



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 3, 2024 – 01:00 am GMT

PDB ID : 5DGE
Title : Coping with proline stalling: structural basis of hypusine-induced protein synthesis by the eukaryotic ribosome
Authors : Melnikov, S.; Mailliot, J.; Shin, B.-S.; Rigger, L.; Yusupova, G.; Micura, R.; Dever, T.E.; Yusupov, M.
Deposited on : 2015-08-27
Resolution : 3.45 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

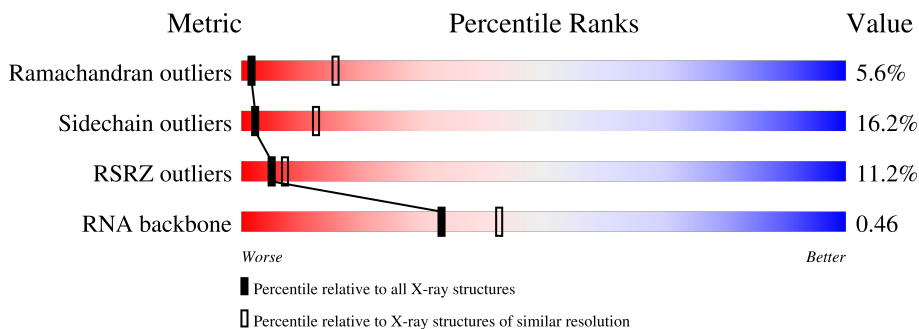
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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.



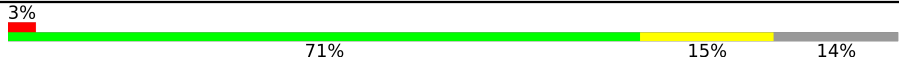
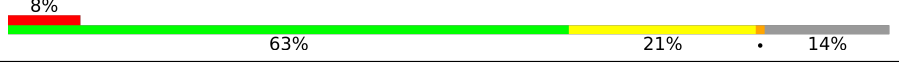
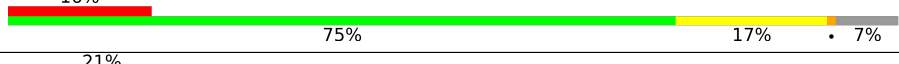



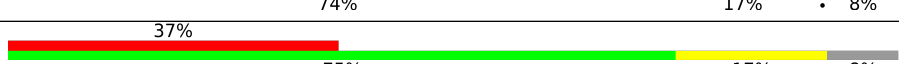
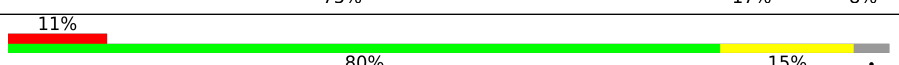
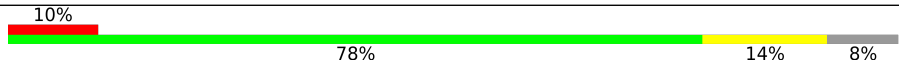


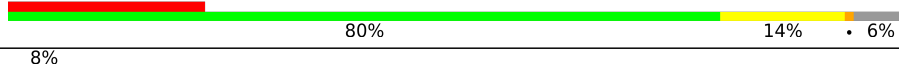
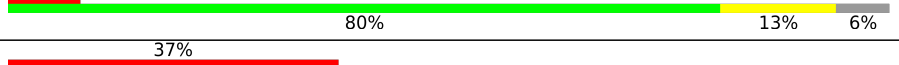

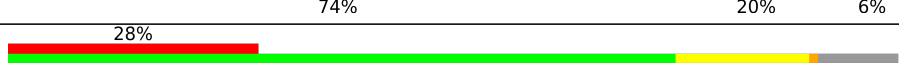




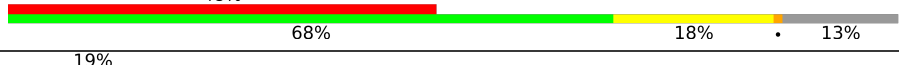





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)
RNA backbone	3102	1036 (3.96-2.96)

