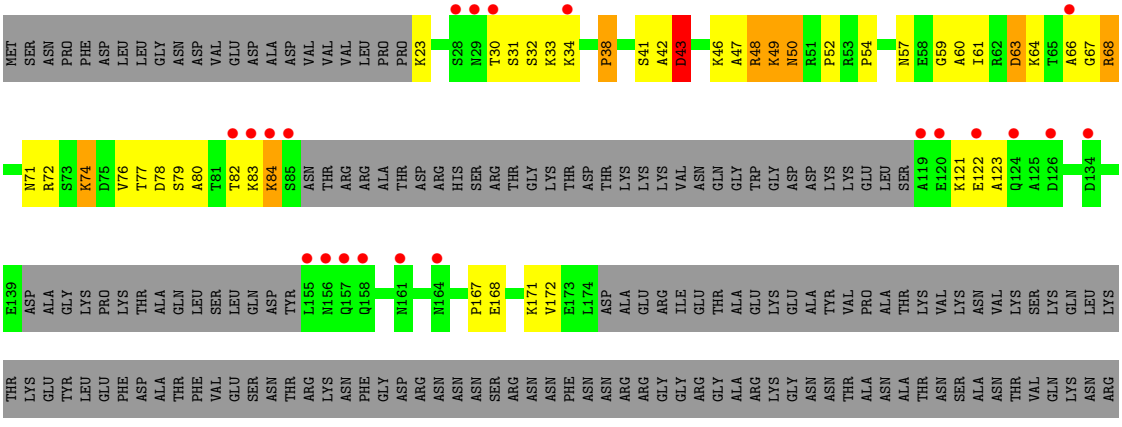
• Molecule 35: Suppressor protein STM1

Chain SM:



• Molecule 35: Suppressor protein STM1

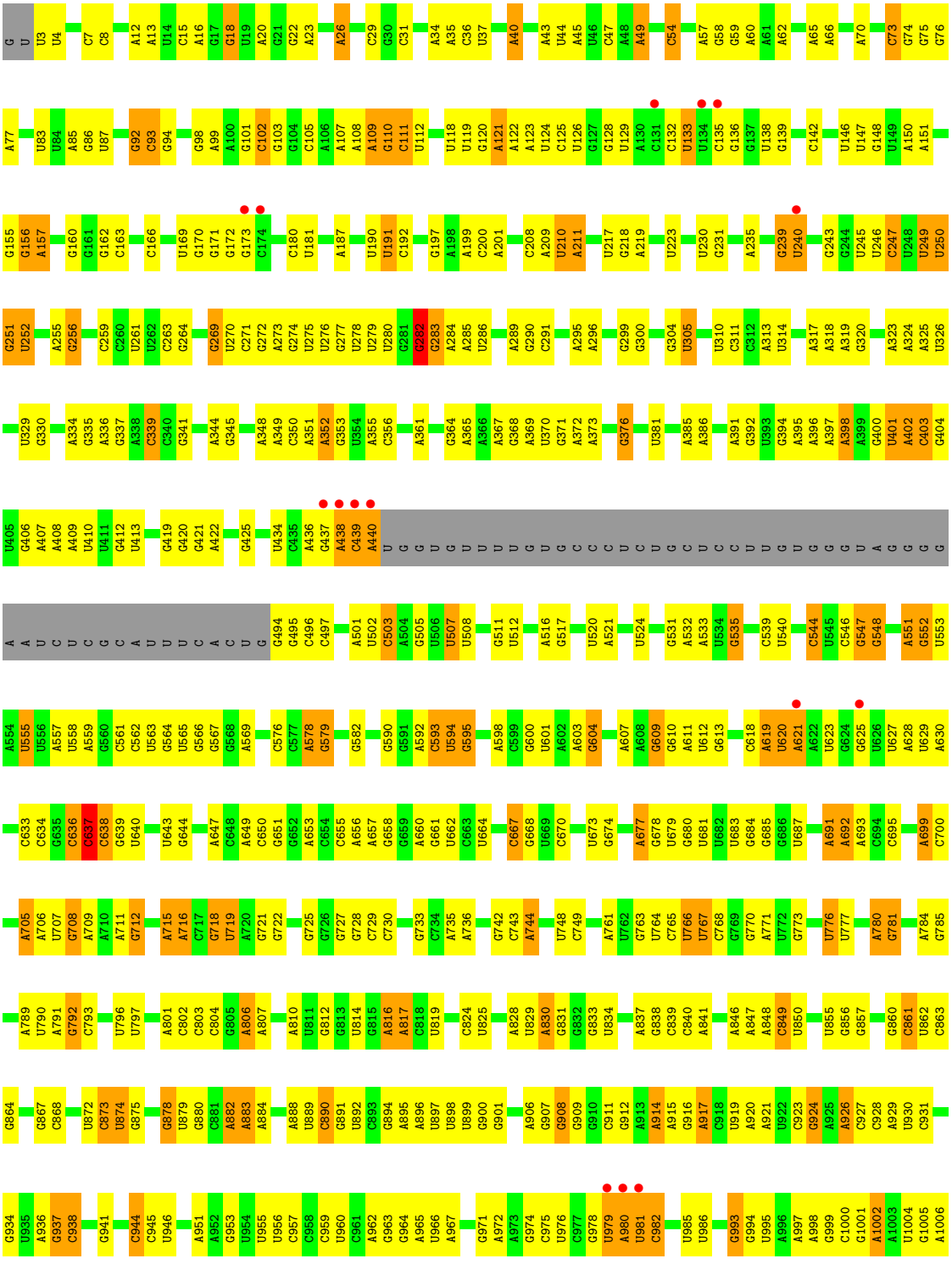
Chain sM:

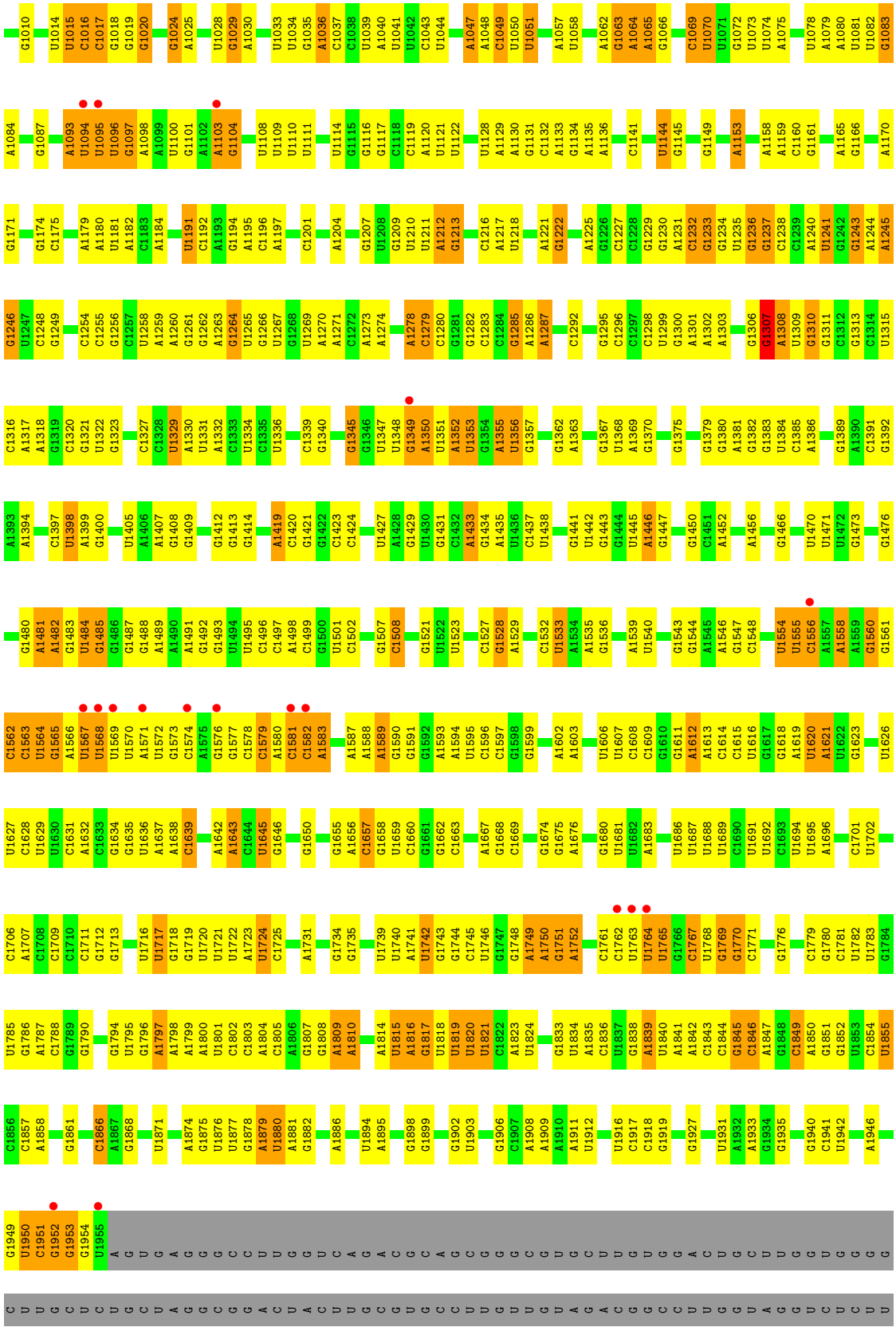


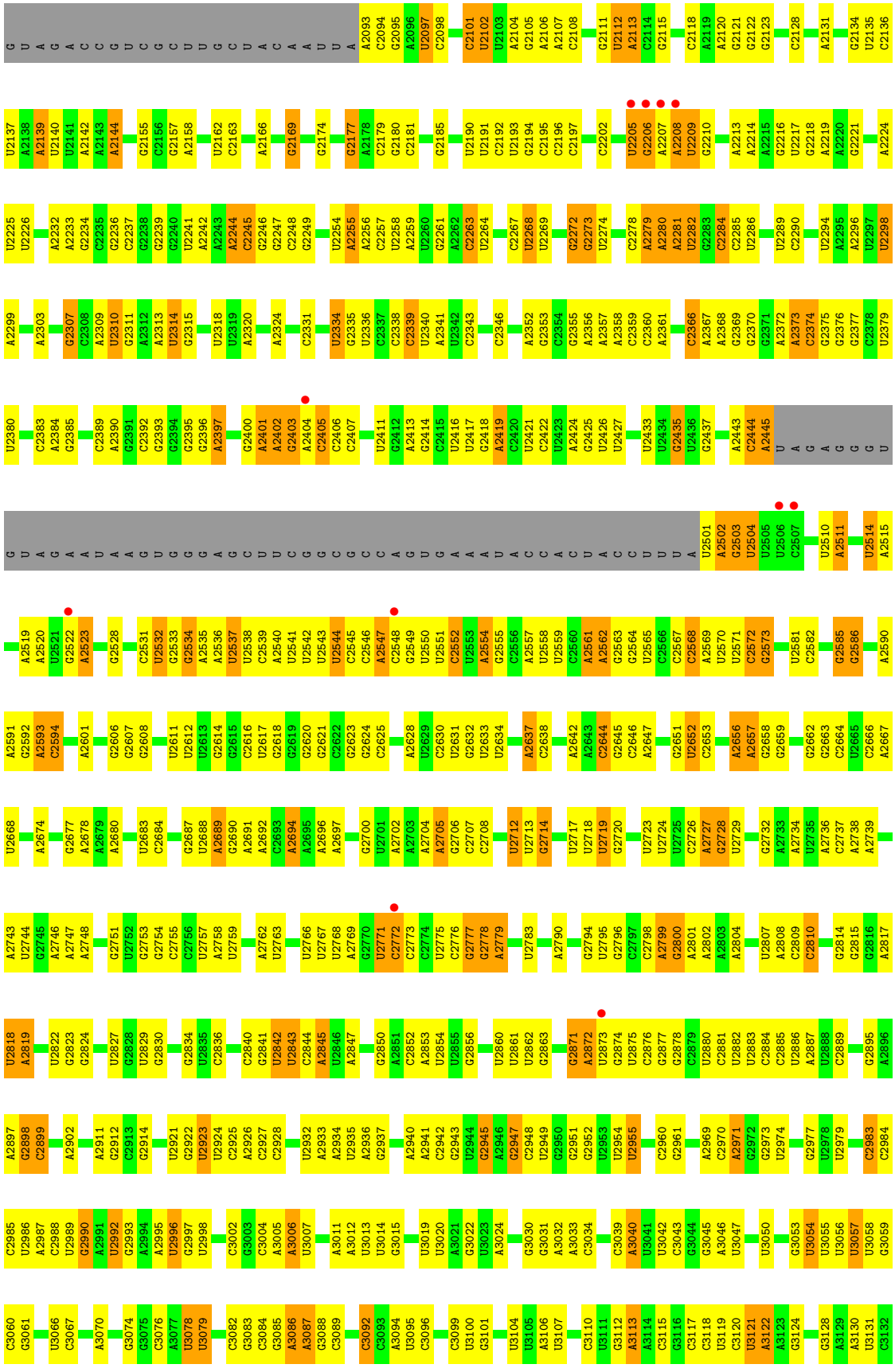
ASN
ILE
ASP
VAL
SER
ASN
LEU
PRO
SER
LEU
ALA

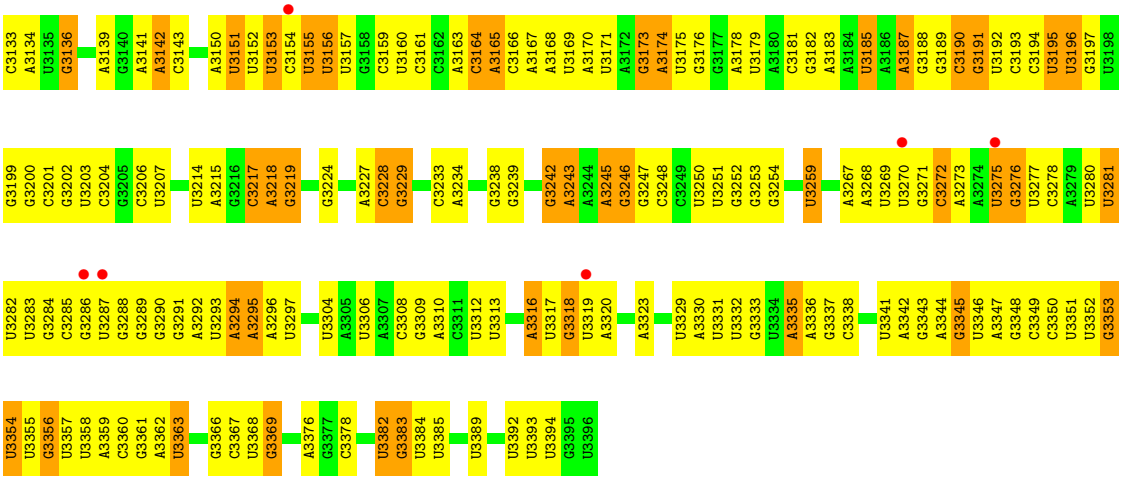
• Molecule 36: 25S ribosomal RNA

Chain 1:



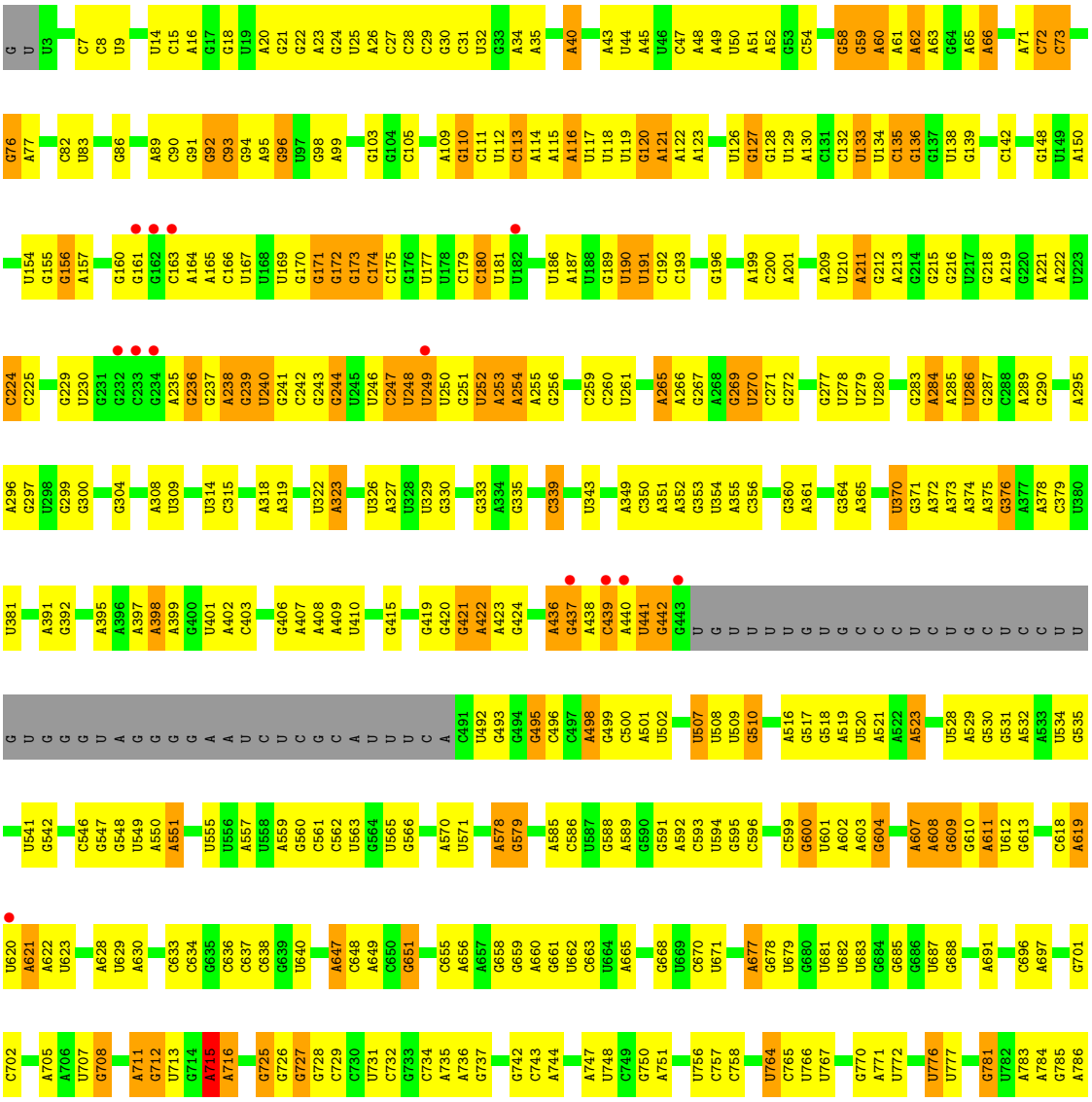


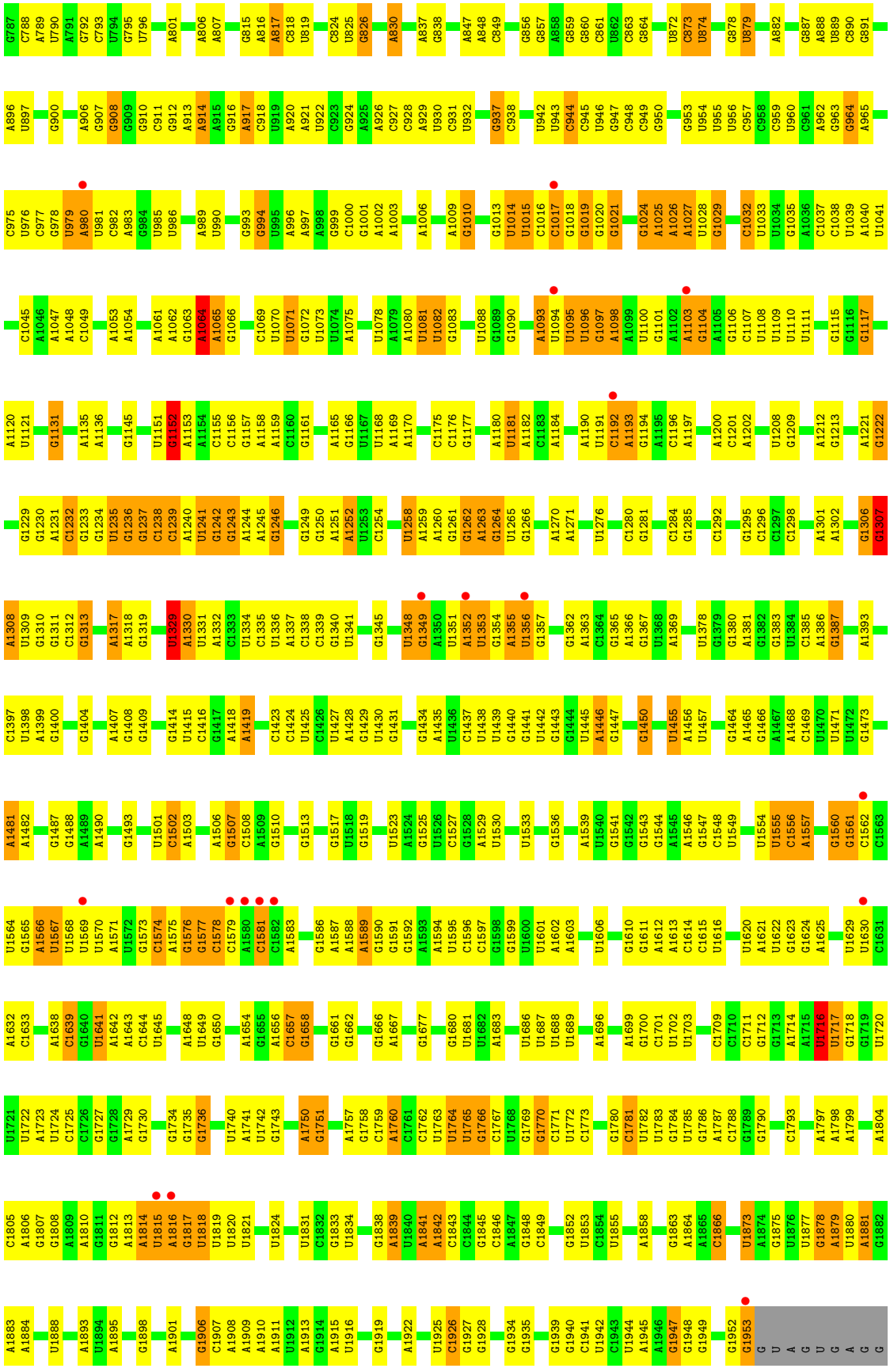


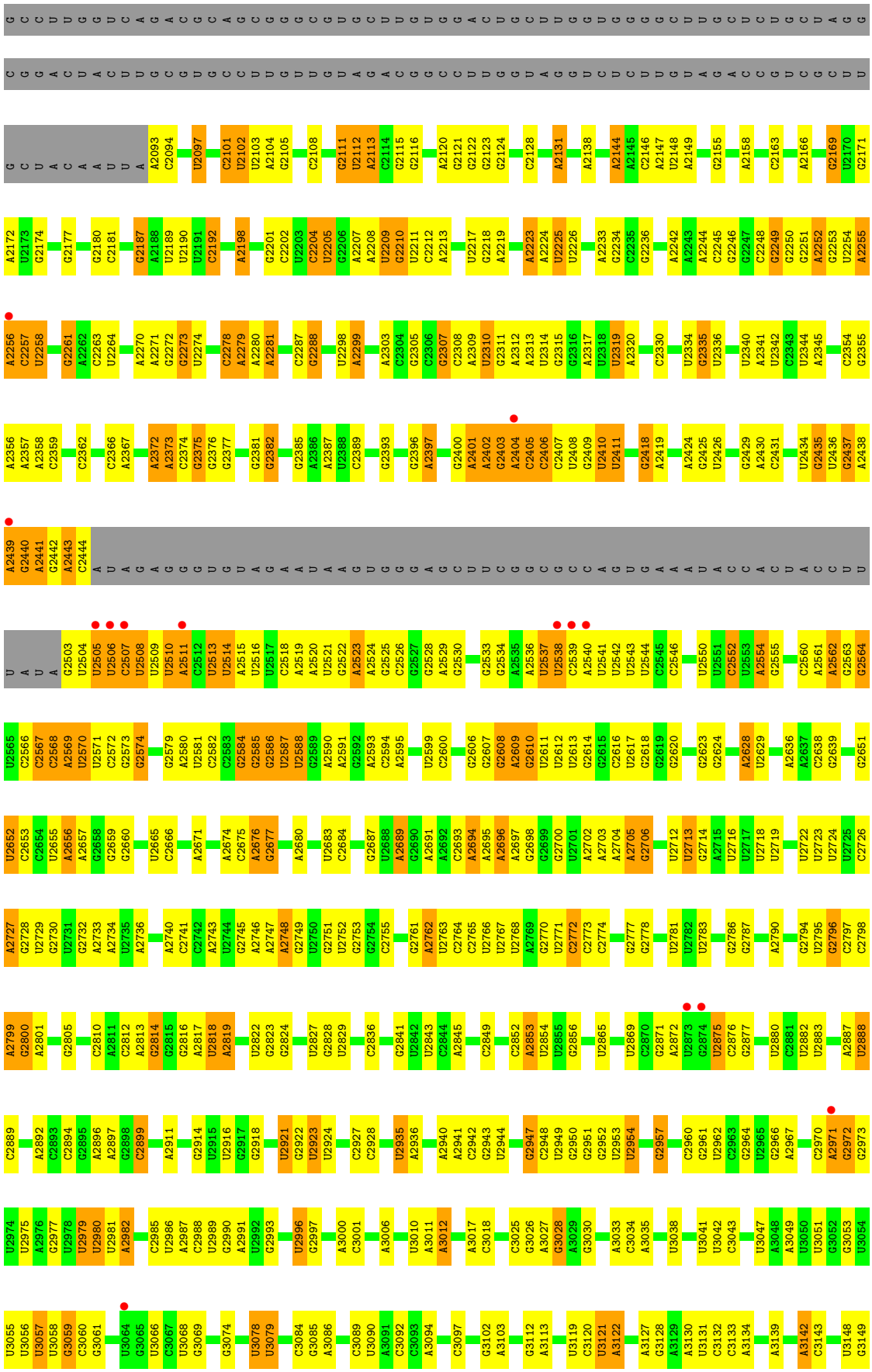


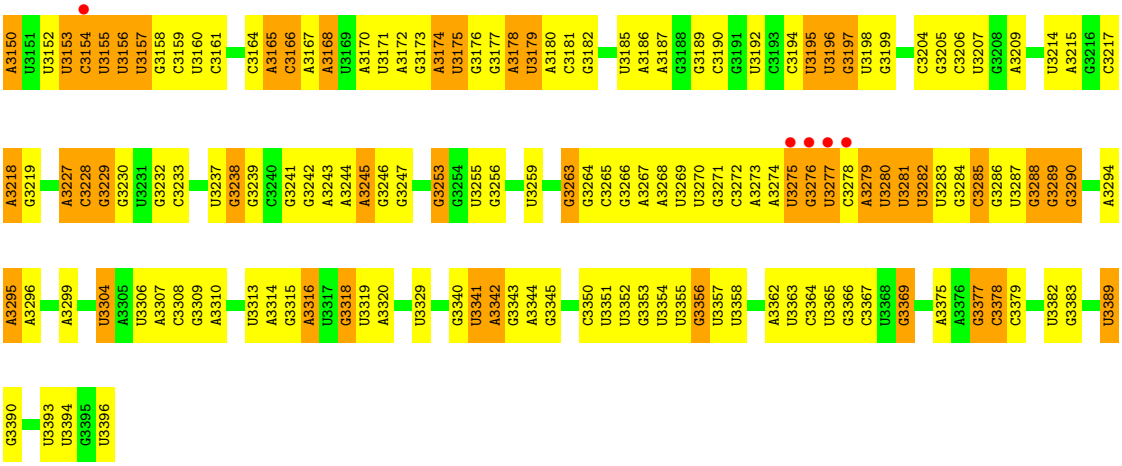
• Molecule 36: 25S ribosomal RNA

Chain 5:



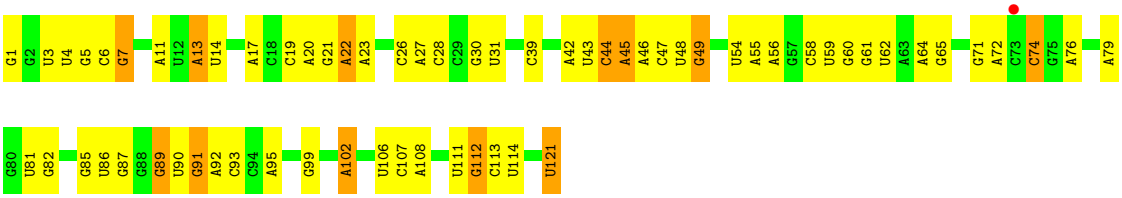






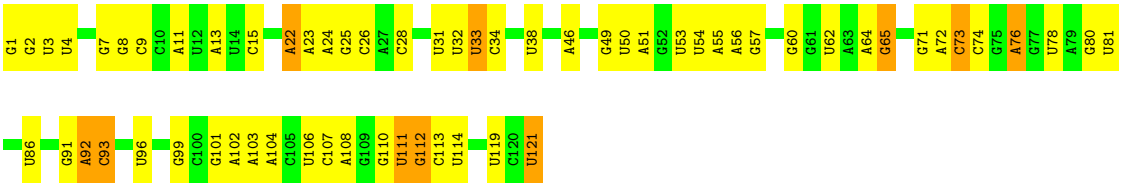
• Molecule 37: 5S ribosomal RNA

Chain 3:



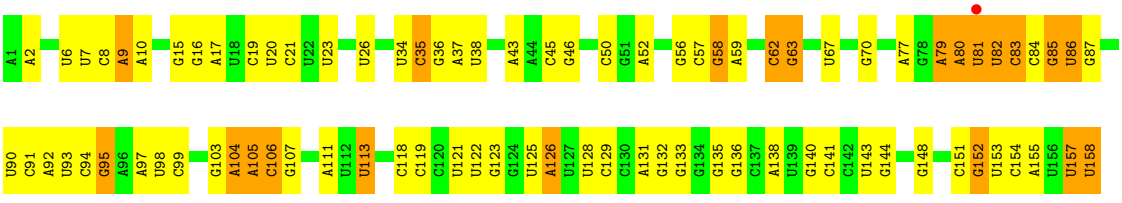
• Molecule 37: 5S ribosomal RNA

Chain 7:



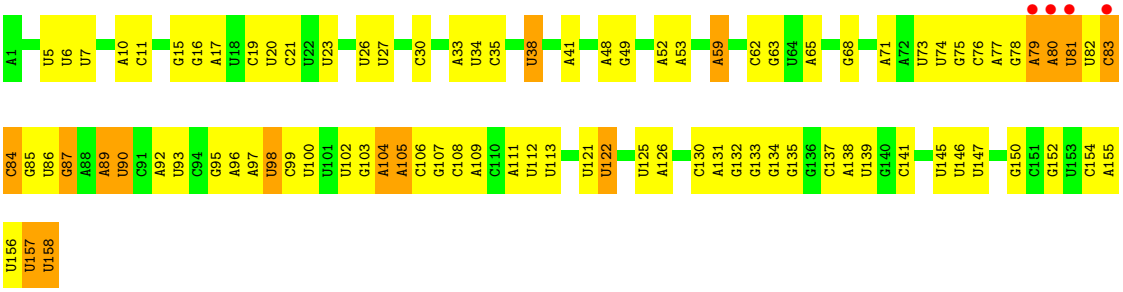
• Molecule 38: 5.8S ribosomal RNA

Chain 4:



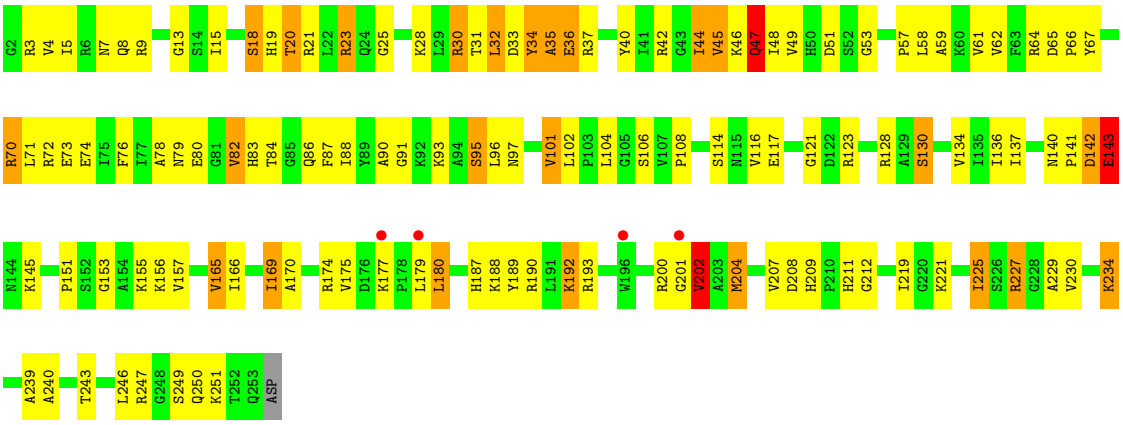
• Molecule 38: 5.8S ribosomal RNA

Chain 8:



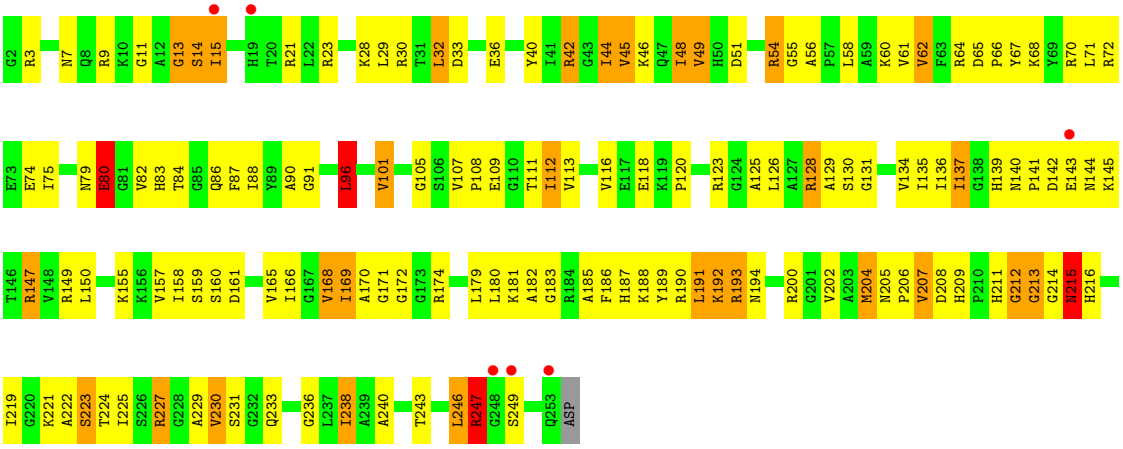
• Molecule 39: 60S ribosomal protein L2-A

Chain L2:



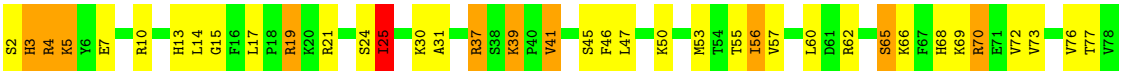
• Molecule 39: 60S ribosomal protein L2-A

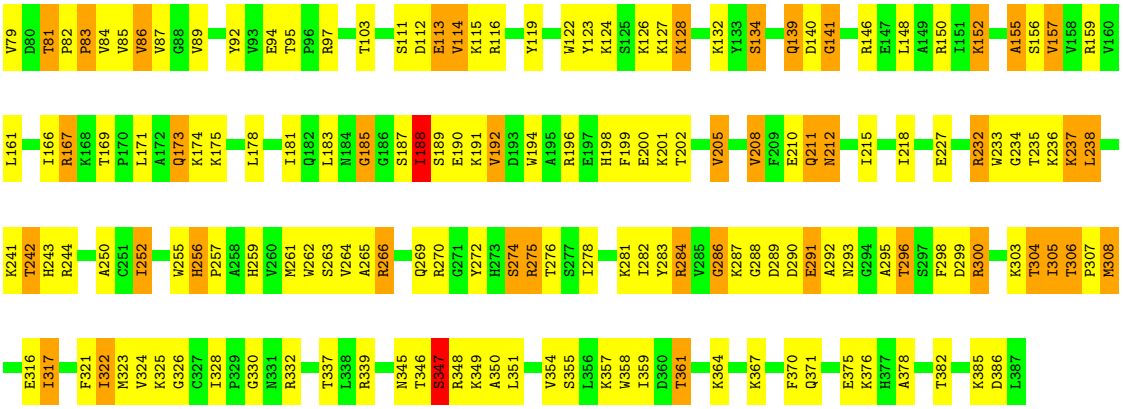
Chain l2:



• Molecule 40: 60S ribosomal protein L3

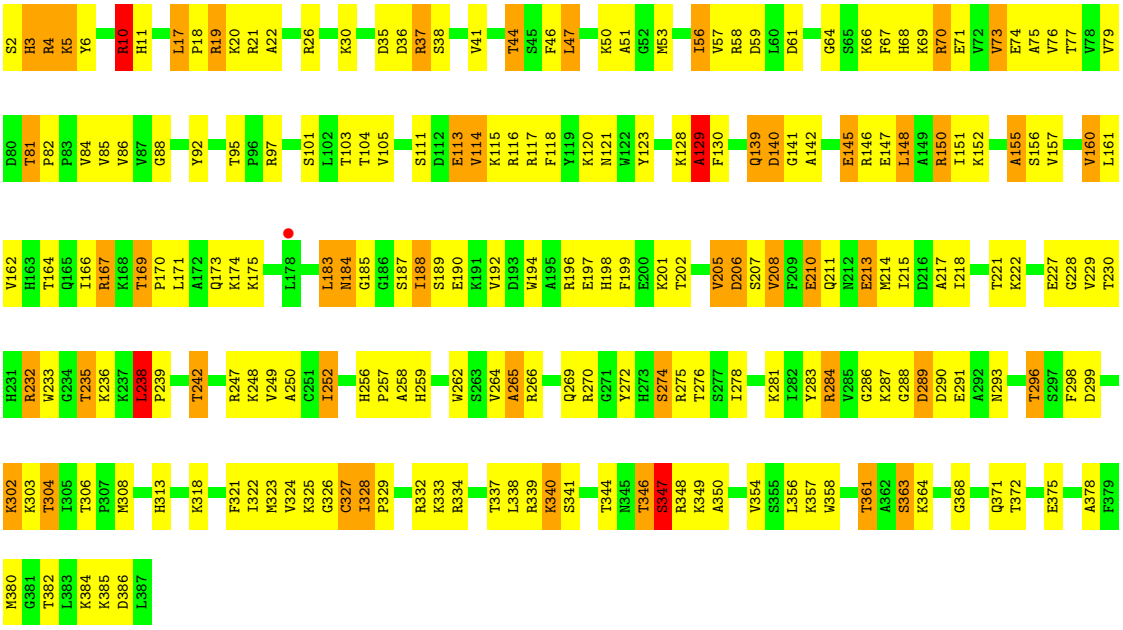
Chain L3:





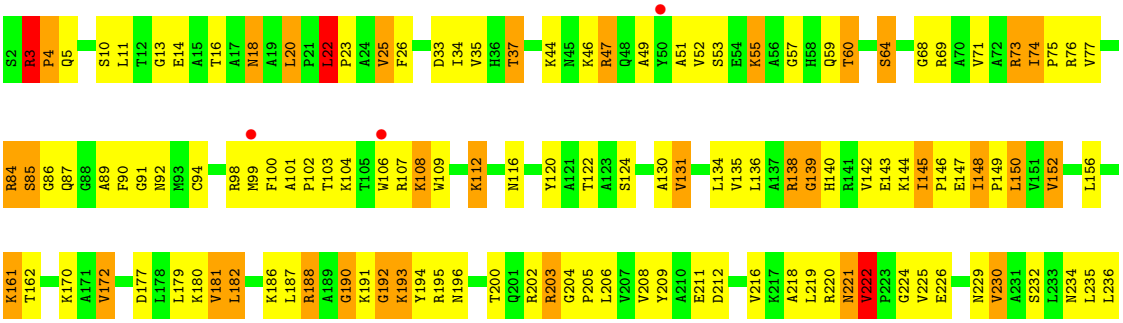
• Molecule 40: 60S ribosomal protein L3

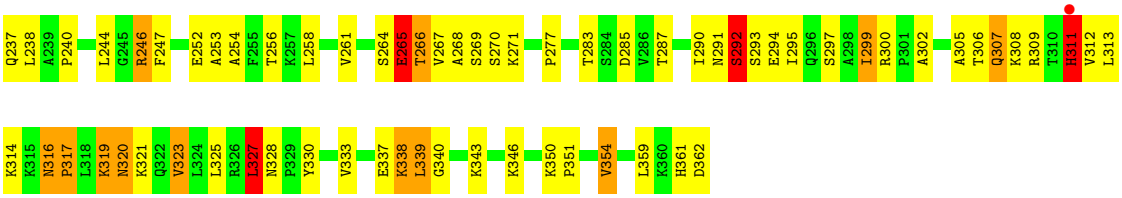
Chain l3:



• Molecule 41: 60S ribosomal protein L4-A

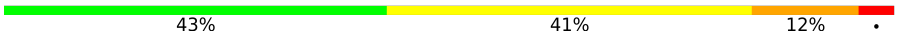
Chain L4:

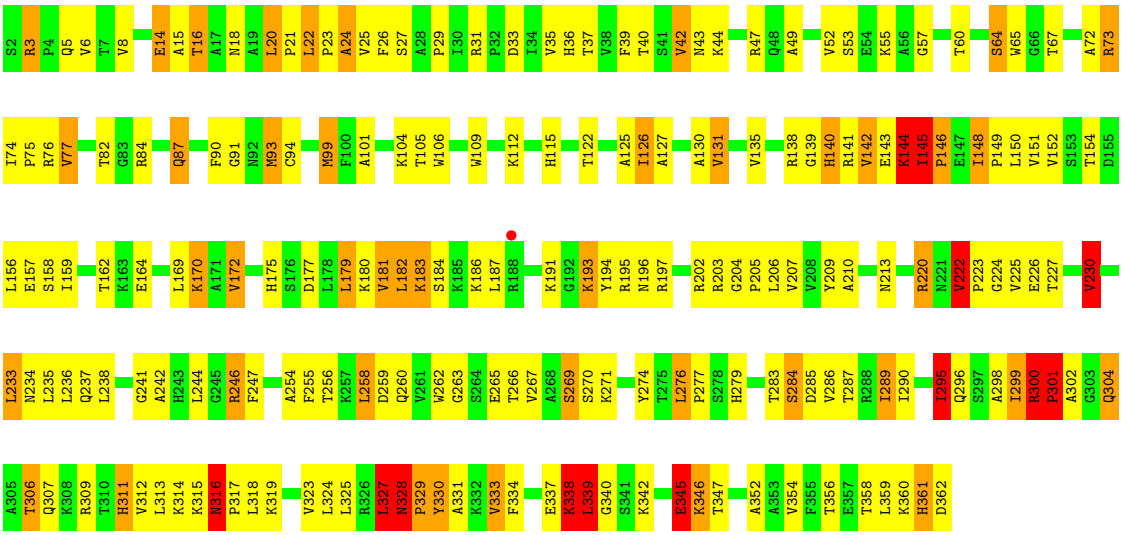




• Molecule 41: 60S ribosomal protein L4-A

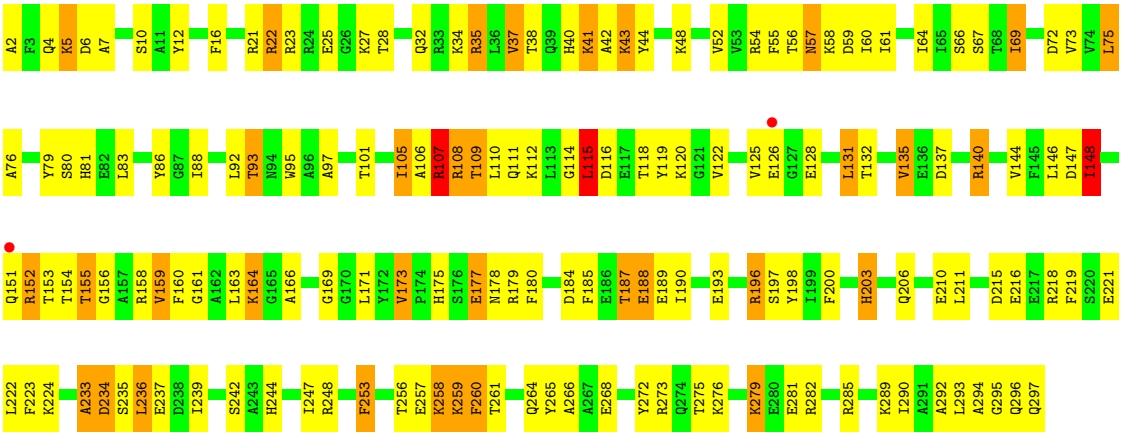
Chain l4:





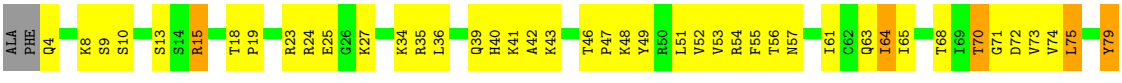
• Molecule 42: 60S ribosomal protein L5

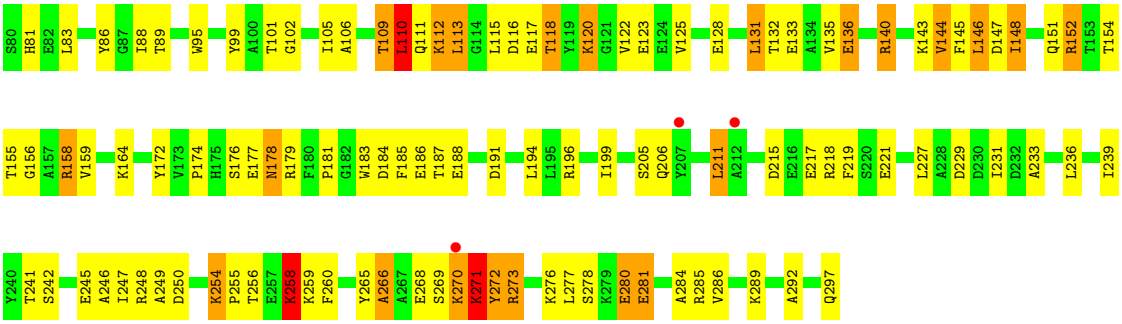
Chain L5:



• Molecule 42: 60S ribosomal protein L5

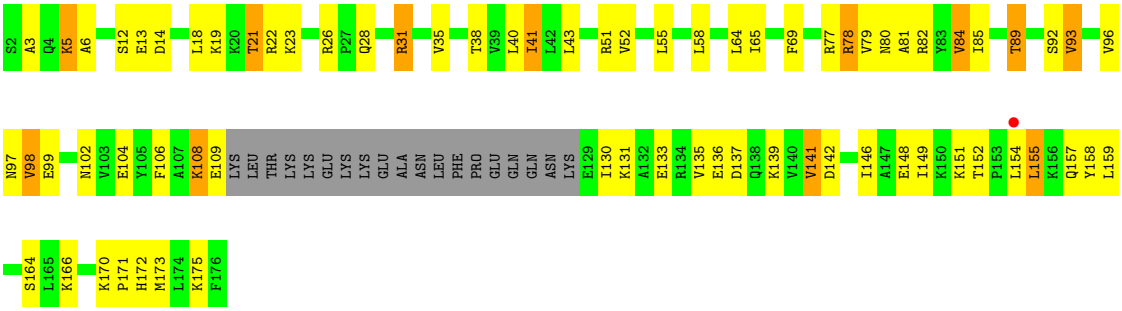
Chain l5:





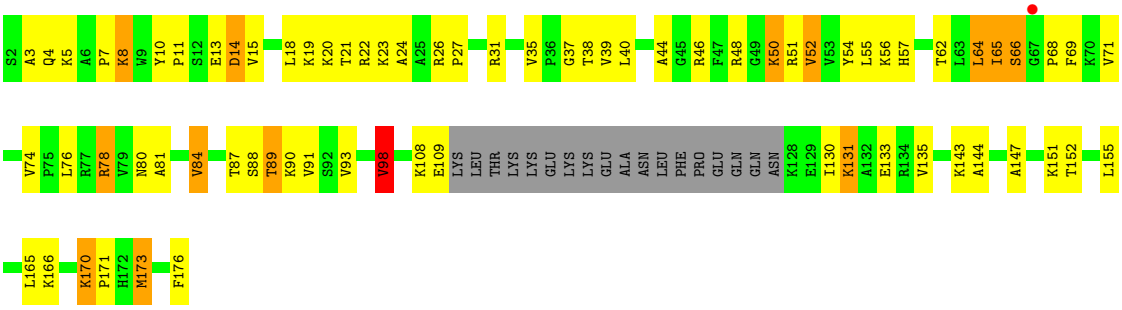
• Molecule 43: 60S ribosomal protein L6-A

Chain L6:



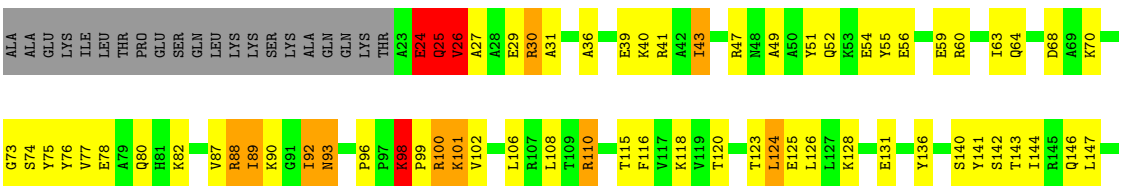
• Molecule 43: 60S ribosomal protein L6-A

Chain l6:



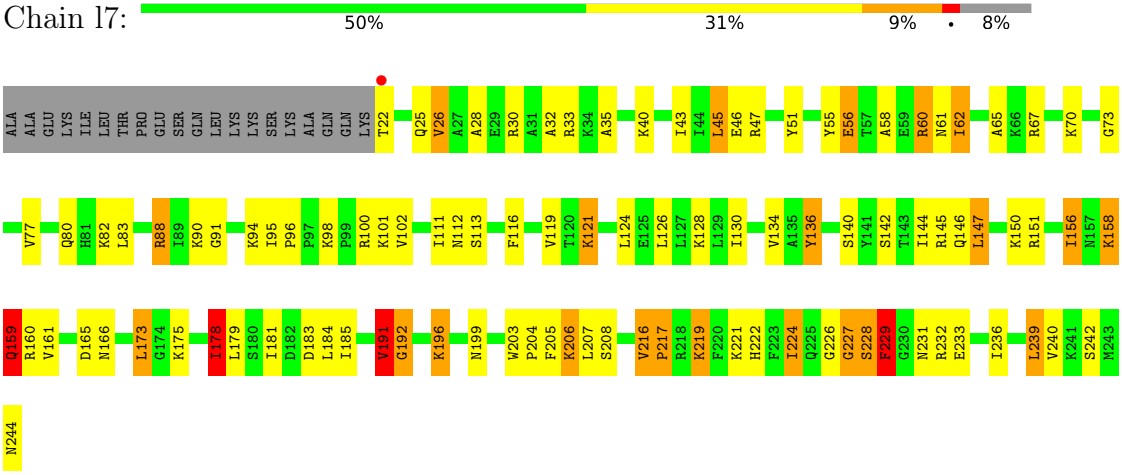
• Molecule 44: 60S ribosomal protein L7-A

Chain L7:



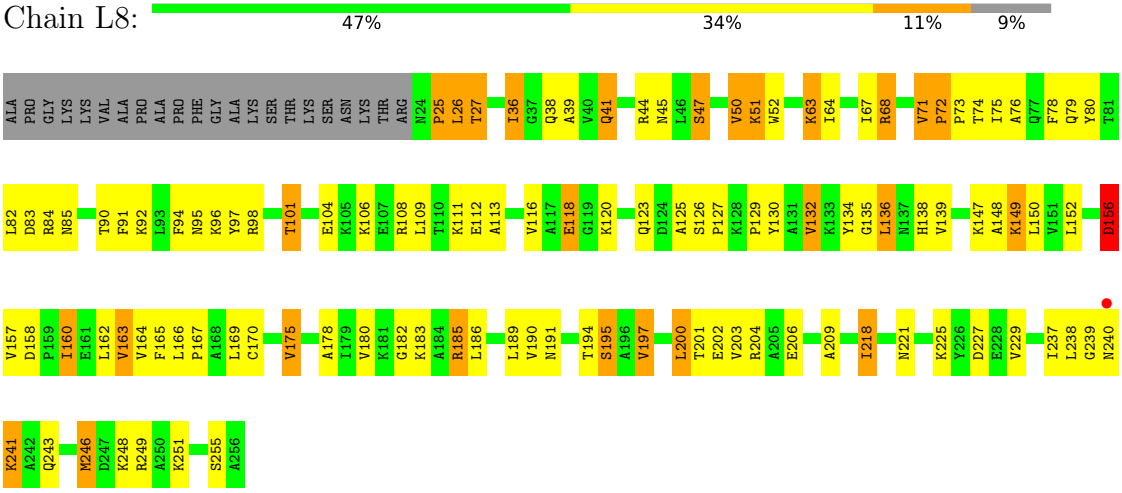
• Molecule 44: 60S ribosomal protein L7-A

Chain l7:



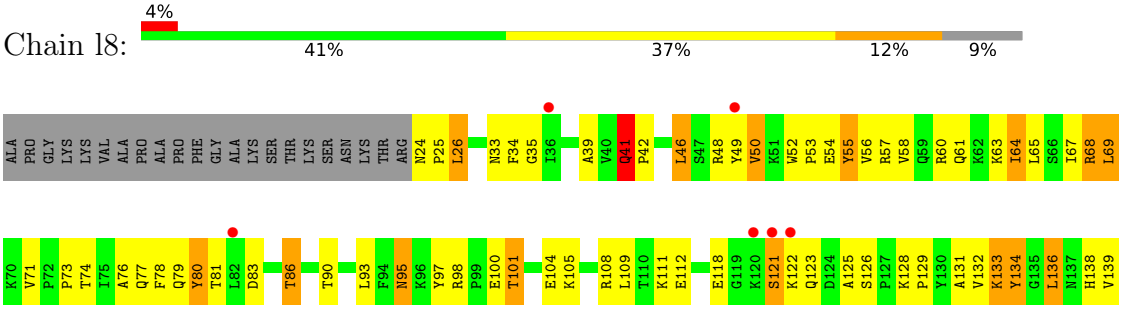
• Molecule 45: 60S ribosomal protein L8-A

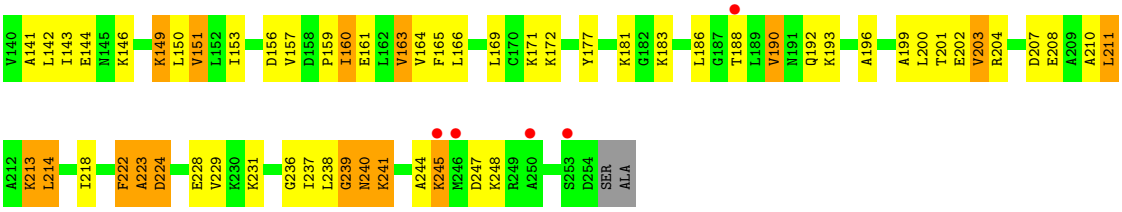
Chain L8:



• Molecule 45: 60S ribosomal protein L8-A

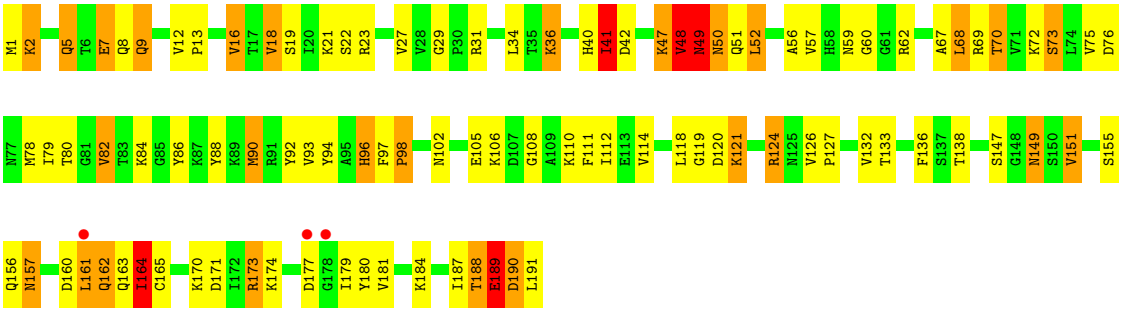
Chain l8:





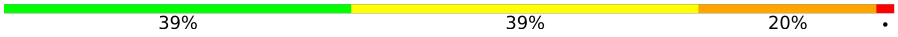
• Molecule 46: 60S ribosomal protein L9-A

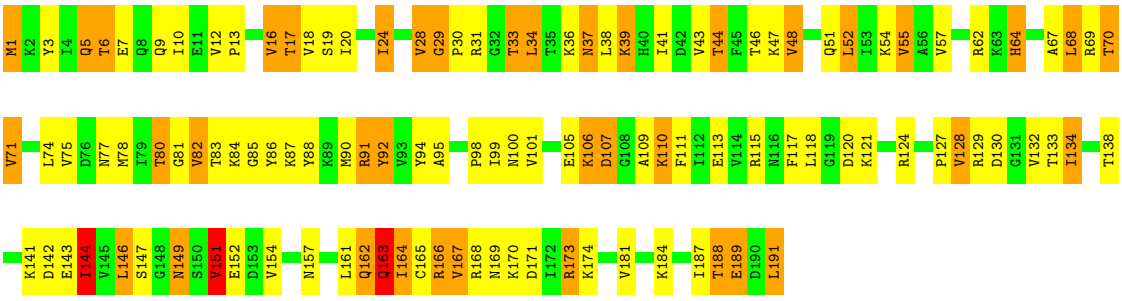
Chain L9:



• Molecule 46: 60S ribosomal protein L9-A

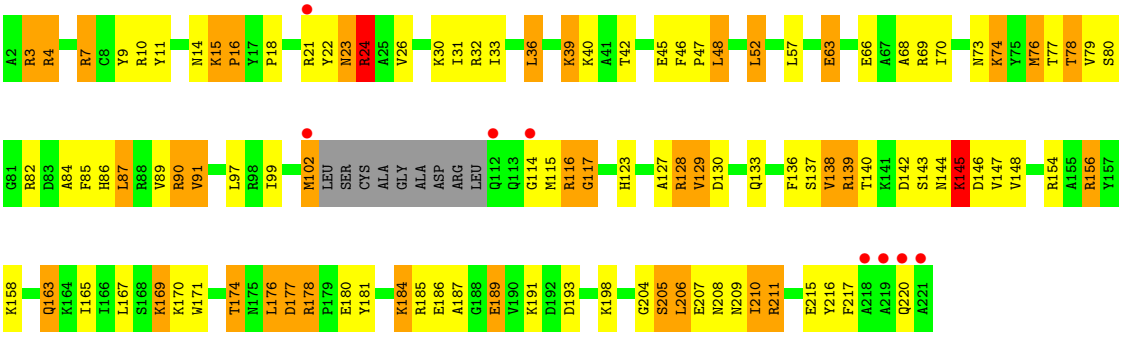
Chain l9:





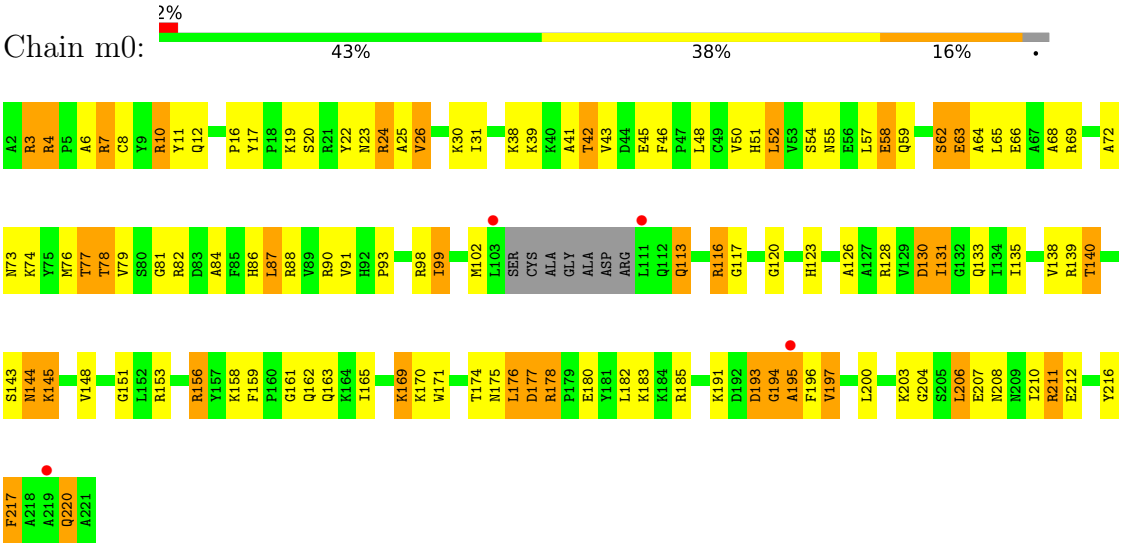
• Molecule 47: 60S ribosomal protein L10