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

Mol	Chain	Length	Quality of chain
1	2	1800	
1	6	1800	
2	S0	251	
2	s0	251	
3	S1	254	
3	s1	254	

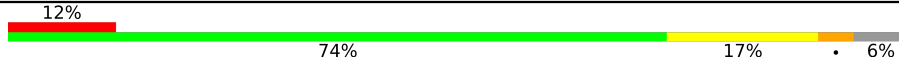
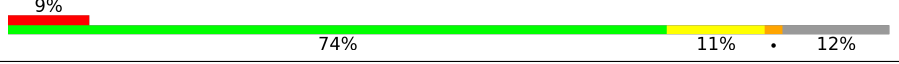
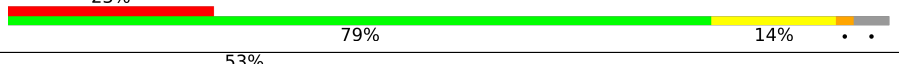


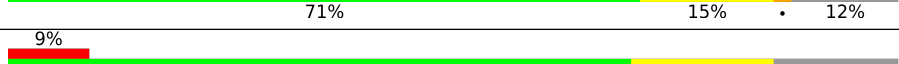
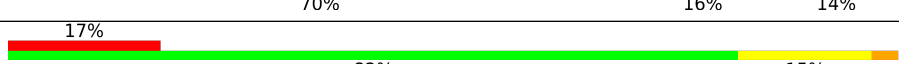
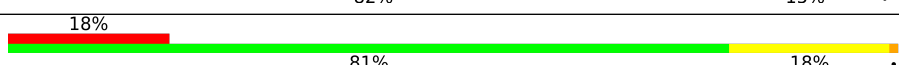

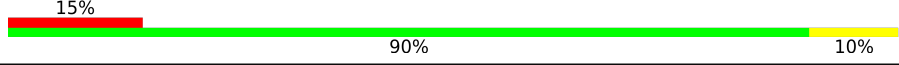

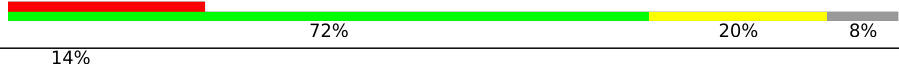
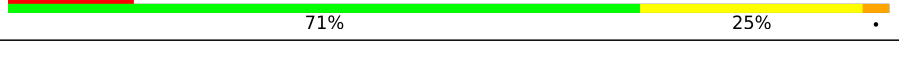

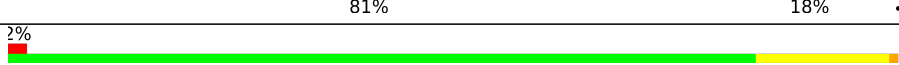




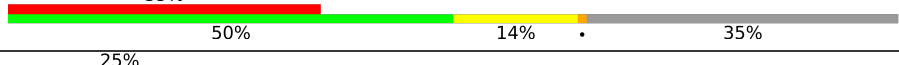





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Mol	Chain	Length	Quality of chain
4	S2	253	
4	s2	253	
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
12	c0	105	
13	C1	155	
13	c1	155	
14	C2	142	
14	c2	142	
15	C3	150	
15	c3	150	
16	C4	136	

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Mol	Chain	Length	Quality of chain
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	
28	D6	97	
28	d6	97	

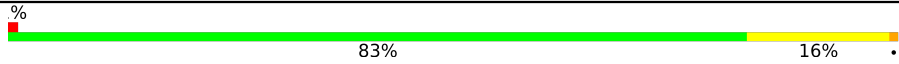
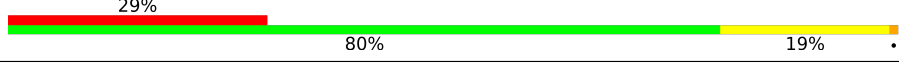
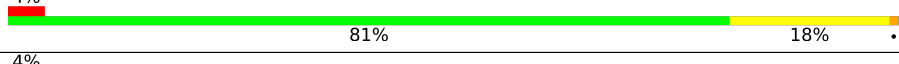


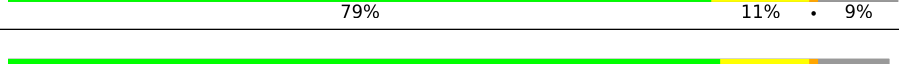
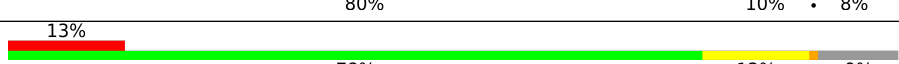
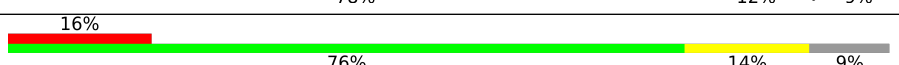
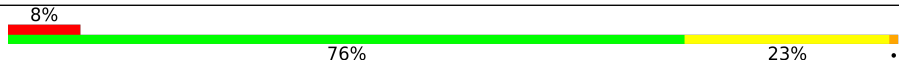


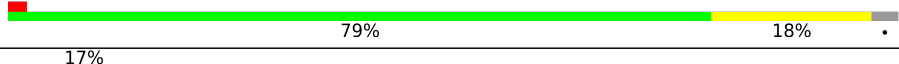
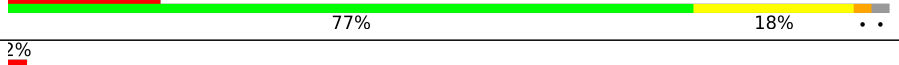

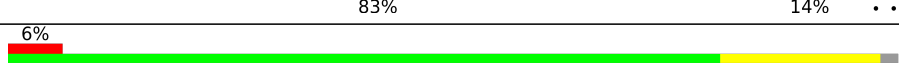




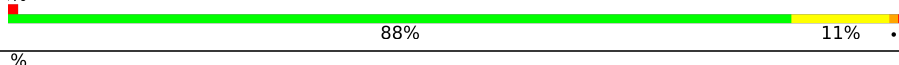
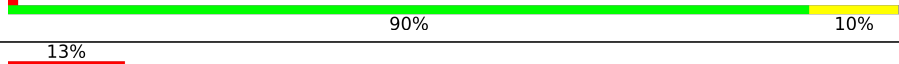




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Mol	Chain	Length	Quality of chain
29	D7	81	36% 91% 9%
29	d7	81	19% 79% 19%
30	D8	66	42% 74% 20% 5%
30	d8	66	41% 67% 27% 5%
31	D9	55	18% 76% 20%
31	d9	55	42% 73% 24%
32	E0	63	49% 81% 13% 5%
32	e0	63	27% 67% 25% 6%
33	E1	76	28% 67% 25% 7%
33	e1	76	49% 58% 38%
34	SR	318	26% 89% 10%
34	sR	318	48% 90% 9%
35	SM	273	16% 46% 11% 42%
35	sM	273	9% 31% 7% 62%
36	1	3396	2% 69% 22% 7%
36	5	3396	0% 69% 22% 7%
37	3	121	82% 18%
37	7	121	84% 14%
38	4	158	0% 76% 24%
38	8	158	79% 19%
39	L2	253	5% 82% 16%
39	l2	253	0% 82% 16%
40	L3	386	2% 79% 20%
40	l3	386	2% 83% 16%
41	L4	361	0% 82% 17%