Chain M0:



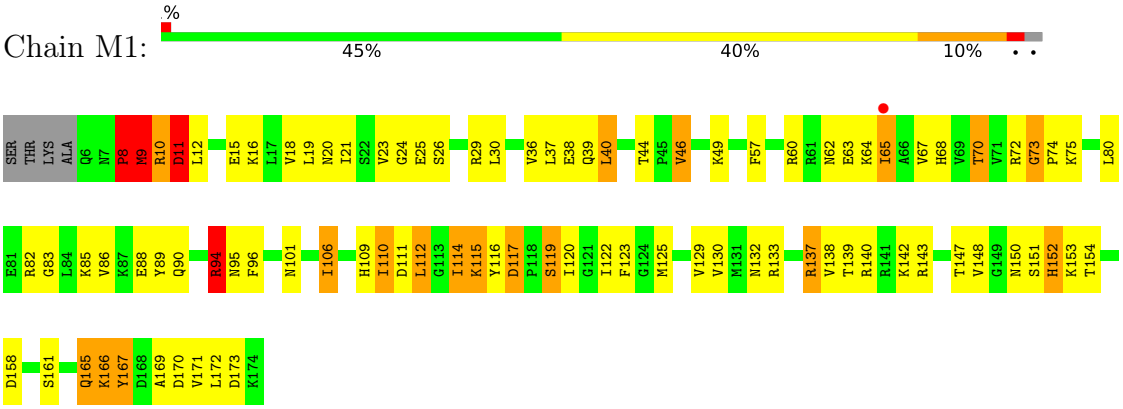
• Molecule 47: 60S ribosomal protein L10

Chain m0:



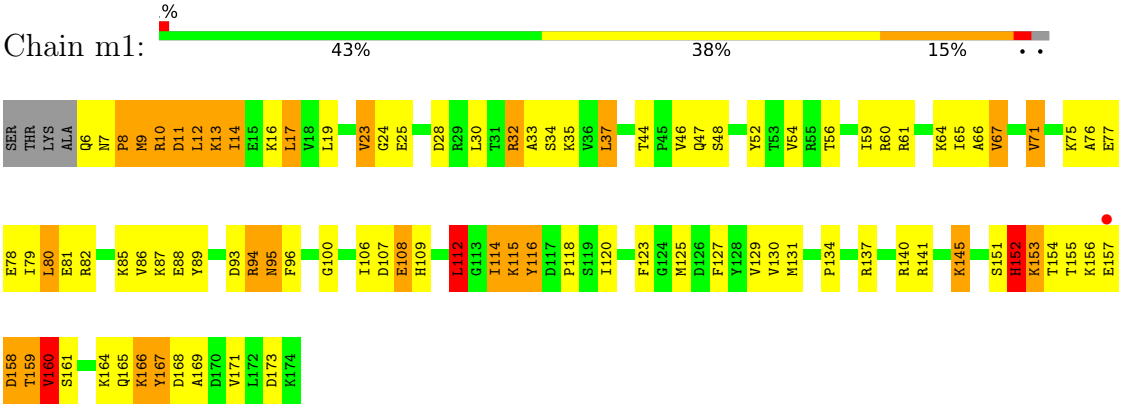
• Molecule 48: 60S ribosomal protein L11-B

Chain M1:



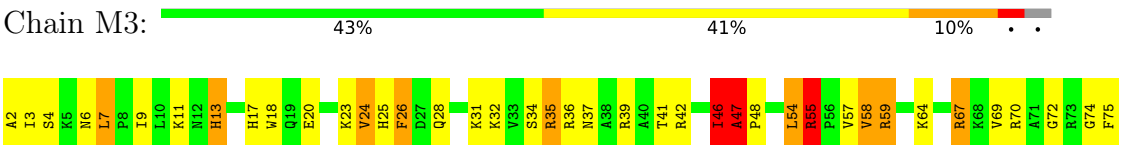
• Molecule 48: 60S ribosomal protein L11-B

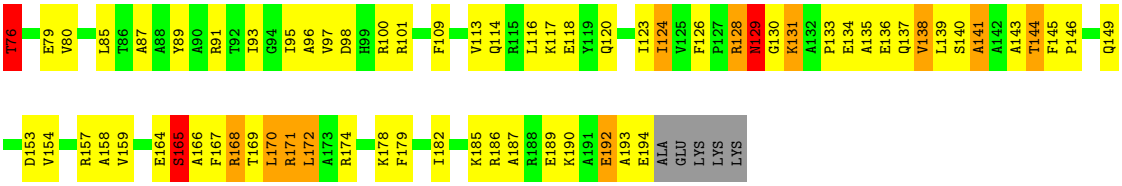
Chain m1:



• Molecule 49: 60S ribosomal protein L13-A

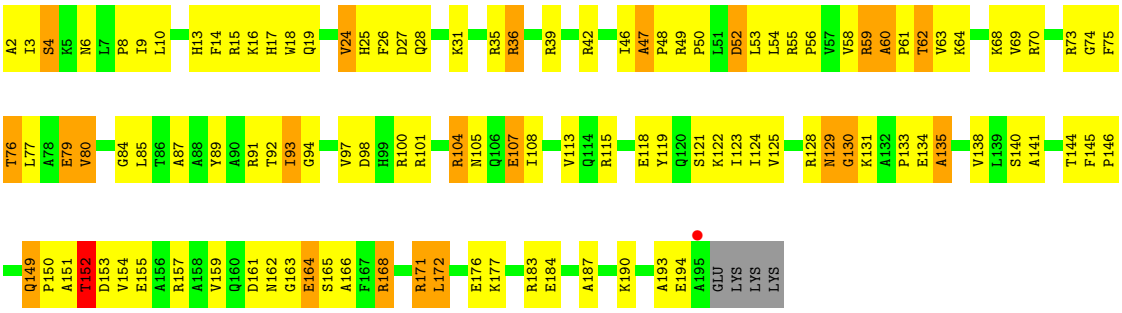
Chain M3:





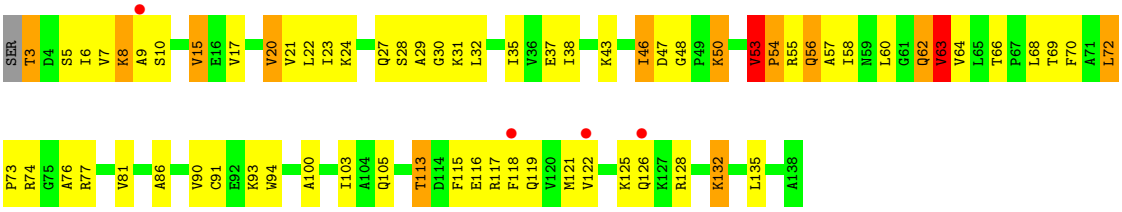
• Molecule 49: 60S ribosomal protein L13-A

Chain m3:



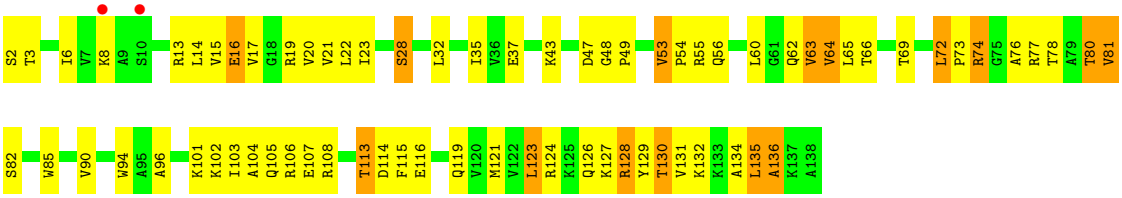
• Molecule 50: 60S ribosomal protein L14-A

Chain M4:



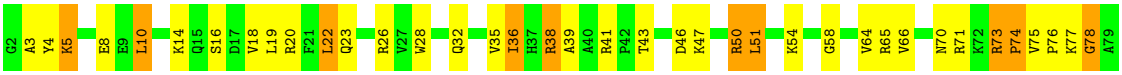
• Molecule 50: 60S ribosomal protein L14-A

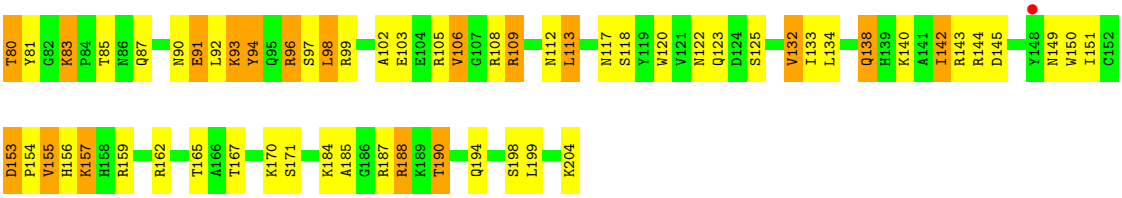
Chain m4:



• Molecule 51: 60S ribosomal protein L15-A

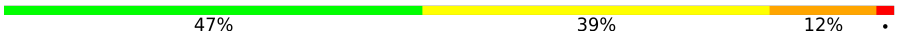
Chain M5:

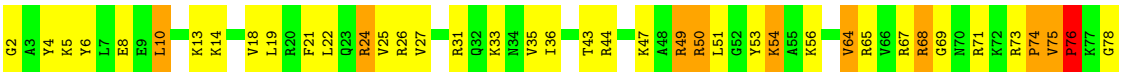


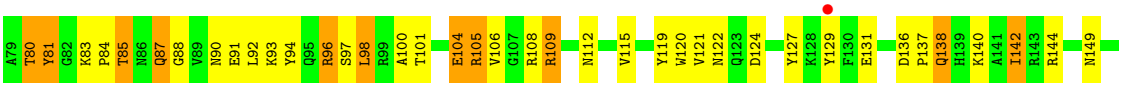


• Molecule 51: 60S ribosomal protein L15-A

Chain m5:

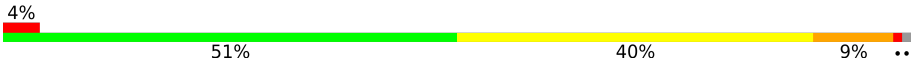


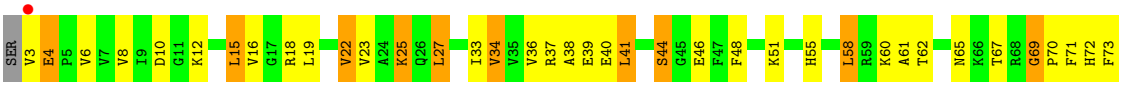


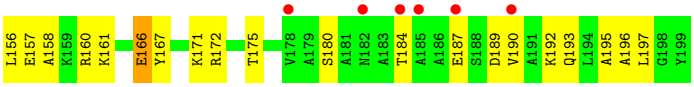


• Molecule 52: 60S ribosomal protein L16-A

Chain M6:

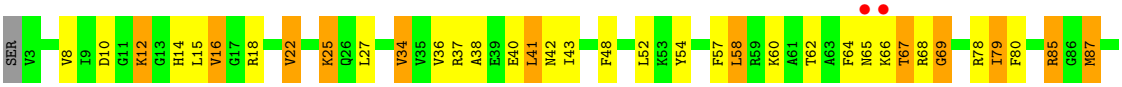


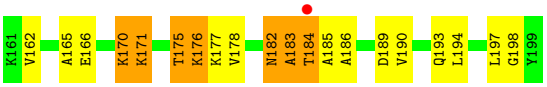




• Molecule 52: 60S ribosomal protein L16-A

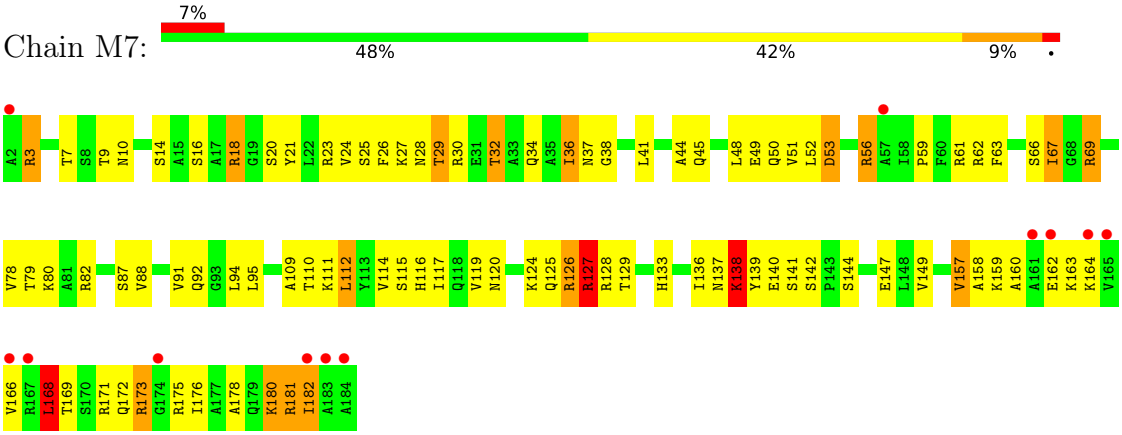
Chain m6:





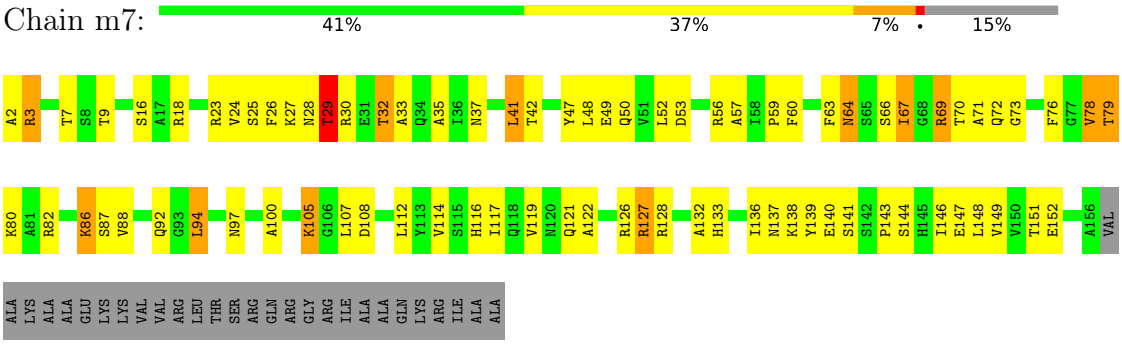
• Molecule 53: 60S ribosomal protein L17-A

Chain M7:



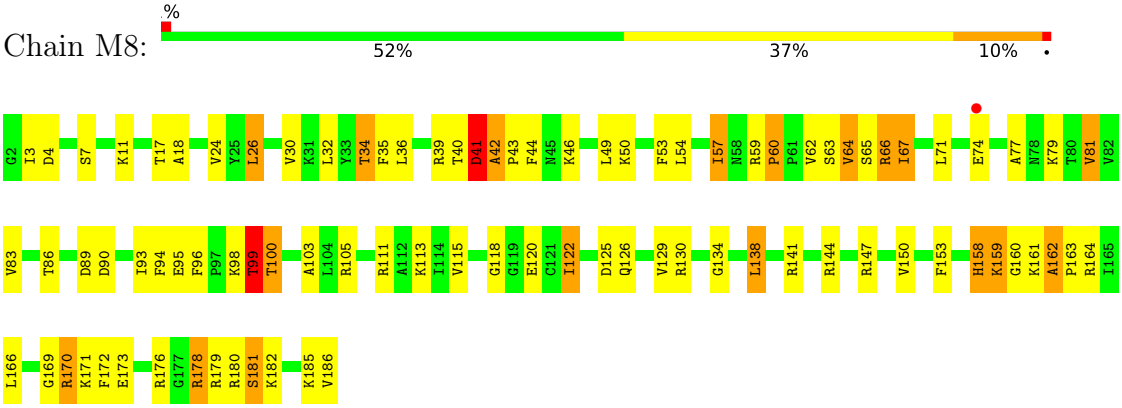
• Molecule 53: 60S ribosomal protein L17-A

Chain m7:



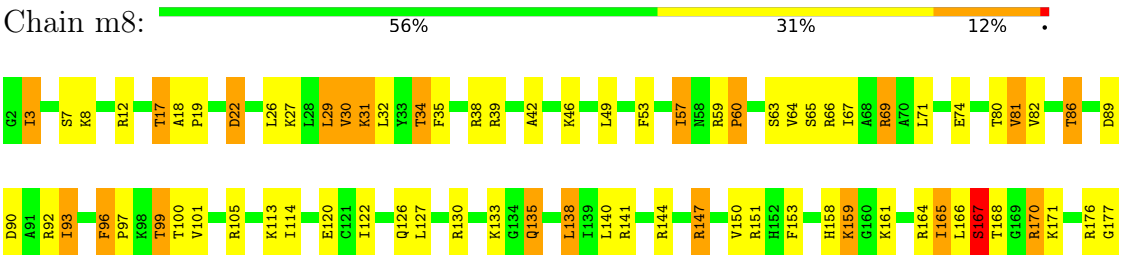
• Molecule 54: 60S ribosomal protein L18-A

Chain M8:



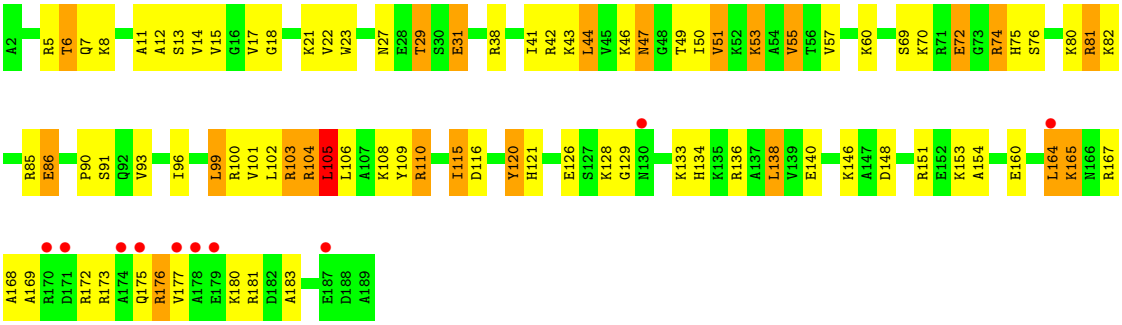
• Molecule 54: 60S ribosomal protein L18-A

Chain m8:



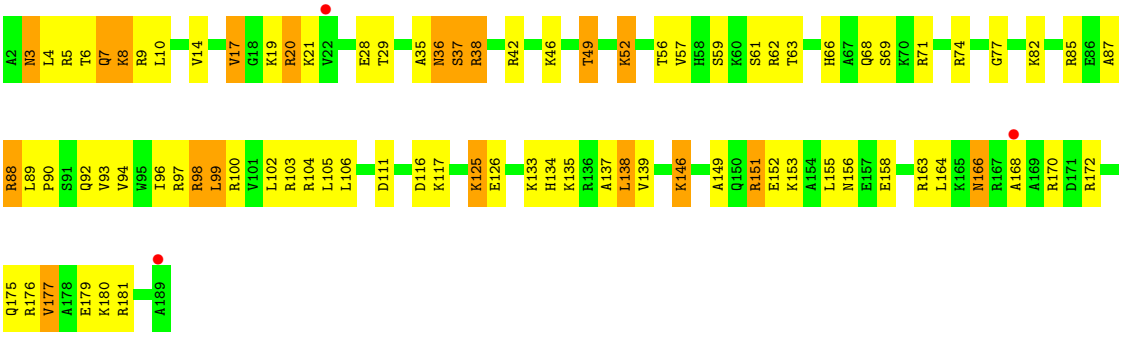
• Molecule 55: 60S ribosomal protein L19-A

Chain M9:



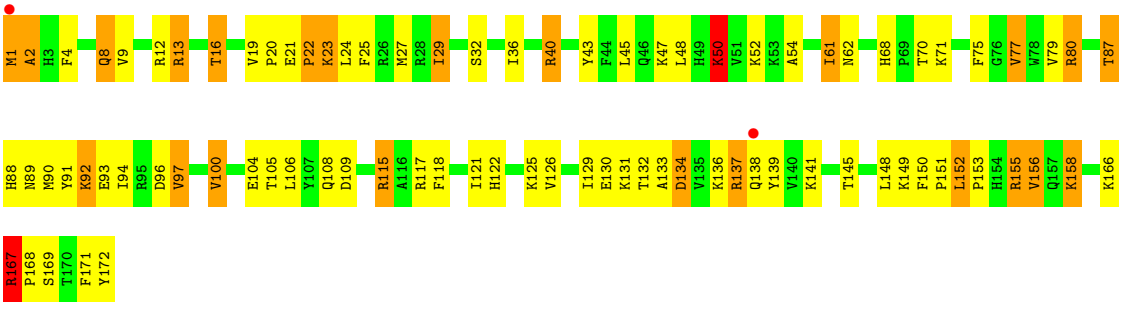
• Molecule 55: 60S ribosomal protein L19-A

Chain m9:



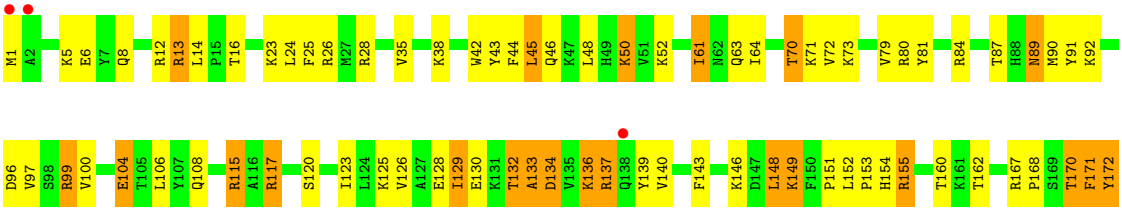
• Molecule 56: 60S ribosomal protein L20-A

Chain N0:



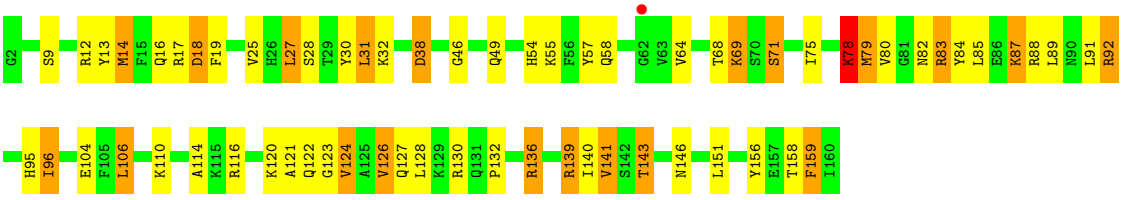
• Molecule 56: 60S ribosomal protein L20-A

Chain n0:



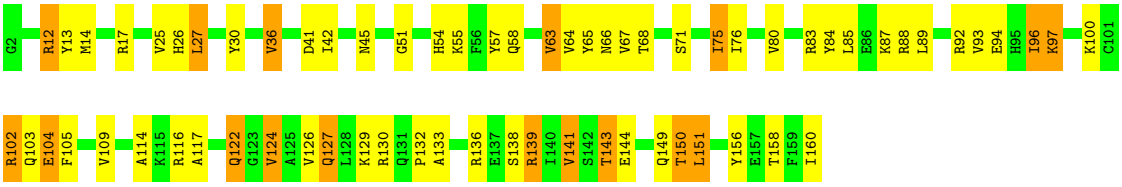
• Molecule 57: 60S ribosomal protein L21-A

Chain N1:



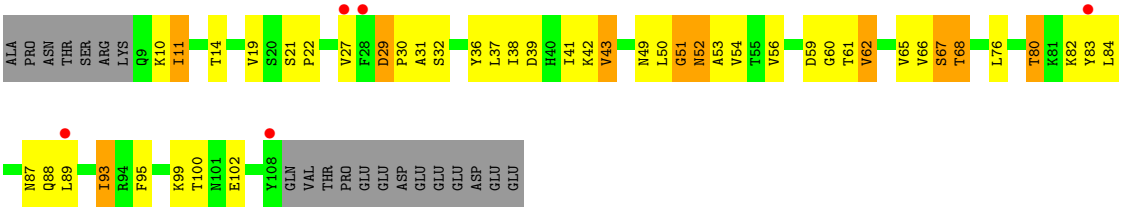
• Molecule 57: 60S ribosomal protein L21-A

Chain n1:



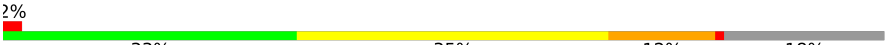
• Molecule 58: 60S ribosomal protein L22-A

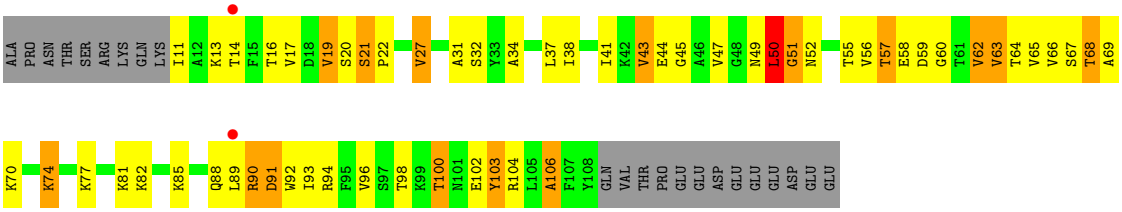
Chain N2:



• Molecule 58: 60S ribosomal protein L22-A

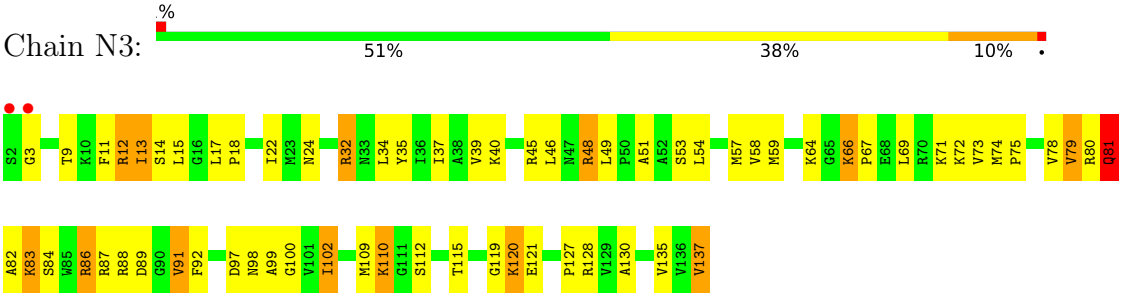
Chain n2:





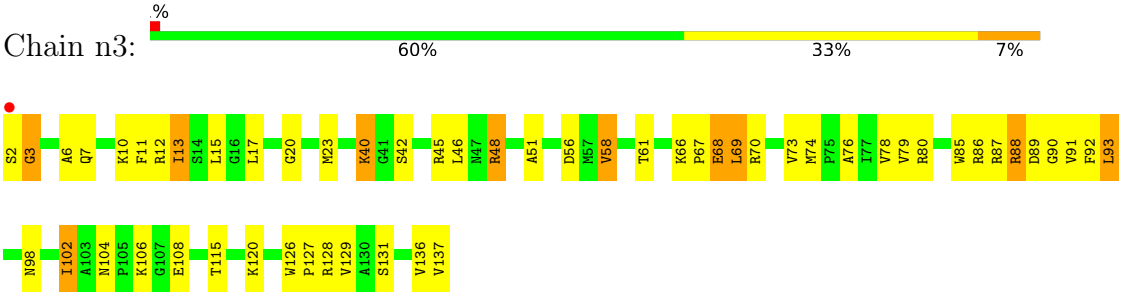
• Molecule 59: 60S ribosomal protein L23-A

Chain N3:



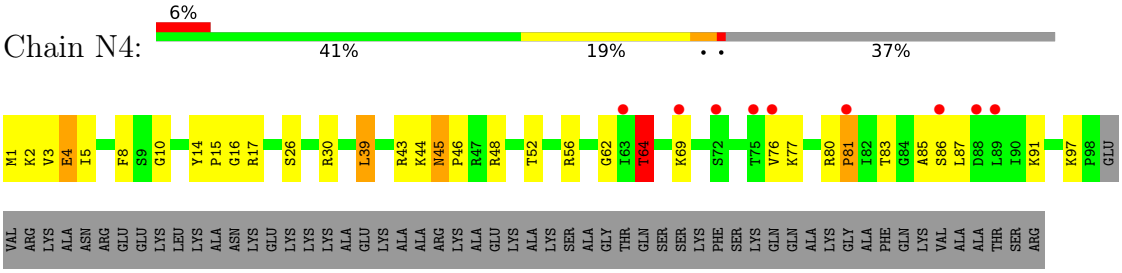
• Molecule 59: 60S ribosomal protein L23-A

Chain n3:



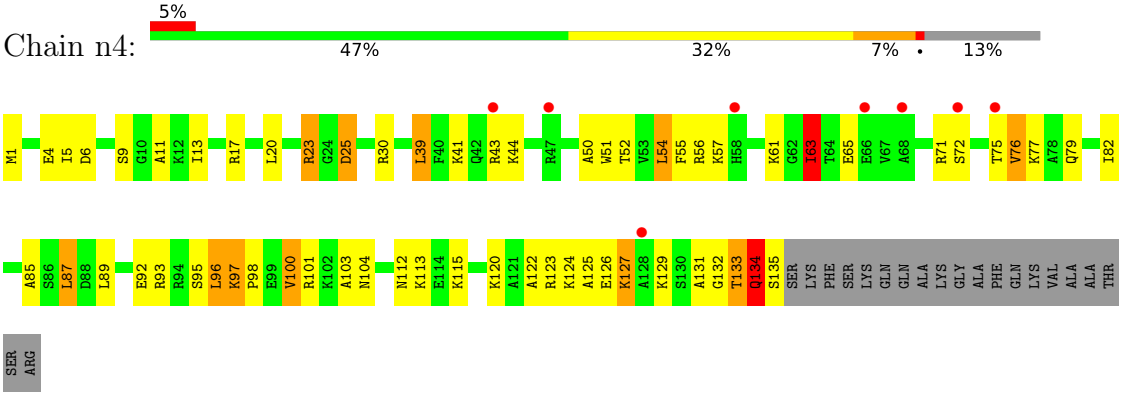
• Molecule 60: 60S ribosomal protein L24-A

Chain N4:



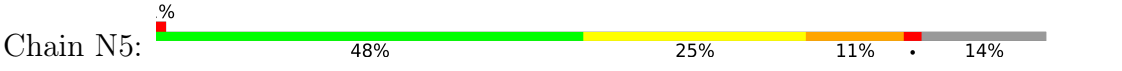
• Molecule 60: 60S ribosomal protein L24-A

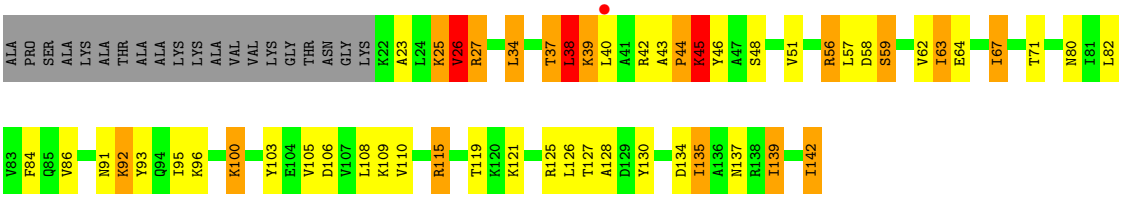
Chain n4:

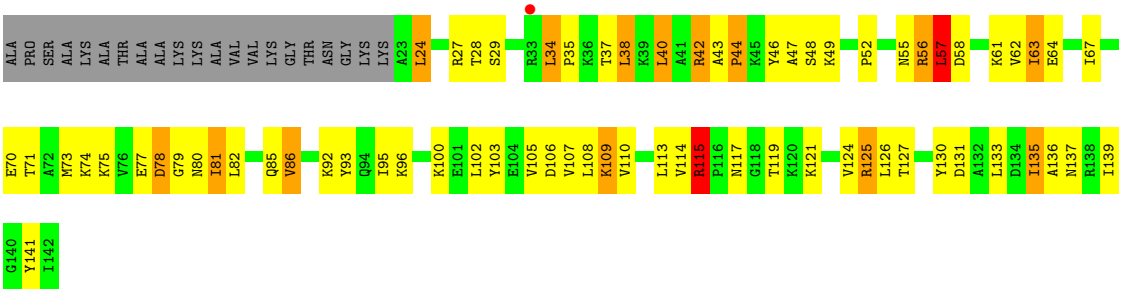


• Molecule 61: 60S ribosomal protein L25

Chain N5:

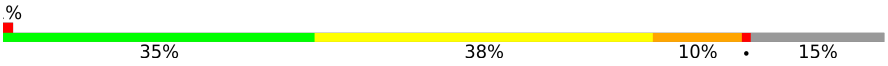






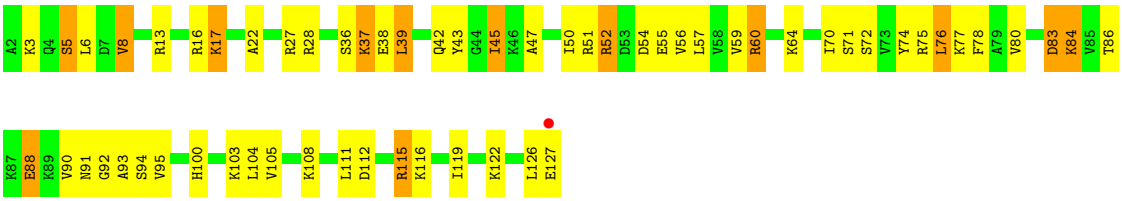
• Molecule 61: 60S ribosomal protein L25

Chain n5:



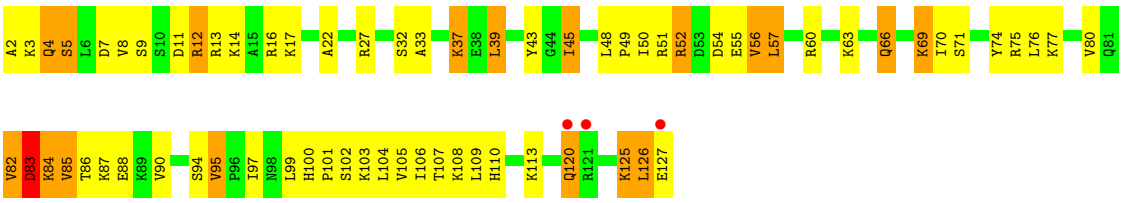
• Molecule 62: 60S ribosomal protein L26-A

Chain N6:



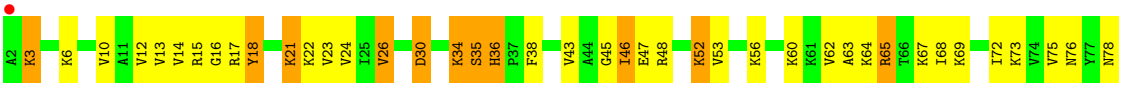
• Molecule 62: 60S ribosomal protein L26-A

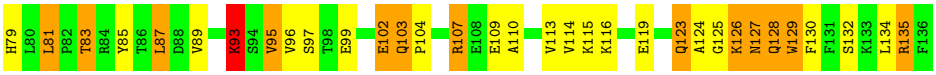
Chain n6:



• Molecule 63: 60S ribosomal protein L27-A

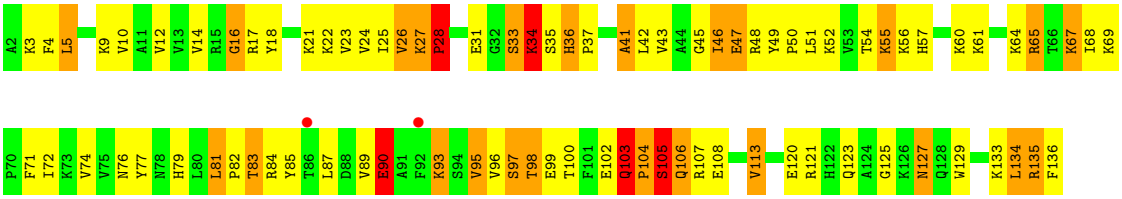
Chain N7:





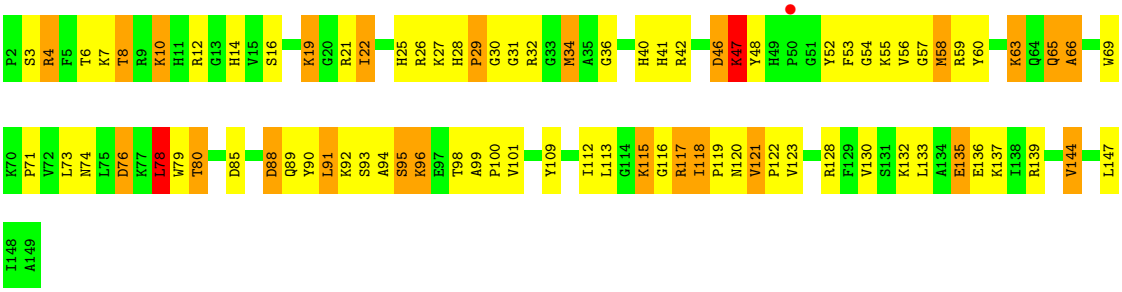
• Molecule 63: 60S ribosomal protein L27-A

Chain n7:



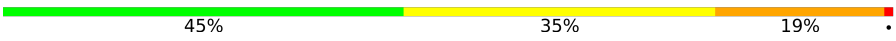
• Molecule 64: 60S ribosomal protein L28

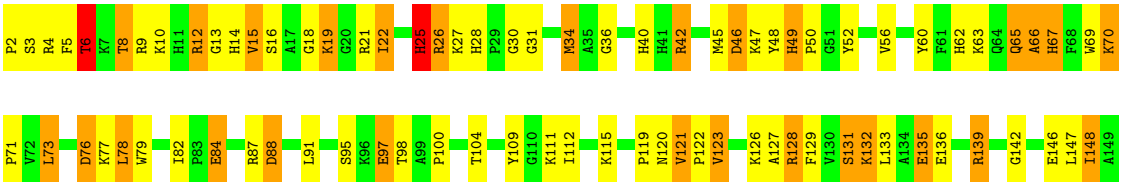
Chain N8:



• Molecule 64: 60S ribosomal protein L28

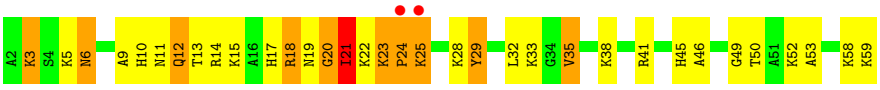
Chain n8:





• Molecule 65: 60S ribosomal protein L29

Chain N9:

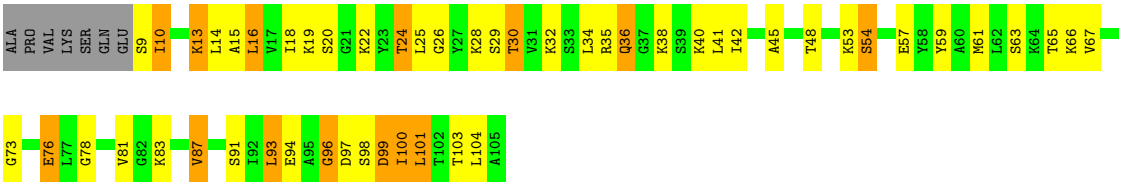


• Molecule 65: 60S ribosomal protein L29

Chain n9:

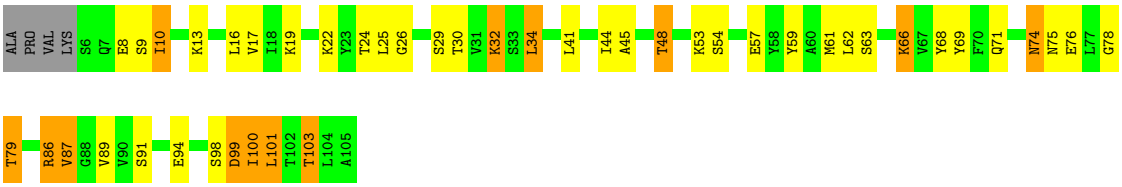
• Molecule 66: 60S ribosomal protein L30

Chain O0:



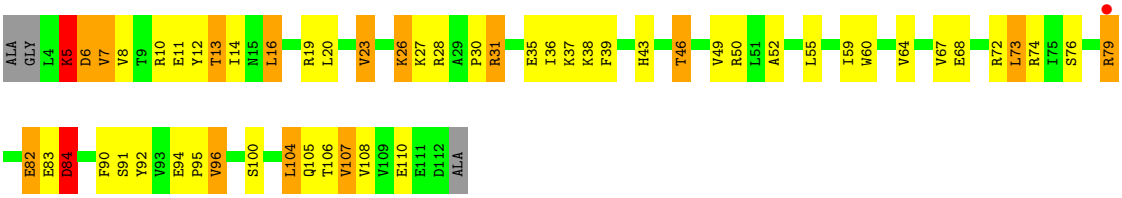
• Molecule 66: 60S ribosomal protein L30

Chain o0:



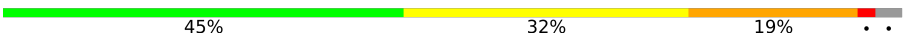
• Molecule 67: 60S ribosomal protein L31-A

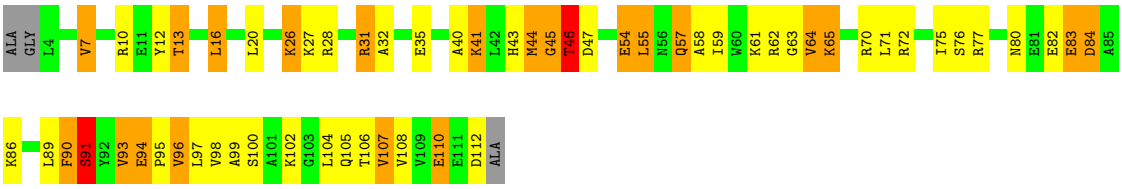
Chain O1:



• Molecule 67: 60S ribosomal protein L31-A

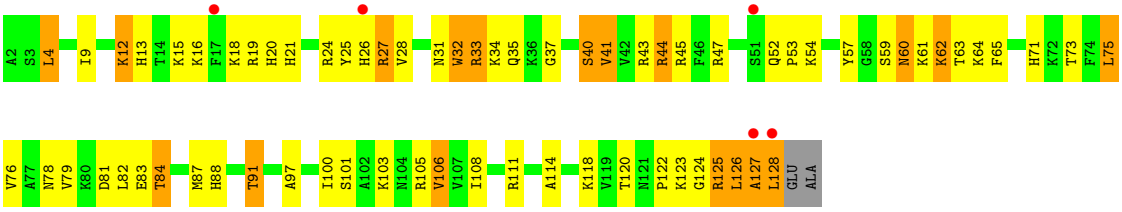
Chain o1:





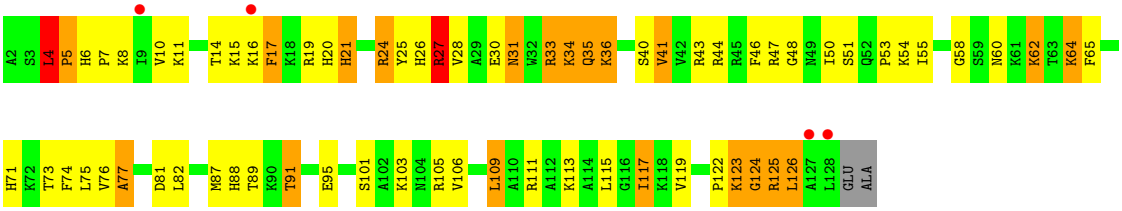
• Molecule 68: 60S ribosomal protein L32

Chain O2:



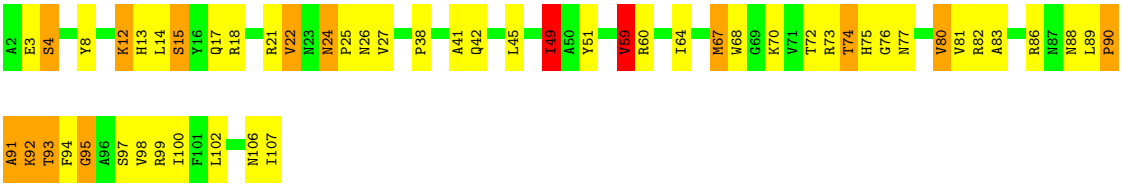
• Molecule 68: 60S ribosomal protein L32

Chain o2:



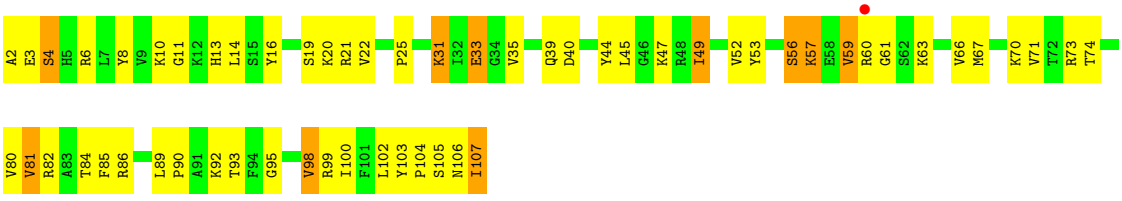
• Molecule 69: 60S ribosomal protein L33-A

Chain O3:



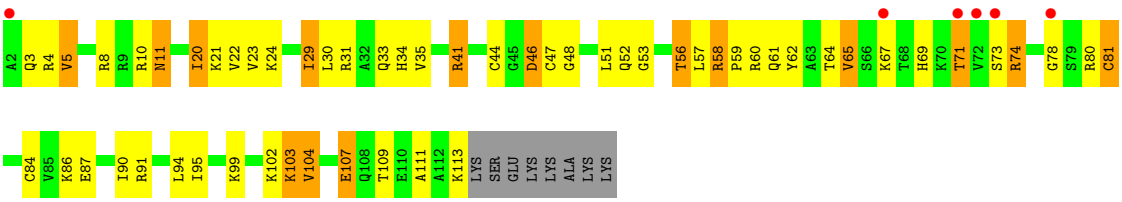
• Molecule 69: 60S ribosomal protein L33-A

Chain o3:



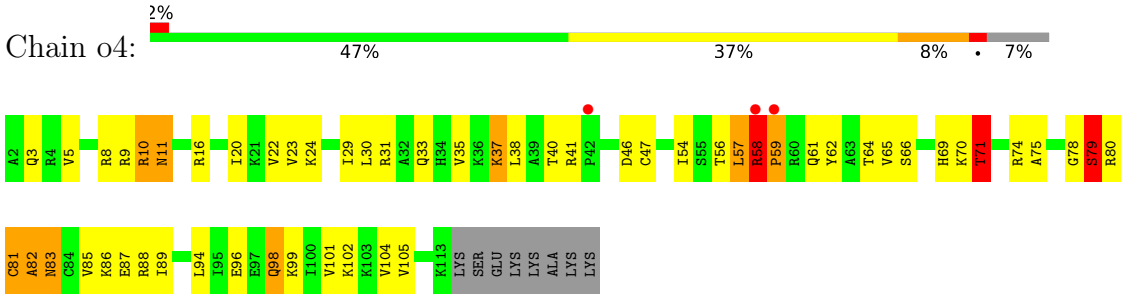
• Molecule 70: 60S ribosomal protein L34-A

Chain O4:



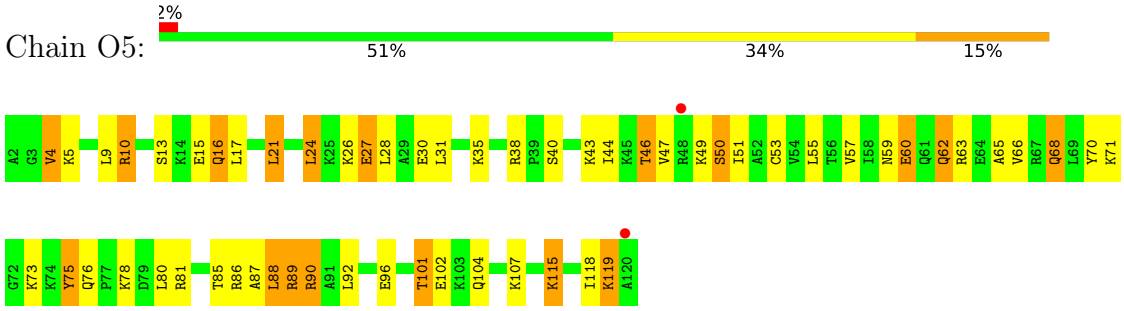
• Molecule 70: 60S ribosomal protein L34-A

Chain o4:



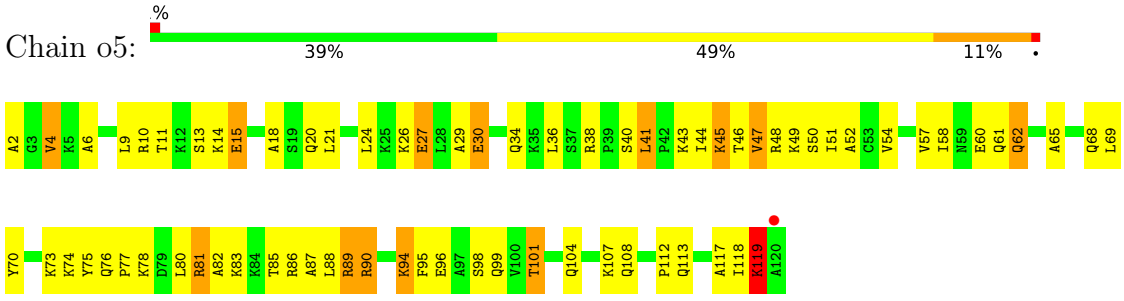
• Molecule 71: 60S ribosomal protein L35-A

Chain O5:



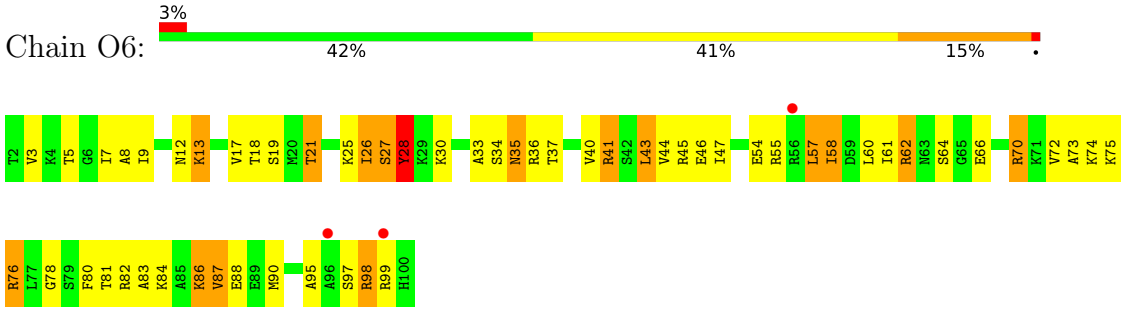
• Molecule 71: 60S ribosomal protein L35-A

Chain o5:



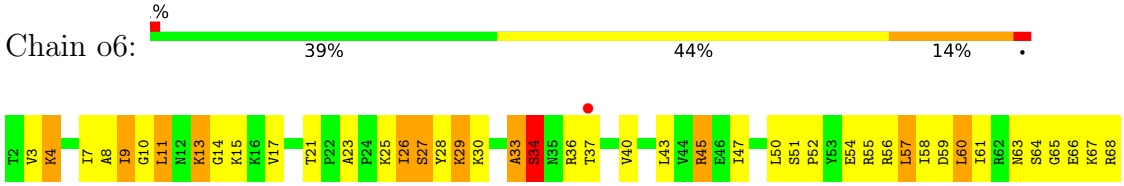
• Molecule 72: 60S ribosomal protein L36-A

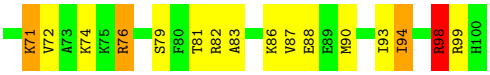
Chain O6:



• Molecule 72: 60S ribosomal protein L36-A

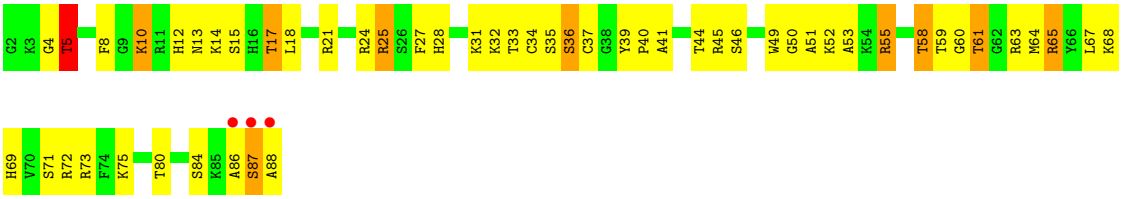
Chain o6:





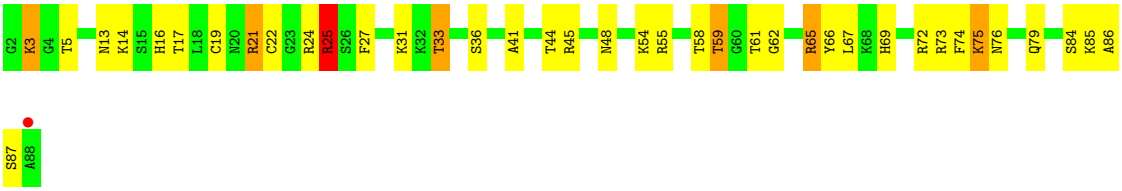
• Molecule 73: 60S ribosomal protein L37-A

Chain O7:



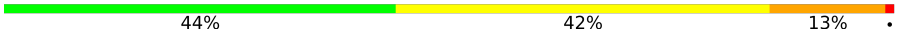
• Molecule 73: 60S ribosomal protein L37-A

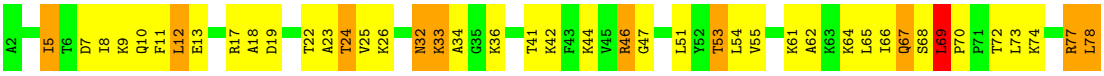
Chain o7:



• Molecule 74: 60S ribosomal protein L38

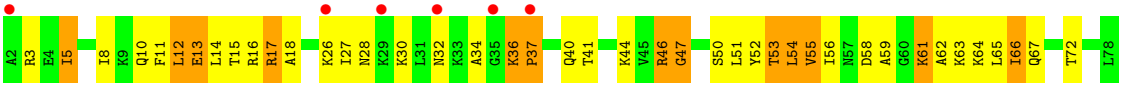
Chain O8:





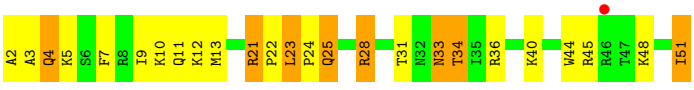
• Molecule 74: 60S ribosomal protein L38

Chain o8:



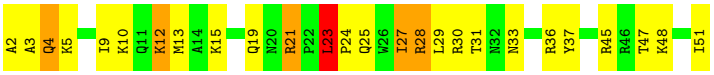
• Molecule 75: 60S ribosomal protein L39

Chain O9:



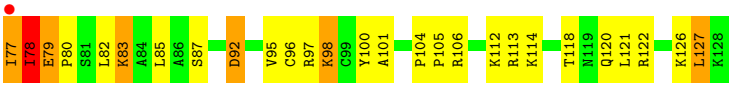
• Molecule 75: 60S ribosomal protein L39

Chain o9:



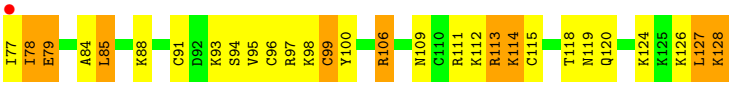
• Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:



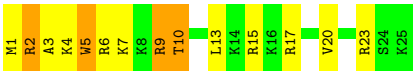
• Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:



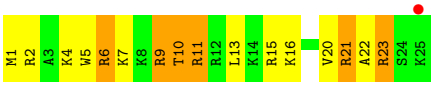
• Molecule 77: 60S ribosomal protein L41-A

Chain Q1:



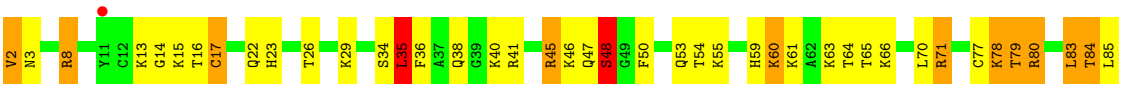
• Molecule 77: 60S ribosomal protein L41-A

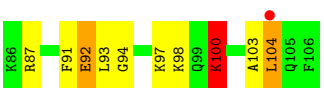
Chain q1:



• Molecule 78: 60S ribosomal protein L42-A

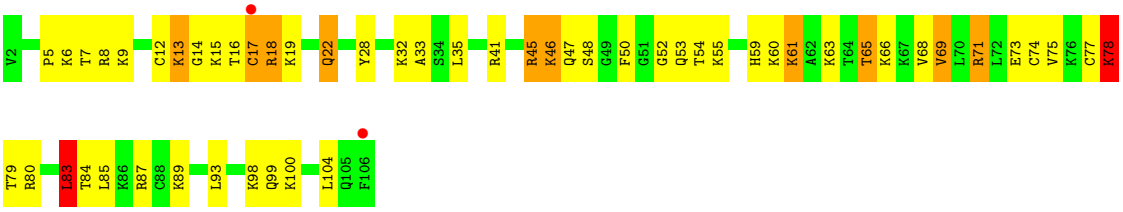
Chain Q2:





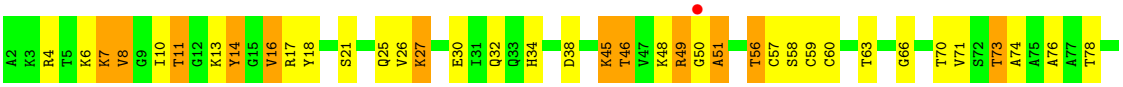
• Molecule 78: 60S ribosomal protein L42-A

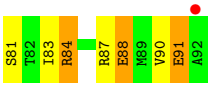
Chain q2:



• Molecule 79: 60S ribosomal protein L43-A

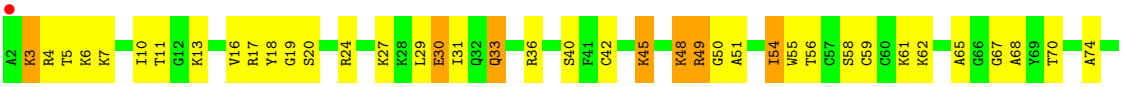
Chain Q3:

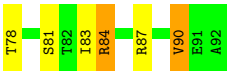




• Molecule 79: 60S ribosomal protein L43-A

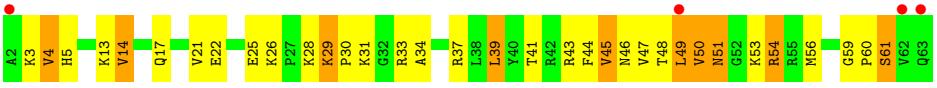
Chain q3:





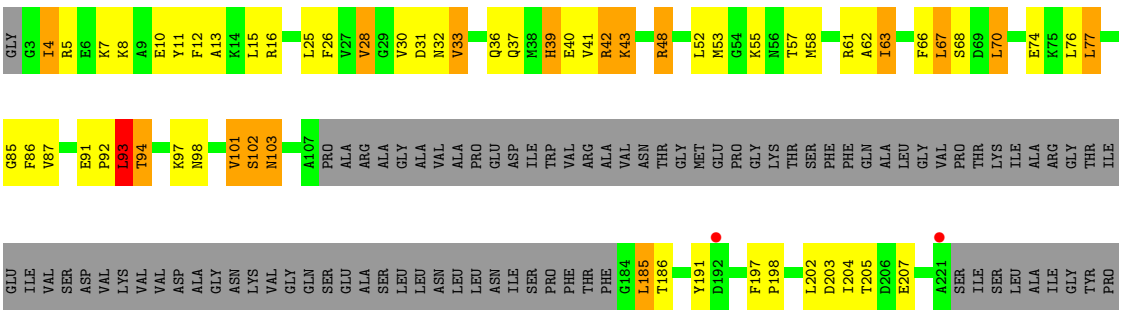
• Molecule 80: 40S ribosomal protein S30-A