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Mol	Chain	Length	Quality of chain
41	l4	361	 % 83% 16%
42	L5	296	 29% 80% 19%
42	l5	296	 4% 81% 18%
43	L6	175	 4% 77% 12% 11%
43	l6	175	 5% 74% 15% 10%
44	L7	243	 79% 11% 9%
44	l7	243	 80% 10% 8%
45	L8	255	 13% 78% 12% 9%
45	l8	255	 16% 76% 14% 9%
46	L9	191	 8% 76% 23%
46	l9	191	 2% 81% 17%
47	M0	220	 7% 79% 16%
47	m0	220	 2% 79% 18%
48	M1	173	 17% 77% 18%
48	m1	173	 2% 77% 20%
49	M3	198	 2% 83% 14%
49	m3	198	 6% 80% 18%
50	M4	137	 82% 18%
50	m4	137	 83% 16%
51	M5	203	 8% 83% 17%
51	m5	203	 19% 87% 12%
52	M6	198	 % 88% 11%
52	m6	198	 % 90% 10%
53	M7	183	 13% 80% 19%
53	m7	183	 % 72% 13% 15%

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Mol	Chain	Length	Quality of chain
54	M8	185	2% 85% 14%
54	m8	185	2% 86% 12%
55	M9	188	16% 89% 11%
55	m9	188	5% 86% 13%
56	N0	172	3% 81% 19%
56	n0	172	% 78% 21%
57	N1	159	% 81% 18%
57	n1	159	% 81% 18%
58	N2	120	22% 70% 13% 17%
58	n2	120	17% 66% 16% 18%
59	N3	136	2% 88% 12%
59	n3	136	% 88% 12%
60	N4	155	18% 55% 8% 37%
60	n4	155	13% 75% 10% 13%
61	N5	141	9% 66% 20% 14%
61	n5	141	6% 71% 13% 15%
62	N6	126	7% 82% 16%
62	n6	126	87% 13%
63	N7	135	49% 85% 13%
63	n7	135	17% 80% 19%
64	N8	148	7% 84% 14%
64	n8	148	9% 79% 20%
65	N9	58	83% 16%
65	n9	58	83% 16%
66	O0	104	13% 75% 17% 7%

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Mol	Chain	Length	Quality of chain
66	o0	104	8% 84% 12% .
67	O1	112	29% 78% 19% ..
67	o1	112	16% 79% 19% .
68	O2	129	2% 81% 16% ..
68	o2	129	2% 76% 22% ..
69	O3	106	91% 8% .
69	o3	106	3% 88% 11% .
70	O4	121	33% 78% 14% . 7%
70	o4	121	20% 78% 15% 7%
71	O5	119	% 83% 16% .
71	o5	119	2% 82% 17% .
72	O6	99	13% 77% 21% .
72	o6	99	13% 78% 19% .
73	O7	87	79% 21%
73	o7	87	78% 21% .
74	O8	77	4% 78% 22%
74	o8	77	42% 83% 17%
75	O9	50	82% 16% .
75	o9	50	2% 90% 10%
76	Q0	52	13% 83% 15% .
76	q0	52	2% 75% 25%
77	Q1	25	76% 24%
77	q1	25	76% 24%
78	Q2	105	8% 79% 19% ..
78	q2	105	% 76% 23% .

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Mol	Chain	Length	Quality of chain
79	Q3	91	
79	q3	91	
80	m2	165	
81	p0	311	
82	p1	106	
82	p2	106	
83	f	157	
84	B	3	
84	C	3	