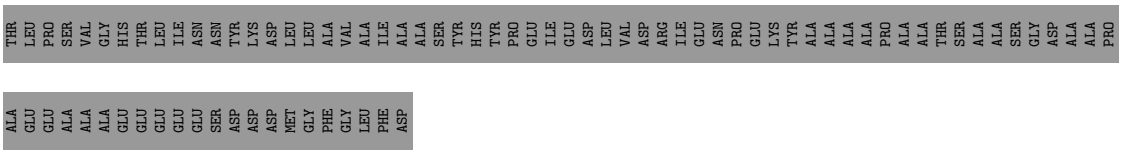
Chain e0:



• Molecule 81: 60S acidic ribosomal protein P0

Chain p0:



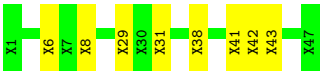


• Molecule 82: Unknown protein chain m2

Chain m2:

• Molecule 83: Unknown protein chain p1

Chain p1:



• Molecule 84: Unknown protein chain p2

Chain p2:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	435.15Å 287.07Å 303.24Å 90.00° 98.87° 90.00°	Depositor
Resolution (Å)	99.87 – 3.20 99.87 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (99.87-3.20) 99.9 (99.87-3.20)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.194 , 0.246 0.195 , 0.245	Depositor DCC
R_{free} test set	24121 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	88.0	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 92.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	411206	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

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

[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, MG, 3K8

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	2	0.43	0/41698	0.62	4/64972 (0.0%)
1	6	0.49	0/42765	0.64	3/66634 (0.0%)
2	S0	0.64	0/1617	1.10	9/2215 (0.4%)
2	s0	0.63	0/1623	1.12	9/2222 (0.4%)
3	S1	0.53	0/1735	0.96	4/2335 (0.2%)
3	s1	0.65	0/1748	1.06	5/2352 (0.2%)
4	S2	0.65	0/1665	1.04	4/2263 (0.2%)
4	s2	0.79	1/1665 (0.1%)	1.12	13/2263 (0.6%)
5	S3	0.65	0/1759	1.08	6/2368 (0.3%)
5	s3	0.56	0/1759	0.97	5/2368 (0.2%)
6	S4	0.66	0/2109	1.05	10/2839 (0.4%)
6	s4	0.68	0/2109	1.11	13/2839 (0.5%)
7	S5	0.54	0/1629	0.97	4/2202 (0.2%)
7	s5	0.61	0/1629	1.08	9/2202 (0.4%)
8	S6	0.63	0/1823	1.02	7/2439 (0.3%)
8	s6	0.72	0/1779	1.09	9/2379 (0.4%)
9	S7	0.58	0/1506	1.11	10/2028 (0.5%)
9	s7	0.62	0/1516	1.01	4/2043 (0.2%)
10	S8	0.78	0/1514	1.10	5/2021 (0.2%)
10	s8	0.82	0/1514	1.01	4/2021 (0.2%)
11	S9	0.60	0/1519	1.04	5/2035 (0.2%)
11	s9	0.69	0/1519	1.14	10/2035 (0.5%)
12	C0	0.53	0/790	1.01	5/1069 (0.5%)
12	c0	0.51	0/777	1.04	5/1049 (0.5%)
13	C1	0.77	0/1240	1.12	7/1675 (0.4%)
13	c1	0.85	0/1194	1.13	5/1610 (0.3%)
14	C2	0.53	0/900	0.95	0/1224
14	c2	0.44	0/900	0.88	0/1224
15	C3	0.67	0/1215	1.06	5/1638 (0.3%)
15	c3	0.77	0/1215	1.03	2/1638 (0.1%)
16	C4	0.61	0/901	1.02	2/1217 (0.2%)
16	c4	0.73	0/960	1.12	4/1290 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	C5	0.61	0/998	1.05	3/1341 (0.2%)
17	c5	0.63	1/1060 (0.1%)	1.20	12/1426 (0.8%)
18	C6	0.58	0/1125	1.01	5/1510 (0.3%)
18	c6	0.63	0/1131	1.04	1/1518 (0.1%)
19	C7	0.61	0/935	1.01	3/1254 (0.2%)
19	c7	0.61	0/914	1.11	2/1224 (0.2%)
20	C8	0.59	0/1211	1.01	5/1628 (0.3%)
20	c8	0.63	0/1211	1.00	1/1628 (0.1%)
21	C9	0.56	0/1130	0.97	4/1517 (0.3%)
21	c9	0.63	0/1130	1.00	3/1517 (0.2%)
22	D0	0.65	0/865	0.98	0/1169
22	d0	0.62	0/892	1.05	4/1205 (0.3%)
23	D1	0.62	0/693	0.99	2/935 (0.2%)
23	d1	0.66	0/693	0.94	0/935
24	D2	0.68	0/1038	1.09	4/1395 (0.3%)
24	d2	0.84	0/1038	1.10	3/1395 (0.2%)
25	D3	0.83	0/1139	1.16	6/1518 (0.4%)
25	d3	0.93	0/1139	1.16	6/1518 (0.4%)
26	D4	0.59	0/1087	1.02	4/1449 (0.3%)
26	d4	0.65	0/1087	1.05	2/1449 (0.1%)
27	D5	0.55	0/571	1.15	4/768 (0.5%)
27	d5	0.57	0/566	1.09	2/761 (0.3%)
28	D6	0.65	0/782	1.04	2/1047 (0.2%)
28	d6	0.71	0/782	1.04	1/1047 (0.1%)
29	D7	0.60	0/620	1.07	3/838 (0.4%)
29	d7	0.64	0/620	1.16	5/838 (0.6%)
30	D8	0.47	0/499	0.89	0/670
30	d8	0.55	0/499	1.04	1/670 (0.1%)
31	D9	0.67	0/452	0.99	1/600 (0.2%)
31	d9	0.60	0/452	0.98	2/600 (0.3%)
32	E0	0.60	0/483	0.98	0/643
33	E1	0.63	0/577	1.15	3/770 (0.4%)
33	e1	0.59	0/619	1.09	4/822 (0.5%)
34	SR	0.56	1/2494 (0.0%)	0.96	6/3393 (0.2%)
34	sR	0.50	0/2495	0.88	3/3395 (0.1%)
35	SM	0.76	1/1113 (0.1%)	1.13	4/1502 (0.3%)
35	sM	0.64	0/682	1.12	6/921 (0.7%)
36	1	0.67	0/75394	0.78	11/117545 (0.0%)
36	5	0.68	0/75414	0.78	13/117575 (0.0%)
37	3	0.56	0/2883	0.67	0/4491
37	7	0.64	0/2883	0.79	0/4491
38	4	0.65	0/3746	0.77	0/5832
38	8	0.58	0/3746	0.70	0/5832

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
39	L2	1.04	0/1948	1.25	13/2617 (0.5%)
39	l2	0.96	0/1946	1.28	10/2614 (0.4%)
40	L3	0.97	2/3146 (0.1%)	1.19	20/4228 (0.5%)
40	l3	1.10	4/3146 (0.1%)	1.29	19/4228 (0.4%)
41	L4	1.07	0/2800	1.34	24/3790 (0.6%)
41	l4	1.04	3/2800 (0.1%)	1.36	30/3790 (0.8%)
42	L5	0.70	0/2425	1.09	9/3271 (0.3%)
42	l5	0.87	0/2408	1.13	11/3248 (0.3%)
43	L6	1.01	1/1260 (0.1%)	1.15	3/1694 (0.2%)
43	l6	1.01	0/1269	1.22	9/1705 (0.5%)
44	L7	1.06	1/1821 (0.1%)	1.30	10/2451 (0.4%)
44	l7	1.11	1/1828 (0.1%)	1.35	17/2461 (0.7%)
45	L8	0.74	0/1836	1.13	8/2481 (0.3%)
45	l8	0.69	0/1795	1.10	8/2429 (0.3%)
46	L9	0.87	0/1539	1.17	6/2073 (0.3%)
46	l9	1.05	1/1539 (0.1%)	1.27	13/2073 (0.6%)
47	M0	0.94	1/1741 (0.1%)	1.19	7/2335 (0.3%)
47	m0	0.96	0/1758	1.25	15/2358 (0.6%)
48	M1	0.65	0/1374	0.99	2/1842 (0.1%)
48	m1	0.86	0/1374	1.17	5/1842 (0.3%)
49	M3	1.04	2/1568 (0.1%)	1.31	13/2106 (0.6%)
49	m3	0.94	0/1573	1.20	9/2113 (0.4%)
50	M4	1.02	0/1068	1.29	8/1438 (0.6%)
50	m4	1.15	0/1074	1.22	2/1446 (0.1%)
51	M5	0.99	0/1757	1.18	6/2354 (0.3%)
51	m5	0.88	1/1757 (0.1%)	1.23	9/2354 (0.4%)
52	M6	1.12	0/1585	1.31	9/2128 (0.4%)
52	m6	1.23	0/1585	1.32	8/2128 (0.4%)
53	M7	1.05	0/1443	1.18	8/1944 (0.4%)
53	m7	1.16	1/1250 (0.1%)	1.27	5/1683 (0.3%)
54	M8	1.07	1/1465 (0.1%)	1.31	11/1965 (0.6%)
54	m8	0.97	0/1465	1.30	15/1965 (0.8%)
55	M9	0.79	0/1538	1.05	4/2050 (0.2%)
55	m9	0.83	0/1538	1.06	4/2050 (0.2%)
56	N0	1.05	1/1481 (0.1%)	1.24	8/1990 (0.4%)
56	n0	1.12	1/1481 (0.1%)	1.30	7/1990 (0.4%)
57	N1	0.97	0/1300	1.18	5/1743 (0.3%)
57	n1	1.06	2/1300 (0.2%)	1.19	0/1743
58	N2	0.52	0/812	0.93	2/1099 (0.2%)
58	n2	0.63	0/794	1.10	6/1076 (0.6%)
59	N3	0.98	0/1018	1.24	5/1369 (0.4%)
59	n3	1.09	0/1018	1.32	1/1369 (0.1%)
60	N4	0.83	0/712	1.34	5/958 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
60	n4	0.87	0/1052	1.14	4/1398 (0.3%)
61	N5	0.88	0/979	1.24	6/1321 (0.5%)
61	n5	0.84	0/974	1.18	4/1314 (0.3%)
62	N6	0.94	0/1004	1.25	5/1341 (0.4%)
62	n6	0.90	0/1004	1.21	5/1341 (0.4%)
63	N7	0.66	0/1118	1.06	1/1497 (0.1%)
63	n7	0.62	0/1118	1.06	4/1497 (0.3%)
64	N8	1.03	0/1204	1.30	6/1612 (0.4%)
64	n8	0.99	1/1204 (0.1%)	1.31	15/1612 (0.9%)
65	N9	0.94	0/473	1.22	4/629 (0.6%)
65	n9	1.07	1/473 (0.2%)	1.42	4/629 (0.6%)
66	O0	0.66	0/751	1.01	1/1008 (0.1%)
66	o0	0.65	0/775	1.02	2/1040 (0.2%)
67	O1	0.87	0/890	1.13	3/1196 (0.3%)
67	o1	0.93	0/897	1.22	4/1205 (0.3%)
68	O2	1.15	2/1041 (0.2%)	1.27	3/1394 (0.2%)
68	o2	1.13	2/1041 (0.2%)	1.29	3/1394 (0.2%)
69	O3	1.13	1/868 (0.1%)	1.25	3/1168 (0.3%)
69	o3	1.18	1/868 (0.1%)	1.29	5/1168 (0.4%)
70	O4	0.85	0/890	1.23	8/1189 (0.7%)
70	o4	0.79	0/890	1.23	9/1189 (0.8%)
71	O5	0.96	0/978	1.24	3/1301 (0.2%)
71	o5	0.78	0/974	1.04	2/1297 (0.2%)
72	O6	0.83	0/778	1.20	0/1034
72	o6	0.76	0/777	1.17	2/1033 (0.2%)
73	O7	1.10	0/696	1.40	5/923 (0.5%)
73	o7	0.92	0/696	1.26	2/923 (0.2%)
74	O8	0.67	0/618	1.11	2/826 (0.2%)
74	o8	0.62	0/614	1.06	4/822 (0.5%)
75	O9	1.03	1/443 (0.2%)	1.22	0/588
75	o9	0.97	0/443	1.29	3/588 (0.5%)
76	Q0	0.92	0/423	1.21	4/562 (0.7%)
76	q0	1.08	1/423 (0.2%)	1.16	0/562
77	Q1	0.85	0/234	1.17	1/300 (0.3%)
77	q1	0.99	0/234	1.14	0/300
78	Q2	0.95	1/860 (0.1%)	1.14	2/1136 (0.2%)
78	q2	0.95	2/860 (0.2%)	1.09	2/1136 (0.2%)
79	Q3	0.98	1/701 (0.1%)	1.18	4/934 (0.4%)
79	q3	0.92	0/701	1.16	2/934 (0.2%)
80	e0	0.69	0/499	1.11	0/665
81	p0	0.54	0/1091	0.99	2/1472 (0.1%)
All	All	0.71	41/430072 (0.0%)	0.91	856/631360 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	s0	0	1
7	S5	0	1
7	s5	0	2
9	S7	0	2
9	s7	0	1
10	S8	0	1
16	C4	0	3
16	c4	0	1
17	c5	0	1
18	C6	0	1
18	c6	0	1
19	C7	0	1
24	d2	0	1
26	d4	0	1
27	D5	0	3
28	D6	0	1
39	L2	0	1
39	l2	0	4
44	l7	0	2
46	L9	0	1
48	M1	0	1
52	M6	0	1
52	m6	0	1
56	N0	0	1
56	n0	0	1
57	N1	0	1
59	n3	0	1
64	N8	0	2
64	n8	0	3
65	N9	0	1
67	O1	0	1
80	e0	0	1
82	m2	0	1
All	All	0	46

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	q2	17	CYS	CB-SG	7.79	2.06	1.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	7.74	2.06	1.81
56	N0	100	VAL	CA-CB	-7.29	1.45	1.54
44	l7	216	VAL	CA-CB	-6.90	1.45	1.54
34	SR	161	LYS	CA-C	6.88	1.61	1.52

The worst 5 of 856 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	N4	80	ARG	CA-C-N	15.67	139.43	119.84
60	N4	80	ARG	C-N-CA	15.67	139.43	119.84
73	o7	5	THR	CA-C-N	-13.51	106.02	120.47
73	o7	5	THR	C-N-CA	-13.51	106.02	120.47
41	L4	3	ARG	CA-C-N	12.31	135.23	119.84

There are no chirality outliers.

5 of 46 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	38	THR	Peptide
7	S5	44	ASN	Peptide
9	S7	131	PHE	Peptide
9	S7	31	SER	Peptide
10	S8	147	ALA	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	37283	0	18757	994	1
1	6	38238	0	19241	960	0
2	S0	1577	0	1567	97	0
2	s0	1583	0	1578	98	0
3	S1	1709	0	1784	129	0
3	s1	1722	0	1793	72	0
4	S2	1635	0	1723	88	0
4	s2	1635	0	1723	78	0
5	S3	1734	0	1817	59	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	s3	1734	0	1817	79	0
6	S4	2068	0	2154	89	0
6	s4	2068	0	2154	95	0
7	S5	1609	0	1675	75	0
7	s5	1609	0	1675	97	0
8	S6	1799	0	1878	83	0
8	s6	1755	0	1846	81	0
9	S7	1481	0	1572	67	0
9	s7	1491	0	1578	63	0
10	S8	1489	0	1525	70	0
10	s8	1489	0	1525	64	0
11	S9	1494	0	1573	67	0
11	s9	1494	0	1573	87	0
12	C0	773	0	729	40	0
12	c0	762	0	699	35	0
13	C1	1214	0	1259	47	0
13	c1	1168	0	1231	42	0
14	C2	892	0	891	34	0
14	c2	892	0	891	26	0
15	C3	1192	0	1255	63	0
15	c3	1192	0	1255	64	0
16	C4	891	0	883	79	0
16	c4	949	0	985	50	0
17	C5	977	0	1002	50	0
17	c5	1039	0	1050	58	0
18	C6	1105	0	1166	72	0
18	c6	1111	0	1171	73	0
19	C7	926	0	930	55	0
19	c7	906	0	909	50	0
20	C8	1192	0	1222	57	0
20	c8	1192	0	1222	72	0
21	C9	1112	0	1124	56	0
21	c9	1112	0	1124	40	0
22	D0	855	0	917	54	0
22	d0	882	0	939	43	0
23	D1	684	0	672	39	0
23	d1	684	0	672	35	0
24	D2	1021	0	1060	52	0
24	d2	1021	0	1060	50	0
25	D3	1121	0	1196	61	0
25	d3	1121	0	1196	50	0
26	D4	1073	0	1132	51	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	d4	1073	0	1132	51	0
27	D5	563	0	603	37	0
27	d5	558	0	598	28	0
28	D6	769	0	815	61	0
28	d6	769	0	814	45	0
29	D7	610	0	630	25	0
29	d7	610	0	631	33	0
30	D8	497	0	535	22	0
30	d8	497	0	535	31	0
31	D9	442	0	428	23	0
31	d9	442	0	428	26	0
32	E0	475	0	525	13	0
33	E1	566	0	603	30	0
33	e1	608	0	656	41	0
34	SR	2441	0	2397	121	0
34	sR	2442	0	2392	95	0
35	SM	1104	0	996	46	0
35	sM	679	0	603	28	0
36	1	67355	0	33839	1386	0
36	5	67376	0	33855	1341	1
37	3	2579	0	1304	64	0
37	7	2579	0	1304	50	0
38	4	3353	0	1695	69	0
38	8	3353	0	1695	68	0
39	L2	1914	0	1981	76	0
39	l2	1912	0	1976	98	0
40	L3	3075	0	3142	147	0
40	l3	3075	0	3142	175	0
41	L4	2748	0	2859	138	0
41	l4	2748	0	2859	149	0
42	L5	2375	0	2325	125	0
42	l5	2359	0	2311	99	0
43	L6	1239	0	1326	47	0
43	l6	1248	0	1339	51	0
44	L7	1784	0	1862	93	0
44	l7	1791	0	1869	68	0
45	L8	1804	0	1877	71	0
45	l8	1763	0	1819	85	0
46	L9	1518	0	1587	88	0
46	l9	1518	0	1587	78	0
47	M0	1705	0	1735	90	0
47	m0	1722	0	1755	75	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	M1	1353	0	1383	62	0
48	m1	1353	0	1383	58	0
49	M3	1543	0	1608	85	0
49	m3	1548	0	1613	81	0
50	M4	1053	0	1149	55	0
50	m4	1059	0	1154	52	0
51	M5	1720	0	1779	70	0
51	m5	1720	0	1779	87	0
52	M6	1555	0	1659	73	0
52	m6	1555	0	1659	64	0
53	M7	1420	0	1437	65	0
53	m7	1227	0	1236	53	0
54	M8	1441	0	1543	65	0
54	m8	1441	0	1543	58	0
55	M9	1521	0	1617	70	0
55	m9	1521	0	1617	57	0
56	N0	1445	0	1487	62	0
56	n0	1445	0	1487	63	0
57	N1	1276	0	1323	60	0
57	n1	1276	0	1323	61	0
58	N2	796	0	812	28	0
58	n2	778	0	791	35	0
59	N3	1003	0	1048	55	0
59	n3	1003	0	1048	46	0
60	N4	699	0	640	15	0
60	n4	1038	0	1071	37	0
61	N5	964	0	1025	42	0
61	n5	959	0	1023	50	0
62	N6	993	0	1081	33	0
62	n6	993	0	1081	52	0
63	N7	1092	0	1155	47	0
63	n7	1092	0	1155	58	0
64	N8	1173	0	1215	80	0
64	n8	1173	0	1215	67	0
65	N9	462	0	491	24	0
65	n9	462	0	491	19	0
66	O0	743	0	797	36	0
66	o0	767	0	816	30	0
67	O1	876	0	912	33	0
67	o1	883	0	918	37	0
68	O2	1020	0	1090	45	0
68	o2	1020	0	1090	49	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	O3	850	0	880	41	0
69	o3	850	0	880	30	0
70	O4	880	0	945	33	0
70	o4	880	0	945	43	0
71	O5	969	0	1078	45	0
71	o5	965	0	1067	57	0
72	O6	771	0	849	37	0
72	o6	770	0	846	42	0
73	O7	681	0	682	41	0
73	o7	681	0	683	25	0
74	O8	612	0	682	28	0
74	o8	608	0	671	24	0
75	O9	436	0	475	30	0
75	o9	436	0	475	28	0
76	Q0	417	0	456	16	0
76	q0	417	0	456	18	0
77	Q1	233	0	284	15	0
77	q1	233	0	284	17	0
78	Q2	847	0	917	29	0
78	q2	847	0	918	39	0
79	Q3	694	0	734	30	0
79	q3	694	0	734	32	0
80	e0	491	0	542	21	0
81	p0	1076	0	1040	35	0
82	m2	750	0	170	14	0
83	p1	235	0	52	4	0
84	p2	230	0	51	2	0
85	1	469	0	0	0	0
85	2	125	0	0	0	0
85	3	14	0	0	0	0
85	4	21	0	0	0	0
85	5	505	0	0	0	0
85	6	148	0	0	0	0
85	7	17	0	0	0	0
85	8	14	0	0	0	0
85	D0	1	0	0	0	0
85	D3	1	0	0	0	0
85	L2	1	0	0	0	0
85	L3	3	0	0	0	0
85	L4	1	0	0	0	0
85	L5	2	0	0	0	0
85	L7	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	L8	1	0	0	0	0
85	M0	3	0	0	0	0
85	M1	1	0	0	0	0
85	M3	3	0	0	0	0
85	M5	1	0	0	0	0
85	M6	1	0	0	0	0
85	M7	5	0	0	0	0
85	M9	1	0	0	0	0
85	N0	1	0	0	0	0
85	N3	2	0	0	0	0
85	N5	1	0	0	0	0
85	N6	2	0	0	0	0
85	N8	5	0	0	0	0
85	O2	1	0	0	0	0
85	O4	1	0	0	0	0
85	O5	1	0	0	0	0
85	O7	3	0	0	0	0
85	Q2	1	0	0	0	0
85	S4	1	0	0	0	0
85	S8	1	0	0	0	0
85	SM	1	0	0	0	0
85	c1	1	0	0	0	0
85	c7	1	0	0	0	0
85	c8	1	0	0	0	0
85	c9	1	0	0	0	0
85	d3	1	0	0	0	0
85	d4	1	0	0	0	0
85	d6	1	0	0	0	0
85	l2	1	0	0	0	0
85	l3	1	0	0	0	0
85	l4	1	0	0	0	0
85	l5	2	0	0	0	0
85	l7	1	0	0	0	0
85	l9	1	0	0	0	0
85	m0	1	0	0	0	0
85	m1	1	0	0	0	0
85	m5	2	0	0	0	0
85	m6	1	0	0	0	0
85	m7	5	0	0	0	0
85	n0	2	0	0	0	0
85	n3	2	0	0	0	0
85	n6	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	n8	4	0	0	0	0
85	n9	1	0	0	0	0
85	o1	1	0	0	0	0
85	o3	1	0	0	0	0
85	o4	2	0	0	0	0
85	o7	1	0	0	0	0
85	q0	1	0	0	0	0
85	q1	1	0	0	0	0
85	q3	1	0	0	0	0
85	s1	1	0	0	0	0
85	s6	1	0	0	0	0
85	s8	2	0	0	0	0
85	sM	2	0	0	0	0
86	1	2457	0	0	229	0
86	2	1092	0	0	109	0
86	3	77	0	0	5	0
86	4	98	0	0	7	0
86	5	2478	0	0	240	0
86	6	1106	0	0	107	0
86	7	77	0	0	10	0
86	8	119	0	0	18	0
86	C1	7	0	0	0	0
86	C3	7	0	0	0	0
86	C5	7	0	0	3	0
86	C8	7	0	0	0	0
86	D9	7	0	0	1	0
86	L3	21	0	0	1	0
86	L4	7	0	0	0	0
86	M0	7	0	0	1	0
86	M5	7	0	0	1	0
86	M7	14	0	0	2	0
86	M8	7	0	0	0	0
86	M9	7	0	0	0	0
86	N1	7	0	0	1	0
86	N9	7	0	0	0	0
86	O1	7	0	0	6	0
86	O2	7	0	0	0	0
86	O3	7	0	0	1	0
86	O7	14	0	0	6	0
86	O9	7	0	0	1	0
86	S8	7	0	0	0	0
86	SR	7	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	c3	7	0	0	1	0
86	c5	7	0	0	2	0
86	c8	7	0	0	0	0
86	d4	7	0	0	0	0
86	d9	7	0	0	0	0
86	l3	21	0	0	2	0
86	l4	14	0	0	0	0
86	l5	21	0	0	0	0
86	l9	7	0	0	0	0
86	m0	14	0	0	4	0
86	m1	7	0	0	1	0
86	m4	7	0	0	0	0
86	m5	7	0	0	1	0
86	m6	7	0	0	0	0
86	m7	7	0	0	0	0
86	m8	7	0	0	0	0
86	m9	7	0	0	0	0
86	n1	7	0	0	1	0
86	n3	7	0	0	0	0
86	n9	7	0	0	0	0
86	o3	7	0	0	1	0
86	q2	7	0	0	3	0
86	s1	14	0	0	0	0
86	s4	7	0	0	1	0
86	s8	7	0	0	1	0
86	s9	7	0	0	2	0
86	sR	7	0	0	0	0
87	2	28	0	27	4	0
87	6	28	0	27	1	0
88	D6	1	0	0	0	0
88	D7	1	0	0	0	0
88	D9	1	0	0	0	0
88	E1	1	0	0	0	0
88	O7	1	0	0	0	0
88	Q0	1	0	0	0	0
88	Q2	1	0	0	0	0
88	Q3	1	0	0	0	0
88	d6	1	0	0	0	0
88	d7	1	0	0	0	0
88	d9	1	0	0	0	0
88	e1	1	0	0	0	0
88	o7	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	q0	1	0	0	0	0
88	q2	1	0	0	0	0
88	q3	1	0	0	0	0
All	All	411206	0	297328	11845	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

The worst 5 of 11845 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:q2:17:CYS:SG	78:q2:17:CYS:CB	2.07	1.43
78:Q2:17:CYS:SG	78:Q2:17:CYS:CB	2.06	1.41
40:l3:41:VAL:HA	40:l3:185:GLY:HA3	1.23	1.07
36:5:3274:A:H3'	36:5:3275:U:H5"	1.38	1.04
42:l5:111:GLN:HA	42:l5:116:ASP:HB3	1.39	1.02

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1353:U:O2'	36:5:3165:A:OP1[2_546]	2.18	0.02

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	S0	204/251 (81%)	148 (72%)	39 (19%)	17 (8%)	0 4
2	s0	204/251 (81%)	148 (72%)	32 (16%)	24 (12%)	0 1
3	S1	212/254 (84%)	149 (70%)	34 (16%)	29 (14%)	0 1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	s1	214/254 (84%)	178 (83%)	23 (11%)	13 (6%)	1 9
4	S2	215/253 (85%)	178 (83%)	26 (12%)	11 (5%)	1 13
4	s2	215/253 (85%)	169 (79%)	30 (14%)	16 (7%)	1 6
5	S3	221/239 (92%)	173 (78%)	28 (13%)	20 (9%)	0 3
5	s3	221/239 (92%)	176 (80%)	29 (13%)	16 (7%)	1 6
6	S4	258/260 (99%)	203 (79%)	38 (15%)	17 (7%)	1 7
6	s4	258/260 (99%)	209 (81%)	29 (11%)	20 (8%)	1 5
7	S5	204/224 (91%)	155 (76%)	28 (14%)	21 (10%)	0 2
7	s5	204/224 (91%)	156 (76%)	26 (13%)	22 (11%)	0 2
8	S6	224/236 (95%)	191 (85%)	22 (10%)	11 (5%)	1 13
8	s6	216/236 (92%)	179 (83%)	22 (10%)	15 (7%)	1 7
9	S7	182/189 (96%)	137 (75%)	25 (14%)	20 (11%)	0 2
9	s7	184/189 (97%)	140 (76%)	28 (15%)	16 (9%)	0 3
10	S8	184/200 (92%)	154 (84%)	21 (11%)	9 (5%)	1 13
10	s8	184/200 (92%)	161 (88%)	12 (6%)	11 (6%)	1 10
11	S9	183/196 (93%)	147 (80%)	24 (13%)	12 (7%)	1 7
11	s9	183/196 (93%)	149 (81%)	26 (14%)	8 (4%)	2 15
12	C0	94/105 (90%)	70 (74%)	18 (19%)	6 (6%)	1 8
12	c0	92/105 (88%)	66 (72%)	11 (12%)	15 (16%)	0 0
13	C1	153/155 (99%)	118 (77%)	17 (11%)	18 (12%)	0 1
13	c1	144/155 (93%)	114 (79%)	24 (17%)	6 (4%)	2 16
14	C2	122/142 (86%)	75 (62%)	21 (17%)	26 (21%)	0 0
14	c2	122/142 (86%)	71 (58%)	31 (25%)	20 (16%)	0 0
15	C3	148/150 (99%)	123 (83%)	12 (8%)	13 (9%)	0 3
15	c3	148/150 (99%)	115 (78%)	22 (15%)	11 (7%)	1 6
16	C4	125/136 (92%)	95 (76%)	15 (12%)	15 (12%)	0 1
16	c4	126/136 (93%)	104 (82%)	16 (13%)	6 (5%)	2 14
17	C5	122/141 (86%)	81 (66%)	28 (23%)	13 (11%)	0 2
17	c5	133/141 (94%)	90 (68%)	26 (20%)	17 (13%)	0 1
18	C6	139/142 (98%)	109 (78%)	20 (14%)	10 (7%)	1 6
18	c6	140/142 (99%)	112 (80%)	16 (11%)	12 (9%)	0 3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
19	C7	116/136 (85%)	82 (71%)	25 (22%)	9 (8%)	1 5
19	c7	113/136 (83%)	87 (77%)	14 (12%)	12 (11%)	0 2
20	C8	143/145 (99%)	115 (80%)	15 (10%)	13 (9%)	0 3
20	c8	143/145 (99%)	117 (82%)	20 (14%)	6 (4%)	2 16
21	C9	141/143 (99%)	115 (82%)	20 (14%)	6 (4%)	2 16
21	c9	141/143 (99%)	115 (82%)	22 (16%)	4 (3%)	4 25
22	D0	105/120 (88%)	82 (78%)	20 (19%)	3 (3%)	3 24
22	d0	108/120 (90%)	84 (78%)	14 (13%)	10 (9%)	0 3
23	D1	85/87 (98%)	64 (75%)	15 (18%)	6 (7%)	1 6
23	d1	85/87 (98%)	70 (82%)	8 (9%)	7 (8%)	0 4
24	D2	127/129 (98%)	105 (83%)	20 (16%)	2 (2%)	7 36
24	d2	127/129 (98%)	113 (89%)	13 (10%)	1 (1%)	16 50
25	D3	142/144 (99%)	115 (81%)	14 (10%)	13 (9%)	0 3
25	d3	142/144 (99%)	123 (87%)	13 (9%)	6 (4%)	2 16
26	D4	132/134 (98%)	107 (81%)	19 (14%)	6 (4%)	2 15
26	d4	132/134 (98%)	100 (76%)	21 (16%)	11 (8%)	0 4
27	D5	68/107 (64%)	45 (66%)	13 (19%)	10 (15%)	0 1
27	d5	67/107 (63%)	52 (78%)	12 (18%)	3 (4%)	2 15
28	D6	95/97 (98%)	61 (64%)	17 (18%)	17 (18%)	0 0
28	d6	95/97 (98%)	71 (75%)	16 (17%)	8 (8%)	0 4
29	D7	79/81 (98%)	62 (78%)	11 (14%)	6 (8%)	1 5
29	d7	79/81 (98%)	59 (75%)	15 (19%)	5 (6%)	1 8
30	D8	61/66 (92%)	45 (74%)	11 (18%)	5 (8%)	0 4
30	d8	61/66 (92%)	46 (75%)	10 (16%)	5 (8%)	0 4
31	D9	51/55 (93%)	41 (80%)	7 (14%)	3 (6%)	1 10
31	d9	51/55 (93%)	37 (72%)	8 (16%)	6 (12%)	0 1
32	E0	58/60 (97%)	42 (72%)	12 (21%)	4 (7%)	1 7
33	E1	69/76 (91%)	34 (49%)	11 (16%)	24 (35%)	0 0
33	e1	74/76 (97%)	34 (46%)	22 (30%)	18 (24%)	0 0
34	SR	316/318 (99%)	238 (75%)	56 (18%)	22 (7%)	1 6
34	sR	316/318 (99%)	261 (83%)	39 (12%)	16 (5%)	1 13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
35	SM	155/273 (57%)	109 (70%)	26 (17%)	20 (13%)	0 1
35	sM	98/273 (36%)	61 (62%)	23 (24%)	14 (14%)	0 1
39	L2	250/253 (99%)	218 (87%)	22 (9%)	10 (4%)	2 17
39	l2	250/253 (99%)	209 (84%)	26 (10%)	15 (6%)	1 10
40	L3	384/386 (100%)	333 (87%)	34 (9%)	17 (4%)	2 15
40	l3	384/386 (100%)	339 (88%)	32 (8%)	13 (3%)	3 20
41	L4	359/361 (99%)	302 (84%)	40 (11%)	17 (5%)	2 14
41	l4	359/361 (99%)	293 (82%)	40 (11%)	26 (7%)	1 6
42	L5	294/296 (99%)	239 (81%)	34 (12%)	21 (7%)	1 6
42	l5	292/296 (99%)	252 (86%)	32 (11%)	8 (3%)	4 25
43	L6	152/175 (87%)	134 (88%)	16 (10%)	2 (1%)	9 40
43	l6	153/175 (87%)	127 (83%)	23 (15%)	3 (2%)	6 31
44	L7	220/243 (90%)	195 (89%)	19 (9%)	6 (3%)	4 25
44	l7	221/243 (91%)	193 (87%)	23 (10%)	5 (2%)	5 29
45	L8	231/255 (91%)	188 (81%)	36 (16%)	7 (3%)	3 23
45	l8	229/255 (90%)	181 (79%)	31 (14%)	17 (7%)	1 6
46	L9	189/191 (99%)	156 (82%)	25 (13%)	8 (4%)	2 16
46	l9	189/191 (99%)	162 (86%)	23 (12%)	4 (2%)	5 31
47	M0	207/220 (94%)	172 (83%)	21 (10%)	14 (7%)	1 7
47	m0	209/220 (95%)	165 (79%)	30 (14%)	14 (7%)	1 7
48	M1	167/173 (96%)	127 (76%)	24 (14%)	16 (10%)	0 3
48	m1	167/173 (96%)	142 (85%)	10 (6%)	15 (9%)	0 3
49	M3	191/198 (96%)	156 (82%)	23 (12%)	12 (6%)	1 8
49	m3	192/198 (97%)	149 (78%)	25 (13%)	18 (9%)	0 3
50	M4	134/137 (98%)	115 (86%)	12 (9%)	7 (5%)	1 12
50	m4	135/137 (98%)	120 (89%)	13 (10%)	2 (2%)	8 37
51	M5	201/203 (99%)	179 (89%)	17 (8%)	5 (2%)	4 27
51	m5	201/203 (99%)	175 (87%)	17 (8%)	9 (4%)	2 15
52	M6	195/198 (98%)	176 (90%)	14 (7%)	5 (3%)	4 26
52	m6	195/198 (98%)	170 (87%)	18 (9%)	7 (4%)	2 19
53	M7	181/183 (99%)	150 (83%)	22 (12%)	9 (5%)	1 13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
53	m7	153/183 (84%)	136 (89%)	12 (8%)	5 (3%)	3 21
54	M8	183/185 (99%)	157 (86%)	20 (11%)	6 (3%)	3 21
54	m8	183/185 (99%)	158 (86%)	23 (13%)	2 (1%)	11 43
55	M9	186/188 (99%)	158 (85%)	23 (12%)	5 (3%)	4 25
55	m9	186/188 (99%)	165 (89%)	20 (11%)	1 (0%)	24 59
56	N0	170/172 (99%)	150 (88%)	17 (10%)	3 (2%)	6 34
56	n0	170/172 (99%)	154 (91%)	15 (9%)	1 (1%)	21 56
57	N1	157/159 (99%)	132 (84%)	19 (12%)	6 (4%)	2 18
57	n1	157/159 (99%)	143 (91%)	13 (8%)	1 (1%)	21 56
58	N2	98/120 (82%)	77 (79%)	17 (17%)	4 (4%)	2 17
58	n2	96/120 (80%)	76 (79%)	14 (15%)	6 (6%)	1 8
59	N3	134/136 (98%)	120 (90%)	12 (9%)	2 (2%)	8 37
59	n3	134/136 (98%)	122 (91%)	9 (7%)	3 (2%)	5 29
60	N4	96/155 (62%)	69 (72%)	17 (18%)	10 (10%)	0 2
60	n4	133/155 (86%)	106 (80%)	17 (13%)	10 (8%)	1 5
61	N5	119/141 (84%)	103 (87%)	10 (8%)	6 (5%)	1 13
61	n5	118/141 (84%)	94 (80%)	15 (13%)	9 (8%)	1 5
62	N6	124/126 (98%)	110 (89%)	11 (9%)	3 (2%)	4 28
62	n6	124/126 (98%)	112 (90%)	7 (6%)	5 (4%)	2 17
63	N7	133/135 (98%)	108 (81%)	12 (9%)	13 (10%)	0 2
63	n7	133/135 (98%)	101 (76%)	21 (16%)	11 (8%)	0 4
64	N8	146/148 (99%)	120 (82%)	19 (13%)	7 (5%)	2 14
64	n8	146/148 (99%)	117 (80%)	21 (14%)	8 (6%)	1 11
65	N9	56/58 (97%)	47 (84%)	5 (9%)	4 (7%)	1 6
65	n9	56/58 (97%)	37 (66%)	13 (23%)	6 (11%)	0 2
66	O0	95/104 (91%)	86 (90%)	8 (8%)	1 (1%)	11 43
66	o0	98/104 (94%)	88 (90%)	9 (9%)	1 (1%)	12 45
67	O1	107/112 (96%)	96 (90%)	5 (5%)	6 (6%)	1 11
67	o1	107/112 (96%)	84 (78%)	15 (14%)	8 (8%)	1 5
68	O2	125/129 (97%)	106 (85%)	14 (11%)	5 (4%)	2 17
68	o2	125/129 (97%)	105 (84%)	15 (12%)	5 (4%)	2 17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
69	O3	104/106 (98%)	94 (90%)	6 (6%)	4 (4%)	2 18
69	o3	104/106 (98%)	94 (90%)	7 (7%)	3 (3%)	3 24
70	O4	110/120 (92%)	90 (82%)	19 (17%)	1 (1%)	14 47
70	o4	110/120 (92%)	97 (88%)	10 (9%)	3 (3%)	4 25
71	O5	117/119 (98%)	104 (89%)	10 (8%)	3 (3%)	4 26
71	o5	117/119 (98%)	100 (86%)	14 (12%)	3 (3%)	4 26
72	O6	97/99 (98%)	72 (74%)	17 (18%)	8 (8%)	0 4
72	o6	97/99 (98%)	81 (84%)	11 (11%)	5 (5%)	1 12
73	O7	85/87 (98%)	72 (85%)	12 (14%)	1 (1%)	10 42
73	o7	85/87 (98%)	68 (80%)	12 (14%)	5 (6%)	1 10
74	O8	75/77 (97%)	61 (81%)	12 (16%)	2 (3%)	4 25
74	o8	75/77 (97%)	64 (85%)	8 (11%)	3 (4%)	2 17
75	O9	48/50 (96%)	42 (88%)	5 (10%)	1 (2%)	5 31
75	o9	48/50 (96%)	40 (83%)	8 (17%)	0	100 100
76	Q0	50/52 (96%)	44 (88%)	4 (8%)	2 (4%)	2 17
76	q0	50/52 (96%)	49 (98%)	0	1 (2%)	6 31
77	Q1	23/25 (92%)	22 (96%)	1 (4%)	0	100 100
77	q1	23/25 (92%)	20 (87%)	2 (9%)	1 (4%)	2 16
78	Q2	103/105 (98%)	76 (74%)	19 (18%)	8 (8%)	1 5
78	q2	103/105 (98%)	86 (84%)	14 (14%)	3 (3%)	3 24
79	Q3	89/91 (98%)	76 (85%)	10 (11%)	3 (3%)	3 20
79	q3	89/91 (98%)	81 (91%)	7 (8%)	1 (1%)	11 43
80	e0	60/62 (97%)	44 (73%)	8 (13%)	8 (13%)	0 1
81	p0	139/311 (45%)	110 (79%)	21 (15%)	8 (6%)	1 10
All	All	22333/24143 (92%)	18176 (81%)	2788 (12%)	1369 (6%)	1 9

5 of 1369 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	39	ASN
2	S0	66	ALA
2	S0	139	VAL
2	S0	158	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	S0	164/209 (78%)	135 (82%)	29 (18%)	2 10
2	s0	165/209 (79%)	129 (78%)	36 (22%)	1 6
3	S1	191/223 (86%)	149 (78%)	42 (22%)	1 6
3	s1	192/223 (86%)	148 (77%)	44 (23%)	1 5
4	S2	176/204 (86%)	134 (76%)	42 (24%)	1 4
4	s2	176/204 (86%)	127 (72%)	49 (28%)	0 2
5	S3	182/194 (94%)	141 (78%)	41 (22%)	1 5
5	s3	182/194 (94%)	138 (76%)	44 (24%)	1 4
6	S4	221/221 (100%)	170 (77%)	51 (23%)	1 5
6	s4	221/221 (100%)	176 (80%)	45 (20%)	1 7
7	S5	173/190 (91%)	140 (81%)	33 (19%)	1 9
7	s5	173/190 (91%)	134 (78%)	39 (22%)	1 5
8	S6	188/201 (94%)	153 (81%)	35 (19%)	1 9
8	s6	187/201 (93%)	150 (80%)	37 (20%)	1 8
9	S7	165/169 (98%)	130 (79%)	35 (21%)	1 6
9	s7	165/169 (98%)	136 (82%)	29 (18%)	2 10
10	S8	150/161 (93%)	127 (85%)	23 (15%)	3 14
10	s8	150/161 (93%)	124 (83%)	26 (17%)	2 10
11	S9	158/165 (96%)	119 (75%)	39 (25%)	1 3
11	s9	158/165 (96%)	123 (78%)	35 (22%)	1 5
12	C0	77/98 (79%)	64 (83%)	13 (17%)	2 11
12	c0	73/98 (74%)	57 (78%)	16 (22%)	1 5
13	C1	129/136 (95%)	107 (83%)	22 (17%)	2 11
13	c1	129/136 (95%)	98 (76%)	31 (24%)	1 4
14	C2	88/118 (75%)	68 (77%)	20 (23%)	1 5
14	c2	88/118 (75%)	61 (69%)	27 (31%)	0 1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	C3	127/127 (100%)	98 (77%)	29 (23%)	1 5
15	c3	127/127 (100%)	98 (77%)	29 (23%)	1 5
16	C4	81/104 (78%)	56 (69%)	25 (31%)	0 1
16	c4	97/104 (93%)	74 (76%)	23 (24%)	1 4
17	C5	101/117 (86%)	85 (84%)	16 (16%)	2 13
17	c5	103/117 (88%)	84 (82%)	19 (18%)	1 9
18	C6	117/118 (99%)	86 (74%)	31 (26%)	0 3
18	c6	118/118 (100%)	90 (76%)	28 (24%)	1 4
19	C7	94/124 (76%)	73 (78%)	21 (22%)	1 5
19	c7	92/124 (74%)	71 (77%)	21 (23%)	1 5
20	C8	128/128 (100%)	101 (79%)	27 (21%)	1 6
20	c8	128/128 (100%)	97 (76%)	31 (24%)	1 4
21	C9	115/115 (100%)	87 (76%)	28 (24%)	1 4
21	c9	115/115 (100%)	97 (84%)	18 (16%)	2 13
22	D0	100/113 (88%)	74 (74%)	26 (26%)	0 3
22	d0	103/113 (91%)	72 (70%)	31 (30%)	0 1
23	D1	74/74 (100%)	56 (76%)	18 (24%)	1 4
23	d1	74/74 (100%)	55 (74%)	19 (26%)	0 3
24	D2	110/110 (100%)	87 (79%)	23 (21%)	1 6
24	d2	110/110 (100%)	94 (86%)	16 (14%)	3 16
25	D3	119/119 (100%)	96 (81%)	23 (19%)	1 8
25	d3	119/119 (100%)	90 (76%)	29 (24%)	1 4
26	D4	112/112 (100%)	85 (76%)	27 (24%)	1 4
26	d4	112/112 (100%)	89 (80%)	23 (20%)	1 7
27	D5	61/88 (69%)	47 (77%)	14 (23%)	1 5
27	d5	61/88 (69%)	49 (80%)	12 (20%)	1 8
28	D6	83/83 (100%)	61 (74%)	22 (26%)	0 3
28	d6	83/83 (100%)	70 (84%)	13 (16%)	2 13
29	D7	70/70 (100%)	57 (81%)	13 (19%)	1 9
29	d7	70/70 (100%)	59 (84%)	11 (16%)	2 13
30	D8	56/59 (95%)	38 (68%)	18 (32%)	0 1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
30	d8	56/59 (95%)	42 (75%)	14 (25%)	0 3
31	D9	47/48 (98%)	38 (81%)	9 (19%)	1 9
31	d9	47/48 (98%)	35 (74%)	12 (26%)	0 3
32	E0	51/51 (100%)	41 (80%)	10 (20%)	1 8
33	E1	62/66 (94%)	45 (73%)	17 (27%)	0 2
33	e1	66/66 (100%)	50 (76%)	16 (24%)	1 4
34	SR	260/261 (100%)	204 (78%)	56 (22%)	1 6
34	sR	260/261 (100%)	231 (89%)	29 (11%)	6 25
35	SM	97/228 (42%)	72 (74%)	25 (26%)	0 3
35	sM	54/228 (24%)	40 (74%)	14 (26%)	0 3
39	L2	193/195 (99%)	144 (75%)	49 (25%)	0 3
39	l2	192/195 (98%)	147 (77%)	45 (23%)	1 4
40	L3	320/322 (99%)	240 (75%)	80 (25%)	0 3
40	l3	320/322 (99%)	247 (77%)	73 (23%)	1 5
41	L4	288/288 (100%)	220 (76%)	68 (24%)	1 4
41	l4	288/288 (100%)	220 (76%)	68 (24%)	1 4
42	L5	244/244 (100%)	190 (78%)	54 (22%)	1 5
42	l5	243/244 (100%)	185 (76%)	58 (24%)	1 4
43	L6	134/152 (88%)	116 (87%)	18 (13%)	4 19
43	l6	135/152 (89%)	109 (81%)	26 (19%)	1 8
44	L7	186/204 (91%)	159 (86%)	27 (14%)	3 16
44	l7	187/204 (92%)	153 (82%)	34 (18%)	2 9
45	L8	187/207 (90%)	144 (77%)	43 (23%)	1 5
45	l8	177/207 (86%)	135 (76%)	42 (24%)	1 4
46	L9	171/171 (100%)	136 (80%)	35 (20%)	1 7
46	l9	171/171 (100%)	118 (69%)	53 (31%)	0 1
47	M0	177/186 (95%)	130 (73%)	47 (27%)	0 3
47	m0	179/186 (96%)	144 (80%)	35 (20%)	1 8
48	M1	147/150 (98%)	122 (83%)	25 (17%)	2 11
48	m1	147/150 (98%)	108 (74%)	39 (26%)	0 3
49	M3	154/158 (98%)	119 (77%)	35 (23%)	1 5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
49	m3	154/158 (98%)	120 (78%)	34 (22%)	1 5
50	M4	107/108 (99%)	86 (80%)	21 (20%)	1 8
50	m4	108/108 (100%)	81 (75%)	27 (25%)	0 3
51	M5	175/175 (100%)	137 (78%)	38 (22%)	1 6
51	m5	175/175 (100%)	141 (81%)	34 (19%)	1 8
52	M6	160/161 (99%)	134 (84%)	26 (16%)	2 12
52	m6	160/161 (99%)	123 (77%)	37 (23%)	1 5
53	M7	140/145 (97%)	103 (74%)	37 (26%)	0 3
53	m7	125/145 (86%)	99 (79%)	26 (21%)	1 7
54	M8	150/150 (100%)	124 (83%)	26 (17%)	2 10
54	m8	150/150 (100%)	116 (77%)	34 (23%)	1 5
55	M9	153/153 (100%)	117 (76%)	36 (24%)	1 4
55	m9	153/153 (100%)	123 (80%)	30 (20%)	1 8
56	N0	156/156 (100%)	125 (80%)	31 (20%)	1 7
56	n0	156/156 (100%)	121 (78%)	35 (22%)	1 5
57	N1	136/136 (100%)	110 (81%)	26 (19%)	1 9
57	n1	136/136 (100%)	107 (79%)	29 (21%)	1 6
58	N2	87/106 (82%)	72 (83%)	15 (17%)	2 10
58	n2	85/106 (80%)	69 (81%)	16 (19%)	1 9
59	N3	104/104 (100%)	80 (77%)	24 (23%)	1 5
59	n3	104/104 (100%)	87 (84%)	17 (16%)	2 12
60	N4	57/129 (44%)	52 (91%)	5 (9%)	9 35
60	n4	100/129 (78%)	80 (80%)	20 (20%)	1 7
61	N5	104/117 (89%)	77 (74%)	27 (26%)	0 3
61	n5	104/117 (89%)	81 (78%)	23 (22%)	1 5
62	N6	109/109 (100%)	83 (76%)	26 (24%)	1 4
62	n6	109/109 (100%)	81 (74%)	28 (26%)	0 3
63	N7	115/115 (100%)	86 (75%)	29 (25%)	0 3
63	n7	115/115 (100%)	81 (70%)	34 (30%)	0 1
64	N8	118/118 (100%)	90 (76%)	28 (24%)	1 4
64	n8	118/118 (100%)	91 (77%)	27 (23%)	1 5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
65	N9	46/46 (100%)	34 (74%)	12 (26%)	0 3
65	n9	46/46 (100%)	30 (65%)	16 (35%)	0 0
66	O0	81/87 (93%)	62 (76%)	19 (24%)	1 4
66	o0	84/87 (97%)	67 (80%)	17 (20%)	1 7
67	O1	92/96 (96%)	70 (76%)	22 (24%)	1 4
67	o1	94/96 (98%)	63 (67%)	31 (33%)	0 1
68	O2	109/110 (99%)	84 (77%)	25 (23%)	1 5
68	o2	109/110 (99%)	75 (69%)	34 (31%)	0 1
69	O3	90/90 (100%)	73 (81%)	17 (19%)	1 9
69	o3	90/90 (100%)	73 (81%)	17 (19%)	1 9
70	O4	95/102 (93%)	70 (74%)	25 (26%)	0 3
70	o4	95/102 (93%)	74 (78%)	21 (22%)	1 5
71	O5	104/104 (100%)	80 (77%)	24 (23%)	1 5
71	o5	103/104 (99%)	79 (77%)	24 (23%)	1 5
72	O6	81/81 (100%)	55 (68%)	26 (32%)	0 1
72	o6	80/81 (99%)	50 (62%)	30 (38%)	0 0
73	O7	70/70 (100%)	54 (77%)	16 (23%)	1 5
73	o7	70/70 (100%)	57 (81%)	13 (19%)	1 9
74	O8	68/68 (100%)	50 (74%)	18 (26%)	0 3
74	o8	67/68 (98%)	49 (73%)	18 (27%)	0 2
75	O9	45/45 (100%)	36 (80%)	9 (20%)	1 7
75	o9	45/45 (100%)	36 (80%)	9 (20%)	1 7
76	Q0	47/47 (100%)	35 (74%)	12 (26%)	0 3
76	q0	47/47 (100%)	34 (72%)	13 (28%)	0 2
77	Q1	23/23 (100%)	19 (83%)	4 (17%)	2 10
77	q1	23/23 (100%)	15 (65%)	8 (35%)	0 0
78	Q2	90/90 (100%)	63 (70%)	27 (30%)	0 1
78	q2	90/90 (100%)	69 (77%)	21 (23%)	1 5
79	Q3	71/71 (100%)	54 (76%)	17 (24%)	1 4
79	q3	71/71 (100%)	55 (78%)	16 (22%)	1 5
80	e0	53/53 (100%)	41 (77%)	12 (23%)	1 5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
81	p0	105/253 (42%)	83 (79%)	22 (21%)	1 6
All	All	18728/20241 (92%)	14564 (78%)	4164 (22%)	1 5

5 of 4164 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
59	n3	7	GLN
63	n7	93	LYS
58	n2	85	LYS
81	p0	94	THR
55	M9	108	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 188 such sidechains are listed below:

Mol	Chain	Res	Type
15	c3	58	HIS
43	l6	28	GLN
18	c6	77	GLN
27	d5	38	HIS
46	l9	162	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1747/1800 (97%)	513 (29%)	56 (3%)
1	6	1793/1800 (99%)	475 (26%)	48 (2%)
36	1	3145/3396 (92%)	715 (22%)	78 (2%)
36	5	3145/3396 (92%)	691 (21%)	76 (2%)
37	3	120/121 (99%)	17 (14%)	2 (1%)
37	7	120/121 (99%)	24 (20%)	2 (1%)
38	4	157/158 (99%)	36 (22%)	5 (3%)
38	8	157/158 (99%)	38 (24%)	2 (1%)
All	All	10384/10950 (94%)	2509 (24%)	269 (2%)

5 of 2509 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	3	U

Continued on next page...

Continued from previous page...