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
83	5CT	f	51	X	-	-	-
85	MG	1	3407	-	-	-	X
85	MG	1	3423	-	-	-	X
85	MG	1	3449	-	-	-	X
85	MG	1	3459	-	-	-	X
85	MG	1	3491	-	-	-	X
85	MG	1	3523	-	-	-	X
85	MG	1	3608	-	-	-	X
85	MG	1	3617	-	-	-	X
85	MG	1	3634	-	-	-	X
85	MG	1	3639	-	-	-	X
85	MG	1	3642	-	-	-	X
85	MG	1	3662	-	-	-	X
85	MG	1	3663	-	-	-	X
85	MG	1	3665	-	-	-	X
85	MG	1	3692	-	-	-	X
85	MG	1	3708	-	-	-	X
85	MG	1	3714	-	-	-	X
85	MG	1	3723	-	-	-	X
85	MG	1	3729	-	-	-	X
85	MG	1	3737	-	-	-	X
85	MG	1	3742	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	1	3745	-	-	-	X
85	MG	1	3754	-	-	-	X
85	MG	2	1904	-	-	-	X
85	MG	2	1912	-	-	-	X
85	MG	2	1939	-	-	-	X
85	MG	2	1943	-	-	-	X
85	MG	2	1949	-	-	-	X
85	MG	2	1958	-	-	-	X
85	MG	2	1965	-	-	-	X
85	MG	2	1973	-	-	-	X
85	MG	2	1974	-	-	-	X
85	MG	2	1985	-	-	-	X
85	MG	2	1989	-	-	-	X
85	MG	3	203	-	-	-	X
85	MG	4	203	-	-	-	X
85	MG	4	205	-	-	-	X
85	MG	4	214	-	-	-	X
85	MG	5	3418	-	-	-	X
85	MG	5	3426	-	-	-	X
85	MG	5	3444	-	-	-	X
85	MG	5	3446	-	-	-	X
85	MG	5	3448	-	-	-	X
85	MG	5	3460	-	-	-	X
85	MG	5	3468	-	-	-	X
85	MG	5	3469	-	-	-	X
85	MG	5	3483	-	-	-	X
85	MG	5	3503	-	-	-	X
85	MG	5	3543	-	-	-	X
85	MG	5	3552	-	-	-	X
85	MG	5	3599	-	-	-	X
85	MG	5	3600	-	-	-	X
85	MG	5	3613	-	-	-	X
85	MG	5	3625	-	-	-	X
85	MG	5	3637	-	-	-	X
85	MG	5	3638	-	-	-	X
85	MG	5	3649	-	-	-	X
85	MG	5	3672	-	-	-	X
85	MG	5	3680	-	-	-	X
85	MG	5	3685	-	-	-	X
85	MG	5	3690	-	-	-	X
85	MG	5	3698	-	-	-	X
85	MG	5	3714	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	5	3741	-	-	-	X
85	MG	5	3746	-	-	-	X
85	MG	5	3750	-	-	-	X
85	MG	5	3773	-	-	-	X
85	MG	5	3816	-	-	-	X
85	MG	6	1915	-	-	-	X
85	MG	6	1932	-	-	-	X
85	MG	6	1937	-	-	-	X
85	MG	6	1982	-	-	-	X
85	MG	6	1985	-	-	-	X
85	MG	6	1986	-	-	-	X
85	MG	6	1990	-	-	-	X
85	MG	6	1996	-	-	-	X
85	MG	6	2004	-	-	-	X
85	MG	6	2008	-	-	-	X
85	MG	7	207	-	-	-	X
85	MG	8	207	-	-	-	X
85	MG	8	209	-	-	-	X
85	MG	D3	201	-	-	-	X
85	MG	M7	201	-	-	-	X
85	MG	14	401	-	-	-	X
86	OHX	5	4062	-	-	-	X
86	OHX	5	4153	-	-	-	X
86	OHX	5	4166	-	-	-	X
86	OHX	6	2183	-	-	-	X

2 Entry composition [i](#)

There are 90 unique types of molecules in this entry. The entry contains 413121 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
			Total	C	N	O	S			
13	C1	155	1214	775	230	206	3	0	0	0
13	c1	146	1168	747	221	197	3	0	0	0

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			

- 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			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	D7	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			
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			
32	e0	62	Total	C	N	O	S	0	0	0
			491	309	101	80	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
			2436	1541	418	469	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	sR	318	2441	1544	418	471	8	0	0	0