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

5 of 269 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	5	2101	C
36	5	2255	A
36	5	3289	G
36	1	1716	U
36	1	1562	C

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2559 ligands modelled in this entry, 1426 are monoatomic - leaving 1133 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	3919	-	0,6,6	-	-	-		
86	OHX	1	4001	-	0,6,6	-	-	-		
86	OHX	5	4173	-	0,6,6	-	-	-		
86	OHX	O7	106	-	0,6,6	-	-	-		
86	OHX	2	2177	-	0,6,6	-	-	-		
86	OHX	1	4071	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	3968	-	0,6,6	-	-	-		
86	OHX	1	4096	-	0,6,6	-	-	-		
86	OHX	6	2159	-	0,6,6	-	-	-		
86	OHX	6	2125	-	0,6,6	-	-	-		
86	OHX	5	4081	-	0,6,6	-	-	-		
86	OHX	5	4162	-	0,6,6	-	-	-		
86	OHX	5	4014	-	0,6,6	-	-	-		
86	OHX	1	3922	-	0,6,6	-	-	-		
86	OHX	1	4028	-	0,6,6	-	-	-		
86	OHX	1	3997	-	0,6,6	-	-	-		
86	OHX	5	3916	-	0,6,6	-	-	-		
86	OHX	5	4047	-	0,6,6	-	-	-		
86	OHX	5	4113	-	0,6,6	-	-	-		
86	OHX	2	2057	-	0,6,6	-	-	-		
86	OHX	2	2118	-	0,6,6	-	-	-		
86	OHX	2	2173	-	0,6,6	-	-	-		
86	OHX	5	4231	-	0,6,6	-	-	-		
86	OHX	5	4052	-	0,6,6	-	-	-		
86	OHX	5	4157	-	0,6,6	-	-	-		
86	OHX	6	2052	-	0,6,6	-	-	-		
86	OHX	1	3999	-	0,6,6	-	-	-		
86	OHX	5	4170	-	0,6,6	-	-	-		
86	OHX	1	4067	-	0,6,6	-	-	-		
86	OHX	5	4177	-	0,6,6	-	-	-		
86	OHX	6	2079	-	0,6,6	-	-	-		
86	OHX	5	3955	-	0,6,6	-	-	-		
86	OHX	6	2116	-	0,6,6	-	-	-		
86	OHX	2	2078	-	0,6,6	-	-	-		
86	OHX	6	2103	-	0,6,6	-	-	-		
86	OHX	1	4081	-	0,6,6	-	-	-		
86	OHX	5	4093	-	0,6,6	-	-	-		
86	OHX	2	2081	-	0,6,6	-	-	-		
86	OHX	5	4079	-	0,6,6	-	-	-		
86	OHX	5	4082	-	0,6,6	-	-	-		
86	OHX	2	2160	-	0,6,6	-	-	-		
86	OHX	2	2166	-	0,6,6	-	-	-		
86	OHX	5	4221	-	0,6,6	-	-	-		
86	OHX	5	3938	-	0,6,6	-	-	-		
86	OHX	5	4218	-	0,6,6	-	-	-		
86	OHX	5	4137	-	0,6,6	-	-	-		
86	OHX	5	4194	-	0,6,6	-	-	-		
86	OHX	1	3885	-	0,6,6	-	-	-		
86	OHX	1	4191	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	6	2168	-	0,6,6	-	-	-		
86	OHX	5	4220	-	0,6,6	-	-	-		
86	OHX	5	4239	-	0,6,6	-	-	-		
86	OHX	5	3963	-	0,6,6	-	-	-		
86	OHX	5	4204	-	0,6,6	-	-	-		
86	OHX	5	3956	-	0,6,6	-	-	-		
86	OHX	6	2091	-	0,6,6	-	-	-		
86	OHX	5	4186	-	0,6,6	-	-	-		
86	OHX	1	4023	-	0,6,6	-	-	-		
86	OHX	2	2145	-	0,6,6	-	-	-		
86	OHX	3	216	-	0,6,6	-	-	-		
86	OHX	s1	303	-	0,6,6	-	-	-		
86	OHX	1	3907	-	0,6,6	-	-	-		
86	OHX	1	3979	-	0,6,6	-	-	-		
86	OHX	5	4215	-	0,6,6	-	-	-		
86	OHX	6	2128	-	0,6,6	-	-	-		
86	OHX	6	2190	-	0,6,6	-	-	-		
86	OHX	2	2050	-	0,6,6	-	-	-		
86	OHX	1	3953	-	0,6,6	-	-	-		
86	OHX	5	4090	-	0,6,6	-	-	-		
86	OHX	5	4086	-	0,6,6	-	-	-		
86	OHX	5	3933	-	0,6,6	-	-	-		
86	OHX	1	4030	-	0,6,6	-	-	-		
86	OHX	1	4175	-	0,6,6	-	-	-		
86	OHX	1	4006	-	0,6,6	-	-	-		
86	OHX	6	2109	-	0,6,6	-	-	-		
86	OHX	1	4079	-	0,6,6	-	-	-		
86	OHX	6	2177	-	0,6,6	-	-	-		
86	OHX	6	2185	-	0,6,6	-	-	-		
86	OHX	6	2200	-	0,6,6	-	-	-		
86	OHX	5	4224	-	0,6,6	-	-	-		
86	OHX	1	3944	-	0,6,6	-	-	-		
86	OHX	2	2152	-	0,6,6	-	-	-		
86	OHX	5	4189	-	0,6,6	-	-	-		
86	OHX	1	4137	-	0,6,6	-	-	-		
86	OHX	6	2150	-	0,6,6	-	-	-		
86	OHX	5	4025	-	0,6,6	-	-	-		
86	OHX	5	4244	-	0,6,6	-	-	-		
86	OHX	5	4122	-	0,6,6	-	-	-		
86	OHX	1	4204	-	0,6,6	-	-	-		
86	OHX	5	4111	-	0,6,6	-	-	-		
86	OHX	l4	403	-	0,6,6	-	-	-		
86	OHX	6	2100	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	2	2071	-	0,6,6	-	-	-		
86	OHX	6	2175	-	0,6,6	-	-	-		
86	OHX	5	4136	-	0,6,6	-	-	-		
86	OHX	4	234	-	0,6,6	-	-	-		
86	OHX	5	4108	-	0,6,6	-	-	-		
86	OHX	5	4095	-	0,6,6	-	-	-		
86	OHX	1	4057	-	0,6,6	-	-	-		
86	OHX	5	3960	-	0,6,6	-	-	-		
86	OHX	7	225	-	0,6,6	-	-	-		
86	OHX	6	2119	-	0,6,6	-	-	-		
86	OHX	5	4066	-	0,6,6	-	-	-		
86	OHX	5	4022	-	0,6,6	-	-	-		
86	OHX	4	225	-	0,6,6	-	-	-		
86	OHX	7	227	-	0,6,6	-	-	-		
86	OHX	5	4006	-	0,6,6	-	-	-		
86	OHX	6	2187	-	0,6,6	-	-	-		
86	OHX	5	4222	-	0,6,6	-	-	-		
86	OHX	8	215	-	0,6,6	-	-	-		
86	OHX	5	4158	-	0,6,6	-	-	-		
86	OHX	2	2142	-	0,6,6	-	-	-		
86	OHX	5	3905	-	0,6,6	-	-	-		
86	OHX	2	2060	-	0,6,6	-	-	-		
86	OHX	5	4182	-	0,6,6	-	-	-		
86	OHX	2	2178	-	0,6,6	-	-	-		
86	OHX	1	4025	-	0,6,6	-	-	-		
86	OHX	6	2204	-	0,6,6	-	-	-		
86	OHX	1	4043	-	0,6,6	-	-	-		
86	OHX	1	4068	-	0,6,6	-	-	-		
86	OHX	6	2148	-	0,6,6	-	-	-		
86	OHX	8	217	-	0,6,6	-	-	-		
86	OHX	6	2199	-	0,6,6	-	-	-		
86	OHX	5	4000	-	0,6,6	-	-	-		
86	OHX	1	3918	-	0,6,6	-	-	-		
86	OHX	1	3960	-	0,6,6	-	-	-		
86	OHX	5	4117	-	0,6,6	-	-	-		
86	OHX	6	2112	-	0,6,6	-	-	-		
86	OHX	1	4014	-	0,6,6	-	-	-		
86	OHX	4	226	-	0,6,6	-	-	-		
86	OHX	6	2188	-	0,6,6	-	-	-		
86	OHX	5	3940	-	0,6,6	-	-	-		
86	OHX	6	2203	-	0,6,6	-	-	-		
86	OHX	5	4184	-	0,6,6	-	-	-		
86	OHX	1	4124	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	4200	-	0,6,6	-	-	-		
86	OHX	4	228	-	0,6,6	-	-	-		
86	OHX	2	2041	-	0,6,6	-	-	-		
86	OHX	6	2074	-	0,6,6	-	-	-		
86	OHX	5	4119	-	0,6,6	-	-	-		
86	OHX	5	4234	-	0,6,6	-	-	-		
86	OHX	5	4143	-	0,6,6	-	-	-		
86	OHX	5	4104	-	0,6,6	-	-	-		
86	OHX	1	4177	-	0,6,6	-	-	-		
86	OHX	5	4013	-	0,6,6	-	-	-		
86	OHX	5	3966	-	0,6,6	-	-	-		
86	OHX	5	4129	-	0,6,6	-	-	-		
86	OHX	5	4246	-	0,6,6	-	-	-		
86	OHX	1	3892	-	0,6,6	-	-	-		
86	OHX	1	4034	-	0,6,6	-	-	-		
86	OHX	6	2099	-	0,6,6	-	-	-		
86	OHX	2	2029	-	0,6,6	-	-	-		
86	OHX	6	2056	-	0,6,6	-	-	-		
86	OHX	5	4249	-	0,6,6	-	-	-		
86	OHX	6	2121	-	0,6,6	-	-	-		
86	OHX	6	2184	-	0,6,6	-	-	-		
86	OHX	5	3901	-	0,6,6	-	-	-		
86	OHX	5	3987	-	0,6,6	-	-	-		
86	OHX	1	4112	-	0,6,6	-	-	-		
86	OHX	1	4048	-	0,6,6	-	-	-		
86	OHX	5	4171	-	0,6,6	-	-	-		
86	OHX	6	2086	-	0,6,6	-	-	-		
86	OHX	5	4106	-	0,6,6	-	-	-		
86	OHX	1	3966	-	0,6,6	-	-	-		
86	OHX	O3	201	-	0,6,6	-	-	-		
86	OHX	6	2180	-	0,6,6	-	-	-		
86	OHX	2	2121	-	0,6,6	-	-	-		
86	OHX	1	4002	-	0,6,6	-	-	-		
86	OHX	5	3909	-	0,6,6	-	-	-		
86	OHX	5	4253	-	0,6,6	-	-	-		
86	OHX	6	2194	-	0,6,6	-	-	-		
86	OHX	1	3881	-	0,6,6	-	-	-		
86	OHX	5	4077	-	0,6,6	-	-	-		
86	OHX	6	2087	-	0,6,6	-	-	-		
86	OHX	l9	202	-	0,6,6	-	-	-		
86	OHX	6	2048	-	0,6,6	-	-	-		
86	OHX	1	4122	-	0,6,6	-	-	-		
86	OHX	1	4187	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	5	4229	-	0,6,6	-	-	-		
86	OHX	5	4078	-	0,6,6	-	-	-		
86	OHX	1	3911	-	0,6,6	-	-	-		
86	OHX	1	4188	-	0,6,6	-	-	-		
86	OHX	5	3978	-	0,6,6	-	-	-		
86	OHX	1	4029	-	0,6,6	-	-	-		
86	OHX	5	3939	-	0,6,6	-	-	-		
86	OHX	2	2025	-	0,6,6	-	-	-		
86	OHX	1	4171	-	0,6,6	-	-	-		
86	OHX	5	4102	-	0,6,6	-	-	-		
86	OHX	3	219	-	0,6,6	-	-	-		
86	OHX	5	4190	-	0,6,6	-	-	-		
86	OHX	6	2169	-	0,6,6	-	-	-		
86	OHX	2	2089	-	0,6,6	-	-	-		
86	OHX	8	222	-	0,6,6	-	-	-		
86	OHX	1	3991	-	0,6,6	-	-	-		
86	OHX	L3	406	-	0,6,6	-	-	-		
86	OHX	5	4016	-	0,6,6	-	-	-		
86	OHX	1	4120	-	0,6,6	-	-	-		
86	OHX	2	2115	-	0,6,6	-	-	-		
86	OHX	5	4072	-	0,6,6	-	-	-		
86	OHX	5	4061	-	0,6,6	-	-	-		
86	OHX	5	3930	-	0,6,6	-	-	-		
86	OHX	1	4077	-	0,6,6	-	-	-		
86	OHX	5	3903	-	0,6,6	-	-	-		
86	OHX	2	2092	-	0,6,6	-	-	-		
86	OHX	1	4139	-	0,6,6	-	-	-		
86	OHX	5	3972	-	0,6,6	-	-	-		
86	OHX	2	2136	-	0,6,6	-	-	-		
86	OHX	1	3882	-	0,6,6	-	-	-		
86	OHX	1	3959	-	0,6,6	-	-	-		
86	OHX	6	2163	-	0,6,6	-	-	-		
86	OHX	5	4010	-	0,6,6	-	-	-		
86	OHX	2	2077	-	0,6,6	-	-	-		
86	OHX	1	4033	-	0,6,6	-	-	-		
86	OHX	2	2108	-	0,6,6	-	-	-		
86	OHX	5	3917	-	0,6,6	-	-	-		
86	OHX	5	3922	-	0,6,6	-	-	-		
86	OHX	6	2201	-	0,6,6	-	-	-		
86	OHX	1	4087	-	0,6,6	-	-	-		
86	OHX	6	2082	-	0,6,6	-	-	-		
86	OHX	2	2056	-	0,6,6	-	-	-		
86	OHX	2	2097	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	4151	-	0,6,6	-	-	-		
86	OHX	5	3991	-	0,6,6	-	-	-		
86	OHX	1	4016	-	0,6,6	-	-	-		
86	OHX	5	4174	-	0,6,6	-	-	-		
86	OHX	2	2158	-	0,6,6	-	-	-		
86	OHX	1	3924	-	0,6,6	-	-	-		
86	OHX	1	4027	-	0,6,6	-	-	-		
86	OHX	1	4105	-	0,6,6	-	-	-		
86	OHX	5	4142	-	0,6,6	-	-	-		
86	OHX	5	4208	-	0,6,6	-	-	-		
86	OHX	5	4210	-	0,6,6	-	-	-		
86	OHX	1	4121	-	0,6,6	-	-	-		
86	OHX	8	229	-	0,6,6	-	-	-		
86	OHX	1	3935	-	0,6,6	-	-	-		
86	OHX	6	2064	-	0,6,6	-	-	-		
86	OHX	1	4007	-	0,6,6	-	-	-		
86	OHX	1	4161	-	0,6,6	-	-	-		
86	OHX	6	2063	-	0,6,6	-	-	-		
86	OHX	5	4003	-	0,6,6	-	-	-		
86	OHX	5	4028	-	0,6,6	-	-	-		
86	OHX	5	4037	-	0,6,6	-	-	-		
86	OHX	1	4080	-	0,6,6	-	-	-		
86	OHX	5	4065	-	0,6,6	-	-	-		
86	OHX	1	3902	-	0,6,6	-	-	-		
86	OHX	6	2062	-	0,6,6	-	-	-		
86	OHX	5	4103	-	0,6,6	-	-	-		
86	OHX	1	4145	-	0,6,6	-	-	-		
86	OHX	6	2129	-	0,6,6	-	-	-		
86	OHX	SR	401	-	0,6,6	-	-	-		
86	OHX	1	3956	-	0,6,6	-	-	-		
86	OHX	1	4035	-	0,6,6	-	-	-		
86	OHX	5	3913	-	0,6,6	-	-	-		
86	OHX	5	4166	-	0,6,6	-	-	-		
86	OHX	5	4237	-	0,6,6	-	-	-		
86	OHX	1	3873	-	0,6,6	-	-	-		
86	OHX	2	2132	-	0,6,6	-	-	-		
86	OHX	8	225	-	0,6,6	-	-	-		
86	OHX	2	2126	-	0,6,6	-	-	-		
86	OHX	2	2155	-	0,6,6	-	-	-		
86	OHX	1	4114	-	0,6,6	-	-	-		
86	OHX	2	2064	-	0,6,6	-	-	-		
86	OHX	1	4174	-	0,6,6	-	-	-		
86	OHX	O2	202	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	4041	-	0,6,6	-	-	-		
86	OHX	1	4185	-	0,6,6	-	-	-		
86	OHX	5	4105	-	0,6,6	-	-	-		
86	OHX	1	3994	-	0,6,6	-	-	-		
86	OHX	1	3961	-	0,6,6	-	-	-		
86	OHX	6	2120	-	0,6,6	-	-	-		
86	OHX	5	4130	-	0,6,6	-	-	-		
86	OHX	5	4202	-	0,6,6	-	-	-		
86	OHX	1	3868	-	0,6,6	-	-	-		
86	OHX	5	4007	-	0,6,6	-	-	-		
86	OHX	5	4059	-	0,6,6	-	-	-		
86	OHX	5	4241	-	0,6,6	-	-	-		
86	OHX	8	219	-	0,6,6	-	-	-		
86	OHX	5	4154	-	0,6,6	-	-	-		
86	OHX	5	3904	-	0,6,6	-	-	-		
86	OHX	5	4009	-	0,6,6	-	-	-		
86	OHX	6	2123	-	0,6,6	-	-	-		
86	OHX	1	4169	-	0,6,6	-	-	-		
86	OHX	5	4245	-	0,6,6	-	-	-		
86	OHX	5	4180	-	0,6,6	-	-	-		
86	OHX	M0	304	-	0,6,6	-	-	-		
86	OHX	6	2058	-	0,6,6	-	-	-		
86	OHX	1	3875	-	0,6,6	-	-	-		
86	OHX	1	4008	-	0,6,6	-	-	-		
86	OHX	5	3906	-	0,6,6	-	-	-		
86	OHX	2	2162	-	0,6,6	-	-	-		
86	OHX	m4	201	-	0,6,6	-	-	-		
86	OHX	1	3869	-	0,6,6	-	-	-		
86	OHX	2	2147	-	0,6,6	-	-	-		
86	OHX	5	3975	-	0,6,6	-	-	-		
86	OHX	n9	102	-	0,6,6	-	-	-		
86	OHX	5	3994	-	0,6,6	-	-	-		
86	OHX	4	222	-	0,6,6	-	-	-		
86	OHX	6	2196	-	0,6,6	-	-	-		
86	OHX	1	3939	-	0,6,6	-	-	-		
86	OHX	5	3929	-	0,6,6	-	-	-		
86	OHX	5	3945	-	0,6,6	-	-	-		
86	OHX	1	3947	-	0,6,6	-	-	-		
86	OHX	6	2068	-	0,6,6	-	-	-		
86	OHX	2	2073	-	0,6,6	-	-	-		
86	OHX	5	4087	-	0,6,6	-	-	-		
86	OHX	1	3889	-	0,6,6	-	-	-		
86	OHX	1	3954	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	4064	-	0,6,6	-	-	-		
86	OHX	1	4158	-	0,6,6	-	-	-		
86	OHX	C1	201	-	0,6,6	-	-	-		
86	OHX	6	2053	-	0,6,6	-	-	-		
86	OHX	6	2170	-	0,6,6	-	-	-		
86	OHX	5	4120	-	0,6,6	-	-	-		
86	OHX	5	4183	-	0,6,6	-	-	-		
86	OHX	5	4196	-	0,6,6	-	-	-		
86	OHX	2	2054	-	0,6,6	-	-	-		
86	OHX	4	227	-	0,6,6	-	-	-		
86	OHX	1	4178	-	0,6,6	-	-	-		
86	OHX	1	4135	-	0,6,6	-	-	-		
86	OHX	5	4128	-	0,6,6	-	-	-		
86	OHX	1	4179	-	0,6,6	-	-	-		
86	OHX	1	3863	-	0,6,6	-	-	-		
86	OHX	1	4202	-	0,6,6	-	-	-		
86	OHX	5	4038	-	0,6,6	-	-	-		
86	OHX	5	4083	-	0,6,6	-	-	-		
86	OHX	2	2143	-	0,6,6	-	-	-		
86	OHX	5	4005	-	0,6,6	-	-	-		
86	OHX	1	3933	-	0,6,6	-	-	-		
86	OHX	5	4225	-	0,6,6	-	-	-		
87	3K8	2	2179	-	32,32,32	0.82	1 (3%)	44,47,47	0.92	2 (4%)
86	OHX	5	4050	-	0,6,6	-	-	-		
86	OHX	2	2062	-	0,6,6	-	-	-		
86	OHX	2	2111	-	0,6,6	-	-	-		
86	OHX	6	2189	-	0,6,6	-	-	-		
86	OHX	5	4107	-	0,6,6	-	-	-		
86	OHX	1	3986	-	0,6,6	-	-	-		
86	OHX	5	3962	-	0,6,6	-	-	-		
86	OHX	5	3952	-	0,6,6	-	-	-		
86	OHX	1	3915	-	0,6,6	-	-	-		
86	OHX	6	2166	-	0,6,6	-	-	-		
86	OHX	5	3967	-	0,6,6	-	-	-		
86	OHX	5	4209	-	0,6,6	-	-	-		
86	OHX	6	2154	-	0,6,6	-	-	-		
86	OHX	q2	502	-	0,6,6	-	-	-		
86	OHX	2	2157	-	0,6,6	-	-	-		
86	OHX	2	2036	-	0,6,6	-	-	-		
86	OHX	D9	102	-	0,6,6	-	-	-		
86	OHX	5	4195	-	0,6,6	-	-	-		
86	OHX	1	3949	-	0,6,6	-	-	-		
86	OHX	5	4168	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	5	4178	-	0,6,6	-	-	-		
86	OHX	1	4053	-	0,6,6	-	-	-		
86	OHX	1	3963	-	0,6,6	-	-	-		
86	OHX	6	2102	-	0,6,6	-	-	-		
86	OHX	l5	303	-	0,6,6	-	-	-		
86	OHX	1	4128	-	0,6,6	-	-	-		
86	OHX	4	224	-	0,6,6	-	-	-		
86	OHX	1	4083	-	0,6,6	-	-	-		
86	OHX	5	4096	-	0,6,6	-	-	-		
86	OHX	5	4199	-	0,6,6	-	-	-		
86	OHX	1	4004	-	0,6,6	-	-	-		
86	OHX	1	3877	-	0,6,6	-	-	-		
86	OHX	2	2070	-	0,6,6	-	-	-		
86	OHX	1	4037	-	0,6,6	-	-	-		
86	OHX	6	2106	-	0,6,6	-	-	-		
86	OHX	5	3923	-	0,6,6	-	-	-		
86	OHX	1	3984	-	0,6,6	-	-	-		
86	OHX	C8	201	-	0,6,6	-	-	-		
86	OHX	7	221	-	0,6,6	-	-	-		
86	OHX	1	4144	-	0,6,6	-	-	-		
86	OHX	1	3862	-	0,6,6	-	-	-		
86	OHX	5	4230	-	0,6,6	-	-	-		
86	OHX	1	3962	-	0,6,6	-	-	-		
86	OHX	2	2047	-	0,6,6	-	-	-		
86	OHX	6	2165	-	0,6,6	-	-	-		
86	OHX	m0	302	-	0,6,6	-	-	-		
86	OHX	5	3907	-	0,6,6	-	-	-		
86	OHX	2	2069	-	0,6,6	-	-	-		
86	OHX	5	4011	-	0,6,6	-	-	-		
86	OHX	5	4069	-	0,6,6	-	-	-		
86	OHX	2	2172	-	0,6,6	-	-	-		
86	OHX	5	4214	-	0,6,6	-	-	-		
86	OHX	7	218	-	0,6,6	-	-	-		
86	OHX	5	3953	-	0,6,6	-	-	-		
86	OHX	5	3973	-	0,6,6	-	-	-		
86	OHX	5	4251	-	0,6,6	-	-	-		
86	OHX	7	223	-	0,6,6	-	-	-		
86	OHX	5	4165	-	0,6,6	-	-	-		
86	OHX	6	2118	-	0,6,6	-	-	-		
86	OHX	1	3971	-	0,6,6	-	-	-		
86	OHX	5	4030	-	0,6,6	-	-	-		
86	OHX	1	3957	-	0,6,6	-	-	-		
86	OHX	5	4149	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	3950	-	0,6,6	-	-	-		
86	OHX	1	4163	-	0,6,6	-	-	-		
86	OHX	1	4199	-	0,6,6	-	-	-		
86	OHX	2	2082	-	0,6,6	-	-	-		
86	OHX	5	3910	-	0,6,6	-	-	-		
86	OHX	2	2170	-	0,6,6	-	-	-		
86	OHX	5	3914	-	0,6,6	-	-	-		
86	OHX	6	2071	-	0,6,6	-	-	-		
86	OHX	6	2139	-	0,6,6	-	-	-		
86	OHX	6	2192	-	0,6,6	-	-	-		
86	OHX	5	4040	-	0,6,6	-	-	-		
86	OHX	5	4138	-	0,6,6	-	-	-		
86	OHX	1	3958	-	0,6,6	-	-	-		
86	OHX	2	2034	-	0,6,6	-	-	-		
86	OHX	m6	202	-	0,6,6	-	-	-		
86	OHX	6	2130	-	0,6,6	-	-	-		
86	OHX	1	3880	-	0,6,6	-	-	-		
86	OHX	5	4063	-	0,6,6	-	-	-		
86	OHX	l3	403	-	0,6,6	-	-	-		
86	OHX	1	4104	-	0,6,6	-	-	-		
86	OHX	1	3975	-	0,6,6	-	-	-		
86	OHX	M9	202	-	0,6,6	-	-	-		
86	OHX	5	3921	-	0,6,6	-	-	-		
86	OHX	1	3865	-	0,6,6	-	-	-		
86	OHX	n1	201	-	0,6,6	-	-	-		
86	OHX	2	2037	-	0,6,6	-	-	-		
86	OHX	2	2139	-	0,6,6	-	-	-		
86	OHX	5	4019	-	0,6,6	-	-	-		
86	OHX	6	2072	-	0,6,6	-	-	-		
86	OHX	1	4000	-	0,6,6	-	-	-		
86	OHX	2	2129	-	0,6,6	-	-	-		
86	OHX	4	223	-	0,6,6	-	-	-		
86	OHX	5	3961	-	0,6,6	-	-	-		
86	OHX	2	2138	-	0,6,6	-	-	-		
86	OHX	m5	303	-	0,6,6	-	-	-		
86	OHX	6	2067	-	0,6,6	-	-	-		
86	OHX	3	221	-	0,6,6	-	-	-		
86	OHX	5	4110	-	0,6,6	-	-	-		
86	OHX	5	4236	-	0,6,6	-	-	-		
86	OHX	5	4021	-	0,6,6	-	-	-		
86	OHX	8	226	-	0,6,6	-	-	-		
86	OHX	5	4235	-	0,6,6	-	-	-		
86	OHX	8	231	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	2	2051	-	0,6,6	-	-	-		
86	OHX	1	3926	-	0,6,6	-	-	-		
86	OHX	s9	201	-	0,6,6	-	-	-		
87	3K8	6	2205	-	32,32,32	0.54	0	44,47,47	0.90	3 (6%)
86	OHX	4	235	-	0,6,6	-	-	-		
86	OHX	6	2181	-	0,6,6	-	-	-		
86	OHX	2	2150	-	0,6,6	-	-	-		
86	OHX	5	4043	-	0,6,6	-	-	-		
86	OHX	1	4051	-	0,6,6	-	-	-		
86	OHX	L4	402	-	0,6,6	-	-	-		
86	OHX	1	4150	-	0,6,6	-	-	-		
86	OHX	2	2100	-	0,6,6	-	-	-		
86	OHX	2	2120	-	0,6,6	-	-	-		
86	OHX	1	4063	-	0,6,6	-	-	-		
86	OHX	3	218	-	0,6,6	-	-	-		
86	OHX	1	3921	-	0,6,6	-	-	-		
86	OHX	6	2076	-	0,6,6	-	-	-		
86	OHX	1	4085	-	0,6,6	-	-	-		
86	OHX	2	2067	-	0,6,6	-	-	-		
86	OHX	1	3983	-	0,6,6	-	-	-		
86	OHX	6	2137	-	0,6,6	-	-	-		
86	OHX	2	2106	-	0,6,6	-	-	-		
86	OHX	1	3914	-	0,6,6	-	-	-		
86	OHX	1	4044	-	0,6,6	-	-	-		
86	OHX	1	4109	-	0,6,6	-	-	-		
86	OHX	1	4091	-	0,6,6	-	-	-		
86	OHX	5	4088	-	0,6,6	-	-	-		
86	OHX	5	4217	-	0,6,6	-	-	-		
86	OHX	5	4207	-	0,6,6	-	-	-		
86	OHX	8	224	-	0,6,6	-	-	-		
86	OHX	1	4110	-	0,6,6	-	-	-		
86	OHX	2	2128	-	0,6,6	-	-	-		
86	OHX	2	2165	-	0,6,6	-	-	-		
86	OHX	2	2032	-	0,6,6	-	-	-		
86	OHX	5	3941	-	0,6,6	-	-	-		
86	OHX	1	4061	-	0,6,6	-	-	-		
86	OHX	5	4232	-	0,6,6	-	-	-		
86	OHX	5	3976	-	0,6,6	-	-	-		
86	OHX	5	4118	-	0,6,6	-	-	-		
86	OHX	1	3995	-	0,6,6	-	-	-		
86	OHX	1	4125	-	0,6,6	-	-	-		
86	OHX	1	4152	-	0,6,6	-	-	-		
86	OHX	5	4226	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	6	2069	-	0,6,6	-	-	-		
86	OHX	1	4193	-	0,6,6	-	-	-		
86	OHX	1	4167	-	0,6,6	-	-	-		
86	OHX	1	3980	-	0,6,6	-	-	-		
86	OHX	2	2068	-	0,6,6	-	-	-		
86	OHX	2	2093	-	0,6,6	-	-	-		
86	OHX	M5	302	-	0,6,6	-	-	-		
86	OHX	1	4100	-	0,6,6	-	-	-		
86	OHX	6	2131	-	0,6,6	-	-	-		
86	OHX	s4	301	-	0,6,6	-	-	-		
86	OHX	5	3983	-	0,6,6	-	-	-		
86	OHX	1	3890	-	0,6,6	-	-	-		
86	OHX	1	4190	-	0,6,6	-	-	-		
86	OHX	5	4056	-	0,6,6	-	-	-		
86	OHX	1	4166	-	0,6,6	-	-	-		
86	OHX	1	4133	-	0,6,6	-	-	-		
86	OHX	6	2094	-	0,6,6	-	-	-		
86	OHX	6	2096	-	0,6,6	-	-	-		
86	OHX	1	4132	-	0,6,6	-	-	-		
86	OHX	2	2174	-	0,6,6	-	-	-		
86	OHX	1	4055	-	0,6,6	-	-	-		
86	OHX	1	4143	-	0,6,6	-	-	-		
86	OHX	1	4198	-	0,6,6	-	-	-		
86	OHX	1	3941	-	0,6,6	-	-	-		
86	OHX	1	3988	-	0,6,6	-	-	-		
86	OHX	1	4054	-	0,6,6	-	-	-		
86	OHX	4	229	-	0,6,6	-	-	-		
86	OHX	6	2075	-	0,6,6	-	-	-		
86	OHX	5	3989	-	0,6,6	-	-	-		
86	OHX	l5	304	-	0,6,6	-	-	-		
86	OHX	2	2161	-	0,6,6	-	-	-		
86	OHX	5	4049	-	0,6,6	-	-	-		
86	OHX	2	2086	-	0,6,6	-	-	-		
86	OHX	2	2164	-	0,6,6	-	-	-		
86	OHX	6	2081	-	0,6,6	-	-	-		
86	OHX	5	4018	-	0,6,6	-	-	-		
86	OHX	1	3937	-	0,6,6	-	-	-		
86	OHX	1	4210	-	0,6,6	-	-	-		
86	OHX	1	4082	-	0,6,6	-	-	-		
86	OHX	5	3919	-	0,6,6	-	-	-		
86	OHX	5	4001	-	0,6,6	-	-	-		
86	OHX	8	220	-	0,6,6	-	-	-		
86	OHX	6	2104	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	5	4002	-	0,6,6	-	-	-		
86	OHX	2	2169	-	0,6,6	-	-	-		
86	OHX	6	2114	-	0,6,6	-	-	-		
86	OHX	5	3948	-	0,6,6	-	-	-		
86	OHX	5	3968	-	0,6,6	-	-	-		
86	OHX	5	4193	-	0,6,6	-	-	-		
86	OHX	O7	105	-	0,6,6	-	-	-		
86	OHX	5	4252	-	0,6,6	-	-	-		
86	OHX	5	3936	-	0,6,6	-	-	-		
86	OHX	1	3927	-	0,6,6	-	-	-		
86	OHX	1	3867	-	0,6,6	-	-	-		
86	OHX	5	4126	-	0,6,6	-	-	-		
86	OHX	1	4076	-	0,6,6	-	-	-		
86	OHX	6	2146	-	0,6,6	-	-	-		
86	OHX	1	4148	-	0,6,6	-	-	-		
86	OHX	3	225	-	0,6,6	-	-	-		
86	OHX	6	2092	-	0,6,6	-	-	-		
86	OHX	1	4049	-	0,6,6	-	-	-		
86	OHX	5	3999	-	0,6,6	-	-	-		
86	OHX	5	4067	-	0,6,6	-	-	-		
86	OHX	2	2137	-	0,6,6	-	-	-		
86	OHX	1	3864	-	0,6,6	-	-	-		
86	OHX	N9	101	-	0,6,6	-	-	-		
86	OHX	5	3990	-	0,6,6	-	-	-		
86	OHX	5	4109	-	0,6,6	-	-	-		
86	OHX	5	4247	-	0,6,6	-	-	-		
86	OHX	1	3977	-	0,6,6	-	-	-		
86	OHX	1	3948	-	0,6,6	-	-	-		
86	OHX	1	4180	-	0,6,6	-	-	-		
86	OHX	2	2044	-	0,6,6	-	-	-		
86	OHX	5	4191	-	0,6,6	-	-	-		
86	OHX	6	2133	-	0,6,6	-	-	-		
86	OHX	5	4070	-	0,6,6	-	-	-		
86	OHX	2	2048	-	0,6,6	-	-	-		
86	OHX	2	2114	-	0,6,6	-	-	-		
86	OHX	1	4126	-	0,6,6	-	-	-		
86	OHX	5	4023	-	0,6,6	-	-	-		
86	OHX	5	4036	-	0,6,6	-	-	-		
86	OHX	5	4124	-	0,6,6	-	-	-		
86	OHX	6	2117	-	0,6,6	-	-	-		
86	OHX	6	2172	-	0,6,6	-	-	-		
86	OHX	1	4116	-	0,6,6	-	-	-		
86	OHX	6	2158	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	5	4089	-	0,6,6	-	-	-		
86	OHX	5	4075	-	0,6,6	-	-	-		
86	OHX	1	4136	-	0,6,6	-	-	-		
86	OHX	5	4100	-	0,6,6	-	-	-		
86	OHX	1	3912	-	0,6,6	-	-	-		
86	OHX	1	4201	-	0,6,6	-	-	-		
86	OHX	5	4151	-	0,6,6	-	-	-		
86	OHX	5	4175	-	0,6,6	-	-	-		
86	OHX	1	4141	-	0,6,6	-	-	-		
86	OHX	6	2191	-	0,6,6	-	-	-		
86	OHX	1	3874	-	0,6,6	-	-	-		
86	OHX	1	3970	-	0,6,6	-	-	-		
86	OHX	5	3944	-	0,6,6	-	-	-		
86	OHX	2	2156	-	0,6,6	-	-	-		
86	OHX	2	2130	-	0,6,6	-	-	-		
86	OHX	l3	402	-	0,6,6	-	-	-		
86	OHX	5	4242	-	0,6,6	-	-	-		
86	OHX	1	3987	-	0,6,6	-	-	-		
86	OHX	1	4118	-	0,6,6	-	-	-		
86	OHX	1	4070	-	0,6,6	-	-	-		
86	OHX	6	2089	-	0,6,6	-	-	-		
86	OHX	5	3935	-	0,6,6	-	-	-		
86	OHX	5	4094	-	0,6,6	-	-	-		
86	OHX	5	4159	-	0,6,6	-	-	-		
86	OHX	8	218	-	0,6,6	-	-	-		
86	OHX	6	2155	-	0,6,6	-	-	-		
86	OHX	6	2115	-	0,6,6	-	-	-		
86	OHX	5	4115	-	0,6,6	-	-	-		
86	OHX	1	3871	-	0,6,6	-	-	-		
86	OHX	2	2104	-	0,6,6	-	-	-		
86	OHX	6	2141	-	0,6,6	-	-	-		
86	OHX	5	4057	-	0,6,6	-	-	-		
86	OHX	2	2084	-	0,6,6	-	-	-		
86	OHX	1	3940	-	0,6,6	-	-	-		
86	OHX	6	2073	-	0,6,6	-	-	-		
86	OHX	1	3998	-	0,6,6	-	-	-		
86	OHX	5	3992	-	0,6,6	-	-	-		
86	OHX	5	4091	-	0,6,6	-	-	-		
86	OHX	5	4203	-	0,6,6	-	-	-		
86	OHX	6	2077	-	0,6,6	-	-	-		
86	OHX	m1	202	-	0,6,6	-	-	-		
86	OHX	2	2074	-	0,6,6	-	-	-		
86	OHX	6	2107	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	2	2033	-	0,6,6	-	-	-		
86	OHX	2	2026	-	0,6,6	-	-	-		
86	OHX	1	3974	-	0,6,6	-	-	-		
86	OHX	5	3908	-	0,6,6	-	-	-		
86	OHX	2	2154	-	0,6,6	-	-	-		
86	OHX	5	4073	-	0,6,6	-	-	-		
86	OHX	5	4114	-	0,6,6	-	-	-		
86	OHX	2	2055	-	0,6,6	-	-	-		
86	OHX	3	224	-	0,6,6	-	-	-		
86	OHX	1	3938	-	0,6,6	-	-	-		
86	OHX	5	4068	-	0,6,6	-	-	-		
86	OHX	6	2144	-	0,6,6	-	-	-		
86	OHX	1	4094	-	0,6,6	-	-	-		
86	OHX	1	4159	-	0,6,6	-	-	-		
86	OHX	6	2162	-	0,6,6	-	-	-		
86	OHX	7	222	-	0,6,6	-	-	-		
86	OHX	1	3879	-	0,6,6	-	-	-		
86	OHX	1	3899	-	0,6,6	-	-	-		
86	OHX	1	4012	-	0,6,6	-	-	-		
86	OHX	1	4115	-	0,6,6	-	-	-		
86	OHX	1	4147	-	0,6,6	-	-	-		
86	OHX	4	231	-	0,6,6	-	-	-		
86	OHX	6	2111	-	0,6,6	-	-	-		
86	OHX	1	3992	-	0,6,6	-	-	-		
86	OHX	1	3934	-	0,6,6	-	-	-		
86	OHX	M8	201	-	0,6,6	-	-	-		
86	OHX	5	4233	-	0,6,6	-	-	-		
86	OHX	2	2042	-	0,6,6	-	-	-		
86	OHX	6	2095	-	0,6,6	-	-	-		
86	OHX	6	2080	-	0,6,6	-	-	-		
86	OHX	2	2153	-	0,6,6	-	-	-		
86	OHX	2	2105	-	0,6,6	-	-	-		
86	OHX	1	4173	-	0,6,6	-	-	-		
86	OHX	5	4200	-	0,6,6	-	-	-		
86	OHX	6	2054	-	0,6,6	-	-	-		
86	OHX	1	3898	-	0,6,6	-	-	-		
86	OHX	6	2135	-	0,6,6	-	-	-		
86	OHX	5	4027	-	0,6,6	-	-	-		
86	OHX	1	4192	-	0,6,6	-	-	-		
86	OHX	5	4228	-	0,6,6	-	-	-		
86	OHX	1	3896	-	0,6,6	-	-	-		
86	OHX	N1	201	-	0,6,6	-	-	-		
86	OHX	1	3916	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	6	2132	-	0,6,6	-	-	-		
86	OHX	5	3947	-	0,6,6	-	-	-		
86	OHX	6	2126	-	0,6,6	-	-	-		
86	OHX	2	2031	-	0,6,6	-	-	-		
86	OHX	4	233	-	0,6,6	-	-	-		
86	OHX	5	4133	-	0,6,6	-	-	-		
86	OHX	8	230	-	0,6,6	-	-	-		
86	OHX	2	2059	-	0,6,6	-	-	-		
86	OHX	5	4254	-	0,6,6	-	-	-		
86	OHX	5	3925	-	0,6,6	-	-	-		
86	OHX	2	2122	-	0,6,6	-	-	-		
86	OHX	2	2110	-	0,6,6	-	-	-		
86	OHX	5	4092	-	0,6,6	-	-	-		
86	OHX	2	2109	-	0,6,6	-	-	-		
86	OHX	2	2075	-	0,6,6	-	-	-		
86	OHX	6	2197	-	0,6,6	-	-	-		
86	OHX	1	3955	-	0,6,6	-	-	-		
86	OHX	5	3969	-	0,6,6	-	-	-		
86	OHX	2	2040	-	0,6,6	-	-	-		
86	OHX	4	232	-	0,6,6	-	-	-		
86	OHX	1	4117	-	0,6,6	-	-	-		
86	OHX	2	2141	-	0,6,6	-	-	-		
86	OHX	6	2061	-	0,6,6	-	-	-		
86	OHX	2	2090	-	0,6,6	-	-	-		
86	OHX	5	4035	-	0,6,6	-	-	-		
86	OHX	5	4048	-	0,6,6	-	-	-		
86	OHX	1	4194	-	0,6,6	-	-	-		
86	OHX	1	4056	-	0,6,6	-	-	-		
86	OHX	3	222	-	0,6,6	-	-	-		
86	OHX	1	3887	-	0,6,6	-	-	-		
86	OHX	6	2085	-	0,6,6	-	-	-		
86	OHX	5	4212	-	0,6,6	-	-	-		
86	OHX	5	3920	-	0,6,6	-	-	-		
86	OHX	2	2107	-	0,6,6	-	-	-		
86	OHX	1	3897	-	0,6,6	-	-	-		
86	OHX	5	3931	-	0,6,6	-	-	-		
86	OHX	m7	206	-	0,6,6	-	-	-		
86	OHX	1	3925	-	0,6,6	-	-	-		
86	OHX	5	4187	-	0,6,6	-	-	-		
86	OHX	5	3918	-	0,6,6	-	-	-		
86	OHX	1	3866	-	0,6,6	-	-	-		
86	OHX	6	2101	-	0,6,6	-	-	-		
86	OHX	1	3905	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	4086	-	0,6,6	-	-	-		
86	OHX	5	4188	-	0,6,6	-	-	-		
86	OHX	4	230	-	0,6,6	-	-	-		
86	OHX	1	3964	-	0,6,6	-	-	-		
86	OHX	1	3893	-	0,6,6	-	-	-		
86	OHX	1	4084	-	0,6,6	-	-	-		
86	OHX	5	4029	-	0,6,6	-	-	-		
86	OHX	m0	303	-	0,6,6	-	-	-		
86	OHX	5	4015	-	0,6,6	-	-	-		
86	OHX	6	2122	-	0,6,6	-	-	-		
86	OHX	7	217	-	0,6,6	-	-	-		
86	OHX	1	4155	-	0,6,6	-	-	-		
86	OHX	1	3936	-	0,6,6	-	-	-		
86	OHX	1	3888	-	0,6,6	-	-	-		
86	OHX	1	4111	-	0,6,6	-	-	-		
86	OHX	1	4156	-	0,6,6	-	-	-		
86	OHX	5	3943	-	0,6,6	-	-	-		
86	OHX	1	4123	-	0,6,6	-	-	-		
86	OHX	1	3908	-	0,6,6	-	-	-		
86	OHX	2	2080	-	0,6,6	-	-	-		
86	OHX	1	4031	-	0,6,6	-	-	-		
86	OHX	1	4040	-	0,6,6	-	-	-		
86	OHX	1	4046	-	0,6,6	-	-	-		
86	OHX	1	4095	-	0,6,6	-	-	-		
86	OHX	1	4108	-	0,6,6	-	-	-		
86	OHX	5	4213	-	0,6,6	-	-	-		
86	OHX	5	4216	-	0,6,6	-	-	-		
86	OHX	1	3895	-	0,6,6	-	-	-		
86	OHX	1	4066	-	0,6,6	-	-	-		
86	OHX	5	4131	-	0,6,6	-	-	-		
86	OHX	d4	202	-	0,6,6	-	-	-		
86	OHX	2	2151	-	0,6,6	-	-	-		
86	OHX	1	4036	-	0,6,6	-	-	-		
86	OHX	5	4033	-	0,6,6	-	-	-		
86	OHX	2	2045	-	0,6,6	-	-	-		
86	OHX	5	4141	-	0,6,6	-	-	-		
86	OHX	5	4034	-	0,6,6	-	-	-		
86	OHX	1	4182	-	0,6,6	-	-	-		
86	OHX	L3	405	-	0,6,6	-	-	-		
86	OHX	5	3958	-	0,6,6	-	-	-		
86	OHX	5	4243	-	0,6,6	-	-	-		
86	OHX	5	4161	-	0,6,6	-	-	-		
86	OHX	2	2135	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	3876	-	0,6,6	-	-	-		
86	OHX	1	4149	-	0,6,6	-	-	-		
86	OHX	5	4097	-	0,6,6	-	-	-		
86	OHX	5	4054	-	0,6,6	-	-	-		
86	OHX	5	4197	-	0,6,6	-	-	-		
86	OHX	L3	404	-	0,6,6	-	-	-		
86	OHX	6	2059	-	0,6,6	-	-	-		
86	OHX	1	3943	-	0,6,6	-	-	-		
86	OHX	1	3976	-	0,6,6	-	-	-		
86	OHX	1	3996	-	0,6,6	-	-	-		
86	OHX	1	4017	-	0,6,6	-	-	-		
86	OHX	6	2156	-	0,6,6	-	-	-		
86	OHX	1	4093	-	0,6,6	-	-	-		
86	OHX	1	4131	-	0,6,6	-	-	-		
86	OHX	5	4127	-	0,6,6	-	-	-		
86	OHX	5	4211	-	0,6,6	-	-	-		
86	OHX	1	4042	-	0,6,6	-	-	-		
86	OHX	6	2113	-	0,6,6	-	-	-		
86	OHX	5	3924	-	0,6,6	-	-	-		
86	OHX	5	3928	-	0,6,6	-	-	-		
86	OHX	2	2149	-	0,6,6	-	-	-		
86	OHX	6	2134	-	0,6,6	-	-	-		
86	OHX	5	4167	-	0,6,6	-	-	-		
86	OHX	8	223	-	0,6,6	-	-	-		
86	OHX	2	2127	-	0,6,6	-	-	-		
86	OHX	1	4101	-	0,6,6	-	-	-		
86	OHX	1	4184	-	0,6,6	-	-	-		
86	OHX	5	3926	-	0,6,6	-	-	-		
86	OHX	5	4080	-	0,6,6	-	-	-		
86	OHX	5	4250	-	0,6,6	-	-	-		
86	OHX	6	2097	-	0,6,6	-	-	-		
86	OHX	6	2051	-	0,6,6	-	-	-		
86	OHX	5	4051	-	0,6,6	-	-	-		
86	OHX	1	4119	-	0,6,6	-	-	-		
86	OHX	3	215	-	0,6,6	-	-	-		
86	OHX	1	4176	-	0,6,6	-	-	-		
86	OHX	1	4181	-	0,6,6	-	-	-		
86	OHX	1	4203	-	0,6,6	-	-	-		
86	OHX	1	4097	-	0,6,6	-	-	-		
86	OHX	6	2124	-	0,6,6	-	-	-		
86	OHX	2	2119	-	0,6,6	-	-	-		
86	OHX	6	2070	-	0,6,6	-	-	-		
86	OHX	6	2176	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	2	2134	-	0,6,6	-	-	-		
86	OHX	6	2060	-	0,6,6	-	-	-		
86	OHX	2	2046	-	0,6,6	-	-	-		
86	OHX	1	3965	-	0,6,6	-	-	-		
86	OHX	1	4165	-	0,6,6	-	-	-		
86	OHX	6	2171	-	0,6,6	-	-	-		
86	OHX	6	2183	-	0,6,6	-	-	-		
86	OHX	5	4146	-	0,6,6	-	-	-		
86	OHX	2	2066	-	0,6,6	-	-	-		
86	OHX	1	4127	-	0,6,6	-	-	-		
86	OHX	5	3911	-	0,6,6	-	-	-		
86	OHX	5	4044	-	0,6,6	-	-	-		
86	OHX	5	4185	-	0,6,6	-	-	-		
86	OHX	8	216	-	0,6,6	-	-	-		
86	OHX	5	4084	-	0,6,6	-	-	-		
86	OHX	2	2052	-	0,6,6	-	-	-		
86	OHX	5	4240	-	0,6,6	-	-	-		
86	OHX	1	4134	-	0,6,6	-	-	-		
86	OHX	5	3959	-	0,6,6	-	-	-		
86	OHX	l4	402	-	0,6,6	-	-	-		
86	OHX	3	223	-	0,6,6	-	-	-		
86	OHX	1	3972	-	0,6,6	-	-	-		
86	OHX	6	2098	-	0,6,6	-	-	-		
86	OHX	2	2116	-	0,6,6	-	-	-		
86	OHX	2	2087	-	0,6,6	-	-	-		
86	OHX	1	4010	-	0,6,6	-	-	-		
86	OHX	1	4052	-	0,6,6	-	-	-		
86	OHX	5	3995	-	0,6,6	-	-	-		
86	OHX	1	4047	-	0,6,6	-	-	-		
86	OHX	5	4169	-	0,6,6	-	-	-		
86	OHX	5	4176	-	0,6,6	-	-	-		
86	OHX	2	2039	-	0,6,6	-	-	-		
86	OHX	2	2088	-	0,6,6	-	-	-		
86	OHX	5	4008	-	0,6,6	-	-	-		
86	OHX	1	3900	-	0,6,6	-	-	-		
86	OHX	6	2157	-	0,6,6	-	-	-		
86	OHX	1	4146	-	0,6,6	-	-	-		
86	OHX	2	2168	-	0,6,6	-	-	-		
86	OHX	6	2049	-	0,6,6	-	-	-		
86	OHX	6	2066	-	0,6,6	-	-	-		
86	OHX	6	2147	-	0,6,6	-	-	-		
86	OHX	1	3909	-	0,6,6	-	-	-		
86	OHX	5	4153	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	2	2043	-	0,6,6	-	-	-		
86	OHX	1	4162	-	0,6,6	-	-	-		
86	OHX	1	4015	-	0,6,6	-	-	-		
86	OHX	5	4164	-	0,6,6	-	-	-		
86	OHX	5	4064	-	0,6,6	-	-	-		
86	OHX	1	4113	-	0,6,6	-	-	-		
86	OHX	7	219	-	0,6,6	-	-	-		
86	OHX	1	4078	-	0,6,6	-	-	-		
86	OHX	5	3986	-	0,6,6	-	-	-		
86	OHX	3	220	-	0,6,6	-	-	-		
86	OHX	5	3982	-	0,6,6	-	-	-		
86	OHX	5	3996	-	0,6,6	-	-	-		
86	OHX	1	4157	-	0,6,6	-	-	-		
86	OHX	5	4032	-	0,6,6	-	-	-		
86	OHX	5	4135	-	0,6,6	-	-	-		
86	OHX	2	2061	-	0,6,6	-	-	-		
86	OHX	1	3878	-	0,6,6	-	-	-		
86	OHX	1	4170	-	0,6,6	-	-	-		
86	OHX	5	4039	-	0,6,6	-	-	-		
86	OHX	5	4112	-	0,6,6	-	-	-		
86	OHX	5	4179	-	0,6,6	-	-	-		
86	OHX	1	4022	-	0,6,6	-	-	-		
86	OHX	C3	201	-	0,6,6	-	-	-		
86	OHX	2	2175	-	0,6,6	-	-	-		
86	OHX	1	4072	-	0,6,6	-	-	-		
86	OHX	5	3902	-	0,6,6	-	-	-		
86	OHX	5	4099	-	0,6,6	-	-	-		
86	OHX	1	3930	-	0,6,6	-	-	-		
86	OHX	1	4041	-	0,6,6	-	-	-		
86	OHX	1	4026	-	0,6,6	-	-	-		
86	OHX	7	220	-	0,6,6	-	-	-		
86	OHX	1	3903	-	0,6,6	-	-	-		
86	OHX	1	4164	-	0,6,6	-	-	-		
86	OHX	2	2113	-	0,6,6	-	-	-		
86	OHX	6	2093	-	0,6,6	-	-	-		
86	OHX	2	2176	-	0,6,6	-	-	-		
86	OHX	2	2079	-	0,6,6	-	-	-		
86	OHX	1	4197	-	0,6,6	-	-	-		
86	OHX	5	3942	-	0,6,6	-	-	-		
86	OHX	2	2101	-	0,6,6	-	-	-		
86	OHX	2	2171	-	0,6,6	-	-	-		
86	OHX	2	2103	-	0,6,6	-	-	-		
86	OHX	1	4186	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	3982	-	0,6,6	-	-	-		
86	OHX	6	2202	-	0,6,6	-	-	-		
86	OHX	5	3949	-	0,6,6	-	-	-		
86	OHX	7	226	-	0,6,6	-	-	-		
86	OHX	1	3928	-	0,6,6	-	-	-		
86	OHX	6	2142	-	0,6,6	-	-	-		
86	OHX	5	3981	-	0,6,6	-	-	-		
86	OHX	5	4053	-	0,6,6	-	-	-		
86	OHX	5	3977	-	0,6,6	-	-	-		
86	OHX	1	4039	-	0,6,6	-	-	-		
86	OHX	5	4139	-	0,6,6	-	-	-		
86	OHX	5	4160	-	0,6,6	-	-	-		
86	OHX	1	3945	-	0,6,6	-	-	-		
86	OHX	6	2193	-	0,6,6	-	-	-		
86	OHX	c8	202	-	0,6,6	-	-	-		
86	OHX	5	4004	-	0,6,6	-	-	-		
86	OHX	5	3985	-	0,6,6	-	-	-		
86	OHX	6	2083	-	0,6,6	-	-	-		
86	OHX	2	2091	-	0,6,6	-	-	-		
86	OHX	2	2098	-	0,6,6	-	-	-		
86	OHX	6	2164	-	0,6,6	-	-	-		
86	OHX	5	3984	-	0,6,6	-	-	-		
86	OHX	5	4098	-	0,6,6	-	-	-		
86	OHX	1	3901	-	0,6,6	-	-	-		
86	OHX	1	3910	-	0,6,6	-	-	-		
86	OHX	1	4073	-	0,6,6	-	-	-		
86	OHX	1	3870	-	0,6,6	-	-	-		
86	OHX	O1	201	-	0,6,6	-	-	-		
86	OHX	6	2138	-	0,6,6	-	-	-		
86	OHX	1	3894	-	0,6,6	-	-	-		
86	OHX	6	2140	-	0,6,6	-	-	-		
86	OHX	1	3942	-	0,6,6	-	-	-		
86	OHX	5	4017	-	0,6,6	-	-	-		
86	OHX	5	4076	-	0,6,6	-	-	-		
86	OHX	2	2049	-	0,6,6	-	-	-		
86	OHX	1	4003	-	0,6,6	-	-	-		
86	OHX	2	2072	-	0,6,6	-	-	-		
86	OHX	6	2167	-	0,6,6	-	-	-		
86	OHX	5	3937	-	0,6,6	-	-	-		
86	OHX	1	3884	-	0,6,6	-	-	-		
86	OHX	1	4065	-	0,6,6	-	-	-		
86	OHX	5	3912	-	0,6,6	-	-	-		
86	OHX	5	3971	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	1	4160	-	0,6,6	-	-	-		
86	OHX	1	4103	-	0,6,6	-	-	-		
86	OHX	5	4134	-	0,6,6	-	-	-		
86	OHX	1	3913	-	0,6,6	-	-	-		
86	OHX	5	4163	-	0,6,6	-	-	-		
86	OHX	6	2198	-	0,6,6	-	-	-		
86	OHX	1	3985	-	0,6,6	-	-	-		
86	OHX	2	2163	-	0,6,6	-	-	-		
86	OHX	2	2099	-	0,6,6	-	-	-		
86	OHX	2	2167	-	0,6,6	-	-	-		
86	OHX	5	4132	-	0,6,6	-	-	-		
86	OHX	d9	102	-	0,6,6	-	-	-		
86	OHX	1	3978	-	0,6,6	-	-	-		
86	OHX	6	2178	-	0,6,6	-	-	-		
86	OHX	2	2133	-	0,6,6	-	-	-		
86	OHX	1	3981	-	0,6,6	-	-	-		
86	OHX	1	4107	-	0,6,6	-	-	-		
86	OHX	1	4013	-	0,6,6	-	-	-		
86	OHX	O9	101	-	0,6,6	-	-	-		
86	OHX	2	2131	-	0,6,6	-	-	-		
86	OHX	1	3904	-	0,6,6	-	-	-		
86	OHX	1	3993	-	0,6,6	-	-	-		
86	OHX	1	4009	-	0,6,6	-	-	-		
86	OHX	5	3951	-	0,6,6	-	-	-		
86	OHX	5	4206	-	0,6,6	-	-	-		
86	OHX	l5	305	-	0,6,6	-	-	-		
86	OHX	1	4189	-	0,6,6	-	-	-		
86	OHX	5	4181	-	0,6,6	-	-	-		
86	OHX	1	4062	-	0,6,6	-	-	-		
86	OHX	1	4092	-	0,6,6	-	-	-		
86	OHX	2	2148	-	0,6,6	-	-	-		
86	OHX	6	2174	-	0,6,6	-	-	-		
86	OHX	5	4150	-	0,6,6	-	-	-		
86	OHX	2	2112	-	0,6,6	-	-	-		
86	OHX	1	4075	-	0,6,6	-	-	-		
86	OHX	6	2143	-	0,6,6	-	-	-		
86	OHX	5	4012	-	0,6,6	-	-	-		
86	OHX	5	4147	-	0,6,6	-	-	-		
86	OHX	5	4172	-	0,6,6	-	-	-		
86	OHX	1	3973	-	0,6,6	-	-	-		
86	OHX	5	4227	-	0,6,6	-	-	-		
86	OHX	5	4145	-	0,6,6	-	-	-		
86	OHX	5	4192	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	2	2030	-	0,6,6	-	-	-		
86	OHX	1	4183	-	0,6,6	-	-	-		
86	OHX	1	4089	-	0,6,6	-	-	-		
86	OHX	2	2083	-	0,6,6	-	-	-		
86	OHX	1	4196	-	0,6,6	-	-	-		
86	OHX	5	3957	-	0,6,6	-	-	-		
86	OHX	6	2186	-	0,6,6	-	-	-		
86	OHX	2	2095	-	0,6,6	-	-	-		
86	OHX	5	4058	-	0,6,6	-	-	-		
86	OHX	5	4248	-	0,6,6	-	-	-		
86	OHX	1	4208	-	0,6,6	-	-	-		
86	OHX	sR	401	-	0,6,6	-	-	-		
86	OHX	5	3915	-	0,6,6	-	-	-		
86	OHX	1	4038	-	0,6,6	-	-	-		
86	OHX	1	4059	-	0,6,6	-	-	-		
86	OHX	6	2182	-	0,6,6	-	-	-		
86	OHX	1	4005	-	0,6,6	-	-	-		
86	OHX	5	4125	-	0,6,6	-	-	-		
86	OHX	2	2123	-	0,6,6	-	-	-		
86	OHX	1	4050	-	0,6,6	-	-	-		
86	OHX	m9	201	-	0,6,6	-	-	-		
86	OHX	5	4152	-	0,6,6	-	-	-		
86	OHX	1	3872	-	0,6,6	-	-	-		
86	OHX	6	2055	-	0,6,6	-	-	-		
86	OHX	2	2065	-	0,6,6	-	-	-		
86	OHX	1	4024	-	0,6,6	-	-	-		
86	OHX	1	3952	-	0,6,6	-	-	-		
86	OHX	1	4209	-	0,6,6	-	-	-		
86	OHX	1	4153	-	0,6,6	-	-	-		
86	OHX	1	4195	-	0,6,6	-	-	-		
86	OHX	1	4098	-	0,6,6	-	-	-		
86	OHX	1	4168	-	0,6,6	-	-	-		
86	OHX	5	3934	-	0,6,6	-	-	-		
86	OHX	2	2146	-	0,6,6	-	-	-		
86	OHX	2	2023	-	0,6,6	-	-	-		
86	OHX	2	2125	-	0,6,6	-	-	-		
86	OHX	1	3920	-	0,6,6	-	-	-		
86	OHX	6	2136	-	0,6,6	-	-	-		
86	OHX	5	4198	-	0,6,6	-	-	-		
86	OHX	3	217	-	0,6,6	-	-	-		
86	OHX	6	2078	-	0,6,6	-	-	-		
86	OHX	1	4130	-	0,6,6	-	-	-		
86	OHX	6	2179	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	OHX	5	3965	-	0,6,6	-	-	-		
86	OHX	5	3946	-	0,6,6	-	-	-		
86	OHX	2	2085	-	0,6,6	-	-	-		
86	OHX	1	3923	-	0,6,6	-	-	-		
86	OHX	2	2053	-	0,6,6	-	-	-		
86	OHX	1	4021	-	0,6,6	-	-	-		
86	OHX	6	2108	-	0,6,6	-	-	-		
86	OHX	6	2161	-	0,6,6	-	-	-		
86	OHX	2	2024	-	0,6,6	-	-	-		
86	OHX	6	2153	-	0,6,6	-	-	-		
86	OHX	1	4102	-	0,6,6	-	-	-		
86	OHX	M7	206	-	0,6,6	-	-	-		
86	OHX	5	4026	-	0,6,6	-	-	-		
86	OHX	5	4238	-	0,6,6	-	-	-		
86	OHX	s8	303	-	0,6,6	-	-	-		
86	OHX	5	4085	-	0,6,6	-	-	-		
86	OHX	1	4011	-	0,6,6	-	-	-		
86	OHX	1	4069	-	0,6,6	-	-	-		
86	OHX	1	4099	-	0,6,6	-	-	-		
86	OHX	c3	201	-	0,6,6	-	-	-		
86	OHX	1	4032	-	0,6,6	-	-	-		
86	OHX	c5	201	-	0,6,6	-	-	-		
86	OHX	5	3927	-	0,6,6	-	-	-		
86	OHX	1	3883	-	0,6,6	-	-	-		
86	OHX	2	2027	-	0,6,6	-	-	-		
86	OHX	8	227	-	0,6,6	-	-	-		
86	OHX	5	3964	-	0,6,6	-	-	-		
86	OHX	5	4148	-	0,6,6	-	-	-		
86	OHX	1	3946	-	0,6,6	-	-	-		
86	OHX	1	4074	-	0,6,6	-	-	-		
86	OHX	2	2038	-	0,6,6	-	-	-		
86	OHX	1	4138	-	0,6,6	-	-	-		
86	OHX	1	4142	-	0,6,6	-	-	-		
86	OHX	6	2151	-	0,6,6	-	-	-		
86	OHX	1	3951	-	0,6,6	-	-	-		
86	OHX	l3	404	-	0,6,6	-	-	-		
86	OHX	2	2117	-	0,6,6	-	-	-		
86	OHX	1	3891	-	0,6,6	-	-	-		
86	OHX	1	3861	-	0,6,6	-	-	-		
86	OHX	1	3917	-	0,6,6	-	-	-		
86	OHX	5	4156	-	0,6,6	-	-	-		
86	OHX	1	4060	-	0,6,6	-	-	-		
86	OHX	6	2195	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	3950	-	0,6,6	-	-	-		
86	OHX	5	3980	-	0,6,6	-	-	-		
86	OHX	5	4031	-	0,6,6	-	-	-		
86	OHX	5	4123	-	0,6,6	-	-	-		
86	OHX	6	2065	-	0,6,6	-	-	-		
86	OHX	6	2090	-	0,6,6	-	-	-		
86	OHX	2	2140	-	0,6,6	-	-	-		
86	OHX	s1	302	-	0,6,6	-	-	-		
86	OHX	2	2159	-	0,6,6	-	-	-		
86	OHX	1	3906	-	0,6,6	-	-	-		
86	OHX	5	4121	-	0,6,6	-	-	-		
86	OHX	1	4154	-	0,6,6	-	-	-		
86	OHX	1	4090	-	0,6,6	-	-	-		
86	OHX	S8	302	-	0,6,6	-	-	-		
86	OHX	M7	207	-	0,6,6	-	-	-		
86	OHX	5	4055	-	0,6,6	-	-	-		
86	OHX	1	4205	-	0,6,6	-	-	-		
86	OHX	1	4019	-	0,6,6	-	-	-		
86	OHX	1	3969	-	0,6,6	-	-	-		
86	OHX	1	4172	-	0,6,6	-	-	-		
86	OHX	5	4223	-	0,6,6	-	-	-		
86	OHX	7	224	-	0,6,6	-	-	-		
86	OHX	5	4042	-	0,6,6	-	-	-		
86	OHX	5	4116	-	0,6,6	-	-	-		
86	OHX	8	228	-	0,6,6	-	-	-		
86	OHX	5	4024	-	0,6,6	-	-	-		
86	OHX	1	4020	-	0,6,6	-	-	-		
86	OHX	5	4074	-	0,6,6	-	-	-		
86	OHX	6	2057	-	0,6,6	-	-	-		
86	OHX	6	2127	-	0,6,6	-	-	-		
86	OHX	6	2047	-	0,6,6	-	-	-		
86	OHX	1	4140	-	0,6,6	-	-	-		
86	OHX	5	4155	-	0,6,6	-	-	-		
86	OHX	5	4060	-	0,6,6	-	-	-		
86	OHX	2	2124	-	0,6,6	-	-	-		
86	OHX	1	4058	-	0,6,6	-	-	-		
86	OHX	5	3970	-	0,6,6	-	-	-		
86	OHX	1	4129	-	0,6,6	-	-	-		
86	OHX	5	4046	-	0,6,6	-	-	-		
86	OHX	2	2144	-	0,6,6	-	-	-		
86	OHX	5	3979	-	0,6,6	-	-	-		
86	OHX	5	3988	-	0,6,6	-	-	-		
86	OHX	2	2063	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	5	4045	-	0,6,6	-	-	-		
86	OHX	2	2035	-	0,6,6	-	-	-		
86	OHX	m8	201	-	0,6,6	-	-	-		
86	OHX	5	4219	-	0,6,6	-	-	-		
86	OHX	5	4101	-	0,6,6	-	-	-		
86	OHX	2	2096	-	0,6,6	-	-	-		
86	OHX	1	4106	-	0,6,6	-	-	-		
86	OHX	6	2105	-	0,6,6	-	-	-		
86	OHX	1	4088	-	0,6,6	-	-	-		
86	OHX	5	3932	-	0,6,6	-	-	-		
86	OHX	1	4207	-	0,6,6	-	-	-		
86	OHX	6	2160	-	0,6,6	-	-	-		
86	OHX	1	3886	-	0,6,6	-	-	-		
86	OHX	1	3990	-	0,6,6	-	-	-		
86	OHX	6	2050	-	0,6,6	-	-	-		
86	OHX	2	2094	-	0,6,6	-	-	-		
86	OHX	5	4020	-	0,6,6	-	-	-		
86	OHX	5	4062	-	0,6,6	-	-	-		
86	OHX	1	4206	-	0,6,6	-	-	-		
86	OHX	1	3931	-	0,6,6	-	-	-		
86	OHX	6	2173	-	0,6,6	-	-	-		
86	OHX	5	3998	-	0,6,6	-	-	-		
86	OHX	8	221	-	0,6,6	-	-	-		
86	OHX	5	3954	-	0,6,6	-	-	-		
86	OHX	5	4205	-	0,6,6	-	-	-		
86	OHX	5	3974	-	0,6,6	-	-	-		
86	OHX	6	2145	-	0,6,6	-	-	-		
86	OHX	6	2110	-	0,6,6	-	-	-		
86	OHX	5	4071	-	0,6,6	-	-	-		
86	OHX	2	2028	-	0,6,6	-	-	-		
86	OHX	1	4045	-	0,6,6	-	-	-		
86	OHX	o3	202	-	0,6,6	-	-	-		
86	OHX	6	2088	-	0,6,6	-	-	-		
86	OHX	5	3997	-	0,6,6	-	-	-		
86	OHX	6	2084	-	0,6,6	-	-	-		
86	OHX	5	4140	-	0,6,6	-	-	-		
86	OHX	2	2076	-	0,6,6	-	-	-		
86	OHX	1	3932	-	0,6,6	-	-	-		
86	OHX	1	3929	-	0,6,6	-	-	-		
86	OHX	n3	203	-	0,6,6	-	-	-		
86	OHX	1	3967	-	0,6,6	-	-	-		
86	OHX	2	2102	-	0,6,6	-	-	-		
86	OHX	2	2058	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
86	OHX	1	4211	-	0,6,6	-	-	-		
86	OHX	6	2149	-	0,6,6	-	-	-		
86	OHX	6	2152	-	0,6,6	-	-	-		
86	OHX	1	3989	-	0,6,6	-	-	-		
86	OHX	5	4144	-	0,6,6	-	-	-		
86	OHX	5	3993	-	0,6,6	-	-	-		
86	OHX	5	4201	-	0,6,6	-	-	-		
86	OHX	1	4018	-	0,6,6	-	-	-		
86	OHX	C5	201	-	0,6,6	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	3K8	2	2179	-	-	0/6/25/25	0/5/5/5
87	3K8	6	2205	-	-	0/6/25/25	0/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	2	2179	3K8	C7-C8	3.82	1.42	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	2	2179	3K8	C15-C7-C4	-3.28	116.14	120.36
87	6	2205	3K8	C11-C10-N	3.11	118.55	110.58
87	2	2179	3K8	C11-C10-N	3.08	118.48	110.58
87	6	2205	3K8	C20-C19-C18	-2.21	117.97	120.06
87	6	2205	3K8	C17-C18-C19	2.13	122.08	120.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

497 monomers are involved in 763 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	O7	106	OHX	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	3968	OHX	7	0
86	6	2159	OHX	1	0
86	6	2125	OHX	1	0
86	5	4231	OHX	1	0
86	5	4052	OHX	1	0
86	5	4157	OHX	1	0
86	1	3999	OHX	1	0
86	5	4170	OHX	1	0
86	5	3955	OHX	1	0
86	2	2078	OHX	1	0
86	6	2103	OHX	1	0
86	1	4081	OHX	1	0
86	5	4093	OHX	6	0
86	5	4221	OHX	1	0
86	5	3938	OHX	1	0
86	5	4194	OHX	1	0
86	1	3885	OHX	1	0
86	6	2168	OHX	1	0
86	5	4239	OHX	1	0
86	5	3956	OHX	1	0
86	5	4186	OHX	1	0
86	2	2145	OHX	7	0
86	3	216	OHX	1	0
86	1	3979	OHX	1	0
86	6	2190	OHX	1	0
86	1	3953	OHX	2	0
86	5	4090	OHX	2	0
86	1	4030	OHX	1	0
86	6	2109	OHX	1	0
86	1	4079	OHX	5	0
86	1	3944	OHX	1	0
86	5	4189	OHX	1	0
86	1	4137	OHX	1	0
86	6	2150	OHX	2	0
86	5	4025	OHX	3	0
86	5	4122	OHX	1	0
86	1	4204	OHX	1	0
86	6	2175	OHX	1	0
86	5	4108	OHX	1	0
86	5	4095	OHX	1	0
86	1	4057	OHX	1	0
86	5	3960	OHX	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	4022	OHX	6	0
86	4	225	OHX	1	0
86	8	215	OHX	1	0
86	5	4182	OHX	1	0
86	1	4025	OHX	6	0
86	6	2204	OHX	1	0
86	1	4043	OHX	1	0
86	8	217	OHX	1	0
86	6	2112	OHX	1	0
86	1	4014	OHX	1	0
86	6	2188	OHX	1	0
86	1	4124	OHX	1	0
86	4	228	OHX	1	0
86	5	4104	OHX	1	0
86	5	4013	OHX	6	0
86	5	4129	OHX	1	0
86	6	2056	OHX	1	0
86	5	4249	OHX	1	0
86	6	2121	OHX	8	0
86	5	3901	OHX	2	0
86	O3	201	OHX	1	0
86	5	3909	OHX	3	0
86	1	3881	OHX	1	0
86	5	4077	OHX	1	0
86	6	2087	OHX	1	0
86	6	2048	OHX	1	0
86	1	4187	OHX	1	0
86	5	3978	OHX	1	0
86	1	4029	OHX	5	0
86	1	4171	OHX	10	0
86	5	4102	OHX	1	0
86	2	2089	OHX	5	0
86	5	4016	OHX	1	0
86	5	3903	OHX	1	0
86	2	2092	OHX	1	0
86	1	4139	OHX	3	0
86	2	2136	OHX	1	0
86	1	3959	OHX	1	0
86	5	4010	OHX	1	0
86	2	2108	OHX	2	0
86	5	3917	OHX	1	0
86	6	2201	OHX	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	4087	OHX	2	0
86	5	3991	OHX	1	0
86	1	4016	OHX	1	0
86	5	4174	OHX	1	0
86	2	2158	OHX	1	0
86	1	4027	OHX	1	0
86	1	4121	OHX	2	0
86	1	4007	OHX	1	0
86	6	2063	OHX	1	0
86	5	4003	OHX	6	0
86	5	4028	OHX	1	0
86	5	4037	OHX	5	0
86	1	3902	OHX	1	0
86	6	2062	OHX	2	0
86	1	4145	OHX	7	0
86	6	2129	OHX	1	0
86	1	3956	OHX	3	0
86	1	4035	OHX	2	0
86	1	3873	OHX	2	0
86	2	2132	OHX	1	0
86	8	225	OHX	6	0
86	2	2064	OHX	1	0
86	1	4174	OHX	1	0
86	5	4041	OHX	2	0
86	5	4105	OHX	2	0
86	1	3994	OHX	1	0
86	1	3961	OHX	1	0
86	6	2120	OHX	1	0
86	5	4130	OHX	1	0
86	5	4202	OHX	7	0
86	5	4007	OHX	1	0
86	5	4241	OHX	1	0
86	5	4009	OHX	2	0
86	6	2123	OHX	1	0
86	5	4245	OHX	7	0
86	M0	304	OHX	1	0
86	6	2058	OHX	1	0
86	1	3875	OHX	1	0
86	1	3869	OHX	1	0
86	5	3975	OHX	6	0
86	4	222	OHX	1	0
86	6	2196	OHX	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	3947	OHX	1	0
86	2	2073	OHX	1	0
86	1	3889	OHX	1	0
86	1	3954	OHX	4	0
86	1	4064	OHX	1	0
86	1	4158	OHX	1	0
86	5	4120	OHX	1	0
86	5	4183	OHX	1	0
86	2	2054	OHX	2	0
86	4	227	OHX	1	0
86	1	4179	OHX	1	0
86	1	3863	OHX	1	0
86	1	4202	OHX	1	0
86	5	4083	OHX	5	0
86	5	4005	OHX	1	0
86	5	4225	OHX	1	0
87	2	2179	3K8	4	0
86	2	2062	OHX	1	0
86	6	2189	OHX	3	0
86	1	3986	OHX	1	0
86	5	3962	OHX	1	0
86	6	2154	OHX	2	0
86	q2	502	OHX	3	0
86	2	2036	OHX	2	0
86	D9	102	OHX	1	0
86	5	4195	OHX	1	0
86	1	4053	OHX	6	0
86	4	224	OHX	1	0
86	1	4083	OHX	5	0
86	5	4096	OHX	2	0
86	5	4199	OHX	2	0
86	1	3877	OHX	1	0
86	2	2070	OHX	2	0
86	1	4037	OHX	1	0
86	6	2106	OHX	1	0
86	1	3862	OHX	1	0
86	5	4230	OHX	1	0
86	1	3962	OHX	1	0
86	2	2047	OHX	1	0
86	6	2165	OHX	1	0
86	m0	302	OHX	2	0
86	5	3907	OHX	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	4011	OHX	1	0
86	5	4069	OHX	1	0
86	5	4251	OHX	2	0
86	6	2118	OHX	1	0
86	1	3971	OHX	2	0
86	5	4030	OHX	1	0
86	5	4149	OHX	1	0
86	1	3950	OHX	1	0
86	1	4163	OHX	2	0
86	2	2082	OHX	2	0
86	5	3914	OHX	2	0
86	6	2071	OHX	1	0
86	6	2139	OHX	1	0
86	6	2192	OHX	1	0
86	2	2034	OHX	1	0
86	1	3880	OHX	2	0
86	1	3975	OHX	1	0
86	5	3921	OHX	2	0
86	1	3865	OHX	1	0
86	n1	201	OHX	1	0
86	5	4019	OHX	1	0
86	6	2072	OHX	2	0
86	1	4000	OHX	8	0
86	2	2129	OHX	1	0
86	5	3961	OHX	1	0
86	2	2138	OHX	1	0
86	m5	303	OHX	1	0
86	6	2067	OHX	2	0
86	3	221	OHX	1	0
86	5	4110	OHX	1	0
86	5	4236	OHX	6	0
86	5	4021	OHX	2	0
86	8	226	OHX	4	0
86	2	2051	OHX	1	0
86	s9	201	OHX	2	0
87	6	2205	3K8	1	0
86	2	2120	OHX	1	0
86	3	218	OHX	1	0
86	1	3921	OHX	1	0
86	6	2076	OHX	1	0
86	6	2137	OHX	1	0
86	1	4109	OHX	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	4061	OHX	1	0
86	5	4226	OHX	1	0
86	6	2069	OHX	1	0
86	1	4193	OHX	1	0
86	1	4167	OHX	1	0
86	1	3980	OHX	2	0
86	2	2093	OHX	2	0
86	M5	302	OHX	1	0
86	6	2131	OHX	2	0
86	s4	301	OHX	1	0
86	5	4056	OHX	1	0
86	1	4166	OHX	2	0
86	6	2094	OHX	1	0
86	6	2096	OHX	1	0
86	1	4055	OHX	2	0
86	1	3988	OHX	2	0
86	1	4054	OHX	5	0
86	6	2075	OHX	1	0
86	5	3989	OHX	1	0
86	2	2161	OHX	6	0
86	2	2086	OHX	1	0
86	8	220	OHX	1	0
86	6	2104	OHX	1	0
86	5	4193	OHX	6	0
86	O7	105	OHX	5	0
86	1	3927	OHX	2	0
86	6	2146	OHX	1	0
86	1	4148	OHX	1	0
86	3	225	OHX	2	0
86	6	2092	OHX	1	0
86	1	4180	OHX	3	0
86	2	2044	OHX	7	0
86	5	4191	OHX	6	0
86	5	4070	OHX	1	0
86	2	2048	OHX	1	0
86	2	2114	OHX	1	0
86	5	4036	OHX	3	0
86	5	4075	OHX	1	0
86	5	4100	OHX	2	0
86	1	4201	OHX	3	0
86	5	3944	OHX	7	0
86	2	2156	OHX	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	2	2130	OHX	1	0
86	l3	402	OHX	1	0
86	5	4242	OHX	1	0
86	6	2089	OHX	1	0
86	5	4094	OHX	1	0
86	8	218	OHX	1	0
86	6	2115	OHX	1	0
86	1	3871	OHX	1	0
86	2	2104	OHX	1	0
86	5	4057	OHX	6	0
86	2	2084	OHX	1	0
86	1	3998	OHX	1	0
86	5	4091	OHX	1	0
86	5	4203	OHX	3	0
86	m1	202	OHX	1	0
86	2	2074	OHX	2	0
86	2	2033	OHX	1	0
86	2	2026	OHX	2	0
86	1	3974	OHX	2	0
86	2	2154	OHX	1	0
86	5	4114	OHX	1	0
86	5	4068	OHX	7	0
86	6	2144	OHX	1	0
86	1	4094	OHX	1	0
86	6	2162	OHX	1	0
86	7	222	OHX	1	0
86	1	3879	OHX	1	0
86	1	4012	OHX	1	0
86	4	231	OHX	2	0
86	1	3992	OHX	1	0
86	2	2042	OHX	1	0
86	2	2105	OHX	1	0
86	1	4173	OHX	1	0
86	5	4200	OHX	11	0
86	5	4228	OHX	1	0
86	N1	201	OHX	1	0
86	5	3947	OHX	1	0
86	6	2126	OHX	3	0
86	2	2031	OHX	7	0
86	5	4133	OHX	1	0
86	8	230	OHX	2	0
86	2	2110	OHX	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	2	2109	OHX	1	0
86	2	2075	OHX	6	0
86	1	4117	OHX	1	0
86	2	2141	OHX	1	0
86	2	2090	OHX	5	0
86	5	4035	OHX	5	0
86	5	4048	OHX	1	0
86	1	4194	OHX	1	0
86	1	3887	OHX	1	0
86	2	2107	OHX	1	0
86	1	3897	OHX	1	0
86	5	4187	OHX	1	0
86	5	3918	OHX	2	0
86	6	2101	OHX	3	0
86	1	3964	OHX	1	0
86	1	4084	OHX	2	0
86	5	4029	OHX	1	0
86	m0	303	OHX	2	0
86	5	4015	OHX	1	0
86	6	2122	OHX	1	0
86	1	4155	OHX	6	0
86	1	3936	OHX	1	0
86	1	3908	OHX	1	0
86	1	4031	OHX	1	0
86	1	4095	OHX	1	0
86	5	4213	OHX	1	0
86	1	4066	OHX	1	0
86	5	4131	OHX	2	0
86	1	4036	OHX	2	0
86	5	4033	OHX	1	0
86	2	2045	OHX	1	0
86	5	4141	OHX	1	0
86	1	4182	OHX	1	0
86	L3	405	OHX	1	0
86	5	3958	OHX	1	0
86	5	4161	OHX	2	0
86	1	3876	OHX	1	0
86	1	4149	OHX	5	0
86	5	4197	OHX	1	0
86	1	3943	OHX	1	0
86	1	3996	OHX	1	0
86	1	4042	OHX	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	6	2113	OHX	1	0
86	8	223	OHX	1	0
86	2	2127	OHX	1	0
86	5	3926	OHX	1	0
86	5	4250	OHX	1	0
86	6	2097	OHX	1	0
86	5	4051	OHX	1	0
86	1	4119	OHX	1	0
86	1	4097	OHX	2	0
86	6	2124	OHX	2	0
86	6	2176	OHX	1	0
86	2	2134	OHX	1	0
86	6	2060	OHX	7	0
86	2	2046	OHX	1	0
86	1	4165	OHX	1	0
86	6	2171	OHX	8	0
86	6	2183	OHX	1	0
86	5	4146	OHX	6	0
86	1	4127	OHX	1	0
86	8	216	OHX	7	0
86	2	2052	OHX	1	0
86	5	4240	OHX	5	0
86	1	4134	OHX	1	0
86	5	3959	OHX	2	0
86	1	3972	OHX	1	0
86	1	4010	OHX	2	0
86	2	2039	OHX	2	0
86	1	4146	OHX	1	0
86	2	2168	OHX	1	0
86	6	2066	OHX	1	0
86	6	2147	OHX	7	0
86	1	4162	OHX	5	0
86	5	4164	OHX	1	0
86	1	4113	OHX	1	0
86	7	219	OHX	7	0
86	5	3986	OHX	1	0
86	3	220	OHX	1	0
86	1	4157	OHX	1	0
86	5	4032	OHX	1	0
86	1	3878	OHX	3	0
86	5	4179	OHX	1	0
86	1	4072	OHX	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	4099	OHX	1	0
86	1	3930	OHX	1	0
86	1	4041	OHX	4	0
86	7	220	OHX	2	0
86	1	4164	OHX	1	0
86	6	2093	OHX	1	0
86	1	4197	OHX	1	0
86	2	2171	OHX	1	0
86	2	2103	OHX	1	0
86	6	2202	OHX	1	0
86	7	226	OHX	6	0
86	5	4053	OHX	1	0
86	5	4004	OHX	4	0
86	2	2091	OHX	1	0
86	2	2098	OHX	7	0
86	5	3984	OHX	1	0
86	O1	201	OHX	6	0
86	6	2138	OHX	2	0
86	1	3942	OHX	1	0
86	5	4017	OHX	1	0
86	5	4076	OHX	1	0
86	1	4003	OHX	2	0
86	1	3884	OHX	1	0
86	1	4065	OHX	1	0
86	5	3912	OHX	1	0
86	5	3971	OHX	1	0
86	5	4134	OHX	1	0
86	5	4163	OHX	1	0
86	2	2167	OHX	1	0
86	1	3978	OHX	1	0
86	6	2178	OHX	1	0
86	1	3981	OHX	1	0
86	O9	101	OHX	1	0
86	2	2131	OHX	7	0
86	1	4062	OHX	1	0
86	2	2148	OHX	1	0
86	5	4147	OHX	1	0
86	1	3973	OHX	4	0
86	5	4192	OHX	1	0
86	1	4183	OHX	1	0
86	1	4089	OHX	1	0
86	2	2083	OHX	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	1	4196	OHX	6	0
86	6	2186	OHX	1	0
86	2	2095	OHX	2	0
86	1	4038	OHX	1	0
86	6	2182	OHX	1	0
86	1	4005	OHX	1	0
86	6	2055	OHX	1	0
86	2	2065	OHX	1	0
86	1	4024	OHX	1	0
86	1	4153	OHX	3	0
86	1	4098	OHX	1	0
86	2	2023	OHX	1	0
86	2	2125	OHX	1	0
86	6	2078	OHX	1	0
86	6	2179	OHX	1	0
86	2	2085	OHX	2	0
86	1	3923	OHX	2	0
86	6	2108	OHX	2	0
86	2	2024	OHX	1	0
86	M7	206	OHX	1	0
86	5	4026	OHX	2	0
86	s8	303	OHX	1	0
86	1	4099	OHX	1	0
86	c3	201	OHX	1	0
86	c5	201	OHX	2	0
86	5	3927	OHX	1	0
86	1	3883	OHX	1	0
86	5	3964	OHX	4	0
86	5	4148	OHX	2	0
86	1	4074	OHX	1	0
86	2	2038	OHX	1	0
86	1	4138	OHX	3	0
86	1	4142	OHX	3	0
86	6	2151	OHX	1	0
86	l3	404	OHX	1	0
86	1	4060	OHX	2	0
86	6	2195	OHX	1	0
86	5	3950	OHX	1	0
86	5	3980	OHX	9	0
86	5	4031	OHX	1	0
86	5	4123	OHX	1	0
86	2	2159	OHX	1	0

Continued on next page...

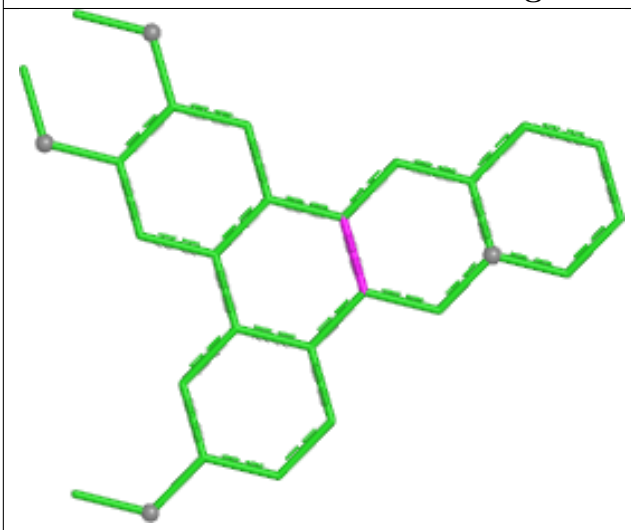
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	5	4121	OHX	2	0
86	1	4154	OHX	4	0
86	M7	207	OHX	1	0
86	1	3969	OHX	1	0
86	5	4223	OHX	1	0
86	1	4020	OHX	1	0
86	5	4074	OHX	1	0
86	6	2127	OHX	2	0
86	1	4140	OHX	1	0
86	5	4155	OHX	1	0
86	2	2144	OHX	1	0
86	2	2035	OHX	1	0
86	5	4219	OHX	8	0
86	2	2096	OHX	2	0
86	1	4106	OHX	1	0
86	6	2160	OHX	1	0
86	6	2050	OHX	2	0
86	5	3998	OHX	1	0
86	5	4205	OHX	5	0
86	5	3974	OHX	2	0
86	6	2110	OHX	1	0
86	1	4045	OHX	2	0
86	o3	202	OHX	1	0
86	6	2084	OHX	1	0
86	5	4140	OHX	1	0
86	2	2076	OHX	1	0
86	1	3929	OHX	2	0
86	2	2058	OHX	1	0
86	6	2149	OHX	1	0
86	5	4144	OHX	1	0
86	5	3993	OHX	3	0
86	5	4201	OHX	7	0
86	1	4018	OHX	1	0
86	C5	201	OHX	3	0

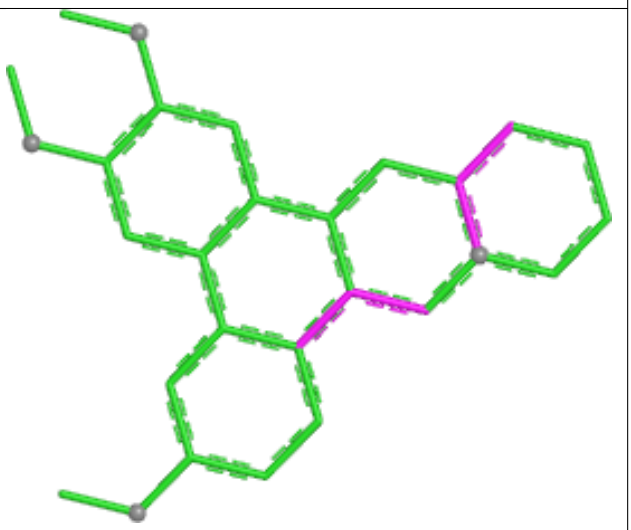
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

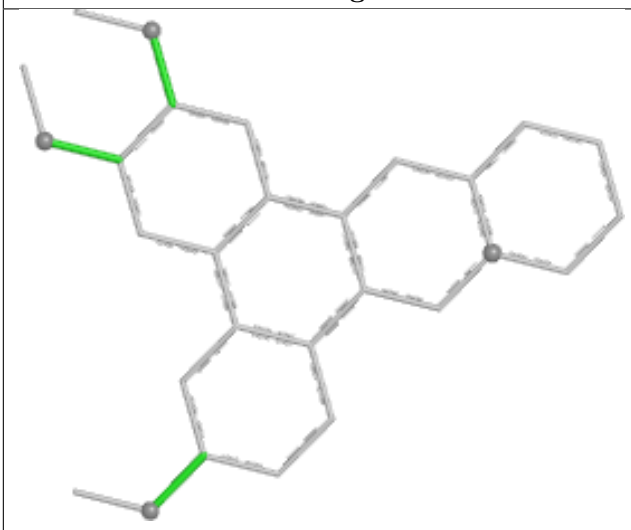
Ligand 3K8 2 2179



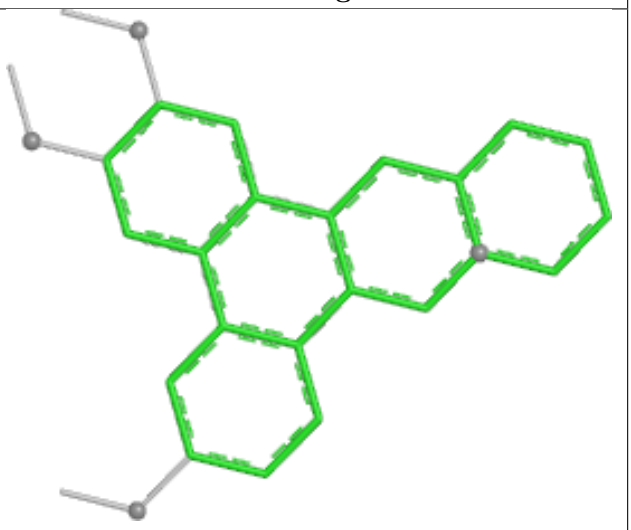
Bond lengths



Bond angles

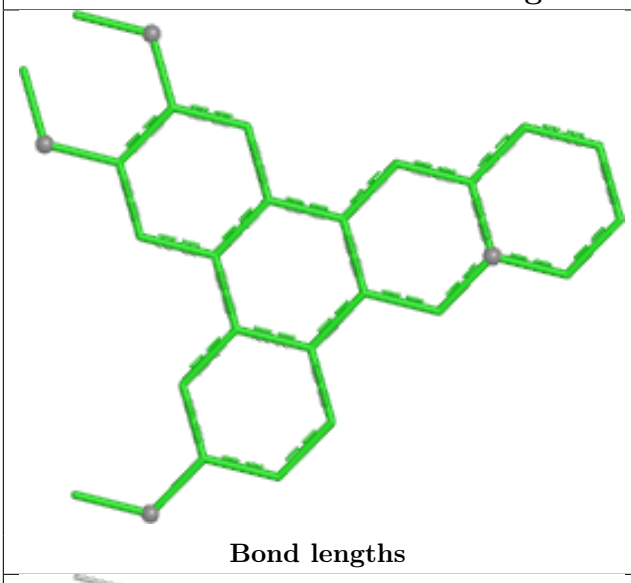


Torsions

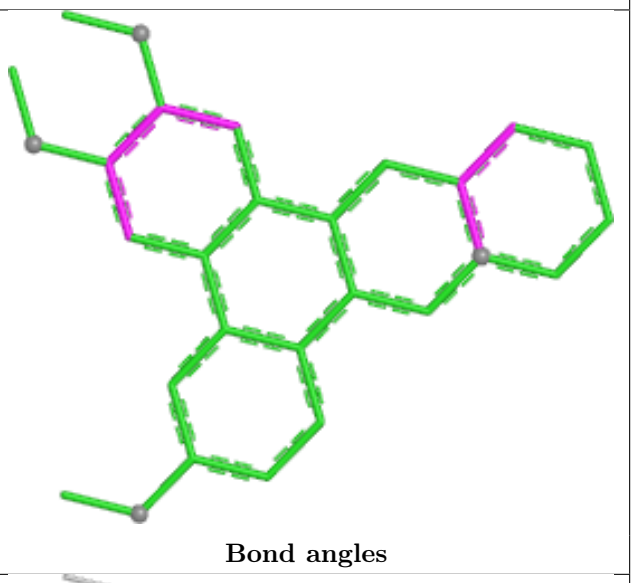


Rings

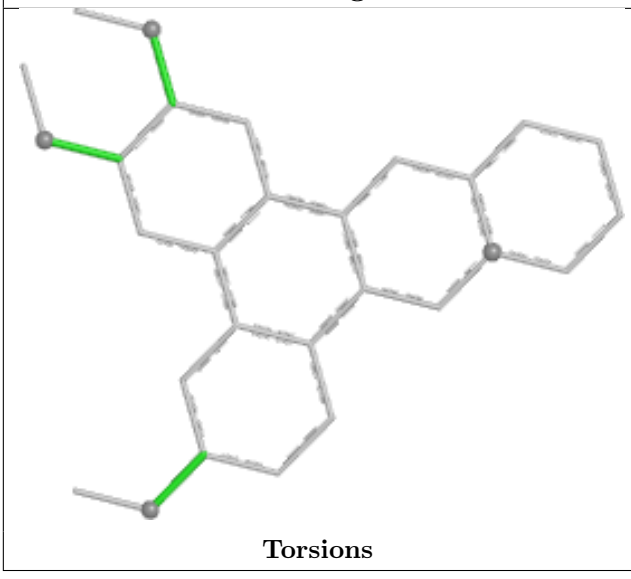
Ligand 3K8 6 2205



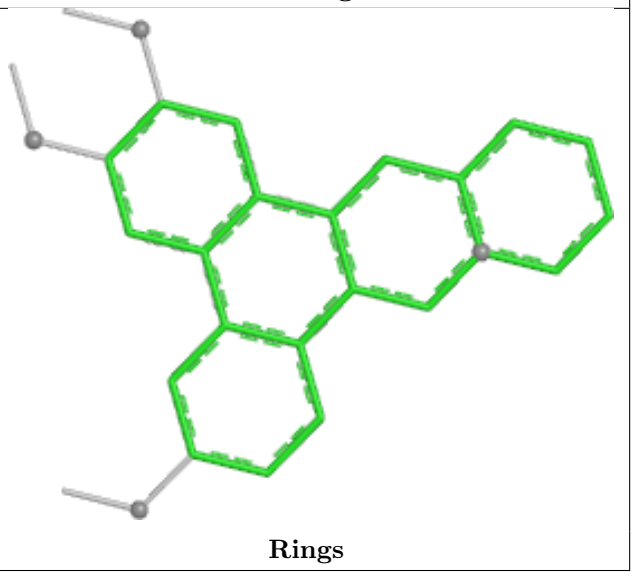
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	2	1750/1800 (97%)	0.05	48 (2%) 56 36	55, 90, 172, 265	0
1	6	1795/1800 (99%)	0.01	42 (2%) 61 41	44, 80, 191, 285	0
2	S0	206/251 (82%)	0.31	7 (3%) 48 30	94, 111, 124, 153	0
2	s0	206/251 (82%)	0.45	11 (5%) 32 20	78, 99, 115, 126	0
3	S1	214/254 (84%)	0.54	15 (7%) 22 14	94, 126, 153, 157	0
3	s1	216/254 (85%)	0.17	8 (3%) 45 28	69, 86, 109, 122	0
4	S2	217/253 (85%)	0.27	4 (1%) 67 48	72, 88, 108, 126	0
4	s2	217/253 (85%)	0.19	6 (2%) 55 35	58, 76, 97, 109	0
5	S3	223/239 (93%)	0.49	13 (5%) 29 18	79, 94, 128, 148	0
5	s3	223/239 (93%)	0.86	28 (12%) 8 6	80, 114, 137, 146	0
6	S4	260/260 (100%)	0.28	6 (2%) 61 41	63, 89, 102, 129	0
6	s4	260/260 (100%)	0.07	4 (1%) 72 52	57, 79, 97, 124	0
7	S5	206/224 (91%)	0.71	18 (8%) 16 11	98, 119, 139, 154	0
7	s5	206/224 (91%)	0.37	8 (3%) 43 27	71, 97, 123, 147	0
8	S6	226/236 (95%)	0.74	31 (13%) 6 5	65, 101, 120, 153	0
8	s6	218/236 (92%)	0.52	17 (7%) 19 12	56, 83, 111, 135	0
9	S7	184/189 (97%)	0.29	3 (1%) 70 51	86, 118, 146, 158	0
9	s7	186/189 (98%)	0.32	5 (2%) 56 36	75, 109, 141, 156	0
10	S8	188/200 (94%)	0.31	5 (2%) 56 36	56, 73, 113, 131	0
10	s8	188/200 (94%)	0.32	6 (3%) 50 31	48, 70, 116, 134	0
11	S9	185/196 (94%)	0.63	16 (8%) 16 11	83, 99, 134, 164	0
11	s9	185/196 (94%)	0.28	10 (5%) 31 20	69, 84, 121, 158	0
12	C0	96/105 (91%)	0.73	15 (15%) 5 4	83, 106, 146, 165	0
12	c0	96/105 (91%)	1.05	17 (17%) 4 3	107, 139, 160, 189	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	C1	155/155 (100%)	0.52	11 (7%) 22 14	59, 71, 129, 137	0
13	c1	146/155 (94%)	0.20	6 (4%) 41 25	51, 68, 104, 128	0
14	C2	124/142 (87%)	0.51	5 (4%) 42 26	134, 149, 164, 175	0
14	c2	124/142 (87%)	0.81	9 (7%) 21 13	186, 202, 221, 224	0
15	C3	150/150 (100%)	0.25	5 (3%) 49 30	67, 88, 106, 111	0
15	c3	150/150 (100%)	0.11	2 (1%) 75 55	58, 76, 96, 114	0
16	C4	127/136 (93%)	0.72	9 (7%) 22 14	70, 116, 138, 148	0
16	c4	128/136 (94%)	0.14	0 100 100	58, 81, 92, 101	0
17	C5	124/141 (87%)	0.54	4 (3%) 50 31	80, 96, 134, 149	0
17	c5	135/141 (95%)	0.92	20 (14%) 5 4	83, 108, 136, 172	0
18	C6	141/142 (99%)	0.68	12 (8%) 16 11	83, 108, 118, 122	0
18	c6	142/142 (100%)	0.61	14 (9%) 13 8	70, 90, 110, 137	0
19	C7	120/136 (88%)	0.49	5 (4%) 40 25	94, 112, 137, 140	0
19	c7	117/136 (86%)	0.35	3 (2%) 57 37	81, 100, 125, 130	0
20	C8	145/145 (100%)	0.45	6 (4%) 41 25	81, 109, 133, 143	0
20	c8	145/145 (100%)	0.18	4 (2%) 55 35	75, 92, 117, 136	0
21	C9	143/143 (100%)	0.69	16 (11%) 10 7	92, 107, 125, 139	0
21	c9	143/143 (100%)	0.12	1 (0%) 84 69	69, 84, 108, 127	0
22	D0	107/120 (89%)	0.86	12 (11%) 10 7	75, 115, 152, 155	0
22	d0	110/120 (91%)	0.93	13 (11%) 9 6	74, 113, 155, 187	0
23	D1	87/87 (100%)	0.35	2 (2%) 61 41	89, 98, 117, 132	0
23	d1	87/87 (100%)	0.06	1 (1%) 78 61	73, 83, 106, 121	0
24	D2	129/129 (100%)	0.14	1 (0%) 82 67	70, 81, 90, 103	0
24	d2	129/129 (100%)	0.06	3 (2%) 61 41	55, 68, 76, 91	0
25	D3	144/144 (100%)	0.34	6 (4%) 40 25	59, 65, 78, 97	0
25	d3	144/144 (100%)	-0.01	1 (0%) 84 69	48, 55, 67, 83	0
26	D4	134/134 (100%)	0.42	5 (3%) 45 28	76, 103, 121, 130	0
26	d4	134/134 (100%)	0.29	5 (3%) 45 28	61, 88, 103, 137	0
27	D5	70/107 (65%)	0.52	2 (2%) 53 35	113, 131, 143, 147	0
27	d5	69/107 (64%)	0.15	0 100 100	84, 114, 131, 139	0
28	D6	97/97 (100%)	0.64	10 (10%) 12 8	74, 94, 142, 150	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	d6	97/97 (100%)	0.44	4 (4%) 41 25	60, 76, 98, 108	0
29	D7	81/81 (100%)	0.26	1 (1%) 76 58	83, 101, 140, 146	0
29	d7	81/81 (100%)	0.13	0 100 100	72, 88, 134, 143	0
30	D8	63/66 (95%)	0.79	7 (11%) 10 7	113, 131, 148, 162	0
30	d8	63/66 (95%)	0.33	1 (1%) 70 51	90, 108, 127, 147	0
31	D9	53/55 (96%)	0.16	2 (3%) 44 27	77, 83, 105, 118	0
31	d9	53/55 (96%)	0.81	5 (9%) 14 9	77, 90, 134, 149	0
32	E0	60/60 (100%)	0.39	2 (3%) 49 30	70, 96, 145, 151	0
33	E1	71/76 (93%)	0.71	6 (8%) 16 11	109, 129, 150, 157	0
33	e1	76/76 (100%)	1.08	12 (15%) 5 4	132, 173, 186, 188	0
34	SR	318/318 (100%)	0.36	13 (4%) 41 25	69, 121, 144, 166	0
34	sR	318/318 (100%)	0.44	15 (4%) 36 23	102, 124, 143, 162	0
35	SM	159/273 (58%)	0.97	33 (20%) 2 2	65, 93, 144, 146	0
35	sM	104/273 (38%)	1.21	21 (20%) 3 2	67, 106, 192, 201	0
36	1	3149/3396 (92%)	-0.34	50 (1%) 70 51	28, 52, 140, 267	0
36	5	3150/3396 (92%)	-0.36	50 (1%) 70 51	28, 52, 127, 268	0
37	3	121/121 (100%)	-0.47	1 (0%) 82 67	42, 71, 88, 93	0
37	7	121/121 (100%)	-0.68	0 100 100	34, 56, 69, 79	0
38	4	158/158 (100%)	-0.42	1 (0%) 85 73	35, 53, 93, 136	0
38	8	158/158 (100%)	-0.34	4 (2%) 58 39	39, 60, 105, 132	0
39	L2	252/253 (99%)	-0.04	4 (1%) 70 51	35, 49, 65, 77	0
39	l2	252/253 (99%)	0.11	6 (2%) 59 40	36, 55, 77, 88	0
40	L3	386/386 (100%)	-0.15	0 100 100	35, 55, 70, 106	0
40	l3	386/386 (100%)	-0.35	1 (0%) 90 81	29, 43, 59, 97	0
41	L4	361/361 (100%)	-0.20	4 (1%) 78 61	29, 44, 64, 71	0
41	l4	361/361 (100%)	-0.21	1 (0%) 90 81	35, 50, 70, 83	0
42	L5	296/296 (100%)	0.07	2 (0%) 84 69	54, 79, 99, 128	0
42	l5	294/296 (99%)	-0.16	3 (1%) 79 63	43, 60, 87, 137	0
43	L6	156/175 (89%)	-0.19	1 (0%) 85 73	40, 49, 71, 101	0
43	l6	157/175 (89%)	-0.16	1 (0%) 85 73	42, 50, 73, 88	0
44	L7	222/243 (91%)	-0.24	2 (0%) 81 64	34, 42, 78, 134	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	l7	223/243 (91%)	-0.30	1 (0%) 88 79	31, 39, 84, 129	0
45	L8	233/255 (91%)	0.05	1 (0%) 88 79	55, 71, 108, 122	0
45	l8	231/255 (90%)	0.40	11 (4%) 35 22	70, 82, 115, 124	0
46	L9	191/191 (100%)	0.08	3 (1%) 70 51	48, 62, 80, 95	0
46	l9	191/191 (100%)	-0.15	0 100 100	39, 47, 72, 101	0
47	M0	211/220 (95%)	-0.10	8 (3%) 44 27	41, 54, 94, 134	0
47	m0	213/220 (96%)	-0.01	4 (1%) 66 46	35, 58, 87, 102	0
48	M1	169/173 (97%)	0.08	1 (0%) 85 73	62, 86, 100, 111	0
48	m1	169/173 (97%)	-0.11	1 (0%) 85 73	44, 65, 81, 93	0
49	M3	193/198 (97%)	-0.11	0 100 100	36, 55, 104, 132	0
49	m3	194/198 (97%)	-0.02	1 (0%) 87 76	45, 64, 109, 142	0
50	M4	136/137 (99%)	-0.19	4 (2%) 53 35	44, 50, 64, 76	0
50	m4	137/137 (100%)	-0.24	2 (1%) 72 52	36, 43, 66, 82	0
51	M5	203/203 (100%)	-0.02	1 (0%) 87 76	33, 46, 58, 61	0
51	m5	203/203 (100%)	0.02	1 (0%) 87 76	41, 57, 70, 75	0
52	M6	197/198 (99%)	-0.01	8 (4%) 41 25	34, 40, 61, 67	0
52	m6	197/198 (99%)	-0.18	3 (1%) 72 52	28, 34, 62, 68	0
53	M7	183/183 (100%)	0.13	12 (6%) 24 15	38, 46, 132, 154	0
53	m7	155/183 (84%)	-0.30	0 100 100	30, 42, 53, 84	0
54	M8	185/185 (100%)	-0.11	1 (0%) 87 76	37, 45, 61, 79	0
54	m8	185/185 (100%)	-0.20	0 100 100	38, 51, 61, 65	0
55	M9	188/188 (100%)	0.32	10 (5%) 32 20	51, 68, 166, 175	0
55	m9	188/188 (100%)	0.10	3 (1%) 70 51	49, 63, 150, 163	0
56	N0	172/172 (100%)	-0.20	2 (1%) 76 58	40, 48, 64, 73	0
56	n0	172/172 (100%)	-0.29	3 (1%) 69 49	33, 40, 52, 67	0
57	N1	159/159 (100%)	0.03	1 (0%) 85 73	40, 50, 96, 104	0
57	n1	159/159 (100%)	-0.16	0 100 100	38, 44, 82, 88	0
58	N2	100/120 (83%)	0.56	5 (5%) 34 22	80, 100, 118, 137	0
58	n2	98/120 (81%)	0.14	2 (2%) 65 45	73, 90, 102, 106	0
59	N3	136/136 (100%)	-0.16	2 (1%) 72 52	40, 51, 66, 77	0
59	n3	136/136 (100%)	-0.30	1 (0%) 84 69	31, 41, 59, 63	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
60	N4	98/155 (63%)	0.57	9 (9%) 14 9	51, 65, 162, 173	0
60	n4	135/155 (87%)	0.39	8 (5%) 28 18	43, 90, 133, 148	0
61	N5	121/141 (85%)	0.06	1 (0%) 82 67	46, 59, 85, 123	0
61	n5	120/141 (85%)	0.15	1 (0%) 82 67	50, 65, 89, 96	0
62	N6	126/126 (100%)	-0.29	1 (0%) 82 67	44, 56, 67, 81	0
62	n6	126/126 (100%)	-0.06	3 (2%) 59 40	48, 60, 78, 88	0
63	N7	135/135 (100%)	-0.04	1 (0%) 84 69	68, 83, 98, 106	0
63	n7	135/135 (100%)	0.17	2 (1%) 72 52	78, 94, 115, 128	0
64	N8	148/148 (100%)	-0.10	1 (0%) 84 69	30, 45, 72, 86	0
64	n8	148/148 (100%)	-0.10	0 100 100	37, 51, 74, 76	0
65	N9	58/58 (100%)	0.24	2 (3%) 48 30	41, 55, 107, 125	0
65	n9	58/58 (100%)	0.07	1 (1%) 69 49	36, 54, 87, 101	0
66	O0	97/104 (93%)	-0.07	0 100 100	67, 78, 105, 117	0
66	o0	100/104 (96%)	0.09	0 100 100	74, 85, 115, 127	0
67	O1	109/112 (97%)	0.04	1 (0%) 81 64	45, 62, 105, 123	0
67	o1	109/112 (97%)	-0.11	0 100 100	40, 54, 98, 119	0
68	O2	127/129 (98%)	-0.09	5 (3%) 43 27	28, 43, 56, 74	0
68	o2	127/129 (98%)	-0.04	4 (3%) 51 32	29, 48, 62, 89	0
69	O3	106/106 (100%)	-0.27	0 100 100	35, 41, 69, 84	0
69	o3	106/106 (100%)	-0.21	1 (0%) 81 64	32, 39, 70, 85	0
70	O4	112/120 (93%)	0.30	6 (5%) 31 20	46, 64, 113, 130	0
70	o4	112/120 (93%)	0.30	3 (2%) 56 36	48, 68, 118, 127	0
71	O5	119/119 (100%)	-0.01	2 (1%) 69 49	45, 63, 72, 74	0
71	o5	119/119 (100%)	-0.00	1 (0%) 82 67	52, 68, 84, 91	0
72	O6	99/99 (100%)	0.02	3 (3%) 52 33	52, 64, 98, 122	0
72	o6	99/99 (100%)	0.20	1 (1%) 79 63	59, 72, 95, 115	0
73	O7	87/87 (100%)	0.05	3 (3%) 48 30	35, 42, 71, 99	0
73	o7	87/87 (100%)	0.03	1 (1%) 78 61	40, 45, 84, 120	0
74	O8	77/77 (100%)	-0.12	0 100 100	71, 84, 112, 123	0
74	o8	77/77 (100%)	0.35	6 (7%) 19 12	74, 89, 104, 110	0
75	O9	50/50 (100%)	-0.06	1 (2%) 65 45	43, 49, 56, 60	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
75	o9	50/50 (100%)	0.00	0 100 100	49, 53, 64, 75	0
76	Q0	52/52 (100%)	-0.19	1 (1%) 66 46	44, 52, 79, 91	0
76	q0	52/52 (100%)	-0.39	1 (1%) 66 46	34, 40, 54, 63	0
77	Q1	25/25 (100%)	-0.08	0 100 100	54, 58, 62, 67	0
77	q1	25/25 (100%)	0.04	1 (4%) 42 26	48, 51, 65, 71	0
78	Q2	105/105 (100%)	-0.05	2 (1%) 66 46	43, 58, 85, 128	0
78	q2	105/105 (100%)	-0.13	2 (1%) 66 46	45, 58, 85, 117	0
79	Q3	91/91 (100%)	-0.05	2 (2%) 62 42	43, 52, 70, 88	0
79	q3	91/91 (100%)	0.12	1 (1%) 78 61	41, 57, 73, 84	0
80	e0	62/62 (100%)	0.30	4 (6%) 25 16	62, 85, 126, 146	0
81	p0	143/311 (45%)	0.36	2 (1%) 73 54	87, 109, 183, 194	0
82	m2	0/160	-	-	-	-
83	p1	0/47	-	-	-	-
84	p2	0/46	-	-	-	-
All	All	33063/35346 (93%)	0.05	965 (2%) 53 35	28, 70, 137, 285	0

The worst 5 of 965 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	s3	145	ALA	7.9
17	c5	4	ALA	7.5
35	sM	83	LYS	7.1
35	SM	88	ARG	6.7
58	N2	89	LEU	6.5