- Molecule 35 is a protein called Suppressor protein STM1.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
39	L2	252	1914	1191	388	334	1	0	0	0
39	l2	252	1912	1190	388	333	1	0	0	0

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	L8	233	1804	1151	323	327	3	0	0	0
45	l8	231	1764	1131	316	314	3	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L8	119	ALA	GLY	conflict	UNP P17076
l8	119	ALA	GLY	conflict	UNP P17076

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M1	3	THR	ALA	conflict	UNP P0C0W9
m1	3	THR	ALA	conflict	UNP P0C0W9

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			742	479	124	138	1			
66	o0	100	Total	C	N	O	S	0	0	0
			766	492	128	145	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			

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

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

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

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

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

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

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

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

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

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

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

- Molecule 76 is a protein called 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 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
80	m2	150	Total	C	N	O	0	0	0
			739	439	150	150			

- 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
			1077	687	192	195	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
82	p1	47	Total	C	N	O	0	0	0
			235	141	47	47			
82	p2	46	Total	C	N	O	0	0	0
			230	138	46	46			

- Molecule 83 is a protein called Eukaryotic translation initiation factor 5A-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
83	f	148	Total	C	N	O	S	0	0	0
			1122	696	189	228	9			

- Molecule 84 is a RNA chain called DNA (5'-R(*CP*CP*(NA))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
84	B	3	Total	C	N	O	P	0	0	0
			59	28	12	17	2			
84	C	3	Total	C	N	O	P	0	0	0
			62	28	12	19	3			

- Molecule 85 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	2	90	Total	Mg	0	0
			90	90		
85	S2	1	Total	Mg	0	0
			1	1		
85	D3	1	Total	Mg	0	0
			1	1		
85	SM	1	Total	Mg	0	0
			1	1		
85	1	361	Total	Mg	0	0
			361	361		
85	3	8	Total	Mg	0	0
			8	8		
85	4	15	Total	Mg	0	0
			15	15		
85	L2	2	Total	Mg	0	0
			2	2		
85	L3	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	L6	1	Total 1	Mg 1	0	0
85	L7	3	Total 3	Mg 3	0	0
85	M0	2	Total 2	Mg 2	0	0
85	M5	2	Total 2	Mg 2	0	0
85	M6	3	Total 3	Mg 3	0	0
85	M7	4	Total 4	Mg 4	0	0
85	M9	1	Total 1	Mg 1	0	0
85	N3	1	Total 1	Mg 1	0	0
85	N6	1	Total 1	Mg 1	0	0
85	N8	3	Total 3	Mg 3	0	0
85	O4	1	Total 1	Mg 1	0	0
85	O7	2	Total 2	Mg 2	0	0
85	Q2	1	Total 1	Mg 1	0	0
85	6	111	Total 111	Mg 111	0	0
85	s4	1	Total 1	Mg 1	0	0
85	s8	2	Total 2	Mg 2	0	0
85	c8	2	Total 2	Mg 2	0	0
85	c9	1	Total 1	Mg 1	0	0
85	d2	1	Total 1	Mg 1	0	0
85	d3	1	Total 1	Mg 1	0	0
85	d6	1	Total 1	Mg 1	0	0