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 oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3803	1/1	-0.25	0.33	203,203,203,203	0
85	MG	2	1994	1/1	0.03	0.32	122,122,122,122	0
85	MG	2	2002	1/1	0.09	0.32	126,126,126,126	0
85	MG	6	2014	1/1	0.17	0.22	171,171,171,171	0
85	MG	1	3813	1/1	0.19	0.34	127,127,127,127	0
85	MG	2	1968	1/1	0.33	0.46	121,121,121,121	0
85	MG	1	3849	1/1	0.35	0.43	111,111,111,111	0
85	MG	5	3777	1/1	0.38	0.34	105,105,105,105	0
85	MG	6	1940	1/1	0.46	0.34	97,97,97,97	0
85	MG	2	1963	1/1	0.47	0.18	150,150,150,150	0
85	MG	1	3650	1/1	0.47	0.41	101,101,101,101	0
85	MG	5	3448	1/1	0.48	0.32	58,58,58,58	0
85	MG	5	3796	1/1	0.48	0.34	101,101,101,101	0
85	MG	5	3885	1/1	0.48	0.42	85,85,85,85	0
85	MG	2	1952	1/1	0.49	0.27	100,100,100,100	0
85	MG	5	3808	1/1	0.50	0.15	161,161,161,161	0
85	MG	6	1924	1/1	0.50	0.33	106,106,106,106	0
85	MG	2	1959	1/1	0.51	0.47	98,98,98,98	0
85	MG	2	2022	1/1	0.51	0.30	120,120,120,120	0
85	MG	2	1954	1/1	0.53	0.28	103,103,103,103	0
85	MG	2	1958	1/1	0.53	0.40	97,97,97,97	0
85	MG	6	1909	1/1	0.54	0.27	121,121,121,121	0
85	MG	1	3627	1/1	0.56	0.17	57,57,57,57	0
85	MG	6	2039	1/1	0.57	0.37	88,88,88,88	0
85	MG	6	2000	1/1	0.57	0.34	109,109,109,109	0
85	MG	6	1963	1/1	0.58	0.17	110,110,110,110	0
85	MG	5	3467	1/1	0.59	0.28	92,92,92,92	0
85	MG	2	2018	1/1	0.59	0.34	79,79,79,79	0
85	MG	2	1975	1/1	0.59	0.47	82,82,82,82	0
85	MG	1	3696	1/1	0.59	0.27	77,77,77,77	0
85	MG	M3	202	1/1	0.59	0.35	102,102,102,102	0
85	MG	2	1991	1/1	0.61	0.35	98,98,98,98	0
85	MG	1	3633	1/1	0.62	0.31	69,69,69,69	0
85	MG	6	2040	1/1	0.62	0.39	97,97,97,97	0
85	MG	6	1985	1/1	0.63	0.23	82,82,82,82	0
85	MG	5	3680	1/1	0.63	0.23	96,96,96,96	0
85	MG	2	1980	1/1	0.63	0.29	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	2	2016	1/1	0.64	0.42	94,94,94,94	0
85	MG	2	1987	1/1	0.64	0.35	101,101,101,101	0
85	MG	2	1926	1/1	0.64	0.46	97,97,97,97	0
85	MG	5	3431	1/1	0.65	0.31	83,83,83,83	0
85	MG	2	1943	1/1	0.65	0.18	69,69,69,69	0
86	OHX	1	4187	7/7	0.66	0.27	151,151,151,151	0
85	MG	1	3405	1/1	0.67	0.36	93,93,93,93	0
85	MG	6	1907	1/1	0.67	0.31	76,76,76,76	0
85	MG	1	3420	1/1	0.67	0.40	87,87,87,87	0
85	MG	2	1972	1/1	0.67	0.31	88,88,88,88	0
85	MG	2	1915	1/1	0.68	0.34	75,75,75,75	0
85	MG	6	1967	1/1	0.68	0.24	89,89,89,89	0
85	MG	5	3799	1/1	0.68	0.41	81,81,81,81	0
85	MG	6	1968	1/1	0.68	0.35	76,76,76,76	0
85	MG	1	3702	1/1	0.68	0.32	62,62,62,62	0
85	MG	5	3735	1/1	0.68	0.32	67,67,67,67	0
85	MG	5	3676	1/1	0.69	0.21	70,70,70,70	0
85	MG	5	3862	1/1	0.69	0.23	87,87,87,87	0
85	MG	2	1908	1/1	0.69	0.38	74,74,74,74	0
85	MG	7	205	1/1	0.69	0.32	64,64,64,64	0
85	MG	2	1989	1/1	0.69	0.31	89,89,89,89	0
86	OHX	5	4238	7/7	0.69	0.22	157,157,157,157	0
85	MG	5	3810	1/1	0.70	0.27	101,101,101,101	0
85	MG	2	1969	1/1	0.70	0.34	98,98,98,98	0
85	MG	6	1953	1/1	0.70	0.45	70,70,70,70	0
85	MG	2	1928	1/1	0.70	0.45	76,76,76,76	0
85	MG	1	3413	1/1	0.70	0.43	59,59,59,59	0
85	MG	2	1974	1/1	0.70	0.32	75,75,75,75	0
85	MG	2	1924	1/1	0.71	0.53	86,86,86,86	0
85	MG	2	2017	1/1	0.71	0.26	79,79,79,79	0
85	MG	6	2043	1/1	0.71	0.29	54,54,54,54	0
85	MG	1	3751	1/1	0.71	0.28	86,86,86,86	0
85	MG	5	3784	1/1	0.71	0.35	90,90,90,90	0
86	OHX	1	4184	7/7	0.71	0.18	195,195,195,195	0
85	MG	6	2001	1/1	0.71	0.15	59,59,59,59	0
85	MG	M1	201	1/1	0.71	0.18	76,76,76,76	0
85	MG	2	1930	1/1	0.72	0.32	67,67,67,67	0
85	MG	5	3711	1/1	0.72	0.30	89,89,89,89	0
85	MG	6	2006	1/1	0.72	0.27	102,102,102,102	0
85	MG	6	1902	1/1	0.73	0.26	59,59,59,59	0
85	MG	6	1904	1/1	0.73	0.28	75,75,75,75	0
85	MG	2	1978	1/1	0.73	0.26	96,96,96,96	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3816	1/1	0.73	0.12	87,87,87,87	0
85	MG	O7	102	1/1	0.73	0.38	70,70,70,70	0
86	OHX	l4	402	7/7	0.73	0.17	171,171,171,171	0
85	MG	2	1950	1/1	0.74	0.41	81,81,81,81	0
85	MG	1	3664	1/1	0.74	0.30	68,68,68,68	0
85	MG	5	3420	1/1	0.74	0.29	71,71,71,71	0
85	MG	2	1951	1/1	0.74	0.31	98,98,98,98	0
85	MG	D0	201	1/1	0.74	0.34	79,79,79,79	0
85	MG	2	1940	1/1	0.74	0.21	63,63,63,63	0
86	OHX	L4	402	7/7	0.74	0.19	154,154,154,154	0
86	OHX	s1	303	7/7	0.74	0.18	173,173,173,173	0
85	MG	6	2029	1/1	0.74	0.42	92,92,92,92	0
86	OHX	5	4244	7/7	0.74	0.14	246,246,246,246	0
85	MG	6	1923	1/1	0.74	0.31	72,72,72,72	0
85	MG	2	1999	1/1	0.75	0.30	76,76,76,76	0
85	MG	1	3492	1/1	0.75	0.27	83,83,83,83	0
85	MG	5	3421	1/1	0.75	0.26	104,104,104,104	0
85	MG	1	3669	1/1	0.75	0.40	60,60,60,60	0
85	MG	1	3857	1/1	0.75	0.23	125,125,125,125	0
85	MG	5	3454	1/1	0.75	0.14	34,34,34,34	0
85	MG	1	3520	1/1	0.75	0.35	75,75,75,75	0
85	MG	5	3886	1/1	0.75	0.24	48,48,48,48	0
85	MG	5	3636	1/1	0.75	0.29	88,88,88,88	0
86	OHX	1	4174	7/7	0.75	0.19	161,161,161,161	0
85	MG	1	3697	1/1	0.75	0.28	44,44,44,44	0
85	MG	6	1951	1/1	0.75	0.33	76,76,76,76	0
85	MG	6	2020	1/1	0.75	0.18	117,117,117,117	0
86	OHX	O9	101	7/7	0.75	0.26	134,134,134,134	0
85	MG	2	1904	1/1	0.75	0.30	68,68,68,68	0
85	MG	5	3746	1/1	0.75	0.30	35,35,35,35	0
85	MG	2	1984	1/1	0.75	0.18	77,77,77,77	0
85	MG	6	1965	1/1	0.75	0.21	72,72,72,72	0
85	MG	2	1945	1/1	0.76	0.29	80,80,80,80	0
85	MG	6	1931	1/1	0.76	0.34	68,68,68,68	0
85	MG	5	3481	1/1	0.76	0.35	62,62,62,62	0
85	MG	M9	201	1/1	0.76	0.28	70,70,70,70	0
85	MG	2	2005	1/1	0.76	0.14	67,67,67,67	0
85	MG	O7	103	1/1	0.76	0.34	65,65,65,65	0
85	MG	7	216	1/1	0.76	0.23	55,55,55,55	0
85	MG	l5	302	1/1	0.76	0.20	65,65,65,65	0
85	MG	o4	201	1/1	0.76	0.35	56,56,56,56	0
86	OHX	2	2162	7/7	0.76	0.17	171,171,171,171	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	2	1993	1/1	0.76	0.24	75,75,75,75	0
85	MG	2	1966	1/1	0.76	0.22	85,85,85,85	0
85	MG	2	1961	1/1	0.76	0.29	61,61,61,61	0
85	MG	6	2046	1/1	0.76	0.20	72,72,72,72	0
85	MG	3	201	1/1	0.76	0.25	75,75,75,75	0
85	MG	5	3789	1/1	0.76	0.30	86,86,86,86	0
85	MG	6	1920	1/1	0.76	0.40	56,56,56,56	0
85	MG	6	1986	1/1	0.76	0.22	87,87,87,87	0
85	MG	1	3729	1/1	0.76	0.15	86,86,86,86	0
86	OHX	l4	403	7/7	0.76	0.16	184,184,184,184	0
88	ZN	d7	101	1/1	0.76	0.20	162,162,162,162	0
85	MG	1	3708	1/1	0.77	0.24	62,62,62,62	0
85	MG	5	3482	1/1	0.77	0.21	68,68,68,68	0
85	MG	2	1913	1/1	0.77	0.22	88,88,88,88	0
85	MG	2	1962	1/1	0.77	0.36	81,81,81,81	0
86	OHX	6	2156	7/7	0.77	0.15	196,196,196,196	0
85	MG	6	1966	1/1	0.77	0.35	88,88,88,88	0
86	OHX	5	4237	7/7	0.77	0.19	163,163,163,163	0
85	MG	1	3649	1/1	0.77	0.23	65,65,65,65	0
85	MG	3	209	1/1	0.77	0.26	68,68,68,68	0
86	OHX	2	2159	7/7	0.77	0.22	145,145,145,145	0
85	MG	5	3470	1/1	0.77	0.15	111,111,111,111	0
85	MG	5	3826	1/1	0.77	0.21	99,99,99,99	0
85	MG	1	3448	1/1	0.78	0.17	42,42,42,42	0
85	MG	6	2031	1/1	0.78	0.21	77,77,77,77	0
85	MG	5	3653	1/1	0.78	0.20	99,99,99,99	0
85	MG	2	2021	1/1	0.78	0.65	99,99,99,99	0
85	MG	2	2001	1/1	0.78	0.21	105,105,105,105	0
85	MG	1	3536	1/1	0.78	0.35	43,43,43,43	0
85	MG	5	3730	1/1	0.78	0.17	94,94,94,94	0
85	MG	1	3540	1/1	0.78	0.12	60,60,60,60	0
85	MG	s6	301	1/1	0.78	0.41	77,77,77,77	0
85	MG	s8	301	1/1	0.78	0.21	62,62,62,62	0
85	MG	2	1977	1/1	0.78	0.32	85,85,85,85	0
85	MG	2	1910	1/1	0.78	0.34	57,57,57,57	0
85	MG	5	3422	1/1	0.78	0.33	40,40,40,40	0
86	OHX	6	2170	7/7	0.78	0.16	167,167,167,167	0
85	MG	6	1935	1/1	0.78	0.12	57,57,57,57	0
86	OHX	5	4190	7/7	0.78	0.17	170,170,170,170	0
86	OHX	5	4224	7/7	0.78	0.18	168,168,168,168	0
85	MG	2	2019	1/1	0.78	0.30	78,78,78,78	0
85	MG	6	2004	1/1	0.78	0.34	83,83,83,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	2	2020	1/1	0.78	0.40	77,77,77,77	0
85	MG	1	3651	1/1	0.78	0.23	76,76,76,76	0
85	MG	5	3477	1/1	0.78	0.24	85,85,85,85	0
86	OHX	m4	201	7/7	0.78	0.12	221,221,221,221	0
85	MG	6	1954	1/1	0.78	0.35	51,51,51,51	0
85	MG	5	3774	1/1	0.79	0.15	105,105,105,105	0
85	MG	2	1996	1/1	0.79	0.30	97,97,97,97	0
86	OHX	2	2163	7/7	0.79	0.22	150,150,150,150	0
85	MG	2	1912	1/1	0.79	0.24	73,73,73,73	0
85	MG	6	1929	1/1	0.79	0.36	58,58,58,58	0
85	MG	1	3479	1/1	0.79	0.26	66,66,66,66	0
85	MG	6	1970	1/1	0.79	0.26	69,69,69,69	0
85	MG	6	1934	1/1	0.79	0.26	78,78,78,78	0
86	OHX	6	2137	7/7	0.79	0.18	148,148,148,148	0
85	MG	6	2045	1/1	0.79	0.30	83,83,83,83	0
85	MG	5	3625	1/1	0.79	0.32	44,44,44,44	0
86	OHX	6	2190	7/7	0.79	0.19	157,157,157,157	0
86	OHX	6	2191	7/7	0.79	0.18	175,175,175,175	0
85	MG	1	3631	1/1	0.79	0.32	76,76,76,76	0
86	OHX	5	4167	7/7	0.79	0.15	195,195,195,195	0
85	MG	1	3695	1/1	0.79	0.12	54,54,54,54	0
85	MG	1	3408	1/1	0.79	0.33	37,37,37,37	0
86	OHX	5	4231	7/7	0.79	0.27	135,135,135,135	0
85	MG	5	3401	1/1	0.79	0.26	57,57,57,57	0
85	MG	5	3895	1/1	0.79	0.23	56,56,56,56	0
86	OHX	5	4243	7/7	0.79	0.16	196,196,196,196	0
85	MG	1	3637	1/1	0.79	0.29	55,55,55,55	0
85	MG	1	3638	1/1	0.79	0.33	60,60,60,60	0
85	MG	6	2007	1/1	0.79	0.26	65,65,65,65	0
85	MG	2	1914	1/1	0.79	0.30	71,71,71,71	0
85	MG	o4	202	1/1	0.79	0.24	63,63,63,63	0
86	OHX	1	4140	7/7	0.80	0.22	150,150,150,150	0
85	MG	6	1932	1/1	0.80	0.32	48,48,48,48	0
85	MG	5	3628	1/1	0.80	0.16	66,66,66,66	0
85	MG	2	1937	1/1	0.80	0.33	61,61,61,61	0
86	OHX	1	4193	7/7	0.80	0.17	143,143,143,143	0
86	OHX	1	4198	7/7	0.80	0.18	171,171,171,171	0
85	MG	5	3813	1/1	0.80	0.15	76,76,76,76	0
85	MG	1	3607	1/1	0.80	0.34	74,74,74,74	0
86	OHX	6	2107	7/7	0.80	0.18	154,154,154,154	0
85	MG	6	1972	1/1	0.80	0.29	75,75,75,75	0
85	MG	1	3642	1/1	0.80	0.21	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3865	1/1	0.80	0.10	47,47,47,47	0
86	OHX	6	2184	7/7	0.80	0.20	150,150,150,150	0
86	OHX	6	2188	7/7	0.80	0.18	161,161,161,161	0
85	MG	5	3869	1/1	0.80	0.16	42,42,42,42	0
85	MG	5	3879	1/1	0.80	0.24	47,47,47,47	0
85	MG	5	3688	1/1	0.80	0.38	67,67,67,67	0
85	MG	5	3434	1/1	0.80	0.28	86,86,86,86	0
85	MG	4	220	1/1	0.80	0.39	81,81,81,81	0
85	MG	6	2042	1/1	0.80	0.27	76,76,76,76	0
85	MG	1	3761	1/1	0.80	0.12	61,61,61,61	0
85	MG	2	2006	1/1	0.80	0.42	81,81,81,81	0
85	MG	n3	202	1/1	0.80	0.22	54,54,54,54	0
86	OHX	5	4240	7/7	0.80	0.19	162,162,162,162	0
85	MG	2	1947	1/1	0.80	0.45	59,59,59,59	0
85	MG	1	3820	1/1	0.80	0.15	64,64,64,64	0
86	OHX	5	4250	7/7	0.80	0.19	154,154,154,154	0
86	OHX	2	2158	7/7	0.80	0.18	159,159,159,159	0
85	MG	1	3470	1/1	0.80	0.15	42,42,42,42	0
85	MG	5	3793	1/1	0.80	0.16	54,54,54,54	0
85	MG	5	3616	1/1	0.80	0.15	55,55,55,55	0
85	MG	5	3460	1/1	0.81	0.35	31,31,31,31	0
85	MG	5	3466	1/1	0.81	0.18	61,61,61,61	0
85	MG	5	3737	1/1	0.81	0.29	77,77,77,77	0
85	MG	6	1992	1/1	0.81	0.27	85,85,85,85	0
85	MG	2	1909	1/1	0.81	0.37	70,70,70,70	0
85	MG	1	3524	1/1	0.81	0.24	43,43,43,43	0
85	MG	5	3783	1/1	0.81	0.28	74,74,74,74	0
86	OHX	6	2185	7/7	0.81	0.13	188,188,188,188	0
85	MG	m1	201	1/1	0.81	0.27	62,62,62,62	0
85	MG	6	1922	1/1	0.81	0.37	61,61,61,61	0
85	MG	o1	201	1/1	0.81	0.11	93,93,93,93	0
85	MG	2	1938	1/1	0.81	0.34	69,69,69,69	0
85	MG	5	3504	1/1	0.81	0.26	46,46,46,46	0
86	OHX	2	2099	7/7	0.81	0.16	163,163,163,163	0
86	OHX	5	4221	7/7	0.81	0.20	143,143,143,143	0
86	OHX	5	4223	7/7	0.81	0.19	148,148,148,148	0
85	MG	c7	201	1/1	0.81	0.31	87,87,87,87	0
85	MG	2	1917	1/1	0.81	0.38	59,59,59,59	0
85	MG	N5	201	1/1	0.81	0.32	71,71,71,71	0
85	MG	1	3732	1/1	0.81	0.18	51,51,51,51	0
86	OHX	1	4126	7/7	0.81	0.17	153,153,153,153	0
85	MG	2	1983	1/1	0.81	0.21	78,78,78,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3658	1/1	0.81	0.22	58,58,58,58	0
85	MG	1	3512	1/1	0.81	0.28	25,25,25,25	0
85	MG	3	212	1/1	0.81	0.20	78,78,78,78	0
86	OHX	1	4192	7/7	0.81	0.17	152,152,152,152	0
86	OHX	l5	305	7/7	0.81	0.18	156,156,156,156	0
85	MG	3	213	1/1	0.81	0.29	59,59,59,59	0
85	MG	6	1946	1/1	0.81	0.44	73,73,73,73	0
85	MG	5	3876	1/1	0.82	0.28	41,41,41,41	0
85	MG	6	1918	1/1	0.82	0.28	71,71,71,71	0
86	OHX	1	4195	7/7	0.82	0.19	139,139,139,139	0
85	MG	1	3801	1/1	0.82	0.24	43,43,43,43	0
86	OHX	1	4200	7/7	0.82	0.21	151,151,151,151	0
86	OHX	1	4202	7/7	0.82	0.20	142,142,142,142	0
86	OHX	4	235	7/7	0.82	0.21	143,143,143,143	0
85	MG	2	1907	1/1	0.82	0.37	55,55,55,55	0
85	MG	5	3889	1/1	0.82	0.26	63,63,63,63	0
85	MG	2	1932	1/1	0.82	0.23	65,65,65,65	0
85	MG	5	3897	1/1	0.82	0.33	57,57,57,57	0
86	OHX	6	2148	7/7	0.82	0.17	140,140,140,140	0
85	MG	1	3506	1/1	0.82	0.36	32,32,32,32	0
85	MG	1	3624	1/1	0.82	0.33	89,89,89,89	0
86	OHX	6	2183	7/7	0.82	0.17	148,148,148,148	0
85	MG	8	210	1/1	0.82	0.30	59,59,59,59	0
85	MG	5	3483	1/1	0.82	0.29	41,41,41,41	0
85	MG	5	3496	1/1	0.82	0.16	42,42,42,42	0
85	MG	5	3411	1/1	0.82	0.30	41,41,41,41	0
85	MG	5	3555	1/1	0.82	0.28	37,37,37,37	0
86	OHX	6	2200	7/7	0.82	0.18	160,160,160,160	0
86	OHX	6	2204	7/7	0.82	0.17	156,156,156,156	0
85	MG	5	3560	1/1	0.82	0.30	36,36,36,36	0
85	MG	5	3418	1/1	0.82	0.33	24,24,24,24	0
85	MG	1	3727	1/1	0.82	0.29	40,40,40,40	0
86	OHX	5	4198	7/7	0.82	0.17	155,155,155,155	0
86	OHX	5	4209	7/7	0.82	0.20	150,150,150,150	0
85	MG	2	1971	1/1	0.82	0.31	70,70,70,70	0
85	MG	6	1933	1/1	0.82	0.49	70,70,70,70	0
85	MG	6	2035	1/1	0.82	0.22	90,90,90,90	0
85	MG	3	207	1/1	0.82	0.32	61,61,61,61	0
86	OHX	5	4233	7/7	0.82	0.15	167,167,167,167	0
86	OHX	5	4234	7/7	0.82	0.21	144,144,144,144	0
86	OHX	2	2176	7/7	0.82	0.15	185,185,185,185	0
86	OHX	1	4094	7/7	0.82	0.14	149,149,149,149	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3464	1/1	0.82	0.19	54,54,54,54	0
85	MG	5	3836	1/1	0.82	0.11	75,75,75,75	0
86	OHX	1	4170	7/7	0.82	0.23	144,144,144,144	0
85	MG	2	1905	1/1	0.82	0.33	68,68,68,68	0
86	OHX	1	4181	7/7	0.82	0.17	149,149,149,149	0
85	MG	1	3530	1/1	0.82	0.29	68,68,68,68	0
86	OHX	1	4186	7/7	0.82	0.19	137,137,137,137	0
85	MG	5	3691	1/1	0.82	0.21	53,53,53,53	0
86	OHX	1	4190	7/7	0.82	0.14	159,159,159,159	0
85	MG	2	2008	1/1	0.83	0.33	51,51,51,51	0
85	MG	5	3666	1/1	0.83	0.49	59,59,59,59	0
85	MG	5	3472	1/1	0.83	0.28	38,38,38,38	0
85	MG	5	3818	1/1	0.83	0.16	70,70,70,70	0
85	MG	1	3756	1/1	0.83	0.14	54,54,54,54	0
85	MG	6	2025	1/1	0.83	0.14	69,69,69,69	0
85	MG	5	3689	1/1	0.83	0.27	78,78,78,78	0
86	OHX	1	4137	7/7	0.83	0.18	143,143,143,143	0
85	MG	2	2010	1/1	0.83	0.37	76,76,76,76	0
86	OHX	1	4167	7/7	0.83	0.22	126,126,126,126	0
85	MG	1	3555	1/1	0.83	0.39	38,38,38,38	0
85	MG	5	3486	1/1	0.83	0.15	66,66,66,66	0
86	OHX	1	4176	7/7	0.83	0.16	161,161,161,161	0
85	MG	6	1979	1/1	0.83	0.16	77,77,77,77	0
85	MG	1	3557	1/1	0.83	0.38	49,49,49,49	0
86	OHX	1	4185	7/7	0.83	0.17	148,148,148,148	0
86	OHX	5	4222	7/7	0.83	0.13	177,177,177,177	0
85	MG	5	3743	1/1	0.83	0.21	36,36,36,36	0
85	MG	1	3573	1/1	0.83	0.31	39,39,39,39	0
85	MG	5	3755	1/1	0.83	0.19	45,45,45,45	0
85	MG	5	3759	1/1	0.83	0.14	53,53,53,53	0
85	MG	5	4259	1/1	0.83	0.28	37,37,37,37	0
85	MG	1	3592	1/1	0.83	0.28	62,62,62,62	0
85	MG	5	3775	1/1	0.83	0.21	83,83,83,83	0
85	MG	1	3837	1/1	0.83	0.31	62,62,62,62	0
86	OHX	5	4242	7/7	0.83	0.17	156,156,156,156	0
85	MG	5	3619	1/1	0.83	0.15	51,51,51,51	0
85	MG	1	3474	1/1	0.83	0.29	74,74,74,74	0
85	MG	2	1990	1/1	0.83	0.31	57,57,57,57	0
86	OHX	5	4251	7/7	0.83	0.18	142,142,142,142	0
86	OHX	7	227	7/7	0.83	0.16	142,142,142,142	0
86	OHX	M9	202	7/7	0.83	0.13	181,181,181,181	0
85	MG	6	1930	1/1	0.83	0.23	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3458	1/1	0.83	0.41	77,77,77,77	0
86	OHX	m1	202	7/7	0.83	0.16	163,163,163,163	0
85	MG	5	3656	1/1	0.83	0.19	41,41,41,41	0
88	ZN	D7	101	1/1	0.83	0.18	166,166,166,166	0
85	MG	5	3657	1/1	0.83	0.18	70,70,70,70	0
85	MG	6	2034	1/1	0.84	0.29	63,63,63,63	0
85	MG	1	3712	1/1	0.84	0.13	46,46,46,46	0
86	OHX	M7	206	7/7	0.84	0.27	118,118,118,118	0
85	MG	1	3647	1/1	0.84	0.13	49,49,49,49	0
85	MG	1	4214	1/1	0.84	0.23	73,73,73,73	0
85	MG	1	3496	1/1	0.84	0.33	42,42,42,42	0
85	MG	8	212	1/1	0.84	0.26	105,105,105,105	0
85	MG	5	3752	1/1	0.84	0.34	37,37,37,37	0
85	MG	1	3612	1/1	0.84	0.30	56,56,56,56	0
85	MG	1	3535	1/1	0.84	0.30	53,53,53,53	0
85	MG	1	3625	1/1	0.84	0.23	39,39,39,39	0
85	MG	5	3498	1/1	0.84	0.12	36,36,36,36	0
85	MG	5	3776	1/1	0.84	0.20	73,73,73,73	0
86	OHX	6	2186	7/7	0.84	0.17	153,153,153,153	0
85	MG	6	2207	1/1	0.84	0.11	76,76,76,76	0
85	MG	5	3538	1/1	0.84	0.32	33,33,33,33	0
85	MG	1	3497	1/1	0.84	0.40	36,36,36,36	0
86	OHX	6	2193	7/7	0.84	0.14	188,188,188,188	0
85	MG	5	3786	1/1	0.84	0.10	61,61,61,61	0
85	MG	3	214	1/1	0.84	0.26	70,70,70,70	0
85	MG	5	3592	1/1	0.84	0.28	48,48,48,48	0
86	OHX	d9	102	7/7	0.84	0.14	179,179,179,179	0
86	OHX	5	4145	7/7	0.84	0.16	143,143,143,143	0
86	OHX	5	4156	7/7	0.84	0.21	131,131,131,131	0
85	MG	4	211	1/1	0.84	0.20	58,58,58,58	0
86	OHX	5	4181	7/7	0.84	0.16	156,156,156,156	0
86	OHX	1	4099	7/7	0.84	0.15	164,164,164,164	0
86	OHX	1	4108	7/7	0.84	0.16	147,147,147,147	0
86	OHX	5	4206	7/7	0.84	0.18	149,149,149,149	0
85	MG	sM	302	1/1	0.84	0.16	51,51,51,51	0
86	OHX	5	4215	7/7	0.84	0.16	154,154,154,154	0
85	MG	6	1988	1/1	0.84	0.14	70,70,70,70	0
85	MG	1	3410	1/1	0.84	0.23	44,44,44,44	0
86	OHX	1	4145	7/7	0.84	0.17	140,140,140,140	0
86	OHX	1	4158	7/7	0.84	0.15	158,158,158,158	0
86	OHX	5	4226	7/7	0.84	0.23	138,138,138,138	0
86	OHX	1	4163	7/7	0.84	0.18	141,141,141,141	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3455	1/1	0.84	0.44	57,57,57,57	0
85	MG	1	3812	1/1	0.84	0.23	53,53,53,53	0
85	MG	2	1965	1/1	0.84	0.37	64,64,64,64	0
85	MG	6	2005	1/1	0.84	0.14	79,79,79,79	0
85	MG	5	3424	1/1	0.84	0.21	60,60,60,60	0
85	MG	5	3861	1/1	0.84	0.28	70,70,70,70	0
85	MG	6	1936	1/1	0.84	0.29	84,84,84,84	0
85	MG	2	2004	1/1	0.84	0.22	73,73,73,73	0
85	MG	1	3835	1/1	0.84	0.34	57,57,57,57	0
85	MG	6	1950	1/1	0.84	0.33	49,49,49,49	0
85	MG	1	3528	1/1	0.84	0.32	47,47,47,47	0
85	MG	1	3843	1/1	0.84	0.20	46,46,46,46	0
86	OHX	1	4194	7/7	0.84	0.15	165,165,165,165	0
85	MG	1	3844	1/1	0.84	0.19	52,52,52,52	0
85	MG	5	3715	1/1	0.84	0.14	75,75,75,75	0
85	MG	5	3890	1/1	0.84	0.24	51,51,51,51	0
85	MG	5	3719	1/1	0.84	0.19	62,62,62,62	0
86	OHX	4	232	7/7	0.84	0.16	154,154,154,154	0
86	OHX	6	2173	7/7	0.85	0.17	163,163,163,163	0
86	OHX	6	2179	7/7	0.85	0.14	157,157,157,157	0
86	OHX	2	2175	7/7	0.85	0.13	182,182,182,182	0
85	MG	1	3561	1/1	0.85	0.36	27,27,27,27	0
86	OHX	2	2178	7/7	0.85	0.17	172,172,172,172	0
85	MG	1	3717	1/1	0.85	0.19	56,56,56,56	0
85	MG	5	3659	1/1	0.85	0.17	45,45,45,45	0
85	MG	5	3662	1/1	0.85	0.23	30,30,30,30	0
85	MG	5	3665	1/1	0.85	0.33	51,51,51,51	0
85	MG	5	3825	1/1	0.85	0.16	48,48,48,48	0
86	OHX	6	2199	7/7	0.85	0.18	156,156,156,156	0
85	MG	6	1911	1/1	0.85	0.20	94,94,94,94	0
85	MG	1	3724	1/1	0.85	0.53	41,41,41,41	0
86	OHX	1	4148	7/7	0.85	0.14	162,162,162,162	0
86	OHX	s9	201	7/7	0.85	0.20	139,139,139,139	0
85	MG	5	3678	1/1	0.85	0.20	49,49,49,49	0
85	MG	2	2000	1/1	0.85	0.24	85,85,85,85	0
86	OHX	1	4164	7/7	0.85	0.10	220,220,220,220	0
85	MG	1	3586	1/1	0.85	0.36	38,38,38,38	0
86	OHX	1	4168	7/7	0.85	0.15	162,162,162,162	0
86	OHX	5	4183	7/7	0.85	0.17	144,144,144,144	0
86	OHX	1	4169	7/7	0.85	0.16	168,168,168,168	0
85	MG	1	3589	1/1	0.85	0.45	43,43,43,43	0
85	MG	5	3473	1/1	0.85	0.18	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	4208	7/7	0.85	0.18	150,150,150,150	0
85	MG	5	3709	1/1	0.85	0.31	49,49,49,49	0
85	MG	1	3450	1/1	0.85	0.37	44,44,44,44	0
85	MG	1	3486	1/1	0.85	0.31	42,42,42,42	0
85	MG	1	3608	1/1	0.85	0.38	59,59,59,59	0
85	MG	1	3762	1/1	0.85	0.18	55,55,55,55	0
85	MG	1	3777	1/1	0.85	0.27	48,48,48,48	0
85	MG	6	1994	1/1	0.85	0.23	62,62,62,62	0
86	OHX	5	4227	7/7	0.85	0.18	158,158,158,158	0
86	OHX	5	4228	7/7	0.85	0.15	154,154,154,154	0
85	MG	c9	201	1/1	0.85	0.16	62,62,62,62	0
85	MG	5	3502	1/1	0.85	0.24	32,32,32,32	0
85	MG	1	3656	1/1	0.85	0.35	43,43,43,43	0
85	MG	5	3516	1/1	0.85	0.24	41,41,41,41	0
85	MG	L5	302	1/1	0.85	0.28	67,67,67,67	0
85	MG	2	1964	1/1	0.85	0.18	98,98,98,98	0
85	MG	2	2013	1/1	0.85	0.19	56,56,56,56	0
85	MG	5	3589	1/1	0.85	0.37	52,52,52,52	0
85	MG	2	1953	1/1	0.85	0.28	84,84,84,84	0
86	OHX	5	4248	7/7	0.85	0.18	165,165,165,165	0
86	OHX	5	4249	7/7	0.85	0.18	152,152,152,152	0
85	MG	1	3498	1/1	0.85	0.35	62,62,62,62	0
85	MG	1	3829	1/1	0.85	0.32	55,55,55,55	0
85	MG	1	3424	1/1	0.85	0.25	50,50,50,50	0
86	OHX	2	2148	7/7	0.85	0.13	170,170,170,170	0
86	OHX	2	2152	7/7	0.85	0.13	172,172,172,172	0
85	MG	1	3472	1/1	0.85	0.28	30,30,30,30	0
85	MG	1	3634	1/1	0.85	0.27	80,80,80,80	0
85	MG	5	3442	1/1	0.85	0.14	42,42,42,42	0
86	OHX	6	2167	7/7	0.85	0.11	203,203,203,203	0
85	MG	5	3444	1/1	0.85	0.16	35,35,35,35	0
85	MG	5	3523	1/1	0.86	0.29	34,34,34,34	0
86	OHX	O2	202	7/7	0.86	0.17	153,153,153,153	0
85	MG	n8	201	1/1	0.86	0.10	30,30,30,30	0
85	MG	1	3671	1/1	0.86	0.20	33,33,33,33	0
85	MG	1	3690	1/1	0.86	0.33	50,50,50,50	0
85	MG	6	1943	1/1	0.86	0.38	45,45,45,45	0
85	MG	5	3571	1/1	0.86	0.39	33,33,33,33	0
86	OHX	2	2115	7/7	0.86	0.15	154,154,154,154	0
86	OHX	2	2140	7/7	0.86	0.14	166,166,166,166	0
86	OHX	6	2172	7/7	0.86	0.15	152,152,152,152	0
86	OHX	2	2147	7/7	0.86	0.20	125,125,125,125	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	6	2178	7/7	0.86	0.16	152,152,152,152	0
85	MG	2	1941	1/1	0.86	0.22	76,76,76,76	0
85	MG	5	3590	1/1	0.86	0.33	27,27,27,27	0
86	OHX	2	2154	7/7	0.86	0.16	157,157,157,157	0
86	OHX	2	2157	7/7	0.86	0.09	293,293,293,293	0
85	MG	6	2012	1/1	0.86	0.34	50,50,50,50	0
85	MG	5	3599	1/1	0.86	0.41	31,31,31,31	0
86	OHX	6	2189	7/7	0.86	0.16	151,151,151,151	0
85	MG	5	3426	1/1	0.86	0.25	45,45,45,45	0
85	MG	2	1942	1/1	0.86	0.21	70,70,70,70	0
86	OHX	2	2164	7/7	0.86	0.12	177,177,177,177	0
86	OHX	2	2172	7/7	0.86	0.16	159,159,159,159	0
86	OHX	2	2173	7/7	0.86	0.15	173,173,173,173	0
85	MG	1	3646	1/1	0.86	0.17	47,47,47,47	0
85	MG	5	3441	1/1	0.86	0.27	31,31,31,31	0
85	MG	6	1906	1/1	0.86	0.30	48,48,48,48	0
86	OHX	d4	202	7/7	0.86	0.12	173,173,173,173	0
85	MG	5	3639	1/1	0.86	0.27	52,52,52,52	0
85	MG	5	3640	1/1	0.86	0.25	63,63,63,63	0
86	OHX	5	4155	7/7	0.86	0.22	128,128,128,128	0
85	MG	5	3806	1/1	0.86	0.23	73,73,73,73	0
85	MG	3	206	1/1	0.86	0.38	32,32,32,32	0
85	MG	5	3654	1/1	0.86	0.41	77,77,77,77	0
85	MG	6	1958	1/1	0.86	0.41	51,51,51,51	0
86	OHX	5	4189	7/7	0.86	0.21	124,124,124,124	0
85	MG	5	3449	1/1	0.86	0.21	65,65,65,65	0
85	MG	1	3468	1/1	0.86	0.29	56,56,56,56	0
85	MG	5	3456	1/1	0.86	0.19	99,99,99,99	0
85	MG	6	1910	1/1	0.86	0.32	56,56,56,56	0
85	MG	5	3831	1/1	0.86	0.20	40,40,40,40	0
86	OHX	5	4213	7/7	0.86	0.22	123,123,123,123	0
86	OHX	1	4166	7/7	0.86	0.18	128,128,128,128	0
85	MG	5	3664	1/1	0.86	0.28	37,37,37,37	0
85	MG	1	3562	1/1	0.86	0.29	49,49,49,49	0
85	MG	1	3442	1/1	0.86	0.30	26,26,26,26	0
85	MG	S8	301	1/1	0.86	0.27	62,62,62,62	0
86	OHX	5	4225	7/7	0.86	0.15	151,151,151,151	0
85	MG	1	3817	1/1	0.86	0.10	47,47,47,47	0
86	OHX	1	4175	7/7	0.86	0.21	131,131,131,131	0
85	MG	4	210	1/1	0.86	0.23	56,56,56,56	0
86	OHX	1	4179	7/7	0.86	0.18	141,141,141,141	0
85	MG	5	3683	1/1	0.86	0.13	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3881	1/1	0.86	0.26	28,28,28,28	0
85	MG	5	3684	1/1	0.86	0.25	78,78,78,78	0
85	MG	6	1976	1/1	0.86	0.14	68,68,68,68	0
85	MG	1	3718	1/1	0.86	0.20	45,45,45,45	0
86	OHX	1	4188	7/7	0.86	0.16	148,148,148,148	0
85	MG	4	217	1/1	0.86	0.12	43,43,43,43	0
85	MG	5	3892	1/1	0.86	0.16	37,37,37,37	0
85	MG	5	3696	1/1	0.86	0.25	54,54,54,54	0
85	MG	1	3827	1/1	0.86	0.31	37,37,37,37	0
85	MG	L3	403	1/1	0.86	0.15	52,52,52,52	0
85	MG	2	1906	1/1	0.86	0.34	58,58,58,58	0
86	OHX	7	225	7/7	0.86	0.16	164,164,164,164	0
85	MG	1	3662	1/1	0.86	0.20	56,56,56,56	0
86	OHX	1	4201	7/7	0.86	0.18	139,139,139,139	0
85	MG	5	3721	1/1	0.86	0.31	62,62,62,62	0
85	MG	1	3539	1/1	0.86	0.27	24,24,24,24	0
85	MG	l5	301	1/1	0.86	0.21	70,70,70,70	0
85	MG	5	3403	1/1	0.86	0.31	61,61,61,61	0
85	MG	1	3419	1/1	0.86	0.15	84,84,84,84	0
86	OHX	M7	207	7/7	0.86	0.18	142,142,142,142	0
85	MG	6	2036	1/1	0.87	0.20	78,78,78,78	0
85	MG	7	208	1/1	0.87	0.20	62,62,62,62	0
86	OHX	1	4204	7/7	0.87	0.20	135,135,135,135	0
86	OHX	1	4210	7/7	0.87	0.20	139,139,139,139	0
86	OHX	4	231	7/7	0.87	0.18	124,124,124,124	0
85	MG	5	3474	1/1	0.87	0.13	37,37,37,37	0
86	OHX	4	233	7/7	0.87	0.18	148,148,148,148	0
85	MG	6	2038	1/1	0.87	0.42	70,70,70,70	0
85	MG	1	3616	1/1	0.87	0.15	64,64,64,64	0
85	MG	1	3427	1/1	0.87	0.21	40,40,40,40	0
85	MG	1	3432	1/1	0.87	0.30	41,41,41,41	0
85	MG	1	3481	1/1	0.87	0.21	32,32,32,32	0
85	MG	5	3489	1/1	0.87	0.32	54,54,54,54	0
85	MG	5	3491	1/1	0.87	0.08	30,30,30,30	0
85	MG	5	3494	1/1	0.87	0.29	60,60,60,60	0
85	MG	6	2044	1/1	0.87	0.15	51,51,51,51	0
85	MG	1	3484	1/1	0.87	0.28	46,46,46,46	0
86	OHX	2	2093	7/7	0.87	0.14	157,157,157,157	0
85	MG	5	3501	1/1	0.87	0.30	40,40,40,40	0
86	OHX	2	2111	7/7	0.87	0.12	164,164,164,164	0
85	MG	6	1964	1/1	0.87	0.25	62,62,62,62	0
86	OHX	2	2134	7/7	0.87	0.16	146,146,146,146	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	6	2174	7/7	0.87	0.20	141,141,141,141	0
86	OHX	2	2137	7/7	0.87	0.13	174,174,174,174	0
85	MG	5	3742	1/1	0.87	0.27	59,59,59,59	0
86	OHX	6	2181	7/7	0.87	0.19	147,147,147,147	0
86	OHX	2	2144	7/7	0.87	0.12	177,177,177,177	0
85	MG	1	3437	1/1	0.87	0.26	35,35,35,35	0
85	MG	5	3510	1/1	0.87	0.24	42,42,42,42	0
85	MG	Q2	502	1/1	0.87	0.17	65,65,65,65	0
85	MG	1	3550	1/1	0.87	0.29	42,42,42,42	0
86	OHX	2	2155	7/7	0.87	0.09	246,246,246,246	0
85	MG	5	3526	1/1	0.87	0.30	31,31,31,31	0
85	MG	5	3761	1/1	0.87	0.07	44,44,44,44	0
85	MG	5	3766	1/1	0.87	0.24	82,82,82,82	0
86	OHX	2	2160	7/7	0.87	0.14	158,158,158,158	0
85	MG	1	3636	1/1	0.87	0.20	50,50,50,50	0
85	MG	5	3551	1/1	0.87	0.32	51,51,51,51	0
85	MG	1	3489	1/1	0.87	0.27	62,62,62,62	0
85	MG	2	1946	1/1	0.87	0.27	65,65,65,65	0
85	MG	1	3848	1/1	0.87	0.27	79,79,79,79	0
86	OHX	2	2174	7/7	0.87	0.17	145,145,145,145	0
86	OHX	5	4102	7/7	0.87	0.19	132,132,132,132	0
86	OHX	5	4142	7/7	0.87	0.21	137,137,137,137	0
85	MG	5	3575	1/1	0.87	0.42	37,37,37,37	0
85	MG	2	1921	1/1	0.87	0.33	52,52,52,52	0
86	OHX	2	2177	7/7	0.87	0.19	154,154,154,154	0
85	MG	1	3854	1/1	0.87	0.32	53,53,53,53	0
85	MG	5	3591	1/1	0.87	0.32	34,34,34,34	0
85	MG	5	3414	1/1	0.87	0.29	36,36,36,36	0
85	MG	5	3594	1/1	0.87	0.33	29,29,29,29	0
86	OHX	1	4110	7/7	0.87	0.16	144,144,144,144	0
86	OHX	5	4197	7/7	0.87	0.21	144,144,144,144	0
86	OHX	1	4111	7/7	0.87	0.22	130,130,130,130	0
86	OHX	5	4204	7/7	0.87	0.15	144,144,144,144	0
85	MG	5	3804	1/1	0.87	0.12	39,39,39,39	0
86	OHX	1	4128	7/7	0.87	0.12	176,176,176,176	0
85	MG	5	3595	1/1	0.87	0.28	41,41,41,41	0
85	MG	2	1955	1/1	0.87	0.22	65,65,65,65	0
85	MG	5	3607	1/1	0.87	0.11	34,34,34,34	0
86	OHX	5	4217	7/7	0.87	0.10	204,204,204,204	0
86	OHX	5	4220	7/7	0.87	0.15	145,145,145,145	0
86	OHX	1	4147	7/7	0.87	0.15	142,142,142,142	0
85	MG	5	3612	1/1	0.87	0.23	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3615	1/1	0.87	0.12	34,34,34,34	0
85	MG	5	3817	1/1	0.87	0.14	59,59,59,59	0
85	MG	2	1936	1/1	0.87	0.36	57,57,57,57	0
86	OHX	1	4165	7/7	0.87	0.24	121,121,121,121	0
85	MG	5	3820	1/1	0.87	0.24	47,47,47,47	0
85	MG	6	1991	1/1	0.87	0.25	70,70,70,70	0
85	MG	1	3648	1/1	0.87	0.15	49,49,49,49	0
85	MG	1	3501	1/1	0.87	0.39	42,42,42,42	0
85	MG	1	3755	1/1	0.87	0.12	41,41,41,41	0
85	MG	2	1944	1/1	0.87	0.18	68,68,68,68	0
85	MG	3	210	1/1	0.87	0.17	68,68,68,68	0
85	MG	2	1960	1/1	0.87	0.15	67,67,67,67	0
86	OHX	1	4178	7/7	0.87	0.18	139,139,139,139	0
85	MG	5	3867	1/1	0.87	0.28	48,48,48,48	0
85	MG	1	3599	1/1	0.87	0.24	41,41,41,41	0
86	OHX	5	4247	7/7	0.87	0.18	145,145,145,145	0
85	MG	5	3874	1/1	0.87	0.34	37,37,37,37	0
85	MG	1	3772	1/1	0.87	0.24	57,57,57,57	0
85	MG	4	206	1/1	0.87	0.26	39,39,39,39	0
85	MG	2	1992	1/1	0.87	0.14	61,61,61,61	0
86	OHX	5	4252	7/7	0.87	0.17	153,153,153,153	0
85	MG	1	3783	1/1	0.87	0.09	44,44,44,44	0
85	MG	1	3789	1/1	0.87	0.19	69,69,69,69	0
86	OHX	8	227	7/7	0.87	0.16	137,137,137,137	0
85	MG	6	2028	1/1	0.87	0.39	66,66,66,66	0
85	MG	5	3465	1/1	0.87	0.16	40,40,40,40	0
85	MG	6	1941	1/1	0.87	0.28	52,52,52,52	0
86	OHX	m0	303	7/7	0.87	0.20	134,134,134,134	0
85	MG	2	1979	1/1	0.87	0.30	60,60,60,60	0
85	MG	2	1923	1/1	0.87	0.38	67,67,67,67	0
86	OHX	m7	206	7/7	0.87	0.18	132,132,132,132	0
87	3K8	2	2179	28/28	0.87	0.14	86,86,86,86	0
86	OHX	1	4199	7/7	0.87	0.17	150,150,150,150	0
85	MG	1	3810	1/1	0.87	0.17	50,50,50,50	0
85	MG	5	3758	1/1	0.88	0.14	54,54,54,54	0
86	OHX	2	2119	7/7	0.88	0.16	144,144,144,144	0
86	OHX	2	2129	7/7	0.88	0.12	204,204,204,204	0
86	OHX	2	2133	7/7	0.88	0.11	163,163,163,163	0
85	MG	1	3710	1/1	0.88	0.34	78,78,78,78	0
86	OHX	2	2136	7/7	0.88	0.16	141,141,141,141	0
85	MG	5	3557	1/1	0.88	0.27	37,37,37,37	0
86	OHX	6	2153	7/7	0.88	0.15	150,150,150,150	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3763	1/1	0.88	0.18	65,65,65,65	0
85	MG	6	1960	1/1	0.88	0.32	44,44,44,44	0
85	MG	5	3767	1/1	0.88	0.18	39,39,39,39	0
85	MG	6	1961	1/1	0.88	0.16	85,85,85,85	0
85	MG	d4	201	1/1	0.88	0.16	66,66,66,66	0
85	MG	5	3583	1/1	0.88	0.31	37,37,37,37	0
85	MG	S4	301	1/1	0.88	0.45	79,79,79,79	0
85	MG	1	3456	1/1	0.88	0.20	31,31,31,31	0
85	MG	N6	201	1/1	0.88	0.24	51,51,51,51	0
85	MG	1	3596	1/1	0.88	0.37	27,27,27,27	0
85	MG	1	3721	1/1	0.88	0.09	49,49,49,49	0
85	MG	2	1948	1/1	0.88	0.13	90,90,90,90	0
85	MG	5	3794	1/1	0.88	0.10	58,58,58,58	0
86	OHX	6	2187	7/7	0.88	0.13	172,172,172,172	0
85	MG	5	3596	1/1	0.88	0.31	37,37,37,37	0
86	OHX	2	2168	7/7	0.88	0.16	162,162,162,162	0
85	MG	5	3798	1/1	0.88	0.12	48,48,48,48	0
85	MG	6	1901	1/1	0.88	0.33	46,46,46,46	0
85	MG	5	3803	1/1	0.88	0.26	80,80,80,80	0
85	MG	1	3494	1/1	0.88	0.26	47,47,47,47	0
85	MG	2	1931	1/1	0.88	0.37	57,57,57,57	0
86	OHX	6	2203	7/7	0.88	0.17	158,158,158,158	0
85	MG	6	1977	1/1	0.88	0.23	48,48,48,48	0
85	MG	1	3730	1/1	0.88	0.16	63,63,63,63	0
86	OHX	D9	102	7/7	0.88	0.16	154,154,154,154	0
85	MG	6	1981	1/1	0.88	0.16	80,80,80,80	0
85	MG	5	3623	1/1	0.88	0.27	45,45,45,45	0
86	OHX	5	4099	7/7	0.88	0.14	155,155,155,155	0
85	MG	1	3430	1/1	0.88	0.29	46,46,46,46	0
85	MG	1	3734	1/1	0.88	0.25	63,63,63,63	0
85	MG	1	3743	1/1	0.88	0.17	56,56,56,56	0
86	OHX	1	4124	7/7	0.88	0.20	127,127,127,127	0
85	MG	2	1901	1/1	0.88	0.27	76,76,76,76	0
86	OHX	5	4162	7/7	0.88	0.19	137,137,137,137	0
86	OHX	5	4163	7/7	0.88	0.17	129,129,129,129	0
85	MG	6	1917	1/1	0.88	0.25	63,63,63,63	0
86	OHX	5	4171	7/7	0.88	0.16	146,146,146,146	0
86	OHX	5	4173	7/7	0.88	0.14	175,175,175,175	0
86	OHX	1	4130	7/7	0.88	0.14	169,169,169,169	0
86	OHX	1	4136	7/7	0.88	0.18	130,130,130,130	0
86	OHX	5	4186	7/7	0.88	0.17	134,134,134,134	0
85	MG	1	3618	1/1	0.88	0.33	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	6	1919	1/1	0.88	0.32	46,46,46,46	0
86	OHX	1	4143	7/7	0.88	0.14	165,165,165,165	0
86	OHX	1	4144	7/7	0.88	0.15	150,150,150,150	0
86	OHX	5	4199	7/7	0.88	0.18	131,131,131,131	0
85	MG	5	3848	1/1	0.88	0.17	53,53,53,53	0
85	MG	2	2007	1/1	0.88	0.40	51,51,51,51	0
85	MG	6	2003	1/1	0.88	0.15	57,57,57,57	0
85	MG	1	4220	1/1	0.88	0.13	43,43,43,43	0
86	OHX	1	4159	7/7	0.88	0.14	163,163,163,163	0
85	MG	2	1933	1/1	0.88	0.24	75,75,75,75	0
85	MG	1	3559	1/1	0.88	0.28	40,40,40,40	0
85	MG	6	1925	1/1	0.88	0.45	42,42,42,42	0
85	MG	6	1928	1/1	0.88	0.29	79,79,79,79	0
85	MG	5	3877	1/1	0.88	0.25	40,40,40,40	0
85	MG	1	3768	1/1	0.88	0.23	54,54,54,54	0
85	MG	1	3770	1/1	0.88	0.15	69,69,69,69	0
85	MG	5	3883	1/1	0.88	0.22	35,35,35,35	0
85	MG	1	3771	1/1	0.88	0.18	63,63,63,63	0
85	MG	1	3673	1/1	0.88	0.30	63,63,63,63	0
85	MG	5	3887	1/1	0.88	0.21	53,53,53,53	0
85	MG	2	1939	1/1	0.88	0.26	70,70,70,70	0
85	MG	6	2030	1/1	0.88	0.23	105,105,105,105	0
85	MG	5	3891	1/1	0.88	0.21	43,43,43,43	0
85	MG	5	3685	1/1	0.88	0.11	33,33,33,33	0
85	MG	1	3449	1/1	0.88	0.21	43,43,43,43	0
85	MG	4	202	1/1	0.88	0.35	50,50,50,50	0
85	MG	1	3523	1/1	0.88	0.32	25,25,25,25	0
85	MG	6	1939	1/1	0.88	0.30	69,69,69,69	0
86	OHX	1	4189	7/7	0.88	0.14	158,158,158,158	0
86	OHX	5	4246	7/7	0.88	0.14	165,165,165,165	0
85	MG	5	3708	1/1	0.88	0.17	50,50,50,50	0
85	MG	7	215	1/1	0.88	0.08	48,48,48,48	0
85	MG	6	2037	1/1	0.88	0.25	72,72,72,72	0
85	MG	8	209	1/1	0.88	0.10	65,65,65,65	0
85	MG	1	3793	1/1	0.88	0.19	41,41,41,41	0
85	MG	1	3795	1/1	0.88	0.11	56,56,56,56	0
85	MG	1	3796	1/1	0.88	0.17	87,87,87,87	0
85	MG	6	1944	1/1	0.88	0.35	71,71,71,71	0
85	MG	l9	201	1/1	0.88	0.12	44,44,44,44	0
86	OHX	8	229	7/7	0.88	0.18	137,137,137,137	0
85	MG	5	3725	1/1	0.88	0.20	54,54,54,54	0
86	OHX	1	4203	7/7	0.88	0.17	156,156,156,156	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3800	1/1	0.88	0.16	58,58,58,58	0
85	MG	1	3580	1/1	0.88	0.23	44,44,44,44	0
85	MG	L5	301	1/1	0.88	0.24	64,64,64,64	0
85	MG	6	1952	1/1	0.88	0.24	65,65,65,65	0
85	MG	1	3583	1/1	0.88	0.27	45,45,45,45	0
85	MG	5	3541	1/1	0.88	0.32	29,29,29,29	0
85	MG	2	2003	1/1	0.88	0.43	90,90,90,90	0
85	MG	5	3552	1/1	0.88	0.28	36,36,36,36	0
85	MG	1	3691	1/1	0.89	0.15	49,49,49,49	0
86	OHX	6	2164	7/7	0.89	0.10	203,203,203,203	0
85	MG	1	3443	1/1	0.89	0.33	67,67,67,67	0
86	OHX	6	2169	7/7	0.89	0.14	161,161,161,161	0
85	MG	1	3619	1/1	0.89	0.18	67,67,67,67	0
85	MG	1	3622	1/1	0.89	0.16	47,47,47,47	0
85	MG	4	214	1/1	0.89	0.21	52,52,52,52	0
85	MG	6	2033	1/1	0.89	0.15	57,57,57,57	0
86	OHX	6	2176	7/7	0.89	0.19	117,117,117,117	0
85	MG	5	3671	1/1	0.89	0.12	30,30,30,30	0
86	OHX	1	4024	7/7	0.89	0.18	125,125,125,125	0
86	OHX	1	4078	7/7	0.89	0.17	132,132,132,132	0
86	OHX	1	4079	7/7	0.89	0.18	123,123,123,123	0
85	MG	2	1976	1/1	0.89	0.32	60,60,60,60	0
86	OHX	1	4098	7/7	0.89	0.17	128,128,128,128	0
85	MG	1	3799	1/1	0.89	0.29	59,59,59,59	0
86	OHX	1	4107	7/7	0.89	0.16	130,130,130,130	0
85	MG	5	3487	1/1	0.89	0.18	52,52,52,52	0
85	MG	1	3547	1/1	0.89	0.21	44,44,44,44	0
85	MG	1	3491	1/1	0.89	0.23	61,61,61,61	0
85	MG	1	3711	1/1	0.89	0.11	38,38,38,38	0
85	MG	M0	301	1/1	0.89	0.15	86,86,86,86	0
86	OHX	6	2194	7/7	0.89	0.11	195,195,195,195	0
86	OHX	6	2195	7/7	0.89	0.13	162,162,162,162	0
86	OHX	6	2196	7/7	0.89	0.12	172,172,172,172	0
85	MG	1	3412	1/1	0.89	0.30	46,46,46,46	0
86	OHX	1	4129	7/7	0.89	0.15	149,149,149,149	0
85	MG	1	3556	1/1	0.89	0.12	55,55,55,55	0
86	OHX	1	4133	7/7	0.89	0.16	126,126,126,126	0
85	MG	6	1955	1/1	0.89	0.40	40,40,40,40	0
86	OHX	s8	303	7/7	0.89	0.14	167,167,167,167	0
85	MG	5	3706	1/1	0.89	0.17	73,73,73,73	0
86	OHX	c3	201	7/7	0.89	0.13	160,160,160,160	0
86	OHX	1	4138	7/7	0.89	0.21	120,120,120,120	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	M7	201	1/1	0.89	0.37	67,67,67,67	0
85	MG	6	1959	1/1	0.89	0.40	58,58,58,58	0
85	MG	2	2181	1/1	0.89	0.12	90,90,90,90	0
85	MG	5	3518	1/1	0.89	0.26	39,39,39,39	0
86	OHX	5	4143	7/7	0.89	0.13	150,150,150,150	0
85	MG	5	3716	1/1	0.89	0.17	45,45,45,45	0
86	OHX	5	4149	7/7	0.89	0.19	124,124,124,124	0
86	OHX	5	4154	7/7	0.89	0.14	157,157,157,157	0
85	MG	5	3718	1/1	0.89	0.22	52,52,52,52	0
86	OHX	1	4151	7/7	0.89	0.15	149,149,149,149	0
86	OHX	5	4161	7/7	0.89	0.18	120,120,120,120	0
85	MG	5	3519	1/1	0.89	0.36	22,22,22,22	0
85	MG	N0	201	1/1	0.89	0.33	48,48,48,48	0
86	OHX	5	4164	7/7	0.89	0.17	125,125,125,125	0
86	OHX	1	4161	7/7	0.89	0.14	150,150,150,150	0
86	OHX	5	4169	7/7	0.89	0.15	140,140,140,140	0
85	MG	1	3720	1/1	0.89	0.12	54,54,54,54	0
85	MG	7	211	1/1	0.89	0.14	79,79,79,79	0
86	OHX	5	4179	7/7	0.89	0.17	136,136,136,136	0
85	MG	7	213	1/1	0.89	0.11	78,78,78,78	0
85	MG	1	3454	1/1	0.89	0.29	48,48,48,48	0
86	OHX	5	4185	7/7	0.89	0.15	145,145,145,145	0
85	MG	1	3414	1/1	0.89	0.25	38,38,38,38	0
85	MG	5	3548	1/1	0.89	0.28	47,47,47,47	0
85	MG	1	3416	1/1	0.89	0.24	36,36,36,36	0
86	OHX	5	4191	7/7	0.89	0.18	131,131,131,131	0
86	OHX	5	4194	7/7	0.89	0.17	133,133,133,133	0
85	MG	d3	201	1/1	0.89	0.26	56,56,56,56	0
86	OHX	1	4173	7/7	0.89	0.14	145,145,145,145	0
85	MG	1	3832	1/1	0.89	0.29	53,53,53,53	0
85	MG	1	3570	1/1	0.89	0.36	41,41,41,41	0
86	OHX	5	4205	7/7	0.89	0.20	136,136,136,136	0
85	MG	2	1982	1/1	0.89	0.43	67,67,67,67	0
86	OHX	5	4207	7/7	0.89	0.15	142,142,142,142	0
85	MG	5	3569	1/1	0.89	0.32	24,24,24,24	0
85	MG	m5	301	1/1	0.89	0.27	54,54,54,54	0
86	OHX	1	4180	7/7	0.89	0.20	111,111,111,111	0
85	MG	2	2009	1/1	0.89	0.39	77,77,77,77	0
86	OHX	1	4183	7/7	0.89	0.19	137,137,137,137	0
85	MG	1	3467	1/1	0.89	0.24	44,44,44,44	0
85	MG	1	3517	1/1	0.89	0.34	33,33,33,33	0
85	MG	5	3584	1/1	0.89	0.35	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	2	1995	1/1	0.89	0.27	57,57,57,57	0
85	MG	1	3851	1/1	0.89	0.17	77,77,77,77	0
85	MG	1	3522	1/1	0.89	0.27	75,75,75,75	0
85	MG	1	3593	1/1	0.89	0.31	29,29,29,29	0
85	MG	1	3757	1/1	0.89	0.12	45,45,45,45	0
85	MG	5	3781	1/1	0.89	0.27	59,59,59,59	0
86	OHX	5	4229	7/7	0.89	0.16	141,141,141,141	0
86	OHX	5	4230	7/7	0.89	0.13	163,163,163,163	0
85	MG	1	3401	1/1	0.89	0.27	42,42,42,42	0
86	OHX	5	4232	7/7	0.89	0.10	191,191,191,191	0
86	OHX	2	2131	7/7	0.89	0.18	140,140,140,140	0
86	OHX	1	4197	7/7	0.89	0.17	137,137,137,137	0
86	OHX	5	4235	7/7	0.89	0.12	170,170,170,170	0
85	MG	1	3428	1/1	0.89	0.12	55,55,55,55	0
85	MG	6	1993	1/1	0.89	0.10	59,59,59,59	0
86	OHX	5	4239	7/7	0.89	0.19	141,141,141,141	0
85	MG	5	3600	1/1	0.89	0.24	44,44,44,44	0
85	MG	5	3601	1/1	0.89	0.20	45,45,45,45	0
85	MG	5	3437	1/1	0.89	0.29	46,46,46,46	0
85	MG	3	202	1/1	0.89	0.17	50,50,50,50	0
86	OHX	5	4245	7/7	0.89	0.20	113,113,113,113	0
86	OHX	2	2146	7/7	0.89	0.11	177,177,177,177	0
85	MG	3	203	1/1	0.89	0.14	98,98,98,98	0
86	OHX	1	4211	7/7	0.89	0.17	161,161,161,161	0
86	OHX	3	223	7/7	0.89	0.12	172,172,172,172	0
85	MG	5	3443	1/1	0.89	0.25	28,28,28,28	0
85	MG	5	3800	1/1	0.89	0.18	59,59,59,59	0
85	MG	1	3765	1/1	0.89	0.18	43,43,43,43	0
86	OHX	5	4254	7/7	0.89	0.12	166,166,166,166	0
85	MG	1	3402	1/1	0.89	0.33	50,50,50,50	0
86	OHX	2	2156	7/7	0.89	0.19	128,128,128,128	0
86	OHX	8	226	7/7	0.89	0.17	147,147,147,147	0
85	MG	2	1929	1/1	0.89	0.29	74,74,74,74	0
85	MG	1	3407	1/1	0.89	0.26	42,42,42,42	0
86	OHX	8	230	7/7	0.89	0.16	130,130,130,130	0
86	OHX	M8	201	7/7	0.89	0.16	140,140,140,140	0
85	MG	3	211	1/1	0.89	0.12	80,80,80,80	0
85	MG	5	3458	1/1	0.89	0.19	38,38,38,38	0
85	MG	1	3684	1/1	0.89	0.18	84,84,84,84	0
85	MG	2	2014	1/1	0.89	0.38	65,65,65,65	0
86	OHX	6	2117	7/7	0.89	0.15	150,150,150,150	0
86	OHX	6	2135	7/7	0.89	0.15	140,140,140,140	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	6	2013	1/1	0.89	0.20	76,76,76,76	0
85	MG	1	3781	1/1	0.89	0.10	40,40,40,40	0
85	MG	4	201	1/1	0.89	0.17	46,46,46,46	0
88	ZN	e1	501	1/1	0.89	0.08	186,186,186,186	0
88	ZN	q2	501	1/1	0.89	0.32	97,97,97,97	0
86	OHX	6	2151	7/7	0.90	0.19	127,127,127,127	0
86	OHX	6	2152	7/7	0.90	0.14	158,158,158,158	0
85	MG	1	3725	1/1	0.90	0.13	73,73,73,73	0
85	MG	1	3482	1/1	0.90	0.25	51,51,51,51	0
86	OHX	6	2158	7/7	0.90	0.13	151,151,151,151	0
86	OHX	6	2160	7/7	0.90	0.16	136,136,136,136	0
86	OHX	6	2161	7/7	0.90	0.15	134,134,134,134	0
86	OHX	6	2162	7/7	0.90	0.18	129,129,129,129	0
85	MG	6	1978	1/1	0.90	0.23	50,50,50,50	0
85	MG	1	3552	1/1	0.90	0.30	33,33,33,33	0
85	MG	6	1980	1/1	0.90	0.36	64,64,64,64	0
85	MG	5	3849	1/1	0.90	0.09	40,40,40,40	0
85	MG	5	3851	1/1	0.90	0.10	57,57,57,57	0
85	MG	5	3857	1/1	0.90	0.28	52,52,52,52	0
86	OHX	1	4017	7/7	0.90	0.16	130,130,130,130	0
85	MG	5	3506	1/1	0.90	0.28	53,53,53,53	0
86	OHX	1	4062	7/7	0.90	0.17	133,133,133,133	0
86	OHX	1	4065	7/7	0.90	0.17	124,124,124,124	0
86	OHX	6	2180	7/7	0.90	0.17	144,144,144,144	0
86	OHX	1	4068	7/7	0.90	0.16	126,126,126,126	0
86	OHX	1	4071	7/7	0.90	0.22	116,116,116,116	0
86	OHX	1	4075	7/7	0.90	0.12	142,142,142,142	0
86	OHX	1	4076	7/7	0.90	0.18	132,132,132,132	0
85	MG	1	3615	1/1	0.90	0.27	39,39,39,39	0
85	MG	1	3554	1/1	0.90	0.39	28,28,28,28	0
86	OHX	1	4081	7/7	0.90	0.17	139,139,139,139	0
86	OHX	1	4082	7/7	0.90	0.13	146,146,146,146	0
86	OHX	1	4093	7/7	0.90	0.15	134,134,134,134	0
85	MG	1	3733	1/1	0.90	0.16	36,36,36,36	0
85	MG	5	3868	1/1	0.90	0.19	68,68,68,68	0
85	MG	6	1926	1/1	0.90	0.35	52,52,52,52	0
86	OHX	1	4106	7/7	0.90	0.14	139,139,139,139	0
85	MG	5	3873	1/1	0.90	0.47	43,43,43,43	0
85	MG	4	207	1/1	0.90	0.22	36,36,36,36	0
85	MG	5	3405	1/1	0.90	0.23	31,31,31,31	0
85	MG	5	3529	1/1	0.90	0.23	34,34,34,34	0
86	OHX	1	4112	7/7	0.90	0.11	174,174,174,174	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	1	4114	7/7	0.90	0.15	137,137,137,137	0
86	OHX	1	4117	7/7	0.90	0.15	136,136,136,136	0
86	OHX	1	4119	7/7	0.90	0.16	139,139,139,139	0
85	MG	5	3407	1/1	0.90	0.13	44,44,44,44	0
86	OHX	c5	201	7/7	0.90	0.10	169,169,169,169	0
85	MG	1	3514	1/1	0.90	0.32	39,39,39,39	0
85	MG	5	3542	1/1	0.90	0.30	33,33,33,33	0
85	MG	5	3546	1/1	0.90	0.42	48,48,48,48	0
85	MG	1	3815	1/1	0.90	0.10	54,54,54,54	0
86	OHX	5	4106	7/7	0.90	0.10	164,164,164,164	0
86	OHX	5	4111	7/7	0.90	0.14	141,141,141,141	0
86	OHX	5	4112	7/7	0.90	0.17	127,127,127,127	0
86	OHX	5	4114	7/7	0.90	0.14	139,139,139,139	0
85	MG	5	3550	1/1	0.90	0.43	47,47,47,47	0
85	MG	5	3888	1/1	0.90	0.19	62,62,62,62	0
85	MG	1	3735	1/1	0.90	0.25	56,56,56,56	0
85	MG	4	216	1/1	0.90	0.17	57,57,57,57	0
86	OHX	5	4153	7/7	0.90	0.19	128,128,128,128	0
86	OHX	1	4139	7/7	0.90	0.15	136,136,136,136	0
85	MG	5	3717	1/1	0.90	0.22	51,51,51,51	0
86	OHX	1	4141	7/7	0.90	0.12	142,142,142,142	0
86	OHX	5	4159	7/7	0.90	0.13	146,146,146,146	0
85	MG	1	3819	1/1	0.90	0.18	43,43,43,43	0
85	MG	1	3422	1/1	0.90	0.30	36,36,36,36	0
85	MG	1	3746	1/1	0.90	0.20	51,51,51,51	0
86	OHX	1	4146	7/7	0.90	0.15	144,144,144,144	0
86	OHX	5	4166	7/7	0.90	0.15	149,149,149,149	0
85	MG	5	4257	1/1	0.90	0.48	30,30,30,30	0
85	MG	5	4258	1/1	0.90	0.34	41,41,41,41	0
86	OHX	5	4170	7/7	0.90	0.12	154,154,154,154	0
85	MG	5	3723	1/1	0.90	0.23	51,51,51,51	0
86	OHX	1	4152	7/7	0.90	0.17	144,144,144,144	0
86	OHX	5	4178	7/7	0.90	0.15	145,145,145,145	0
86	OHX	1	4157	7/7	0.90	0.15	138,138,138,138	0
85	MG	7	202	1/1	0.90	0.18	41,41,41,41	0
85	MG	5	3565	1/1	0.90	0.38	33,33,33,33	0
86	OHX	5	4184	7/7	0.90	0.13	154,154,154,154	0
86	OHX	1	4160	7/7	0.90	0.17	144,144,144,144	0
85	MG	1	3828	1/1	0.90	0.26	25,25,25,25	0
86	OHX	5	4187	7/7	0.90	0.16	130,130,130,130	0
86	OHX	1	4162	7/7	0.90	0.12	167,167,167,167	0
85	MG	5	3731	1/1	0.90	0.27	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3570	1/1	0.90	0.34	36,36,36,36	0
85	MG	1	3459	1/1	0.90	0.29	36,36,36,36	0
85	MG	5	3574	1/1	0.90	0.27	32,32,32,32	0
85	MG	8	204	1/1	0.90	0.33	54,54,54,54	0
85	MG	L8	301	1/1	0.90	0.23	50,50,50,50	0
85	MG	6	2009	1/1	0.90	0.23	63,63,63,63	0
85	MG	5	3748	1/1	0.90	0.24	48,48,48,48	0
86	OHX	1	4172	7/7	0.90	0.11	172,172,172,172	0
85	MG	5	3749	1/1	0.90	0.22	63,63,63,63	0
85	MG	6	2011	1/1	0.90	0.20	56,56,56,56	0
85	MG	1	3676	1/1	0.90	0.20	40,40,40,40	0
86	OHX	5	4212	7/7	0.90	0.15	154,154,154,154	0
85	MG	1	3834	1/1	0.90	0.32	39,39,39,39	0
85	MG	2	1970	1/1	0.90	0.29	73,73,73,73	0
85	MG	5	3445	1/1	0.90	0.27	45,45,45,45	0
85	MG	6	2019	1/1	0.90	0.16	52,52,52,52	0
85	MG	1	3426	1/1	0.90	0.20	63,63,63,63	0
86	OHX	1	4182	7/7	0.90	0.14	151,151,151,151	0
85	MG	6	2023	1/1	0.90	0.23	61,61,61,61	0
85	MG	2	2180	1/1	0.90	0.16	72,72,72,72	0
86	OHX	2	2091	7/7	0.90	0.16	154,154,154,154	0
85	MG	6	2027	1/1	0.90	0.13	95,95,95,95	0
85	MG	D3	201	1/1	0.90	0.15	61,61,61,61	0
86	OHX	2	2107	7/7	0.90	0.15	138,138,138,138	0
85	MG	5	3464	1/1	0.90	0.23	52,52,52,52	0
85	MG	5	3780	1/1	0.90	0.29	74,74,74,74	0
85	MG	1	3418	1/1	0.90	0.23	42,42,42,42	0
85	MG	1	3531	1/1	0.90	0.26	27,27,27,27	0
85	MG	2	1949	1/1	0.90	0.22	58,58,58,58	0
85	MG	1	3478	1/1	0.90	0.12	92,92,92,92	0
85	MG	5	3622	1/1	0.90	0.30	52,52,52,52	0
86	OHX	2	2135	7/7	0.90	0.15	137,137,137,137	0
85	MG	2	1920	1/1	0.90	0.21	57,57,57,57	0
85	MG	1	3774	1/1	0.90	0.21	70,70,70,70	0
86	OHX	2	2139	7/7	0.90	0.14	169,169,169,169	0
86	OHX	5	4241	7/7	0.90	0.12	148,148,148,148	0
85	MG	5	3627	1/1	0.90	0.30	32,32,32,32	0
86	OHX	2	2142	7/7	0.90	0.14	153,153,153,153	0
86	OHX	2	2143	7/7	0.90	0.18	137,137,137,137	0
86	OHX	1	4207	7/7	0.90	0.18	138,138,138,138	0
86	OHX	1	4209	7/7	0.90	0.13	163,163,163,163	0
85	MG	1	3502	1/1	0.90	0.30	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3632	1/1	0.90	0.09	45,45,45,45	0
85	MG	5	3634	1/1	0.90	0.13	43,43,43,43	0
86	OHX	3	224	7/7	0.90	0.18	141,141,141,141	0
85	MG	5	3802	1/1	0.90	0.22	49,49,49,49	0
86	OHX	2	2150	7/7	0.90	0.10	187,187,187,187	0
86	OHX	5	4253	7/7	0.90	0.14	152,152,152,152	0
85	MG	1	3779	1/1	0.90	0.28	66,66,66,66	0
86	OHX	2	2153	7/7	0.90	0.13	154,154,154,154	0
86	OHX	L3	406	7/7	0.90	0.12	163,163,163,163	0
85	MG	1	3644	1/1	0.90	0.23	68,68,68,68	0
85	MG	1	3782	1/1	0.90	0.19	56,56,56,56	0
85	MG	5	3644	1/1	0.90	0.33	64,64,64,64	0
85	MG	6	1908	1/1	0.90	0.26	49,49,49,49	0
85	MG	5	3812	1/1	0.90	0.11	43,43,43,43	0
85	MG	1	3543	1/1	0.90	0.34	38,38,38,38	0
85	MG	5	3814	1/1	0.90	0.16	43,43,43,43	0
85	MG	1	3544	1/1	0.90	0.20	38,38,38,38	0
85	MG	1	3457	1/1	0.90	0.25	44,44,44,44	0
86	OHX	6	2121	7/7	0.90	0.17	124,124,124,124	0
86	OHX	6	2134	7/7	0.90	0.14	163,163,163,163	0
86	OHX	m8	201	7/7	0.90	0.17	143,143,143,143	0
85	MG	1	3600	1/1	0.90	0.24	28,28,28,28	0
85	MG	1	3548	1/1	0.90	0.23	48,48,48,48	0
86	OHX	6	2139	7/7	0.90	0.14	130,130,130,130	0
86	OHX	2	2170	7/7	0.90	0.15	150,150,150,150	0
86	OHX	6	2150	7/7	0.90	0.13	153,153,153,153	0
86	OHX	1	4096	7/7	0.91	0.12	153,153,153,153	0
85	MG	1	3630	1/1	0.91	0.12	36,36,36,36	0
86	OHX	6	2182	7/7	0.91	0.15	142,142,142,142	0
85	MG	1	3805	1/1	0.91	0.19	44,44,44,44	0
86	OHX	1	4103	7/7	0.91	0.16	131,131,131,131	0
85	MG	5	3539	1/1	0.91	0.35	39,39,39,39	0
85	MG	1	3678	1/1	0.91	0.14	65,65,65,65	0
85	MG	1	3680	1/1	0.91	0.22	43,43,43,43	0
85	MG	2	2015	1/1	0.91	0.49	63,63,63,63	0
85	MG	5	3893	1/1	0.91	0.18	29,29,29,29	0
85	MG	1	3688	1/1	0.91	0.15	41,41,41,41	0
85	MG	1	3752	1/1	0.91	0.09	50,50,50,50	0
85	MG	5	3417	1/1	0.91	0.23	30,30,30,30	0
86	OHX	1	4118	7/7	0.91	0.17	126,126,126,126	0
85	MG	4	203	1/1	0.91	0.30	53,53,53,53	0
85	MG	5	3553	1/1	0.91	0.19	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	6	2197	7/7	0.91	0.15	146,146,146,146	0
86	OHX	1	4125	7/7	0.91	0.13	150,150,150,150	0
85	MG	5	3726	1/1	0.91	0.12	50,50,50,50	0
86	OHX	1	4127	7/7	0.91	0.15	131,131,131,131	0
85	MG	6	1997	1/1	0.91	0.17	75,75,75,75	0
85	MG	6	1999	1/1	0.91	0.34	59,59,59,59	0
85	MG	7	210	1/1	0.91	0.25	47,47,47,47	0
85	MG	4	204	1/1	0.91	0.33	44,44,44,44	0
85	MG	1	3818	1/1	0.91	0.13	58,58,58,58	0
85	MG	7	214	1/1	0.91	0.13	52,52,52,52	0
85	MG	1	3485	1/1	0.91	0.25	44,44,44,44	0
85	MG	1	3590	1/1	0.91	0.25	34,34,34,34	0
85	MG	8	202	1/1	0.91	0.24	39,39,39,39	0
85	MG	5	3432	1/1	0.91	0.14	35,35,35,35	0
86	OHX	5	4103	7/7	0.91	0.15	133,133,133,133	0
85	MG	5	3573	1/1	0.91	0.30	42,42,42,42	0
86	OHX	5	4109	7/7	0.91	0.17	121,121,121,121	0
85	MG	1	3826	1/1	0.91	0.11	37,37,37,37	0
85	MG	8	211	1/1	0.91	0.22	51,51,51,51	0
85	MG	1	3500	1/1	0.91	0.34	23,23,23,23	0
86	OHX	5	4122	7/7	0.91	0.15	123,123,123,123	0
86	OHX	5	4123	7/7	0.91	0.15	131,131,131,131	0
86	OHX	5	4127	7/7	0.91	0.12	149,149,149,149	0
86	OHX	5	4132	7/7	0.91	0.11	159,159,159,159	0
86	OHX	5	4141	7/7	0.91	0.13	131,131,131,131	0
85	MG	5	3440	1/1	0.91	0.30	41,41,41,41	0
85	MG	1	3551	1/1	0.91	0.30	36,36,36,36	0
86	OHX	5	4144	7/7	0.91	0.16	135,135,135,135	0
85	MG	5	3588	1/1	0.91	0.22	28,28,28,28	0
85	MG	1	3527	1/1	0.91	0.38	35,35,35,35	0
86	OHX	5	4150	7/7	0.91	0.15	141,141,141,141	0
85	MG	1	3701	1/1	0.91	0.25	48,48,48,48	0
85	MG	m7	201	1/1	0.91	0.33	34,34,34,34	0
85	MG	m7	204	1/1	0.91	0.21	38,38,38,38	0
85	MG	1	3444	1/1	0.91	0.29	42,42,42,42	0
86	OHX	5	4158	7/7	0.91	0.14	136,136,136,136	0
85	MG	6	1938	1/1	0.91	0.19	48,48,48,48	0
86	OHX	5	4160	7/7	0.91	0.15	144,144,144,144	0
85	MG	n8	202	1/1	0.91	0.26	50,50,50,50	0
85	MG	5	3771	1/1	0.91	0.15	38,38,38,38	0
85	MG	2	1986	1/1	0.91	0.15	65,65,65,65	0
85	MG	2	1922	1/1	0.91	0.27	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	L7	301	1/1	0.91	0.13	36,36,36,36	0
85	MG	5	3455	1/1	0.91	0.18	45,45,45,45	0
85	MG	6	2021	1/1	0.91	0.14	96,96,96,96	0
86	OHX	2	2105	7/7	0.91	0.15	141,141,141,141	0
85	MG	L7	302	1/1	0.91	0.18	46,46,46,46	0
85	MG	1	3839	1/1	0.91	0.37	58,58,58,58	0
85	MG	5	3608	1/1	0.91	0.22	56,56,56,56	0
86	OHX	2	2117	7/7	0.91	0.12	160,160,160,160	0
85	MG	5	3609	1/1	0.91	0.27	33,33,33,33	0
86	OHX	2	2121	7/7	0.91	0.13	144,144,144,144	0
86	OHX	1	4177	7/7	0.91	0.07	253,253,253,253	0
86	OHX	2	2122	7/7	0.91	0.13	151,151,151,151	0
86	OHX	2	2123	7/7	0.91	0.14	151,151,151,151	0
86	OHX	2	2124	7/7	0.91	0.13	147,147,147,147	0
86	OHX	5	4188	7/7	0.91	0.17	136,136,136,136	0
86	OHX	2	2127	7/7	0.91	0.13	141,141,141,141	0
85	MG	5	3787	1/1	0.91	0.17	30,30,30,30	0
85	MG	5	3788	1/1	0.91	0.14	39,39,39,39	0
86	OHX	5	4193	7/7	0.91	0.15	130,130,130,130	0
86	OHX	2	2132	7/7	0.91	0.12	163,163,163,163	0
86	OHX	5	4195	7/7	0.91	0.16	125,125,125,125	0
85	MG	5	3462	1/1	0.91	0.24	47,47,47,47	0
85	MG	6	2026	1/1	0.91	0.19	90,90,90,90	0
85	MG	1	3841	1/1	0.91	0.45	63,63,63,63	0
85	MG	1	3842	1/1	0.91	0.39	51,51,51,51	0
85	MG	M3	201	1/1	0.91	0.12	43,43,43,43	0
86	OHX	2	2138	7/7	0.91	0.12	145,145,145,145	0
85	MG	1	3534	1/1	0.91	0.34	31,31,31,31	0
85	MG	1	3773	1/1	0.91	0.23	31,31,31,31	0
85	MG	6	2032	1/1	0.91	0.23	55,55,55,55	0
86	OHX	5	4210	7/7	0.91	0.12	161,161,161,161	0
86	OHX	5	4211	7/7	0.91	0.20	134,134,134,134	0
85	MG	M7	204	1/1	0.91	0.12	41,41,41,41	0
85	MG	5	3629	1/1	0.91	0.18	51,51,51,51	0
86	OHX	5	4214	7/7	0.91	0.13	142,142,142,142	0
85	MG	1	3508	1/1	0.91	0.24	45,45,45,45	0
86	OHX	5	4216	7/7	0.91	0.18	127,127,127,127	0
85	MG	5	3478	1/1	0.91	0.22	38,38,38,38	0
85	MG	1	3714	1/1	0.91	0.17	79,79,79,79	0
86	OHX	2	2149	7/7	0.91	0.13	166,166,166,166	0
85	MG	1	3469	1/1	0.91	0.17	46,46,46,46	0
85	MG	1	3513	1/1	0.91	0.28	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3642	1/1	0.91	0.20	38,38,38,38	0
85	MG	5	3484	1/1	0.91	0.21	54,54,54,54	0
85	MG	N8	201	1/1	0.91	0.07	33,33,33,33	0
85	MG	1	3856	1/1	0.91	0.12	68,68,68,68	0
85	MG	5	3488	1/1	0.91	0.33	58,58,58,58	0
85	MG	1	3617	1/1	0.91	0.18	52,52,52,52	0
85	MG	1	3858	1/1	0.91	0.32	47,47,47,47	0
85	MG	1	3563	1/1	0.91	0.24	41,41,41,41	0
85	MG	5	3832	1/1	0.91	0.22	28,28,28,28	0
85	MG	1	3658	1/1	0.91	0.17	43,43,43,43	0
85	MG	5	3497	1/1	0.91	0.25	29,29,29,29	0
85	MG	6	1903	1/1	0.91	0.32	43,43,43,43	0
86	OHX	2	2169	7/7	0.91	0.14	152,152,152,152	0
85	MG	5	3850	1/1	0.91	0.11	36,36,36,36	0
86	OHX	2	2171	7/7	0.91	0.14	153,153,153,153	0
85	MG	1	3417	1/1	0.91	0.18	41,41,41,41	0
85	MG	5	3668	1/1	0.91	0.24	46,46,46,46	0
85	MG	5	3858	1/1	0.91	0.10	76,76,76,76	0
85	MG	5	3860	1/1	0.91	0.13	45,45,45,45	0
85	MG	1	3495	1/1	0.91	0.24	40,40,40,40	0
85	MG	s1	301	1/1	0.91	0.18	80,80,80,80	0
85	MG	6	1975	1/1	0.91	0.19	67,67,67,67	0
86	OHX	S8	302	7/7	0.91	0.12	165,165,165,165	0
85	MG	5	3866	1/1	0.91	0.09	52,52,52,52	0
85	MG	5	3507	1/1	0.91	0.25	33,33,33,33	0
85	MG	1	3667	1/1	0.91	0.14	78,78,78,78	0
86	OHX	1	4033	7/7	0.91	0.15	132,132,132,132	0
86	OHX	1	4056	7/7	0.91	0.17	129,129,129,129	0
86	OHX	1	4060	7/7	0.91	0.12	148,148,148,148	0
86	OHX	1	4061	7/7	0.91	0.16	128,128,128,128	0
85	MG	5	3515	1/1	0.91	0.35	28,28,28,28	0
86	OHX	6	2154	7/7	0.91	0.12	143,143,143,143	0
85	MG	5	3872	1/1	0.91	0.35	49,49,49,49	0
86	OHX	1	4066	7/7	0.91	0.15	135,135,135,135	0
85	MG	c1	201	1/1	0.91	0.23	46,46,46,46	0
86	OHX	1	4069	7/7	0.91	0.12	148,148,148,148	0
86	OHX	8	231	7/7	0.91	0.16	140,140,140,140	0
86	OHX	l3	404	7/7	0.91	0.14	142,142,142,142	0
85	MG	1	3577	1/1	0.91	0.27	27,27,27,27	0
85	MG	1	3483	1/1	0.91	0.15	52,52,52,52	0
86	OHX	l5	304	7/7	0.91	0.13	149,149,149,149	0
86	OHX	6	2165	7/7	0.91	0.13	151,151,151,151	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	l9	202	7/7	0.91	0.16	130,130,130,130	0
85	MG	5	3521	1/1	0.91	0.33	35,35,35,35	0
85	MG	5	3878	1/1	0.91	0.32	42,42,42,42	0
85	MG	5	3695	1/1	0.91	0.12	46,46,46,46	0
86	OHX	1	4080	7/7	0.91	0.12	146,146,146,146	0
85	MG	3	208	1/1	0.91	0.16	49,49,49,49	0
85	MG	5	3703	1/1	0.91	0.13	63,63,63,63	0
86	OHX	6	2175	7/7	0.91	0.12	168,168,168,168	0
86	OHX	1	4091	7/7	0.91	0.11	156,156,156,156	0
85	MG	1	3545	1/1	0.91	0.24	55,55,55,55	0
85	MG	5	3707	1/1	0.91	0.06	47,47,47,47	0
85	MG	n3	201	1/1	0.92	0.25	26,26,26,26	0
86	OHX	5	4119	7/7	0.92	0.11	147,147,147,147	0
86	OHX	5	4121	7/7	0.92	0.15	135,135,135,135	0
85	MG	1	3632	1/1	0.92	0.22	52,52,52,52	0
85	MG	1	3558	1/1	0.92	0.29	27,27,27,27	0
86	OHX	5	4125	7/7	0.92	0.13	145,145,145,145	0
85	MG	2	1997	1/1	0.92	0.09	78,78,78,78	0
86	OHX	5	4131	7/7	0.92	0.14	135,135,135,135	0
85	MG	1	3463	1/1	0.92	0.17	44,44,44,44	0
86	OHX	5	4136	7/7	0.92	0.15	128,128,128,128	0
85	MG	2	1973	1/1	0.92	0.37	74,74,74,74	0
85	MG	6	2008	1/1	0.92	0.05	61,61,61,61	0
86	OHX	1	4077	7/7	0.92	0.15	126,126,126,126	0
85	MG	q3	502	1/1	0.92	0.27	73,73,73,73	0
86	OHX	2	2068	7/7	0.92	0.10	163,163,163,163	0
86	OHX	5	4147	7/7	0.92	0.15	123,123,123,123	0
86	OHX	2	2075	7/7	0.92	0.13	150,150,150,150	0
85	MG	2	1925	1/1	0.92	0.42	64,64,64,64	0
86	OHX	5	4151	7/7	0.92	0.14	136,136,136,136	0
86	OHX	5	4152	7/7	0.92	0.12	151,151,151,151	0
86	OHX	1	4205	7/7	0.92	0.15	131,131,131,131	0
85	MG	1	3639	1/1	0.92	0.12	69,69,69,69	0
86	OHX	1	4208	7/7	0.92	0.18	133,133,133,133	0
86	OHX	1	4085	7/7	0.92	0.14	136,136,136,136	0
86	OHX	1	4086	7/7	0.92	0.16	135,135,135,135	0
85	MG	6	1957	1/1	0.92	0.30	61,61,61,61	0
86	OHX	2	2102	7/7	0.92	0.12	154,154,154,154	0
85	MG	5	3490	1/1	0.92	0.38	32,32,32,32	0
86	OHX	3	225	7/7	0.92	0.13	147,147,147,147	0
86	OHX	1	4095	7/7	0.92	0.10	152,152,152,152	0
85	MG	4	212	1/1	0.92	0.20	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3493	1/1	0.92	0.10	55,55,55,55	0
86	OHX	4	234	7/7	0.92	0.14	135,135,135,135	0
85	MG	4	213	1/1	0.92	0.25	61,61,61,61	0
86	OHX	1	4100	7/7	0.92	0.13	145,145,145,145	0
86	OHX	1	4101	7/7	0.92	0.13	144,144,144,144	0
85	MG	5	3603	1/1	0.92	0.09	65,65,65,65	0
85	MG	6	2018	1/1	0.92	0.32	54,54,54,54	0
85	MG	1	3641	1/1	0.92	0.27	44,44,44,44	0
85	MG	1	3566	1/1	0.92	0.29	33,33,33,33	0
85	MG	1	3740	1/1	0.92	0.22	53,53,53,53	0
86	OHX	O3	201	7/7	0.92	0.17	120,120,120,120	0
85	MG	1	3614	1/1	0.92	0.29	44,44,44,44	0
86	OHX	2	2125	7/7	0.92	0.14	136,136,136,136	0
85	MG	5	3503	1/1	0.92	0.12	44,44,44,44	0
85	MG	4	221	1/1	0.92	0.28	54,54,54,54	0
86	OHX	6	2126	7/7	0.92	0.14	149,149,149,149	0
86	OHX	6	2132	7/7	0.92	0.11	149,149,149,149	0
85	MG	5	3427	1/1	0.92	0.21	39,39,39,39	0
86	OHX	5	4192	7/7	0.92	0.12	141,141,141,141	0
85	MG	2	2012	1/1	0.92	0.36	68,68,68,68	0
86	OHX	6	2136	7/7	0.92	0.11	148,148,148,148	0
86	OHX	1	4120	7/7	0.92	0.13	152,152,152,152	0
86	OHX	5	4196	7/7	0.92	0.10	182,182,182,182	0
85	MG	5	3747	1/1	0.92	0.07	34,34,34,34	0
86	OHX	6	2142	7/7	0.92	0.09	181,181,181,181	0
85	MG	5	3624	1/1	0.92	0.28	74,74,74,74	0
85	MG	6	1921	1/1	0.92	0.29	50,50,50,50	0
85	MG	5	3511	1/1	0.92	0.34	33,33,33,33	0
85	MG	2	1981	1/1	0.92	0.40	58,58,58,58	0
85	MG	1	3423	1/1	0.92	0.37	47,47,47,47	0
85	MG	5	3438	1/1	0.92	0.40	55,55,55,55	0
86	OHX	1	4131	7/7	0.92	0.14	132,132,132,132	0
86	OHX	1	4132	7/7	0.92	0.14	144,144,144,144	0
85	MG	6	1971	1/1	0.92	0.17	77,77,77,77	0
86	OHX	1	4134	7/7	0.92	0.17	122,122,122,122	0
85	MG	1	3471	1/1	0.92	0.19	43,43,43,43	0
85	MG	5	3638	1/1	0.92	0.32	53,53,53,53	0
85	MG	1	3704	1/1	0.92	0.11	43,43,43,43	0
86	OHX	6	2166	7/7	0.92	0.11	154,154,154,154	0
85	MG	1	3706	1/1	0.92	0.08	55,55,55,55	0
86	OHX	6	2168	7/7	0.92	0.18	129,129,129,129	0
85	MG	6	1927	1/1	0.92	0.30	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3532	1/1	0.92	0.28	45,45,45,45	0
85	MG	5	3652	1/1	0.92	0.14	39,39,39,39	0
85	MG	5	3533	1/1	0.92	0.23	35,35,35,35	0
86	OHX	2	2151	7/7	0.92	0.13	154,154,154,154	0
85	MG	1	3415	1/1	0.92	0.12	49,49,49,49	0
85	MG	5	3896	1/1	0.92	0.12	118,118,118,118	0
85	MG	5	3655	1/1	0.92	0.19	34,34,34,34	0
85	MG	5	3782	1/1	0.92	0.11	55,55,55,55	0
85	MG	1	3553	1/1	0.92	0.22	36,36,36,36	0
86	OHX	1	4156	7/7	0.92	0.12	153,153,153,153	0
85	MG	3	204	1/1	0.92	0.38	63,63,63,63	0
85	MG	7	201	1/1	0.92	0.32	40,40,40,40	0
85	MG	1	3623	1/1	0.92	0.24	54,54,54,54	0
85	MG	M5	301	1/1	0.92	0.25	51,51,51,51	0
86	OHX	2	2161	7/7	0.92	0.12	164,164,164,164	0
85	MG	1	3510	1/1	0.92	0.33	48,48,48,48	0
85	MG	1	3473	1/1	0.92	0.26	24,24,24,24	0
85	MG	5	3792	1/1	0.92	0.16	38,38,38,38	0
86	OHX	2	2166	7/7	0.92	0.11	170,170,170,170	0
86	OHX	2	2167	7/7	0.92	0.16	132,132,132,132	0
86	OHX	6	2192	7/7	0.92	0.13	162,162,162,162	0
85	MG	6	1990	1/1	0.92	0.09	95,95,95,95	0
85	MG	1	3591	1/1	0.92	0.32	48,48,48,48	0
85	MG	1	3666	1/1	0.92	0.17	44,44,44,44	0
85	MG	5	3670	1/1	0.92	0.20	35,35,35,35	0
85	MG	2	1935	1/1	0.92	0.36	52,52,52,52	0
86	OHX	6	2198	7/7	0.92	0.15	143,143,143,143	0
85	MG	5	3675	1/1	0.92	0.32	34,34,34,34	0
85	MG	8	206	1/1	0.92	0.22	46,46,46,46	0
86	OHX	6	2201	7/7	0.92	0.15	151,151,151,151	0
85	MG	1	3830	1/1	0.92	0.21	29,29,29,29	0
85	MG	1	3831	1/1	0.92	0.25	41,41,41,41	0
85	MG	6	1998	1/1	0.92	0.13	55,55,55,55	0
85	MG	5	3568	1/1	0.92	0.30	27,27,27,27	0
85	MG	8	213	1/1	0.92	0.25	47,47,47,47	0
86	OHX	C3	201	7/7	0.92	0.11	162,162,162,162	0
85	MG	O4	201	1/1	0.92	0.12	61,61,61,61	0
86	OHX	1	3949	7/7	0.92	0.20	107,107,107,107	0
85	MG	1	3477	1/1	0.92	0.24	42,42,42,42	0
86	OHX	5	4025	7/7	0.92	0.13	115,115,115,115	0
86	OHX	5	4029	7/7	0.92	0.22	107,107,107,107	0
86	OHX	5	4053	7/7	0.92	0.15	116,116,116,116	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	4064	7/7	0.92	0.14	133,133,133,133	0
86	OHX	5	4073	7/7	0.92	0.16	134,134,134,134	0
86	OHX	5	4090	7/7	0.92	0.15	120,120,120,120	0
86	OHX	5	4091	7/7	0.92	0.20	118,118,118,118	0
85	MG	5	3686	1/1	0.92	0.14	35,35,35,35	0
86	OHX	5	4100	7/7	0.92	0.15	125,125,125,125	0
85	MG	1	3723	1/1	0.92	0.16	64,64,64,64	0
86	OHX	1	4055	7/7	0.92	0.17	121,121,121,121	0
86	OHX	m9	201	7/7	0.92	0.16	142,142,142,142	0
86	OHX	5	4104	7/7	0.92	0.12	150,150,150,150	0
85	MG	5	3475	1/1	0.92	0.30	61,61,61,61	0
85	MG	5	3476	1/1	0.92	0.35	52,52,52,52	0
85	MG	c8	201	1/1	0.92	0.32	80,80,80,80	0
85	MG	m7	205	1/1	0.92	0.12	45,45,45,45	0
85	MG	1	3509	1/1	0.93	0.28	28,28,28,28	0
86	OHX	5	4028	7/7	0.93	0.18	115,115,115,115	0
85	MG	1	3635	1/1	0.93	0.11	64,64,64,64	0
86	OHX	5	4034	7/7	0.93	0.15	117,117,117,117	0
85	MG	1	3584	1/1	0.93	0.30	54,54,54,54	0
85	MG	6	1983	1/1	0.93	0.24	55,55,55,55	0
86	OHX	5	4070	7/7	0.93	0.14	122,122,122,122	0
86	OHX	5	4072	7/7	0.93	0.14	137,137,137,137	0
85	MG	5	3406	1/1	0.93	0.13	44,44,44,44	0
86	OHX	5	4081	7/7	0.93	0.15	138,138,138,138	0
85	MG	1	3784	1/1	0.93	0.14	38,38,38,38	0
85	MG	3	205	1/1	0.93	0.31	42,42,42,42	0
85	MG	1	3787	1/1	0.93	0.12	88,88,88,88	0
85	MG	5	3415	1/1	0.93	0.14	53,53,53,53	0
86	OHX	5	4101	7/7	0.93	0.13	144,144,144,144	0
85	MG	5	3416	1/1	0.93	0.14	36,36,36,36	0
85	MG	5	3534	1/1	0.93	0.21	55,55,55,55	0
85	MG	5	3535	1/1	0.93	0.28	36,36,36,36	0
85	MG	1	3431	1/1	0.93	0.24	46,46,46,46	0
86	OHX	5	4108	7/7	0.93	0.17	115,115,115,115	0
85	MG	5	3692	1/1	0.93	0.17	61,61,61,61	0
85	MG	1	3546	1/1	0.93	0.32	67,67,67,67	0
85	MG	5	3419	1/1	0.93	0.26	34,34,34,34	0
85	MG	5	3701	1/1	0.93	0.20	41,41,41,41	0
86	OHX	5	4116	7/7	0.93	0.20	120,120,120,120	0
85	MG	6	1914	1/1	0.93	0.17	78,78,78,78	0
85	MG	5	3544	1/1	0.93	0.28	71,71,71,71	0
85	MG	5	3545	1/1	0.93	0.22	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3882	1/1	0.93	0.21	33,33,33,33	0
85	MG	6	1916	1/1	0.93	0.33	60,60,60,60	0
85	MG	5	3547	1/1	0.93	0.39	48,48,48,48	0
86	OHX	5	4130	7/7	0.93	0.13	130,130,130,130	0
86	OHX	2	2165	7/7	0.93	0.11	170,170,170,170	0
85	MG	1	3794	1/1	0.93	0.12	49,49,49,49	0
86	OHX	5	4135	7/7	0.93	0.09	184,184,184,184	0
85	MG	6	1996	1/1	0.93	0.08	47,47,47,47	0
86	OHX	5	4140	7/7	0.93	0.16	138,138,138,138	0
85	MG	1	3465	1/1	0.93	0.19	51,51,51,51	0
85	MG	1	3466	1/1	0.93	0.21	55,55,55,55	0
85	MG	2	1998	1/1	0.93	0.12	107,107,107,107	0
85	MG	1	3515	1/1	0.93	0.35	41,41,41,41	0
85	MG	5	3556	1/1	0.93	0.34	39,39,39,39	0
85	MG	1	3451	1/1	0.93	0.18	38,38,38,38	0
86	OHX	1	4196	7/7	0.93	0.13	138,138,138,138	0
85	MG	5	3435	1/1	0.93	0.23	31,31,31,31	0
85	MG	6	2002	1/1	0.93	0.10	98,98,98,98	0
85	MG	1	3452	1/1	0.93	0.31	52,52,52,52	0
85	MG	1	3453	1/1	0.93	0.21	38,38,38,38	0
85	MG	1	3601	1/1	0.93	0.23	34,34,34,34	0
85	MG	1	3603	1/1	0.93	0.18	40,40,40,40	0
85	MG	2	2011	1/1	0.93	0.40	63,63,63,63	0
86	OHX	C5	201	7/7	0.93	0.10	168,168,168,168	0
85	MG	1	3653	1/1	0.93	0.28	45,45,45,45	0
86	OHX	1	4206	7/7	0.93	0.17	133,133,133,133	0
85	MG	7	203	1/1	0.93	0.21	27,27,27,27	0
86	OHX	1	3962	7/7	0.93	0.12	125,125,125,125	0
86	OHX	1	3988	7/7	0.93	0.14	112,112,112,112	0
85	MG	1	3438	1/1	0.93	0.24	48,48,48,48	0
85	MG	7	206	1/1	0.93	0.33	25,25,25,25	0
86	OHX	3	222	7/7	0.93	0.11	146,146,146,146	0
86	OHX	5	4168	7/7	0.93	0.14	139,139,139,139	0
85	MG	5	3578	1/1	0.93	0.25	38,38,38,38	0
86	OHX	1	4039	7/7	0.93	0.13	128,128,128,128	0
86	OHX	1	4047	7/7	0.93	0.14	123,123,123,123	0
86	OHX	5	4172	7/7	0.93	0.08	191,191,191,191	0
86	OHX	1	4052	7/7	0.93	0.19	118,118,118,118	0
86	OHX	5	4174	7/7	0.93	0.29	109,109,109,109	0
86	OHX	5	4177	7/7	0.93	0.14	150,150,150,150	0
86	OHX	1	4054	7/7	0.93	0.29	104,104,104,104	0
85	MG	7	209	1/1	0.93	0.24	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	4180	7/7	0.93	0.17	122,122,122,122	0
85	MG	5	3447	1/1	0.93	0.19	46,46,46,46	0
85	MG	1	3657	1/1	0.93	0.28	54,54,54,54	0
85	MG	5	3751	1/1	0.93	0.08	64,64,64,64	0
85	MG	1	3611	1/1	0.93	0.14	45,45,45,45	0
86	OHX	M0	304	7/7	0.93	0.13	121,121,121,121	0
85	MG	5	3754	1/1	0.93	0.09	51,51,51,51	0
85	MG	2	1927	1/1	0.93	0.35	51,51,51,51	0
85	MG	8	201	1/1	0.93	0.13	45,45,45,45	0
85	MG	2	1967	1/1	0.93	0.25	62,62,62,62	0
85	MG	6	2016	1/1	0.93	0.15	74,74,74,74	0
85	MG	1	3665	1/1	0.93	0.20	53,53,53,53	0
85	MG	5	3459	1/1	0.93	0.17	64,64,64,64	0
86	OHX	6	2105	7/7	0.93	0.14	126,126,126,126	0
85	MG	1	3421	1/1	0.93	0.29	36,36,36,36	0
85	MG	1	3446	1/1	0.93	0.19	39,39,39,39	0
85	MG	1	3747	1/1	0.93	0.20	51,51,51,51	0
86	OHX	6	2125	7/7	0.93	0.13	141,141,141,141	0
85	MG	L3	402	1/1	0.93	0.10	66,66,66,66	0
86	OHX	5	4203	7/7	0.93	0.16	123,123,123,123	0
86	OHX	6	2128	7/7	0.93	0.13	129,129,129,129	0
85	MG	l2	301	1/1	0.93	0.21	42,42,42,42	0
86	OHX	6	2133	7/7	0.93	0.16	135,135,135,135	0
85	MG	1	3460	1/1	0.93	0.28	25,25,25,25	0
86	OHX	1	4083	7/7	0.93	0.13	133,133,133,133	0
85	MG	L4	401	1/1	0.93	0.11	34,34,34,34	0
85	MG	5	3604	1/1	0.93	0.26	43,43,43,43	0
86	OHX	1	4088	7/7	0.93	0.12	141,141,141,141	0
85	MG	5	3468	1/1	0.93	0.14	41,41,41,41	0
86	OHX	6	2144	7/7	0.93	0.11	157,157,157,157	0
86	OHX	6	2146	7/7	0.93	0.12	139,139,139,139	0
86	OHX	6	2147	7/7	0.93	0.16	119,119,119,119	0
86	OHX	1	4092	7/7	0.93	0.10	148,148,148,148	0
85	MG	1	3480	1/1	0.93	0.30	44,44,44,44	0
86	OHX	5	4218	7/7	0.93	0.14	156,156,156,156	0
85	MG	m5	302	1/1	0.93	0.10	55,55,55,55	0
85	MG	1	3754	1/1	0.93	0.06	50,50,50,50	0
85	MG	1	3504	1/1	0.93	0.20	39,39,39,39	0
85	MG	6	1949	1/1	0.93	0.30	52,52,52,52	0
85	MG	n0	201	1/1	0.93	0.15	45,45,45,45	0
85	MG	1	3620	1/1	0.93	0.32	49,49,49,49	0
85	MG	1	3569	1/1	0.93	0.20	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	n6	201	1/1	0.93	0.23	55,55,55,55	0
85	MG	1	3758	1/1	0.93	0.12	46,46,46,46	0
85	MG	1	3505	1/1	0.93	0.36	34,34,34,34	0
85	MG	n8	203	1/1	0.93	0.10	44,44,44,44	0
86	OHX	1	4109	7/7	0.93	0.17	118,118,118,118	0
85	MG	5	3479	1/1	0.93	0.19	31,31,31,31	0
85	MG	1	3571	1/1	0.93	0.27	36,36,36,36	0
85	MG	1	3687	1/1	0.93	0.38	54,54,54,54	0
86	OHX	1	4113	7/7	0.93	0.15	129,129,129,129	0
85	MG	q1	101	1/1	0.93	0.22	50,50,50,50	0
85	MG	6	1956	1/1	0.93	0.35	48,48,48,48	0
85	MG	1	3846	1/1	0.93	0.36	58,58,58,58	0
85	MG	1	3767	1/1	0.93	0.10	44,44,44,44	0
86	OHX	2	2076	7/7	0.93	0.14	135,135,135,135	0
86	OHX	6	2177	7/7	0.93	0.17	130,130,130,130	0
86	OHX	1	4122	7/7	0.93	0.13	143,143,143,143	0
86	OHX	1	4123	7/7	0.93	0.12	151,151,151,151	0
86	OHX	2	2080	7/7	0.93	0.09	172,172,172,172	0
86	OHX	2	2081	7/7	0.93	0.12	143,143,143,143	0
85	MG	5	3633	1/1	0.93	0.35	79,79,79,79	0
85	MG	M7	202	1/1	0.93	0.23	33,33,33,33	0
85	MG	6	2041	1/1	0.93	0.26	68,68,68,68	0
85	MG	1	3462	1/1	0.93	0.28	28,28,28,28	0
86	OHX	2	2103	7/7	0.93	0.08	204,204,204,204	0
86	OHX	2	2104	7/7	0.93	0.12	127,127,127,127	0
85	MG	1	3626	1/1	0.93	0.25	37,37,37,37	0
85	MG	1	3575	1/1	0.93	0.26	32,32,32,32	0
85	MG	N3	201	1/1	0.93	0.23	35,35,35,35	0
85	MG	1	3629	1/1	0.93	0.10	35,35,35,35	0
86	OHX	8	223	7/7	0.93	0.16	119,119,119,119	0
85	MG	1	3576	1/1	0.93	0.25	31,31,31,31	0
85	MG	1	3541	1/1	0.93	0.20	29,29,29,29	0
85	MG	N8	204	1/1	0.93	0.13	47,47,47,47	0
85	MG	5	3499	1/1	0.93	0.32	39,39,39,39	0
85	MG	1	3859	1/1	0.93	0.34	63,63,63,63	0
85	MG	O5	201	1/1	0.93	0.13	56,56,56,56	0
85	MG	1	3860	1/1	0.93	0.28	64,64,64,64	0
86	OHX	2	2126	7/7	0.93	0.12	144,144,144,144	0
85	MG	1	3578	1/1	0.93	0.33	36,36,36,36	0
85	MG	5	3827	1/1	0.93	0.20	65,65,65,65	0
85	MG	1	4217	1/1	0.93	0.22	48,48,48,48	0
85	MG	1	4218	1/1	0.93	0.34	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3509	1/1	0.93	0.39	29,29,29,29	0
86	OHX	s4	301	7/7	0.93	0.12	154,154,154,154	0
85	MG	5	3837	1/1	0.93	0.17	38,38,38,38	0
85	MG	5	3838	1/1	0.93	0.11	38,38,38,38	0
85	MG	5	3842	1/1	0.93	0.22	45,45,45,45	0
85	MG	5	3847	1/1	0.93	0.23	46,46,46,46	0
87	3K8	6	2205	28/28	0.93	0.11	67,67,67,67	0
85	MG	2	1911	1/1	0.93	0.35	55,55,55,55	0
85	MG	d6	102	1/1	0.93	0.17	65,65,65,65	0
86	OHX	5	4001	7/7	0.93	0.12	120,120,120,120	0
86	OHX	5	4019	7/7	0.93	0.13	149,149,149,149	0
85	MG	1	3700	1/1	0.94	0.28	48,48,48,48	0
85	MG	1	3526	1/1	0.94	0.25	26,26,26,26	0
86	OHX	sR	401	7/7	0.94	0.10	169,169,169,169	0
86	OHX	5	3996	7/7	0.94	0.11	136,136,136,136	0
86	OHX	5	3997	7/7	0.94	0.11	118,118,118,118	0
85	MG	5	3672	1/1	0.94	0.13	41,41,41,41	0
86	OHX	5	4008	7/7	0.94	0.12	123,123,123,123	0
85	MG	5	3833	1/1	0.94	0.18	52,52,52,52	0
85	MG	5	3673	1/1	0.94	0.10	36,36,36,36	0
86	OHX	1	4149	7/7	0.94	0.14	118,118,118,118	0
85	MG	5	3543	1/1	0.94	0.29	30,30,30,30	0
86	OHX	5	4032	7/7	0.94	0.13	128,128,128,128	0
85	MG	1	4219	1/1	0.94	0.40	31,31,31,31	0
86	OHX	5	4039	7/7	0.94	0.11	130,130,130,130	0
86	OHX	5	4043	7/7	0.94	0.11	163,163,163,163	0
86	OHX	5	4044	7/7	0.94	0.11	134,134,134,134	0
86	OHX	5	4045	7/7	0.94	0.14	122,122,122,122	0
86	OHX	1	4153	7/7	0.94	0.15	135,135,135,135	0
86	OHX	5	4063	7/7	0.94	0.14	114,114,114,114	0
85	MG	5	3839	1/1	0.94	0.19	43,43,43,43	0
86	OHX	5	4065	7/7	0.94	0.12	132,132,132,132	0
85	MG	5	3841	1/1	0.94	0.15	36,36,36,36	0
85	MG	1	3435	1/1	0.94	0.16	44,44,44,44	0
85	MG	5	3679	1/1	0.94	0.09	41,41,41,41	0
86	OHX	5	4077	7/7	0.94	0.15	130,130,130,130	0
86	OHX	5	4078	7/7	0.94	0.13	134,134,134,134	0
85	MG	6	2022	1/1	0.94	0.28	70,70,70,70	0
86	OHX	5	4088	7/7	0.94	0.14	132,132,132,132	0
86	OHX	5	4089	7/7	0.94	0.12	130,130,130,130	0
85	MG	5	3682	1/1	0.94	0.16	50,50,50,50	0
85	MG	N3	202	1/1	0.94	0.26	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	4095	7/7	0.94	0.15	125,125,125,125	0
86	OHX	5	4098	7/7	0.94	0.11	131,131,131,131	0
85	MG	1	3808	1/1	0.94	0.21	45,45,45,45	0
85	MG	5	3852	1/1	0.94	0.28	47,47,47,47	0
85	MG	1	3549	1/1	0.94	0.20	38,38,38,38	0
86	OHX	2	2141	7/7	0.94	0.10	174,174,174,174	0
85	MG	1	3436	1/1	0.94	0.17	47,47,47,47	0
85	MG	5	3859	1/1	0.94	0.17	64,64,64,64	0
85	MG	5	3450	1/1	0.94	0.21	32,32,32,32	0
85	MG	1	3487	1/1	0.94	0.17	38,38,38,38	0
85	MG	5	3690	1/1	0.94	0.08	42,42,42,42	0
85	MG	5	3863	1/1	0.94	0.17	64,64,64,64	0
85	MG	1	3709	1/1	0.94	0.24	55,55,55,55	0
85	MG	1	3816	1/1	0.94	0.09	59,59,59,59	0
86	OHX	5	4115	7/7	0.94	0.14	127,127,127,127	0
85	MG	5	3693	1/1	0.94	0.28	49,49,49,49	0
85	MG	1	3511	1/1	0.94	0.42	31,31,31,31	0
85	MG	1	3488	1/1	0.94	0.21	57,57,57,57	0
85	MG	5	3870	1/1	0.94	0.13	42,42,42,42	0
85	MG	5	3871	1/1	0.94	0.16	35,35,35,35	0
86	OHX	5	4124	7/7	0.94	0.11	148,148,148,148	0
85	MG	5	3698	1/1	0.94	0.24	72,72,72,72	0
85	MG	5	3700	1/1	0.94	0.12	54,54,54,54	0
86	OHX	5	4128	7/7	0.94	0.09	153,153,153,153	0
85	MG	5	3561	1/1	0.94	0.29	36,36,36,36	0
85	MG	6	1962	1/1	0.94	0.14	52,52,52,52	0
85	MG	5	3705	1/1	0.94	0.13	59,59,59,59	0
85	MG	1	3499	1/1	0.94	0.40	76,76,76,76	0
85	MG	5	3463	1/1	0.94	0.27	35,35,35,35	0
86	OHX	5	4137	7/7	0.94	0.13	145,145,145,145	0
86	OHX	5	4139	7/7	0.94	0.12	140,140,140,140	0
85	MG	1	3713	1/1	0.94	0.17	41,41,41,41	0
85	MG	1	3824	1/1	0.94	0.19	30,30,30,30	0
85	MG	1	3404	1/1	0.94	0.39	75,75,75,75	0
86	OHX	1	4191	7/7	0.94	0.10	174,174,174,174	0
85	MG	1	3716	1/1	0.94	0.34	55,55,55,55	0
85	MG	6	1905	1/1	0.94	0.22	59,59,59,59	0
85	MG	5	3576	1/1	0.94	0.24	27,27,27,27	0
86	OHX	5	4148	7/7	0.94	0.14	127,127,127,127	0
85	MG	5	3577	1/1	0.94	0.22	41,41,41,41	0
85	MG	1	3538	1/1	0.94	0.14	42,42,42,42	0
85	MG	5	3720	1/1	0.94	0.15	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3581	1/1	0.94	0.22	37,37,37,37	0
85	MG	1	3672	1/1	0.94	0.08	72,72,72,72	0
85	MG	5	3724	1/1	0.94	0.21	39,39,39,39	0
85	MG	5	3894	1/1	0.94	0.07	93,93,93,93	0
85	MG	1	3490	1/1	0.94	0.24	33,33,33,33	0
85	MG	6	1974	1/1	0.94	0.10	53,53,53,53	0
85	MG	5	3727	1/1	0.94	0.14	35,35,35,35	0
85	MG	5	3898	1/1	0.94	0.15	57,57,57,57	0
85	MG	5	4255	1/1	0.94	0.17	36,36,36,36	0
85	MG	1	3516	1/1	0.94	0.25	31,31,31,31	0
85	MG	1	3677	1/1	0.94	0.10	64,64,64,64	0
85	MG	5	3734	1/1	0.94	0.07	39,39,39,39	0
85	MG	1	3775	1/1	0.94	0.10	45,45,45,45	0
86	OHX	1	3982	7/7	0.94	0.15	111,111,111,111	0
85	MG	6	2206	1/1	0.94	0.20	60,60,60,60	0
86	OHX	1	3997	7/7	0.94	0.14	120,120,120,120	0
86	OHX	1	4000	7/7	0.94	0.13	111,111,111,111	0
86	OHX	1	4005	7/7	0.94	0.13	127,127,127,127	0
86	OHX	1	4013	7/7	0.94	0.09	165,165,165,165	0
86	OHX	1	4014	7/7	0.94	0.11	124,124,124,124	0
85	MG	5	3738	1/1	0.94	0.18	43,43,43,43	0
86	OHX	5	4176	7/7	0.94	0.15	126,126,126,126	0
86	OHX	1	4020	7/7	0.94	0.10	150,150,150,150	0
86	OHX	1	4022	7/7	0.94	0.12	132,132,132,132	0
86	OHX	L3	404	7/7	0.94	0.13	127,127,127,127	0
85	MG	5	3593	1/1	0.94	0.26	24,24,24,24	0
85	MG	6	1912	1/1	0.94	0.31	52,52,52,52	0
86	OHX	1	4034	7/7	0.94	0.10	143,143,143,143	0
85	MG	6	1913	1/1	0.94	0.32	39,39,39,39	0
86	OHX	1	4043	7/7	0.94	0.14	118,118,118,118	0
85	MG	1	3776	1/1	0.94	0.08	54,54,54,54	0
85	MG	4	208	1/1	0.94	0.31	47,47,47,47	0
85	MG	4	209	1/1	0.94	0.08	49,49,49,49	0
85	MG	7	212	1/1	0.94	0.18	68,68,68,68	0
85	MG	5	3750	1/1	0.94	0.26	30,30,30,30	0
86	OHX	6	2095	7/7	0.94	0.12	139,139,139,139	0
86	OHX	6	2097	7/7	0.94	0.10	164,164,164,164	0
86	OHX	6	2100	7/7	0.94	0.10	181,181,181,181	0
86	OHX	1	4057	7/7	0.94	0.09	187,187,187,187	0
86	OHX	1	4058	7/7	0.94	0.12	134,134,134,134	0
85	MG	1	3836	1/1	0.94	0.21	31,31,31,31	0
85	MG	1	3588	1/1	0.94	0.29	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	6	2124	7/7	0.94	0.14	116,116,116,116	0
85	MG	6	1987	1/1	0.94	0.13	51,51,51,51	0
86	OHX	5	4201	7/7	0.94	0.13	123,123,123,123	0
86	OHX	5	4202	7/7	0.94	0.11	131,131,131,131	0
85	MG	7	228	1/1	0.94	0.09	36,36,36,36	0
86	OHX	6	2127	7/7	0.94	0.30	110,110,110,110	0
85	MG	1	3838	1/1	0.94	0.21	48,48,48,48	0
85	MG	6	1989	1/1	0.94	0.11	52,52,52,52	0
85	MG	8	203	1/1	0.94	0.24	56,56,56,56	0
85	MG	SM	301	1/1	0.94	0.07	58,58,58,58	0
86	OHX	1	4073	7/7	0.94	0.13	130,130,130,130	0
86	OHX	1	4074	7/7	0.94	0.12	133,133,133,133	0
85	MG	5	3760	1/1	0.94	0.13	60,60,60,60	0
85	MG	8	207	1/1	0.94	0.14	64,64,64,64	0
86	OHX	6	2140	7/7	0.94	0.12	142,142,142,142	0
86	OHX	6	2141	7/7	0.94	0.13	140,140,140,140	0
85	MG	1	3503	1/1	0.94	0.32	45,45,45,45	0
85	MG	4	215	1/1	0.94	0.23	74,74,74,74	0
85	MG	5	3765	1/1	0.94	0.10	56,56,56,56	0
85	MG	1	3685	1/1	0.94	0.22	51,51,51,51	0
85	MG	5	3618	1/1	0.94	0.15	32,32,32,32	0
85	MG	8	214	1/1	0.94	0.22	34,34,34,34	0
85	MG	5	3768	1/1	0.94	0.08	44,44,44,44	0
85	MG	l3	401	1/1	0.94	0.33	29,29,29,29	0
85	MG	5	3404	1/1	0.94	0.09	53,53,53,53	0
85	MG	5	3620	1/1	0.94	0.22	44,44,44,44	0
85	MG	l7	301	1/1	0.94	0.13	39,39,39,39	0
86	OHX	6	2157	7/7	0.94	0.15	146,146,146,146	0
85	MG	2	1916	1/1	0.94	0.24	53,53,53,53	0
85	MG	4	219	1/1	0.94	0.26	49,49,49,49	0
85	MG	1	3731	1/1	0.94	0.13	29,29,29,29	0
85	MG	5	3778	1/1	0.94	0.07	36,36,36,36	0
86	OHX	6	2163	7/7	0.94	0.12	136,136,136,136	0
85	MG	1	3785	1/1	0.94	0.34	30,30,30,30	0
85	MG	1	3847	1/1	0.94	0.18	45,45,45,45	0
85	MG	1	3786	1/1	0.94	0.13	73,73,73,73	0
85	MG	1	3493	1/1	0.94	0.13	46,46,46,46	0
85	MG	5	3630	1/1	0.94	0.19	69,69,69,69	0
85	MG	2	1919	1/1	0.94	0.34	63,63,63,63	0
86	OHX	1	4105	7/7	0.94	0.13	124,124,124,124	0
86	OHX	6	2171	7/7	0.94	0.17	120,120,120,120	0
85	MG	1	3852	1/1	0.94	0.26	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3792	1/1	0.94	0.21	51,51,51,51	0
85	MG	1	3855	1/1	0.94	0.12	75,75,75,75	0
85	MG	5	3637	1/1	0.94	0.11	58,58,58,58	0
85	MG	5	3514	1/1	0.94	0.26	64,64,64,64	0
85	MG	1	3595	1/1	0.94	0.38	25,25,25,25	0
85	MG	6	1937	1/1	0.94	0.30	42,42,42,42	0
85	MG	o7	101	1/1	0.94	0.14	47,47,47,47	0
85	MG	5	3517	1/1	0.94	0.20	28,28,28,28	0
86	OHX	1	4115	7/7	0.94	0.12	134,134,134,134	0
86	OHX	1	4116	7/7	0.94	0.13	132,132,132,132	0
85	MG	5	3423	1/1	0.94	0.09	44,44,44,44	0
85	MG	5	3647	1/1	0.94	0.10	37,37,37,37	0
85	MG	1	3694	1/1	0.94	0.16	50,50,50,50	0
86	OHX	7	226	7/7	0.94	0.16	117,117,117,117	0
85	MG	1	3567	1/1	0.94	0.15	34,34,34,34	0
86	OHX	1	4121	7/7	0.94	0.17	112,112,112,112	0
85	MG	5	3522	1/1	0.94	0.28	36,36,36,36	0
85	MG	6	2010	1/1	0.94	0.19	52,52,52,52	0
86	OHX	8	228	7/7	0.94	0.11	143,143,143,143	0
86	OHX	2	2088	7/7	0.94	0.13	132,132,132,132	0
85	MG	1	3742	1/1	0.94	0.13	40,40,40,40	0
85	MG	5	3809	1/1	0.94	0.15	34,34,34,34	0
86	OHX	2	2097	7/7	0.94	0.10	155,155,155,155	0
85	MG	1	3597	1/1	0.94	0.41	43,43,43,43	0
86	OHX	2	2100	7/7	0.94	0.10	150,150,150,150	0
86	OHX	l5	303	7/7	0.94	0.10	146,146,146,146	0
85	MG	5	3433	1/1	0.94	0.24	50,50,50,50	0
85	MG	1	4212	1/1	0.94	0.16	29,29,29,29	0
85	MG	5	3660	1/1	0.94	0.18	55,55,55,55	0
85	MG	1	3654	1/1	0.94	0.18	34,34,34,34	0
85	MG	5	3436	1/1	0.94	0.13	35,35,35,35	0
86	OHX	1	4135	7/7	0.94	0.13	114,114,114,114	0
85	MG	5	3537	1/1	0.94	0.31	40,40,40,40	0
85	MG	1	4216	1/1	0.94	0.27	37,37,37,37	0
86	OHX	2	2116	7/7	0.94	0.11	148,148,148,148	0
85	MG	5	3822	1/1	0.94	0.08	68,68,68,68	0
86	OHX	2	2118	7/7	0.94	0.11	147,147,147,147	0
85	MG	5	3667	1/1	0.94	0.28	64,64,64,64	0
88	ZN	Q2	501	1/1	0.94	0.24	95,95,95,95	0
86	OHX	1	4142	7/7	0.94	0.14	119,119,119,119	0
85	MG	6	2017	1/1	0.94	0.18	46,46,46,46	0
86	OHX	c8	202	7/7	0.94	0.11	155,155,155,155	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3452	1/1	0.95	0.16	38,38,38,38	0
85	MG	5	3453	1/1	0.95	0.38	42,42,42,42	0
86	OHX	5	4075	7/7	0.95	0.11	121,121,121,121	0
86	OHX	5	4076	7/7	0.95	0.11	124,124,124,124	0
85	MG	1	3581	1/1	0.95	0.25	38,38,38,38	0
86	OHX	1	3948	7/7	0.95	0.12	113,113,113,113	0
86	OHX	5	4079	7/7	0.95	0.10	163,163,163,163	0
85	MG	1	3750	1/1	0.95	0.15	30,30,30,30	0
86	OHX	5	4086	7/7	0.95	0.10	140,140,140,140	0
86	OHX	5	4087	7/7	0.95	0.12	126,126,126,126	0
86	OHX	1	3958	7/7	0.95	0.09	129,129,129,129	0
86	OHX	1	3959	7/7	0.95	0.13	102,102,102,102	0
85	MG	6	1915	1/1	0.95	0.26	42,42,42,42	0
86	OHX	1	3980	7/7	0.95	0.12	117,117,117,117	0
86	OHX	5	4093	7/7	0.95	0.15	112,112,112,112	0
85	MG	1	3797	1/1	0.95	0.10	54,54,54,54	0
86	OHX	5	4097	7/7	0.95	0.10	134,134,134,134	0
85	MG	1	3582	1/1	0.95	0.29	29,29,29,29	0
86	OHX	1	3993	7/7	0.95	0.11	165,165,165,165	0
85	MG	2	1985	1/1	0.95	0.10	61,61,61,61	0
86	OHX	1	3998	7/7	0.95	0.22	105,105,105,105	0
85	MG	5	3663	1/1	0.95	0.09	36,36,36,36	0
86	OHX	1	4001	7/7	0.95	0.11	128,128,128,128	0
86	OHX	1	4002	7/7	0.95	0.12	122,122,122,122	0
86	OHX	5	4105	7/7	0.95	0.21	109,109,109,109	0
85	MG	5	3461	1/1	0.95	0.18	35,35,35,35	0
86	OHX	5	4107	7/7	0.95	0.11	141,141,141,141	0
86	OHX	1	4008	7/7	0.95	0.11	130,130,130,130	0
86	OHX	1	4012	7/7	0.95	0.12	120,120,120,120	0
86	OHX	5	4110	7/7	0.95	0.14	126,126,126,126	0
85	MG	1	3753	1/1	0.95	0.11	37,37,37,37	0
85	MG	1	3802	1/1	0.95	0.13	40,40,40,40	0
85	MG	5	3795	1/1	0.95	0.23	46,46,46,46	0
85	MG	6	1982	1/1	0.95	0.25	50,50,50,50	0
85	MG	5	3554	1/1	0.95	0.39	38,38,38,38	0
86	OHX	5	4117	7/7	0.95	0.14	122,122,122,122	0
86	OHX	5	4118	7/7	0.95	0.13	129,129,129,129	0
85	MG	1	3521	1/1	0.95	0.36	33,33,33,33	0
86	OHX	5	4120	7/7	0.95	0.26	109,109,109,109	0
86	OHX	1	4028	7/7	0.95	0.12	142,142,142,142	0
86	OHX	1	4030	7/7	0.95	0.14	117,117,117,117	0
85	MG	1	3564	1/1	0.95	0.16	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3668	1/1	0.95	0.24	47,47,47,47	0
86	OHX	1	4035	7/7	0.95	0.13	121,121,121,121	0
86	OHX	5	4126	7/7	0.95	0.11	141,141,141,141	0
85	MG	5	3558	1/1	0.95	0.30	31,31,31,31	0
86	OHX	1	4042	7/7	0.95	0.12	115,115,115,115	0
85	MG	5	3674	1/1	0.95	0.30	54,54,54,54	0
86	OHX	4	228	7/7	0.95	0.10	122,122,122,122	0
85	MG	5	3559	1/1	0.95	0.15	49,49,49,49	0
86	OHX	5	4134	7/7	0.95	0.11	119,119,119,119	0
86	OHX	1	4049	7/7	0.95	0.10	134,134,134,134	0
85	MG	1	3565	1/1	0.95	0.32	34,34,34,34	0
85	MG	m7	202	1/1	0.95	0.17	37,37,37,37	0
85	MG	1	4215	1/1	0.95	0.19	39,39,39,39	0
85	MG	5	3471	1/1	0.95	0.31	46,46,46,46	0
86	OHX	L3	405	7/7	0.95	0.12	116,116,116,116	0
85	MG	5	3567	1/1	0.95	0.24	34,34,34,34	0
85	MG	L7	303	1/1	0.95	0.24	47,47,47,47	0
86	OHX	1	4059	7/7	0.95	0.08	155,155,155,155	0
85	MG	1	3475	1/1	0.95	0.20	38,38,38,38	0
85	MG	1	3759	1/1	0.95	0.24	48,48,48,48	0
85	MG	M0	302	1/1	0.95	0.18	41,41,41,41	0
85	MG	M0	303	1/1	0.95	0.12	53,53,53,53	0
85	MG	1	3760	1/1	0.95	0.15	46,46,46,46	0
86	OHX	1	4067	7/7	0.95	0.15	127,127,127,127	0
85	MG	6	1995	1/1	0.95	0.20	64,64,64,64	0
86	OHX	6	2064	7/7	0.95	0.13	106,106,106,106	0
86	OHX	6	2085	7/7	0.95	0.10	137,137,137,137	0
86	OHX	6	2086	7/7	0.95	0.14	112,112,112,112	0
85	MG	o3	201	1/1	0.95	0.18	37,37,37,37	0
86	OHX	5	4157	7/7	0.95	0.12	121,121,121,121	0
86	OHX	1	4070	7/7	0.95	0.11	148,148,148,148	0
86	OHX	6	2098	7/7	0.95	0.11	129,129,129,129	0
86	OHX	6	2099	7/7	0.95	0.08	172,172,172,172	0
85	MG	1	3537	1/1	0.95	0.36	35,35,35,35	0
86	OHX	6	2103	7/7	0.95	0.12	128,128,128,128	0
85	MG	sM	301	1/1	0.95	0.09	50,50,50,50	0
86	OHX	6	2106	7/7	0.95	0.13	124,124,124,124	0
86	OHX	5	4165	7/7	0.95	0.15	122,122,122,122	0
85	MG	1	3476	1/1	0.95	0.24	46,46,46,46	0
86	OHX	6	2111	7/7	0.95	0.11	133,133,133,133	0