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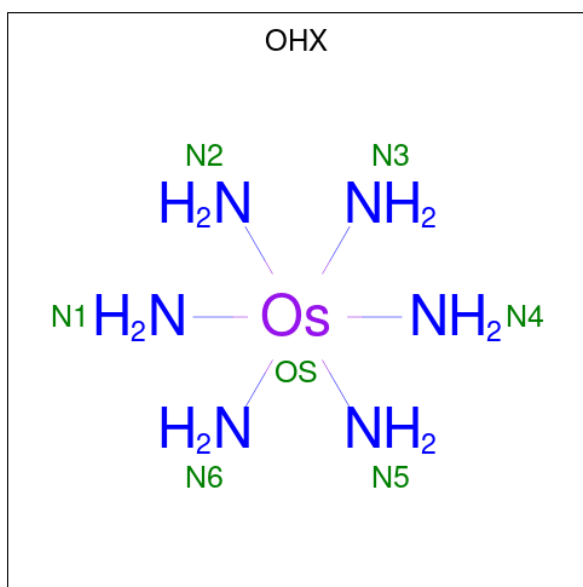
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	5	415	Total Mg 415 415	0	0
85	7	13	Total Mg 13 13	0	0
85	8	10	Total Mg 10 10	0	0
85	12	2	Total Mg 2 2	0	0
85	13	2	Total Mg 2 2	0	0
85	14	1	Total Mg 1 1	0	0
85	15	1	Total Mg 1 1	0	0
85	17	2	Total Mg 2 2	0	0
85	m0	1	Total Mg 1 1	0	0
85	m3	1	Total Mg 1 1	0	0
85	m5	3	Total Mg 3 3	0	0
85	m7	3	Total Mg 3 3	0	0
85	n0	1	Total Mg 1 1	0	0
85	n3	1	Total Mg 1 1	0	0
85	n6	1	Total Mg 1 1	0	0
85	n8	2	Total Mg 2 2	0	0
85	o2	1	Total Mg 1 1	0	0
85	o3	1	Total Mg 1 1	0	0
85	o4	1	Total Mg 1 1	0	0
85	q1	1	Total Mg 1 1	0	0
85	q2	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	q3	1	Total Mg 1 1	0	0
85	f	1	Total Mg 1 1	0	0
85	B	1	Total Mg 1 1	0	0
85	C	1	Total Mg 1 1	0	0

- Molecule 86 is osmium (III) hexammine (three-letter code: OHX) (formula: H₁₂N₆Os).



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	1	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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
86	2	1	7	6	1	0	0
86	2	1	7	6	1	0	0
86	2	1	7	6	1	0	0
86	2	1	7	6	1	0	0
86	2	1	7	6	1	0	0
86	2	1	7	6	1	0	0
86	2	1	7	6	1	0	0
86	2	1	7	6	1	0	0
86	2	1	7	6	1	0	0
86	S1	1	7	6	1	0	0
86	S6	1	7	6	1	0	0
86	S8	1	7	6	1	0	0
86	S9	1	7	6	1	0	0
86	C3	1	7	6	1	0	0
86	C5	1	7	6	1	0	0
86	C8	1	7	6	1	0	0
86	D9	1	7	6	1	0	0
86	SR	1	7	6	1	0	0
86	1	1	7	6	1	1	0
86	1	1	7	6	1	1	0
86	1	1	7	6	1	0	0
86	1	1	7	6	1	1	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
86	3	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	1	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	4	1	7	6	1	0	0
86	L3	1	7	6	1	0	0
86	L3	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
86	L3	1	7	6	1	0	0
86	L4	1	7	6	1	0	0
86	L5	1	7	6	1	0	0
86	M0	1	7	6	1	0	0
86	M0	1	7	6	1	0	0
86	M5	1	7	6	1	0	0
86	M5	1	7	6	1	0	0
86	M6	1	7	6	1	0	0
86	M7	1	7	6	1	0	0
86	M8	1	7	6	1	0	0
86	M9	1	7	6	1	0	0
86	N8	1	7	6	1	0	0
86	N9	1	7	6	1	0	0
86	O1	1	7	6	1	0	0
86	O3	1	7	6	1	0	0
86	O4	1	7	6	1	0	0
86	O7	1	7	6	1	0	0
86	O9	1	7	6	1	0	0
86	Q2	1	7	6	1	0	0
86	6	1	7	6	1	2	0
86	6	1	7	6	1	1	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
86	n3	1	7	6	1	0	0
86	n9	1	7	6	1	0	0
86	o3	1	7	6	1	0	0
86	o6	1	7	6	1	0	0
86	o7	1	7	6	1	0	0
86	o7	1	7	6	1	0	0
86	q2	1	7	6	1	0	0

- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn).