85	MG	5	3828	1/1	0.95	0.23	47,47,47,47	0
86	OHX	6	2118	7/7	0.95	0.13	116,116,116,116	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	6	2119	7/7	0.95	0.10	148,148,148,148	0
85	MG	5	3579	1/1	0.95	0.44	39,39,39,39	0
86	OHX	2	2040	7/7	0.95	0.15	109,109,109,109	0
86	OHX	2	2054	7/7	0.95	0.11	137,137,137,137	0
86	OHX	2	2055	7/7	0.95	0.11	122,122,122,122	0
86	OHX	2	2057	7/7	0.95	0.10	146,146,146,146	0
86	OHX	2	2063	7/7	0.95	0.09	139,139,139,139	0
86	OHX	6	2130	7/7	0.95	0.09	146,146,146,146	0
85	MG	5	3694	1/1	0.95	0.20	43,43,43,43	0
85	MG	1	3763	1/1	0.95	0.30	67,67,67,67	0
86	OHX	1	4084	7/7	0.95	0.08	196,196,196,196	0
85	MG	1	3675	1/1	0.95	0.21	47,47,47,47	0
86	OHX	2	2077	7/7	0.95	0.11	125,125,125,125	0
85	MG	1	3643	1/1	0.95	0.19	45,45,45,45	0
86	OHX	1	4089	7/7	0.95	0.09	156,156,156,156	0
86	OHX	1	4090	7/7	0.95	0.14	126,126,126,126	0
85	MG	5	3586	1/1	0.95	0.33	30,30,30,30	0
86	OHX	2	2082	7/7	0.95	0.10	156,156,156,156	0
86	OHX	2	2085	7/7	0.95	0.10	149,149,149,149	0
85	MG	5	3587	1/1	0.95	0.36	24,24,24,24	0
86	OHX	2	2089	7/7	0.95	0.13	119,119,119,119	0
85	MG	5	3702	1/1	0.95	0.13	37,37,37,37	0
85	MG	M7	203	1/1	0.95	0.29	37,37,37,37	0
85	MG	5	3843	1/1	0.95	0.06	57,57,57,57	0
85	MG	1	3821	1/1	0.95	0.14	48,48,48,48	0
85	MG	M7	205	1/1	0.95	0.21	41,41,41,41	0
86	OHX	1	4102	7/7	0.95	0.12	133,133,133,133	0
86	OHX	2	2101	7/7	0.95	0.10	146,146,146,146	0
85	MG	5	3410	1/1	0.95	0.25	49,49,49,49	0
85	MG	1	3411	1/1	0.95	0.18	33,33,33,33	0
85	MG	5	3492	1/1	0.95	0.31	55,55,55,55	0
85	MG	5	3710	1/1	0.95	0.27	53,53,53,53	0
86	OHX	2	2106	7/7	0.95	0.12	119,119,119,119	0
85	MG	5	3853	1/1	0.95	0.18	57,57,57,57	0
85	MG	5	3854	1/1	0.95	0.18	55,55,55,55	0
86	OHX	2	2112	7/7	0.95	0.11	137,137,137,137	0
86	OHX	2	2113	7/7	0.95	0.10	162,162,162,162	0
85	MG	1	3825	1/1	0.95	0.18	58,58,58,58	0
85	MG	5	3712	1/1	0.95	0.25	47,47,47,47	0
85	MG	5	3713	1/1	0.95	0.13	90,90,90,90	0
85	MG	5	3714	1/1	0.95	0.15	44,44,44,44	0
85	MG	6	1942	1/1	0.95	0.23	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	2	2120	7/7	0.95	0.10	157,157,157,157	0
85	MG	1	3621	1/1	0.95	0.07	36,36,36,36	0
85	MG	5	3598	1/1	0.95	0.32	37,37,37,37	0
85	MG	1	3679	1/1	0.95	0.07	46,46,46,46	0
85	MG	1	3722	1/1	0.95	0.07	47,47,47,47	0
85	MG	6	1948	1/1	0.95	0.27	43,43,43,43	0
85	MG	1	3525	1/1	0.95	0.22	27,27,27,27	0
85	MG	5	3722	1/1	0.95	0.10	66,66,66,66	0
86	OHX	2	2128	7/7	0.95	0.10	153,153,153,153	0
85	MG	N6	202	1/1	0.95	0.12	47,47,47,47	0
85	MG	5	3605	1/1	0.95	0.14	35,35,35,35	0
85	MG	5	3606	1/1	0.95	0.08	26,26,26,26	0
85	MG	1	3683	1/1	0.95	0.19	39,39,39,39	0
85	MG	N8	203	1/1	0.95	0.38	34,34,34,34	0
85	MG	5	3875	1/1	0.95	0.32	50,50,50,50	0
85	MG	5	3728	1/1	0.95	0.18	56,56,56,56	0
85	MG	5	3505	1/1	0.95	0.33	31,31,31,31	0
85	MG	5	3610	1/1	0.95	0.26	30,30,30,30	0
85	MG	5	3732	1/1	0.95	0.36	78,78,78,78	0
85	MG	5	3733	1/1	0.95	0.14	57,57,57,57	0
85	MG	6	2015	1/1	0.95	0.20	51,51,51,51	0
85	MG	1	3572	1/1	0.95	0.30	23,23,23,23	0
85	MG	O2	201	1/1	0.95	0.20	35,35,35,35	0
85	MG	5	3617	1/1	0.95	0.27	48,48,48,48	0
85	MG	5	3429	1/1	0.95	0.19	28,28,28,28	0
85	MG	2	1934	1/1	0.95	0.27	51,51,51,51	0
85	MG	5	3745	1/1	0.95	0.23	39,39,39,39	0
85	MG	5	3513	1/1	0.95	0.28	33,33,33,33	0
85	MG	1	3833	1/1	0.95	0.30	37,37,37,37	0
85	MG	1	3507	1/1	0.95	0.32	25,25,25,25	0
85	MG	1	3429	1/1	0.95	0.47	46,46,46,46	0
86	OHX	1	4150	7/7	0.95	0.12	135,135,135,135	0
85	MG	1	3652	1/1	0.95	0.07	49,49,49,49	0
85	MG	5	3626	1/1	0.95	0.28	41,41,41,41	0
85	MG	1	3425	1/1	0.95	0.12	34,34,34,34	0
86	OHX	1	4155	7/7	0.95	0.11	122,122,122,122	0
85	MG	4	205	1/1	0.95	0.34	51,51,51,51	0
85	MG	5	3520	1/1	0.95	0.26	25,25,25,25	0
86	OHX	7	224	7/7	0.95	0.10	135,135,135,135	0
85	MG	5	3900	1/1	0.95	0.25	50,50,50,50	0
85	MG	5	3756	1/1	0.95	0.26	49,49,49,49	0
85	MG	1	3518	1/1	0.95	0.28	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	8	222	7/7	0.95	0.11	125,125,125,125	0
85	MG	1	3655	1/1	0.95	0.26	38,38,38,38	0
86	OHX	5	3995	7/7	0.95	0.14	109,109,109,109	0
85	MG	1	3579	1/1	0.95	0.32	44,44,44,44	0
85	MG	5	3524	1/1	0.95	0.38	40,40,40,40	0
85	MG	5	3762	1/1	0.95	0.17	56,56,56,56	0
85	MG	1	3739	1/1	0.95	0.15	52,52,52,52	0
85	MG	7	204	1/1	0.95	0.26	55,55,55,55	0
85	MG	1	3604	1/1	0.95	0.09	45,45,45,45	0
85	MG	1	3788	1/1	0.95	0.10	62,62,62,62	0
85	MG	7	207	1/1	0.95	0.08	36,36,36,36	0
86	OHX	5	4031	7/7	0.95	0.22	98,98,98,98	0
85	MG	1	3741	1/1	0.95	0.16	31,31,31,31	0
85	MG	1	3699	1/1	0.95	0.12	39,39,39,39	0
86	OHX	5	4037	7/7	0.95	0.11	130,130,130,130	0
86	OHX	m0	302	7/7	0.95	0.11	130,130,130,130	0
86	OHX	5	4038	7/7	0.95	0.09	137,137,137,137	0
85	MG	1	3533	1/1	0.95	0.11	40,40,40,40	0
85	MG	5	3772	1/1	0.95	0.13	44,44,44,44	0
85	MG	1	3659	1/1	0.95	0.06	35,35,35,35	0
85	MG	6	1973	1/1	0.95	0.28	57,57,57,57	0
85	MG	5	3648	1/1	0.95	0.10	60,60,60,60	0
86	OHX	5	4058	7/7	0.95	0.14	117,117,117,117	0
85	MG	5	3451	1/1	0.95	0.24	41,41,41,41	0
85	MG	5	3540	1/1	0.95	0.24	24,24,24,24	0
85	MG	5	3779	1/1	0.95	0.14	31,31,31,31	0
86	OHX	5	4067	7/7	0.95	0.12	124,124,124,124	0
86	OHX	5	4069	7/7	0.95	0.10	132,132,132,132	0
86	OHX	C1	201	7/7	0.95	0.12	141,141,141,141	0
86	OHX	1	3984	7/7	0.96	0.12	123,123,123,123	0
85	MG	1	3532	1/1	0.96	0.26	35,35,35,35	0
86	OHX	1	3989	7/7	0.96	0.09	136,136,136,136	0
85	MG	1	3715	1/1	0.96	0.08	37,37,37,37	0
85	MG	5	3815	1/1	0.96	0.17	39,39,39,39	0
86	OHX	6	2138	7/7	0.96	0.11	128,128,128,128	0
85	MG	1	3689	1/1	0.96	0.17	42,42,42,42	0
86	OHX	1	3999	7/7	0.96	0.09	126,126,126,126	0
85	MG	1	3840	1/1	0.96	0.21	37,37,37,37	0
85	MG	1	3804	1/1	0.96	0.09	58,58,58,58	0
85	MG	5	3819	1/1	0.96	0.16	42,42,42,42	0
86	OHX	6	2145	7/7	0.96	0.12	138,138,138,138	0
86	OHX	5	4129	7/7	0.96	0.08	137,137,137,137	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3744	1/1	0.96	0.20	53,53,53,53	0
86	OHX	1	4006	7/7	0.96	0.09	133,133,133,133	0
86	OHX	1	4007	7/7	0.96	0.11	135,135,135,135	0
86	OHX	5	4133	7/7	0.96	0.09	145,145,145,145	0
85	MG	5	3821	1/1	0.96	0.10	40,40,40,40	0
86	OHX	1	4009	7/7	0.96	0.10	137,137,137,137	0
86	OHX	1	4011	7/7	0.96	0.10	124,124,124,124	0
85	MG	5	3740	1/1	0.96	0.12	51,51,51,51	0
86	OHX	5	4138	7/7	0.96	0.13	121,121,121,121	0
85	MG	5	3741	1/1	0.96	0.14	47,47,47,47	0
86	OHX	6	2155	7/7	0.96	0.12	121,121,121,121	0
85	MG	5	3446	1/1	0.96	0.05	45,45,45,45	0
86	OHX	1	4015	7/7	0.96	0.09	134,134,134,134	0
85	MG	1	3745	1/1	0.96	0.09	47,47,47,47	0
86	OHX	6	2159	7/7	0.96	0.12	124,124,124,124	0
85	MG	1	3610	1/1	0.96	0.08	44,44,44,44	0
86	OHX	5	4146	7/7	0.96	0.11	138,138,138,138	0
85	MG	1	3811	1/1	0.96	0.19	57,57,57,57	0
85	MG	5	3495	1/1	0.96	0.09	48,48,48,48	0
86	OHX	1	4025	7/7	0.96	0.10	135,135,135,135	0
86	OHX	1	4026	7/7	0.96	0.09	135,135,135,135	0
86	OHX	1	4027	7/7	0.96	0.11	112,112,112,112	0
85	MG	5	3677	1/1	0.96	0.35	56,56,56,56	0
85	MG	5	3835	1/1	0.96	0.10	56,56,56,56	0
86	OHX	1	4032	7/7	0.96	0.27	105,105,105,105	0
85	MG	5	3402	1/1	0.96	0.19	31,31,31,31	0
85	MG	1	3670	1/1	0.96	0.27	49,49,49,49	0
85	MG	6	1947	1/1	0.96	0.30	57,57,57,57	0
86	OHX	1	4036	7/7	0.96	0.12	125,125,125,125	0
86	OHX	1	4037	7/7	0.96	0.11	122,122,122,122	0
85	MG	1	3749	1/1	0.96	0.07	45,45,45,45	0
86	OHX	1	4040	7/7	0.96	0.21	104,104,104,104	0
85	MG	5	3500	1/1	0.96	0.15	37,37,37,37	0
85	MG	1	3778	1/1	0.96	0.30	38,38,38,38	0
86	OHX	1	4044	7/7	0.96	0.13	119,119,119,119	0
86	OHX	1	4046	7/7	0.96	0.09	140,140,140,140	0
85	MG	1	3850	1/1	0.96	0.13	28,28,28,28	0
86	OHX	1	4048	7/7	0.96	0.12	120,120,120,120	0
85	MG	5	3757	1/1	0.96	0.21	37,37,37,37	0
86	OHX	1	4051	7/7	0.96	0.11	136,136,136,136	0
85	MG	M3	203	1/1	0.96	0.15	36,36,36,36	0
86	OHX	1	4053	7/7	0.96	0.08	153,153,153,153	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3457	1/1	0.96	0.27	29,29,29,29	0
86	OHX	2	2130	7/7	0.96	0.12	127,127,127,127	0
85	MG	2	1988	1/1	0.96	0.15	75,75,75,75	0
85	MG	5	3413	1/1	0.96	0.20	45,45,45,45	0
85	MG	1	3780	1/1	0.96	0.36	38,38,38,38	0
85	MG	5	3508	1/1	0.96	0.41	40,40,40,40	0
85	MG	1	3594	1/1	0.96	0.31	24,24,24,24	0
85	MG	1	3406	1/1	0.96	0.18	41,41,41,41	0
85	MG	2	1956	1/1	0.96	0.32	55,55,55,55	0
86	OHX	5	4182	7/7	0.96	0.08	162,162,162,162	0
86	OHX	1	4063	7/7	0.96	0.16	112,112,112,112	0
86	OHX	1	4064	7/7	0.96	0.07	152,152,152,152	0
85	MG	5	3512	1/1	0.96	0.34	27,27,27,27	0
85	MG	5	3770	1/1	0.96	0.07	66,66,66,66	0
85	MG	5	3631	1/1	0.96	0.19	44,44,44,44	0
85	MG	m0	301	1/1	0.96	0.18	37,37,37,37	0
85	MG	5	3699	1/1	0.96	0.21	46,46,46,46	0
85	MG	1	3440	1/1	0.96	0.26	39,39,39,39	0
85	MG	1	3822	1/1	0.96	0.15	49,49,49,49	0
86	OHX	2	2145	7/7	0.96	0.10	132,132,132,132	0
85	MG	1	3441	1/1	0.96	0.22	46,46,46,46	0
85	MG	5	3635	1/1	0.96	0.07	35,35,35,35	0
85	MG	m7	203	1/1	0.96	0.21	49,49,49,49	0
85	MG	5	3704	1/1	0.96	0.10	38,38,38,38	0
85	MG	1	3661	1/1	0.96	0.05	52,52,52,52	0
85	MG	2	1957	1/1	0.96	0.32	69,69,69,69	0
85	MG	5	3469	1/1	0.96	0.08	36,36,36,36	0
85	MG	1	3663	1/1	0.96	0.17	45,45,45,45	0
85	MG	1	3681	1/1	0.96	0.12	44,44,44,44	0
86	OHX	5	3976	7/7	0.96	0.11	113,113,113,113	0
86	OHX	5	3977	7/7	0.96	0.13	104,104,104,104	0
85	MG	5	3641	1/1	0.96	0.32	45,45,45,45	0
85	MG	5	3785	1/1	0.96	0.06	81,81,81,81	0
86	OHX	3	216	7/7	0.96	0.11	118,118,118,118	0
86	OHX	5	3998	7/7	0.96	0.25	103,103,103,103	0
85	MG	5	3580	1/1	0.96	0.20	25,25,25,25	0
86	OHX	5	4005	7/7	0.96	0.09	117,117,117,117	0
85	MG	n9	101	1/1	0.96	0.07	36,36,36,36	0
86	OHX	5	4014	7/7	0.96	0.10	118,118,118,118	0
86	OHX	5	4015	7/7	0.96	0.09	154,154,154,154	0
85	MG	5	3643	1/1	0.96	0.28	54,54,54,54	0
86	OHX	5	4024	7/7	0.96	0.11	113,113,113,113	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3682	1/1	0.96	0.22	47,47,47,47	0
86	OHX	4	227	7/7	0.96	0.13	115,115,115,115	0
85	MG	5	3646	1/1	0.96	0.27	44,44,44,44	0
86	OHX	5	4219	7/7	0.96	0.24	110,110,110,110	0
85	MG	5	3582	1/1	0.96	0.29	33,33,33,33	0
85	MG	2	1918	1/1	0.96	0.39	54,54,54,54	0
86	OHX	5	4033	7/7	0.96	0.09	143,143,143,143	0
85	MG	5	3649	1/1	0.96	0.15	40,40,40,40	0
85	MG	5	3650	1/1	0.96	0.39	48,48,48,48	0
85	MG	1	3403	1/1	0.96	0.30	37,37,37,37	0
86	OHX	2	2043	7/7	0.96	0.14	123,123,123,123	0
86	OHX	5	4040	7/7	0.96	0.08	135,135,135,135	0
86	OHX	1	4097	7/7	0.96	0.13	118,118,118,118	0
86	OHX	2	2053	7/7	0.96	0.10	135,135,135,135	0
85	MG	5	3797	1/1	0.96	0.16	43,43,43,43	0
86	OHX	5	4047	7/7	0.96	0.11	132,132,132,132	0
86	OHX	5	4049	7/7	0.96	0.10	128,128,128,128	0
86	OHX	5	4051	7/7	0.96	0.12	113,113,113,113	0
85	MG	2	1902	1/1	0.96	0.23	38,38,38,38	0
86	OHX	5	4054	7/7	0.96	0.12	112,112,112,112	0
86	OHX	5	4236	7/7	0.96	0.12	113,113,113,113	0
86	OHX	5	4056	7/7	0.96	0.12	116,116,116,116	0
86	OHX	M5	302	7/7	0.96	0.11	120,120,120,120	0
86	OHX	5	4059	7/7	0.96	0.09	132,132,132,132	0
86	OHX	5	4060	7/7	0.96	0.09	144,144,144,144	0
85	MG	5	3525	1/1	0.96	0.29	37,37,37,37	0
86	OHX	2	2062	7/7	0.96	0.10	133,133,133,133	0
85	MG	1	3764	1/1	0.96	0.08	92,92,92,92	0
86	OHX	5	4066	7/7	0.96	0.07	156,156,156,156	0
86	OHX	2	2066	7/7	0.96	0.10	138,138,138,138	0
85	MG	5	3527	1/1	0.96	0.19	47,47,47,47	0
85	MG	6	1969	1/1	0.96	0.29	65,65,65,65	0
86	OHX	5	4071	7/7	0.96	0.09	141,141,141,141	0
86	OHX	O7	105	7/7	0.96	0.12	107,107,107,107	0
85	MG	5	3530	1/1	0.96	0.22	32,32,32,32	0
85	MG	1	3736	1/1	0.96	0.14	48,48,48,48	0
86	OHX	6	2077	7/7	0.96	0.14	118,118,118,118	0
86	OHX	2	2079	7/7	0.96	0.13	126,126,126,126	0
85	MG	5	3807	1/1	0.96	0.08	50,50,50,50	0
85	MG	L2	301	1/1	0.96	0.11	37,37,37,37	0
85	MG	1	3686	1/1	0.96	0.14	40,40,40,40	0
86	OHX	5	4082	7/7	0.96	0.10	122,122,122,122	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	4083	7/7	0.96	0.13	116,116,116,116	0
86	OHX	8	218	7/7	0.96	0.11	113,113,113,113	0
86	OHX	8	220	7/7	0.96	0.09	123,123,123,123	0
86	OHX	8	221	7/7	0.96	0.14	123,123,123,123	0
86	OHX	5	4085	7/7	0.96	0.10	114,114,114,114	0
86	OHX	C8	201	7/7	0.96	0.11	120,120,120,120	0
86	OHX	8	225	7/7	0.96	0.10	130,130,130,130	0
86	OHX	2	2084	7/7	0.96	0.11	129,129,129,129	0
86	OHX	SR	401	7/7	0.96	0.08	174,174,174,174	0
86	OHX	1	3916	7/7	0.96	0.12	113,113,113,113	0
86	OHX	1	3920	7/7	0.96	0.12	98,98,98,98	0
86	OHX	1	3924	7/7	0.96	0.13	102,102,102,102	0
86	OHX	1	3935	7/7	0.96	0.11	103,103,103,103	0
86	OHX	5	4094	7/7	0.96	0.13	114,114,114,114	0
86	OHX	1	3946	7/7	0.96	0.12	125,125,125,125	0
86	OHX	6	2112	7/7	0.96	0.09	125,125,125,125	0
86	OHX	6	2113	7/7	0.96	0.11	114,114,114,114	0
86	OHX	6	2114	7/7	0.96	0.11	136,136,136,136	0
86	OHX	6	2115	7/7	0.96	0.11	134,134,134,134	0
86	OHX	6	2116	7/7	0.96	0.09	137,137,137,137	0
85	MG	1	3542	1/1	0.96	0.22	33,33,33,33	0
86	OHX	2	2086	7/7	0.96	0.12	123,123,123,123	0
85	MG	5	3899	1/1	0.96	0.15	97,97,97,97	0
86	OHX	6	2120	7/7	0.96	0.10	131,131,131,131	0
86	OHX	m5	303	7/7	0.96	0.11	131,131,131,131	0
85	MG	5	3811	1/1	0.96	0.15	38,38,38,38	0
86	OHX	6	2123	7/7	0.96	0.10	146,146,146,146	0
85	MG	O7	104	1/1	0.96	0.26	34,34,34,34	0
86	OHX	1	3967	7/7	0.96	0.12	120,120,120,120	0
86	OHX	1	3976	7/7	0.96	0.11	112,112,112,112	0
86	OHX	1	3977	7/7	0.96	0.11	116,116,116,116	0
85	MG	5	4256	1/1	0.96	0.09	47,47,47,47	0
86	OHX	6	2129	7/7	0.96	0.10	160,160,160,160	0
86	OHX	2	2096	7/7	0.96	0.08	174,174,174,174	0
86	OHX	1	3983	7/7	0.96	0.10	129,129,129,129	0
86	OHX	1	4041	7/7	0.97	0.11	114,114,114,114	0
85	MG	5	3830	1/1	0.97	0.08	38,38,38,38	0
85	MG	1	3461	1/1	0.97	0.27	27,27,27,27	0
85	MG	5	3651	1/1	0.97	0.16	47,47,47,47	0
86	OHX	2	2056	7/7	0.97	0.09	133,133,133,133	0
85	MG	1	3433	1/1	0.97	0.16	36,36,36,36	0
86	OHX	1	4171	7/7	0.97	0.10	111,111,111,111	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3834	1/1	0.97	0.08	77,77,77,77	0
85	MG	1	3698	1/1	0.97	0.15	43,43,43,43	0
85	MG	5	3549	1/1	0.97	0.23	50,50,50,50	0
86	OHX	2	2067	7/7	0.97	0.08	144,144,144,144	0
85	MG	1	3529	1/1	0.97	0.30	34,34,34,34	0
86	OHX	2	2069	7/7	0.97	0.11	121,121,121,121	0
86	OHX	2	2071	7/7	0.97	0.09	132,132,132,132	0
86	OHX	2	2074	7/7	0.97	0.11	122,122,122,122	0
85	MG	1	3814	1/1	0.97	0.08	47,47,47,47	0
85	MG	1	3445	1/1	0.97	0.06	46,46,46,46	0
85	MG	1	3602	1/1	0.97	0.07	39,39,39,39	0
86	OHX	2	2078	7/7	0.97	0.09	130,130,130,130	0
85	MG	5	3425	1/1	0.97	0.19	36,36,36,36	0
85	MG	4	218	1/1	0.97	0.12	38,38,38,38	0
85	MG	5	3845	1/1	0.97	0.12	41,41,41,41	0
85	MG	5	3846	1/1	0.97	0.24	56,56,56,56	0
85	MG	5	3661	1/1	0.97	0.18	49,49,49,49	0
85	MG	1	3766	1/1	0.97	0.14	65,65,65,65	0
85	MG	5	3428	1/1	0.97	0.20	44,44,44,44	0
85	MG	1	3640	1/1	0.97	0.20	35,35,35,35	0
85	MG	5	3430	1/1	0.97	0.08	33,33,33,33	0
86	OHX	2	2090	7/7	0.97	0.09	128,128,128,128	0
85	MG	6	1984	1/1	0.97	0.16	60,60,60,60	0
86	OHX	1	4072	7/7	0.97	0.08	128,128,128,128	0
85	MG	s8	302	1/1	0.97	0.24	46,46,46,46	0
86	OHX	2	2095	7/7	0.97	0.08	157,157,157,157	0
85	MG	5	3562	1/1	0.97	0.29	25,25,25,25	0
85	MG	5	3856	1/1	0.97	0.12	63,63,63,63	0
86	OHX	2	2098	7/7	0.97	0.11	122,122,122,122	0
86	OHX	1	3906	7/7	0.97	0.15	88,88,88,88	0
86	OHX	1	3907	7/7	0.97	0.09	99,99,99,99	0
85	MG	5	3669	1/1	0.97	0.15	49,49,49,49	0
85	MG	1	3703	1/1	0.97	0.17	65,65,65,65	0
85	MG	8	205	1/1	0.97	0.19	43,43,43,43	0
86	OHX	1	3928	7/7	0.97	0.09	110,110,110,110	0
86	OHX	1	3931	7/7	0.97	0.10	106,106,106,106	0
86	OHX	1	3933	7/7	0.97	0.12	94,94,94,94	0
86	OHX	1	3934	7/7	0.97	0.12	94,94,94,94	0
85	MG	1	3769	1/1	0.97	0.14	55,55,55,55	0
86	OHX	1	3941	7/7	0.97	0.10	111,111,111,111	0
86	OHX	1	3943	7/7	0.97	0.09	118,118,118,118	0
86	OHX	3	219	7/7	0.97	0.08	120,120,120,120	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	3	221	7/7	0.97	0.09	132,132,132,132	0
86	OHX	1	3945	7/7	0.97	0.09	122,122,122,122	0
85	MG	L3	401	1/1	0.97	0.19	38,38,38,38	0
86	OHX	6	2202	7/7	0.97	0.06	204,204,204,204	0
85	MG	N8	202	1/1	0.97	0.08	27,27,27,27	0
85	MG	5	3790	1/1	0.97	0.10	46,46,46,46	0
86	OHX	4	225	7/7	0.97	0.08	120,120,120,120	0
86	OHX	4	226	7/7	0.97	0.09	128,128,128,128	0
86	OHX	1	3953	7/7	0.97	0.15	103,103,103,103	0
85	MG	5	3791	1/1	0.97	0.15	51,51,51,51	0
86	OHX	4	229	7/7	0.97	0.07	144,144,144,144	0
86	OHX	4	230	7/7	0.97	0.09	133,133,133,133	0
85	MG	5	3864	1/1	0.97	0.11	68,68,68,68	0
86	OHX	2	2108	7/7	0.97	0.08	157,157,157,157	0
86	OHX	1	3963	7/7	0.97	0.17	107,107,107,107	0
86	OHX	1	3964	7/7	0.97	0.09	129,129,129,129	0
86	OHX	5	3951	7/7	0.97	0.10	103,103,103,103	0
86	OHX	5	3962	7/7	0.97	0.09	80,80,80,80	0
86	OHX	5	3965	7/7	0.97	0.10	101,101,101,101	0
86	OHX	5	3968	7/7	0.97	0.10	107,107,107,107	0
86	OHX	5	3969	7/7	0.97	0.13	102,102,102,102	0
86	OHX	5	3971	7/7	0.97	0.09	106,106,106,106	0
86	OHX	1	3965	7/7	0.97	0.13	107,107,107,107	0
86	OHX	2	2110	7/7	0.97	0.11	126,126,126,126	0
86	OHX	5	3979	7/7	0.97	0.11	100,100,100,100	0
86	OHX	5	3982	7/7	0.97	0.09	114,114,114,114	0
86	OHX	5	3985	7/7	0.97	0.21	104,104,104,104	0
86	OHX	5	3986	7/7	0.97	0.21	99,99,99,99	0
86	OHX	5	3994	7/7	0.97	0.10	111,111,111,111	0
86	OHX	1	3968	7/7	0.97	0.17	108,108,108,108	0
86	OHX	1	4104	7/7	0.97	0.07	141,141,141,141	0
86	OHX	1	3969	7/7	0.97	0.11	112,112,112,112	0
86	OHX	1	3970	7/7	0.97	0.09	122,122,122,122	0
86	OHX	1	3973	7/7	0.97	0.11	113,113,113,113	0
86	OHX	5	4002	7/7	0.97	0.09	118,118,118,118	0
86	OHX	5	4003	7/7	0.97	0.20	108,108,108,108	0
86	OHX	5	4004	7/7	0.97	0.21	79,79,79,79	0
86	OHX	1	3974	7/7	0.97	0.14	96,96,96,96	0
85	MG	1	3748	1/1	0.97	0.13	63,63,63,63	0
86	OHX	5	4013	7/7	0.97	0.20	111,111,111,111	0
85	MG	1	3628	1/1	0.97	0.10	67,67,67,67	0
85	MG	5	3572	1/1	0.97	0.35	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	4017	7/7	0.97	0.10	111,111,111,111	0
86	OHX	2	2114	7/7	0.97	0.10	131,131,131,131	0
86	OHX	5	4022	7/7	0.97	0.21	105,105,105,105	0
85	MG	5	3480	1/1	0.97	0.23	70,70,70,70	0
85	MG	l4	401	1/1	0.97	0.17	41,41,41,41	0
86	OHX	5	4027	7/7	0.97	0.10	117,117,117,117	0
86	OHX	O7	106	7/7	0.97	0.13	105,105,105,105	0
86	OHX	1	3986	7/7	0.97	0.14	102,102,102,102	0
86	OHX	1	3987	7/7	0.97	0.11	117,117,117,117	0
86	OHX	6	2065	7/7	0.97	0.09	115,115,115,115	0
86	OHX	6	2066	7/7	0.97	0.13	121,121,121,121	0
86	OHX	6	2071	7/7	0.97	0.09	112,112,112,112	0
86	OHX	6	2073	7/7	0.97	0.09	146,146,146,146	0
86	OHX	6	2074	7/7	0.97	0.07	156,156,156,156	0
85	MG	6	2024	1/1	0.97	0.25	53,53,53,53	0
86	OHX	6	2081	7/7	0.97	0.18	106,106,106,106	0
86	OHX	5	4041	7/7	0.97	0.24	94,94,94,94	0
86	OHX	5	4042	7/7	0.97	0.10	131,131,131,131	0
85	MG	N8	205	1/1	0.97	0.06	30,30,30,30	0
86	OHX	1	3990	7/7	0.97	0.08	127,127,127,127	0
86	OHX	6	2088	7/7	0.97	0.09	129,129,129,129	0
86	OHX	6	2091	7/7	0.97	0.12	126,126,126,126	0
86	OHX	5	4048	7/7	0.97	0.14	112,112,112,112	0
86	OHX	6	2092	7/7	0.97	0.08	125,125,125,125	0
86	OHX	5	4050	7/7	0.97	0.09	118,118,118,118	0
86	OHX	6	2094	7/7	0.97	0.07	140,140,140,140	0
86	OHX	5	4052	7/7	0.97	0.08	133,133,133,133	0
86	OHX	1	3991	7/7	0.97	0.08	134,134,134,134	0
86	OHX	1	3992	7/7	0.97	0.19	101,101,101,101	0
85	MG	1	3705	1/1	0.97	0.06	55,55,55,55	0
86	OHX	1	3995	7/7	0.97	0.10	118,118,118,118	0
85	MG	5	3681	1/1	0.97	0.17	42,42,42,42	0
86	OHX	6	2101	7/7	0.97	0.08	171,171,171,171	0
86	OHX	5	4061	7/7	0.97	0.09	124,124,124,124	0
86	OHX	5	4062	7/7	0.97	0.07	147,147,147,147	0
85	MG	1	3568	1/1	0.97	0.31	27,27,27,27	0
86	OHX	6	2104	7/7	0.97	0.08	128,128,128,128	0
85	MG	5	3739	1/1	0.97	0.17	41,41,41,41	0
85	MG	5	3485	1/1	0.97	0.31	28,28,28,28	0
85	MG	5	3528	1/1	0.97	0.33	29,29,29,29	0
86	OHX	6	2108	7/7	0.97	0.11	118,118,118,118	0
86	OHX	6	2109	7/7	0.97	0.08	126,126,126,126	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	6	2110	7/7	0.97	0.10	119,119,119,119	0
85	MG	1	3853	1/1	0.97	0.08	90,90,90,90	0
86	OHX	1	4003	7/7	0.97	0.13	109,109,109,109	0
86	OHX	5	4074	7/7	0.97	0.10	123,123,123,123	0
86	OHX	7	223	7/7	0.97	0.11	110,110,110,110	0
86	OHX	1	4004	7/7	0.97	0.09	112,112,112,112	0
85	MG	2	1903	1/1	0.97	0.33	45,45,45,45	0
85	MG	5	3744	1/1	0.97	0.07	61,61,61,61	0
85	MG	5	3687	1/1	0.97	0.14	50,50,50,50	0
85	MG	1	3606	1/1	0.97	0.24	50,50,50,50	0
86	OHX	8	219	7/7	0.97	0.08	131,131,131,131	0
85	MG	1	3674	1/1	0.97	0.25	39,39,39,39	0
86	OHX	1	4010	7/7	0.97	0.09	124,124,124,124	0
85	MG	n0	202	1/1	0.97	0.13	43,43,43,43	0
85	MG	1	3645	1/1	0.97	0.12	40,40,40,40	0
86	OHX	8	224	7/7	0.97	0.08	143,143,143,143	0
86	OHX	6	2122	7/7	0.97	0.08	152,152,152,152	0
85	MG	5	3585	1/1	0.97	0.30	30,30,30,30	0
85	MG	1	3585	1/1	0.97	0.29	47,47,47,47	0
85	MG	5	3409	1/1	0.97	0.28	48,48,48,48	0
85	MG	1	3693	1/1	0.97	0.13	48,48,48,48	0
86	OHX	1	4018	7/7	0.97	0.10	116,116,116,116	0
86	OHX	5	4092	7/7	0.97	0.23	101,101,101,101	0
86	OHX	l3	403	7/7	0.97	0.10	127,127,127,127	0
86	OHX	1	4019	7/7	0.97	0.08	145,145,145,145	0
85	MG	5	3753	1/1	0.97	0.19	54,54,54,54	0
85	MG	n8	204	1/1	0.97	0.06	39,39,39,39	0
86	OHX	5	4096	7/7	0.97	0.10	120,120,120,120	0
86	OHX	6	2131	7/7	0.97	0.09	131,131,131,131	0
85	MG	2	2182	1/1	0.97	0.08	105,105,105,105	0
85	MG	5	3412	1/1	0.97	0.13	35,35,35,35	0
85	MG	5	3697	1/1	0.97	0.10	47,47,47,47	0
85	MG	1	3806	1/1	0.97	0.11	39,39,39,39	0
85	MG	5	3645	1/1	0.97	0.08	42,42,42,42	0
85	MG	5	3823	1/1	0.97	0.15	69,69,69,69	0
86	OHX	1	4031	7/7	0.97	0.07	153,153,153,153	0
85	MG	q0	202	1/1	0.97	0.07	42,42,42,42	0
85	MG	1	4213	1/1	0.97	0.09	31,31,31,31	0
85	MG	1	3807	1/1	0.97	0.08	55,55,55,55	0
86	OHX	o3	202	7/7	0.97	0.20	110,110,110,110	0
86	OHX	2	2033	7/7	0.97	0.12	109,109,109,109	0
86	OHX	2	2037	7/7	0.97	0.12	129,129,129,129	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	1	3587	1/1	0.97	0.29	27,27,27,27	0
86	OHX	1	4038	7/7	0.97	0.08	132,132,132,132	0
85	MG	1	3809	1/1	0.97	0.10	51,51,51,51	0
86	OHX	2	2049	7/7	0.97	0.08	126,126,126,126	0
86	OHX	6	2149	7/7	0.97	0.12	118,118,118,118	0
86	OHX	5	3960	7/7	0.98	0.09	94,94,94,94	0
85	MG	1	3660	1/1	0.98	0.18	43,43,43,43	0
85	MG	1	3728	1/1	0.98	0.09	62,62,62,62	0
86	OHX	5	3966	7/7	0.98	0.08	84,84,84,84	0
85	MG	5	3829	1/1	0.98	0.15	36,36,36,36	0
86	OHX	6	2096	7/7	0.98	0.08	134,134,134,134	0
86	OHX	2	2070	7/7	0.98	0.06	130,130,130,130	0
86	OHX	5	3972	7/7	0.98	0.08	106,106,106,106	0
86	OHX	5	3974	7/7	0.98	0.11	86,86,86,86	0
85	MG	1	3790	1/1	0.98	0.13	42,42,42,42	0
86	OHX	1	3950	7/7	0.98	0.13	99,99,99,99	0
86	OHX	1	3951	7/7	0.98	0.13	102,102,102,102	0
86	OHX	5	3981	7/7	0.98	0.09	100,100,100,100	0
86	OHX	1	3952	7/7	0.98	0.10	107,107,107,107	0
86	OHX	5	3983	7/7	0.98	0.09	91,91,91,91	0
86	OHX	6	2102	7/7	0.98	0.08	121,121,121,121	0
86	OHX	2	2072	7/7	0.98	0.07	126,126,126,126	0
86	OHX	5	3988	7/7	0.98	0.12	96,96,96,96	0
86	OHX	5	3989	7/7	0.98	0.09	100,100,100,100	0
86	OHX	5	3990	7/7	0.98	0.06	122,122,122,122	0
86	OHX	1	3956	7/7	0.98	0.07	113,113,113,113	0
86	OHX	1	3957	7/7	0.98	0.08	101,101,101,101	0
86	OHX	2	2073	7/7	0.98	0.06	148,148,148,148	0
85	MG	m6	201	1/1	0.98	0.07	32,32,32,32	0
85	MG	5	3729	1/1	0.98	0.10	38,38,38,38	0
86	OHX	5	3999	7/7	0.98	0.06	120,120,120,120	0
85	MG	5	3611	1/1	0.98	0.19	33,33,33,33	0
85	MG	1	3791	1/1	0.98	0.14	30,30,30,30	0
85	MG	5	3536	1/1	0.98	0.34	33,33,33,33	0
86	OHX	1	3966	7/7	0.98	0.09	110,110,110,110	0
85	MG	6	1945	1/1	0.98	0.33	42,42,42,42	0
86	OHX	5	4006	7/7	0.98	0.13	104,104,104,104	0
86	OHX	5	4007	7/7	0.98	0.16	110,110,110,110	0
85	MG	1	3845	1/1	0.98	0.18	38,38,38,38	0
86	OHX	5	4012	7/7	0.98	0.10	105,105,105,105	0
85	MG	1	3574	1/1	0.98	0.26	22,22,22,22	0
85	MG	5	3736	1/1	0.98	0.10	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	1	3971	7/7	0.98	0.11	84,84,84,84	0
86	OHX	5	4016	7/7	0.98	0.11	100,100,100,100	0
86	OHX	2	2083	7/7	0.98	0.07	136,136,136,136	0
86	OHX	5	4018	7/7	0.98	0.08	113,113,113,113	0
85	MG	5	3769	1/1	0.98	0.08	42,42,42,42	0
86	OHX	5	4020	7/7	0.98	0.08	124,124,124,124	0
86	OHX	5	4021	7/7	0.98	0.12	107,107,107,107	0
86	OHX	1	3975	7/7	0.98	0.19	93,93,93,93	0
86	OHX	5	4023	7/7	0.98	0.08	114,114,114,114	0
85	MG	5	3840	1/1	0.98	0.05	68,68,68,68	0
85	MG	5	3564	1/1	0.98	0.45	35,35,35,35	0
86	OHX	2	2087	7/7	0.98	0.08	131,131,131,131	0
86	OHX	1	3981	7/7	0.98	0.13	102,102,102,102	0
85	MG	5	3880	1/1	0.98	0.24	40,40,40,40	0
86	OHX	5	4030	7/7	0.98	0.12	92,92,92,92	0
85	MG	5	3805	1/1	0.98	0.13	41,41,41,41	0
85	MG	1	3692	1/1	0.98	0.13	34,34,34,34	0
86	OHX	1	3985	7/7	0.98	0.08	126,126,126,126	0
86	OHX	1	4087	7/7	0.98	0.15	93,93,93,93	0
86	OHX	5	4036	7/7	0.98	0.09	114,114,114,114	0
85	MG	5	3621	1/1	0.98	0.18	46,46,46,46	0
86	OHX	2	2092	7/7	0.98	0.13	116,116,116,116	0
86	OHX	5	4200	7/7	0.98	0.17	92,92,92,92	0
85	MG	5	3884	1/1	0.98	0.29	56,56,56,56	0
86	OHX	2	2094	7/7	0.98	0.07	146,146,146,146	0
85	MG	5	3773	1/1	0.98	0.07	52,52,52,52	0
85	MG	5	3566	1/1	0.98	0.17	28,28,28,28	0
85	MG	5	3408	1/1	0.98	0.23	32,32,32,32	0
85	MG	1	3409	1/1	0.98	0.15	23,23,23,23	0
86	OHX	1	3994	7/7	0.98	0.07	152,152,152,152	0
86	OHX	5	4046	7/7	0.98	0.15	105,105,105,105	0
85	MG	1	3560	1/1	0.98	0.30	38,38,38,38	0
85	MG	1	3609	1/1	0.98	0.07	45,45,45,45	0
85	MG	8	208	1/1	0.98	0.17	54,54,54,54	0
86	OHX	2	2025	7/7	0.98	0.13	91,91,91,91	0
86	OHX	6	2143	7/7	0.98	0.08	139,139,139,139	0
86	OHX	2	2028	7/7	0.98	0.11	100,100,100,100	0
86	OHX	2	2029	7/7	0.98	0.10	108,108,108,108	0
86	OHX	2	2030	7/7	0.98	0.10	100,100,100,100	0
86	OHX	5	4055	7/7	0.98	0.14	106,106,106,106	0
86	OHX	2	2031	7/7	0.98	0.07	116,116,116,116	0
85	MG	1	3719	1/1	0.98	0.17	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
85	MG	5	3597	1/1	0.98	0.27	18,18,18,18	0
86	OHX	2	2109	7/7	0.98	0.07	136,136,136,136	0
86	OHX	2	2038	7/7	0.98	0.09	103,103,103,103	0
86	OHX	2	2039	7/7	0.98	0.10	103,103,103,103	0
86	OHX	3	215	7/7	0.98	0.08	101,101,101,101	0
85	MG	M6	201	1/1	0.98	0.16	49,49,49,49	0
86	OHX	3	217	7/7	0.98	0.08	108,108,108,108	0
86	OHX	3	218	7/7	0.98	0.12	107,107,107,107	0
85	MG	5	3855	1/1	0.98	0.14	46,46,46,46	0
86	OHX	3	220	7/7	0.98	0.07	129,129,129,129	0
86	OHX	2	2048	7/7	0.98	0.06	118,118,118,118	0
85	MG	1	3707	1/1	0.98	0.35	33,33,33,33	0
86	OHX	2	2050	7/7	0.98	0.08	121,121,121,121	0
86	OHX	2	2051	7/7	0.98	0.07	112,112,112,112	0
86	OHX	2	2052	7/7	0.98	0.07	117,117,117,117	0
86	OHX	4	224	7/7	0.98	0.11	107,107,107,107	0
86	OHX	1	4016	7/7	0.98	0.09	113,113,113,113	0
85	MG	1	3447	1/1	0.98	0.10	29,29,29,29	0
85	MG	1	3737	1/1	0.98	0.18	42,42,42,42	0
86	OHX	1	3886	7/7	0.98	0.13	80,80,80,80	0
86	OHX	1	3892	7/7	0.98	0.13	83,83,83,83	0
86	OHX	1	4021	7/7	0.98	0.09	114,114,114,114	0
86	OHX	1	3893	7/7	0.98	0.10	81,81,81,81	0
86	OHX	5	4084	7/7	0.98	0.18	109,109,109,109	0
86	OHX	1	4023	7/7	0.98	0.07	126,126,126,126	0
86	OHX	1	3895	7/7	0.98	0.10	91,91,91,91	0
86	OHX	1	3896	7/7	0.98	0.12	87,87,87,87	0
86	OHX	1	3901	7/7	0.98	0.09	94,94,94,94	0
86	OHX	1	3904	7/7	0.98	0.10	90,90,90,90	0
85	MG	5	3602	1/1	0.98	0.05	48,48,48,48	0
86	OHX	1	4029	7/7	0.98	0.16	107,107,107,107	0
85	MG	1	3434	1/1	0.98	0.08	49,49,49,49	0
86	OHX	1	3911	7/7	0.98	0.07	105,105,105,105	0
86	OHX	1	3912	7/7	0.98	0.10	99,99,99,99	0
86	OHX	1	3913	7/7	0.98	0.09	102,102,102,102	0
86	OHX	7	217	7/7	0.98	0.09	88,88,88,88	0
86	OHX	7	218	7/7	0.98	0.10	98,98,98,98	0
86	OHX	7	220	7/7	0.98	0.14	98,98,98,98	0
86	OHX	7	221	7/7	0.98	0.14	103,103,103,103	0
86	OHX	7	222	7/7	0.98	0.08	109,109,109,109	0
85	MG	5	3439	1/1	0.98	0.33	29,29,29,29	0
86	OHX	1	3917	7/7	0.98	0.11	97,97,97,97	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	2	2058	7/7	0.98	0.09	120,120,120,120	0
86	OHX	O1	201	7/7	0.98	0.08	121,121,121,121	0
86	OHX	1	3922	7/7	0.98	0.11	111,111,111,111	0
86	OHX	8	216	7/7	0.98	0.07	121,121,121,121	0
86	OHX	8	217	7/7	0.98	0.08	108,108,108,108	0
86	OHX	2	2059	7/7	0.98	0.07	127,127,127,127	0
86	OHX	1	3925	7/7	0.98	0.09	107,107,107,107	0
86	OHX	2	2061	7/7	0.98	0.07	132,132,132,132	0
85	MG	1	3439	1/1	0.98	0.27	41,41,41,41	0
86	OHX	6	2051	7/7	0.98	0.12	79,79,79,79	0
86	OHX	6	2055	7/7	0.98	0.11	92,92,92,92	0
86	OHX	6	2059	7/7	0.98	0.09	100,100,100,100	0
86	OHX	6	2061	7/7	0.98	0.09	92,92,92,92	0
86	OHX	1	3932	7/7	0.98	0.08	99,99,99,99	0
85	MG	1	3613	1/1	0.98	0.17	32,32,32,32	0
86	OHX	2	2064	7/7	0.98	0.10	119,119,119,119	0
86	OHX	6	2069	7/7	0.98	0.08	106,106,106,106	0
86	OHX	1	4045	7/7	0.98	0.09	127,127,127,127	0
86	OHX	6	2072	7/7	0.98	0.17	94,94,94,94	0
86	OHX	l3	402	7/7	0.98	0.12	107,107,107,107	0
86	OHX	2	2065	7/7	0.98	0.11	114,114,114,114	0
86	OHX	1	3936	7/7	0.98	0.07	101,101,101,101	0
86	OHX	6	2076	7/7	0.98	0.08	115,115,115,115	0
86	OHX	1	3937	7/7	0.98	0.18	99,99,99,99	0
86	OHX	6	2078	7/7	0.98	0.12	101,101,101,101	0
86	OHX	1	3939	7/7	0.98	0.07	107,107,107,107	0
86	OHX	6	2083	7/7	0.98	0.07	122,122,122,122	0
86	OHX	6	2084	7/7	0.98	0.07	125,125,125,125	0
86	OHX	1	4050	7/7	0.98	0.07	148,148,148,148	0
85	MG	1	3605	1/1	0.98	0.07	54,54,54,54	0
86	OHX	1	3942	7/7	0.98	0.10	93,93,93,93	0
86	OHX	6	2089	7/7	0.98	0.07	133,133,133,133	0
86	OHX	6	2090	7/7	0.98	0.08	116,116,116,116	0
86	OHX	m6	202	7/7	0.98	0.10	98,98,98,98	0
86	OHX	5	3928	7/7	0.98	0.14	78,78,78,78	0
86	OHX	5	3934	7/7	0.98	0.12	92,92,92,92	0
86	OHX	5	3942	7/7	0.98	0.10	90,90,90,90	0
86	OHX	5	3944	7/7	0.98	0.14	101,101,101,101	0
86	OHX	5	3946	7/7	0.98	0.09	90,90,90,90	0
86	OHX	5	3948	7/7	0.98	0.08	76,76,76,76	0
86	OHX	1	4154	7/7	0.98	0.11	108,108,108,108	0
86	OHX	5	3952	7/7	0.98	0.09	87,87,87,87	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	3954	7/7	0.98	0.09	108,108,108,108	0
86	OHX	5	3957	7/7	0.98	0.11	100,100,100,100	0
86	OHX	5	3958	7/7	0.98	0.10	101,101,101,101	0
86	OHX	5	3992	7/7	0.99	0.09	107,107,107,107	0
86	OHX	5	3993	7/7	0.99	0.09	96,96,96,96	0
86	OHX	N1	201	7/7	0.99	0.07	69,69,69,69	0
86	OHX	N9	101	7/7	0.99	0.09	65,65,65,65	0
86	OHX	1	3929	7/7	0.99	0.09	107,107,107,107	0
86	OHX	1	3930	7/7	0.99	0.06	83,83,83,83	0
85	MG	1	3738	1/1	0.99	0.05	43,43,43,43	0
85	MG	5	3801	1/1	0.99	0.07	41,41,41,41	0
86	OHX	5	4000	7/7	0.99	0.07	109,109,109,109	0
85	MG	5	3531	1/1	0.99	0.29	21,21,21,21	0
85	MG	1	3726	1/1	0.99	0.08	33,33,33,33	0
86	OHX	6	2048	7/7	0.99	0.14	78,78,78,78	0
86	OHX	6	2049	7/7	0.99	0.12	70,70,70,70	0
86	OHX	6	2050	7/7	0.99	0.08	77,77,77,77	0
86	OHX	2	2041	7/7	0.99	0.07	100,100,100,100	0
86	OHX	6	2052	7/7	0.99	0.11	72,72,72,72	0
86	OHX	6	2053	7/7	0.99	0.10	81,81,81,81	0
86	OHX	5	4009	7/7	0.99	0.05	126,126,126,126	0
86	OHX	5	4010	7/7	0.99	0.07	76,76,76,76	0
86	OHX	5	4011	7/7	0.99	0.09	100,100,100,100	0
86	OHX	6	2054	7/7	0.99	0.11	84,84,84,84	0
86	OHX	2	2042	7/7	0.99	0.06	103,103,103,103	0
86	OHX	6	2056	7/7	0.99	0.12	77,77,77,77	0
86	OHX	6	2057	7/7	0.99	0.06	82,82,82,82	0
86	OHX	6	2058	7/7	0.99	0.06	94,94,94,94	0
85	MG	1	3598	1/1	0.99	0.38	14,14,14,14	0
86	OHX	5	4175	7/7	0.99	0.17	91,91,91,91	0
86	OHX	6	2060	7/7	0.99	0.08	91,91,91,91	0
86	OHX	1	3938	7/7	0.99	0.12	92,92,92,92	0
86	OHX	6	2062	7/7	0.99	0.07	96,96,96,96	0
86	OHX	6	2063	7/7	0.99	0.07	91,91,91,91	0
86	OHX	2	2044	7/7	0.99	0.10	104,104,104,104	0
86	OHX	1	3940	7/7	0.99	0.07	95,95,95,95	0
86	OHX	2	2045	7/7	0.99	0.06	108,108,108,108	0
86	OHX	6	2067	7/7	0.99	0.10	98,98,98,98	0
86	OHX	5	4026	7/7	0.99	0.06	120,120,120,120	0
86	OHX	6	2068	7/7	0.99	0.09	100,100,100,100	0
86	OHX	1	3865	7/7	0.99	0.12	62,62,62,62	0
86	OHX	6	2070	7/7	0.99	0.10	96,96,96,96	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	1	3866	7/7	0.99	0.12	54,54,54,54	0
86	OHX	1	3944	7/7	0.99	0.07	116,116,116,116	0
86	OHX	1	3867	7/7	0.99	0.10	58,58,58,58	0
86	OHX	1	3868	7/7	0.99	0.10	57,57,57,57	0
86	OHX	6	2075	7/7	0.99	0.06	91,91,91,91	0
86	OHX	5	4035	7/7	0.99	0.12	109,109,109,109	0
86	OHX	1	3947	7/7	0.99	0.07	101,101,101,101	0
86	OHX	1	3869	7/7	0.99	0.12	65,65,65,65	0
86	OHX	1	3870	7/7	0.99	0.09	67,67,67,67	0
86	OHX	6	2079	7/7	0.99	0.06	112,112,112,112	0
86	OHX	6	2080	7/7	0.99	0.09	110,110,110,110	0
86	OHX	1	3871	7/7	0.99	0.11	62,62,62,62	0
86	OHX	6	2082	7/7	0.99	0.06	111,111,111,111	0
86	OHX	1	3875	7/7	0.99	0.09	68,68,68,68	0
86	OHX	1	3876	7/7	0.99	0.10	73,73,73,73	0
86	OHX	1	3877	7/7	0.99	0.05	69,69,69,69	0
86	OHX	1	3954	7/7	0.99	0.11	79,79,79,79	0
86	OHX	6	2087	7/7	0.99	0.06	118,118,118,118	0
86	OHX	1	3955	7/7	0.99	0.06	111,111,111,111	0
86	OHX	1	3878	7/7	0.99	0.07	74,74,74,74	0
86	OHX	1	3879	7/7	0.99	0.12	70,70,70,70	0
86	OHX	1	3881	7/7	0.99	0.08	74,74,74,74	0
86	OHX	1	3882	7/7	0.99	0.10	71,71,71,71	0
86	OHX	6	2093	7/7	0.99	0.07	112,112,112,112	0
86	OHX	1	3960	7/7	0.99	0.12	77,77,77,77	0
86	OHX	1	3961	7/7	0.99	0.10	109,109,109,109	0
86	OHX	2	2046	7/7	0.99	0.06	121,121,121,121	0
86	OHX	5	4057	7/7	0.99	0.08	110,110,110,110	0
86	OHX	1	3887	7/7	0.99	0.06	71,71,71,71	0
86	OHX	1	3889	7/7	0.99	0.07	75,75,75,75	0
86	OHX	1	3890	7/7	0.99	0.12	79,79,79,79	0
86	OHX	1	3891	7/7	0.99	0.08	84,84,84,84	0
86	OHX	2	2047	7/7	0.99	0.04	133,133,133,133	0
86	OHX	s1	302	7/7	0.99	0.07	88,88,88,88	0
85	MG	1	3519	1/1	0.99	0.09	37,37,37,37	0
86	OHX	1	3894	7/7	0.99	0.07	77,77,77,77	0
85	MG	5	3844	1/1	0.99	0.05	77,77,77,77	0
85	MG	5	3563	1/1	0.99	0.32	27,27,27,27	0
86	OHX	5	4068	7/7	0.99	0.06	119,119,119,119	0
86	OHX	1	3972	7/7	0.99	0.07	110,110,110,110	0
86	OHX	1	3897	7/7	0.99	0.07	70,70,70,70	0
86	OHX	1	3898	7/7	0.99	0.06	81,81,81,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	1	3899	7/7	0.99	0.08	81,81,81,81	0
86	OHX	1	3900	7/7	0.99	0.08	76,76,76,76	0
86	OHX	2	2023	7/7	0.99	0.11	76,76,76,76	0
86	OHX	5	3901	7/7	0.99	0.10	52,52,52,52	0
86	OHX	5	3904	7/7	0.99	0.08	56,56,56,56	0
86	OHX	5	3908	7/7	0.99	0.09	66,66,66,66	0
86	OHX	5	3909	7/7	0.99	0.12	64,64,64,64	0
86	OHX	5	3910	7/7	0.99	0.09	63,63,63,63	0
86	OHX	5	4080	7/7	0.99	0.10	95,95,95,95	0
86	OHX	5	3912	7/7	0.99	0.12	66,66,66,66	0
86	OHX	5	3914	7/7	0.99	0.10	64,64,64,64	0
86	OHX	5	3916	7/7	0.99	0.11	63,63,63,63	0
86	OHX	5	3920	7/7	0.99	0.07	76,76,76,76	0
86	OHX	5	3922	7/7	0.99	0.07	70,70,70,70	0
86	OHX	5	3924	7/7	0.99	0.07	69,69,69,69	0
86	OHX	5	3925	7/7	0.99	0.12	75,75,75,75	0
86	OHX	5	3926	7/7	0.99	0.06	72,72,72,72	0
86	OHX	1	3978	7/7	0.99	0.15	84,84,84,84	0
86	OHX	5	3929	7/7	0.99	0.06	80,80,80,80	0
86	OHX	5	3931	7/7	0.99	0.08	84,84,84,84	0
86	OHX	5	3932	7/7	0.99	0.07	70,70,70,70	0
86	OHX	5	3933	7/7	0.99	0.08	78,78,78,78	0
86	OHX	1	3979	7/7	0.99	0.06	116,116,116,116	0
86	OHX	5	3936	7/7	0.99	0.06	84,84,84,84	0
86	OHX	5	3937	7/7	0.99	0.05	83,83,83,83	0
86	OHX	5	3938	7/7	0.99	0.05	72,72,72,72	0
86	OHX	5	3939	7/7	0.99	0.08	77,77,77,77	0
86	OHX	7	219	7/7	0.99	0.11	105,105,105,105	0
86	OHX	5	3940	7/7	0.99	0.11	81,81,81,81	0
86	OHX	5	3941	7/7	0.99	0.09	91,91,91,91	0
86	OHX	1	3902	7/7	0.99	0.07	94,94,94,94	0
86	OHX	5	3943	7/7	0.99	0.08	91,91,91,91	0
86	OHX	1	3903	7/7	0.99	0.07	87,87,87,87	0
86	OHX	5	3945	7/7	0.99	0.08	88,88,88,88	0
86	OHX	2	2024	7/7	0.99	0.10	83,83,83,83	0
86	OHX	5	3947	7/7	0.99	0.07	79,79,79,79	0
86	OHX	8	215	7/7	0.99	0.11	62,62,62,62	0
86	OHX	1	3905	7/7	0.99	0.12	79,79,79,79	0
86	OHX	5	3949	7/7	0.99	0.07	91,91,91,91	0
86	OHX	5	3950	7/7	0.99	0.10	97,97,97,97	0
85	MG	1	3823	1/1	0.99	0.07	60,60,60,60	0
86	OHX	2	2026	7/7	0.99	0.08	87,87,87,87	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	5	3953	7/7	0.99	0.11	106,106,106,106	0
86	OHX	5	4113	7/7	0.99	0.12	100,100,100,100	0
86	OHX	4	223	7/7	0.99	0.07	83,83,83,83	0
86	OHX	5	3956	7/7	0.99	0.06	95,95,95,95	0
86	OHX	1	3908	7/7	0.99	0.06	86,86,86,86	0
86	OHX	1	3909	7/7	0.99	0.06	83,83,83,83	0
86	OHX	5	3959	7/7	0.99	0.06	87,87,87,87	0
86	OHX	1	3910	7/7	0.99	0.08	90,90,90,90	0
86	OHX	5	3961	7/7	0.99	0.07	74,74,74,74	0
85	MG	5	3613	1/1	0.99	0.29	47,47,47,47	0
86	OHX	5	3963	7/7	0.99	0.07	96,96,96,96	0
85	MG	5	3764	1/1	0.99	0.07	46,46,46,46	0
85	MG	5	3614	1/1	0.99	0.03	37,37,37,37	0
86	OHX	5	3967	7/7	0.99	0.08	98,98,98,98	0
86	OHX	1	3914	7/7	0.99	0.07	101,101,101,101	0
86	OHX	1	3915	7/7	0.99	0.06	88,88,88,88	0
86	OHX	5	3970	7/7	0.99	0.07	93,93,93,93	0
85	MG	1	3798	1/1	0.99	0.10	62,62,62,62	0
86	OHX	2	2032	7/7	0.99	0.08	105,105,105,105	0
86	OHX	5	3973	7/7	0.99	0.12	97,97,97,97	0
86	OHX	1	3996	7/7	0.99	0.10	90,90,90,90	0
86	OHX	5	3975	7/7	0.99	0.08	84,84,84,84	0
86	OHX	1	3918	7/7	0.99	0.07	96,96,96,96	0
86	OHX	1	3919	7/7	0.99	0.09	83,83,83,83	0
86	OHX	5	3978	7/7	0.99	0.07	107,107,107,107	0
86	OHX	2	2060	7/7	0.99	0.07	113,113,113,113	0
86	OHX	5	3980	7/7	0.99	0.12	87,87,87,87	0
86	OHX	1	3921	7/7	0.99	0.07	80,80,80,80	0
85	MG	5	3824	1/1	0.99	0.06	56,56,56,56	0
86	OHX	n3	203	7/7	0.99	0.07	97,97,97,97	0
86	OHX	n9	102	7/7	0.99	0.09	70,70,70,70	0
86	OHX	1	3923	7/7	0.99	0.06	88,88,88,88	0
86	OHX	q2	502	7/7	0.99	0.07	85,85,85,85	0
86	OHX	5	3984	7/7	0.99	0.10	88,88,88,88	0
86	OHX	2	2034	7/7	0.99	0.09	106,106,106,106	0
86	OHX	2	2035	7/7	0.99	0.11	103,103,103,103	0
88	ZN	E1	501	1/1	0.99	0.03	124,124,124,124	0
86	OHX	5	3987	7/7	0.99	0.09	89,89,89,89	0
86	OHX	1	3926	7/7	0.99	0.05	94,94,94,94	0
88	ZN	d9	101	1/1	0.99	0.03	92,92,92,92	0
86	OHX	1	3927	7/7	0.99	0.07	91,91,91,91	0
86	OHX	2	2036	7/7	0.99	0.05	98,98,98,98	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	1	3873	7/7	1.00	0.07	65,65,65,65	0
86	OHX	5	3911	7/7	1.00	0.09	52,52,52,52	0
86	OHX	1	3883	7/7	1.00	0.09	72,72,72,72	0
86	OHX	5	3913	7/7	1.00	0.07	59,59,59,59	0
86	OHX	1	3884	7/7	1.00	0.09	78,78,78,78	0
86	OHX	5	3915	7/7	1.00	0.07	70,70,70,70	0
86	OHX	4	222	7/7	1.00	0.09	58,58,58,58	0
86	OHX	5	3917	7/7	1.00	0.08	72,72,72,72	0
86	OHX	5	3918	7/7	1.00	0.05	66,66,66,66	0
86	OHX	5	3919	7/7	1.00	0.06	65,65,65,65	0
86	OHX	1	3885	7/7	1.00	0.08	73,73,73,73	0
86	OHX	5	3921	7/7	1.00	0.07	70,70,70,70	0
86	OHX	1	3874	7/7	1.00	0.05	60,60,60,60	0
86	OHX	5	3923	7/7	1.00	0.07	70,70,70,70	0
86	OHX	5	3955	7/7	1.00	0.06	79,79,79,79	0
86	OHX	1	3862	7/7	1.00	0.12	53,53,53,53	0
86	OHX	6	2047	7/7	1.00	0.10	62,62,62,62	0
86	OHX	5	3991	7/7	1.00	0.05	89,89,89,89	0
86	OHX	1	3888	7/7	1.00	0.05	70,70,70,70	0
86	OHX	5	3927	7/7	1.00	0.05	62,62,62,62	0
86	OHX	1	3863	7/7	1.00	0.08	52,52,52,52	0
86	OHX	n1	201	7/7	1.00	0.07	62,62,62,62	0
86	OHX	1	3864	7/7	1.00	0.11	58,58,58,58	0
86	OHX	5	3930	7/7	1.00	0.04	80,80,80,80	0
86	OHX	2	2027	7/7	1.00	0.08	78,78,78,78	0
86	OHX	5	3964	7/7	1.00	0.04	96,96,96,96	0
86	OHX	5	3902	7/7	1.00	0.10	47,47,47,47	0
86	OHX	5	3903	7/7	1.00	0.10	50,50,50,50	0
88	ZN	D6	500	1/1	1.00	0.03	83,83,83,83	0
86	OHX	1	3861	7/7	1.00	0.10	46,46,46,46	0
88	ZN	D9	101	1/1	1.00	0.04	84,84,84,84	0
86	OHX	5	3935	7/7	1.00	0.06	74,74,74,74	0
88	ZN	O7	101	1/1	1.00	0.02	45,45,45,45	0
88	ZN	Q0	500	1/1	1.00	0.02	50,50,50,50	0
86	OHX	5	3905	7/7	1.00	0.10	56,56,56,56	0
88	ZN	Q3	501	1/1	1.00	0.01	63,63,63,63	0
88	ZN	d6	101	1/1	1.00	0.02	64,64,64,64	0
86	OHX	5	3906	7/7	1.00	0.11	58,58,58,58	0
86	OHX	5	3907	7/7	1.00	0.08	56,56,56,56	0
86	OHX	1	3880	7/7	1.00	0.04	65,65,65,65	0
88	ZN	o7	102	1/1	1.00	0.01	44,44,44,44	0
88	ZN	q0	201	1/1	1.00	0.01	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
86	OHX	1	3872	7/7	1.00	0.07	64,64,64,64	0
88	ZN	q3	501	1/1	1.00	0.02	69,69,69,69	0

6.5 Other polymers (i)

There are no such residues in this entry.