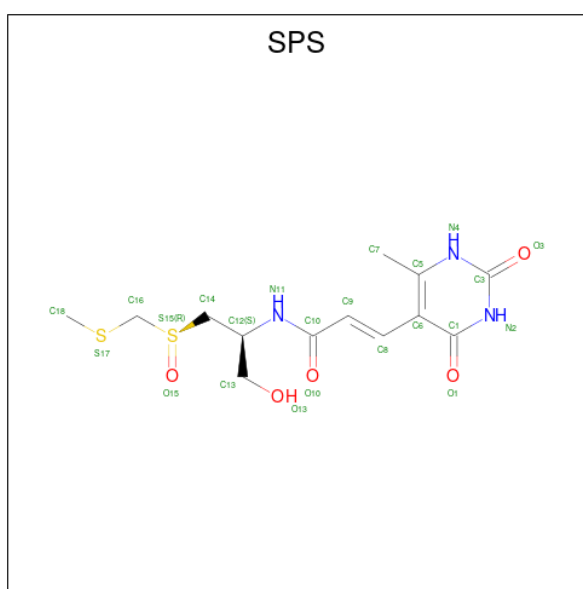
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
87	D6	1	1	1	0	0
87	D7	1	1	1	0	0
87	D9	1	1	1	0	0
87	E1	1	1	1	0	0
87	O7	1	1	1	0	0
87	Q0	1	1	1	0	0
87	Q2	1	1	1	0	0
87	Q3	1	1	1	0	0
87	d6	1	1	1	0	0
87	d7	1	1	1	0	0
87	d9	1	1	1	0	0
87	e1	1	1	1	0	0

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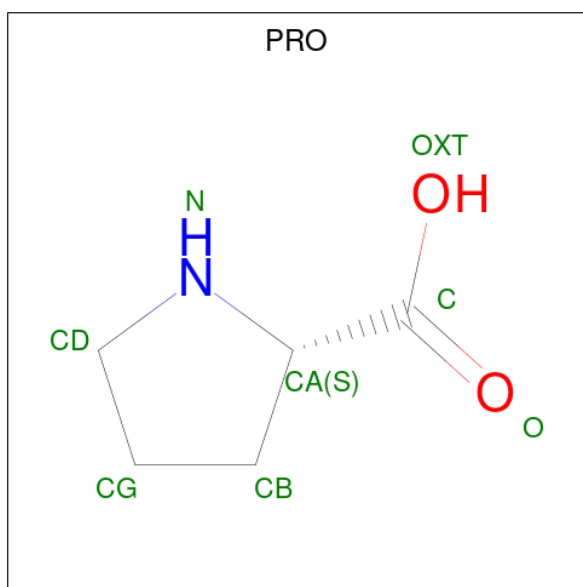
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	o7	1	Total	Zn	0	0
			1	1		
87	q0	1	Total	Zn	0	0
			1	1		
87	q2	1	Total	Zn	0	0
			1	1		
87	q3	1	Total	Zn	0	0
			1	1		

- Molecule 88 is SPARSOMYCIN (three-letter code: SPS) (formula: $C_{13}H_{19}N_3O_5S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
88	1	1	23	13	3	5	2	0	0
88	5	1	23	13	3	5	2	0	0

- Molecule 89 is PROLINE (three-letter code: PRO) (formula: $C_5H_9NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
89	1	1	Total	C	N	O	0	0
			7	5	1	1		
89	5	1	Total	C	N	O	0	0
			7	5	1	1		
89	B	1	Total	C	N	O	0	0
			7	5	1	1		
89	C	1	Total	C	N	O	0	0
			7	5	1	1		

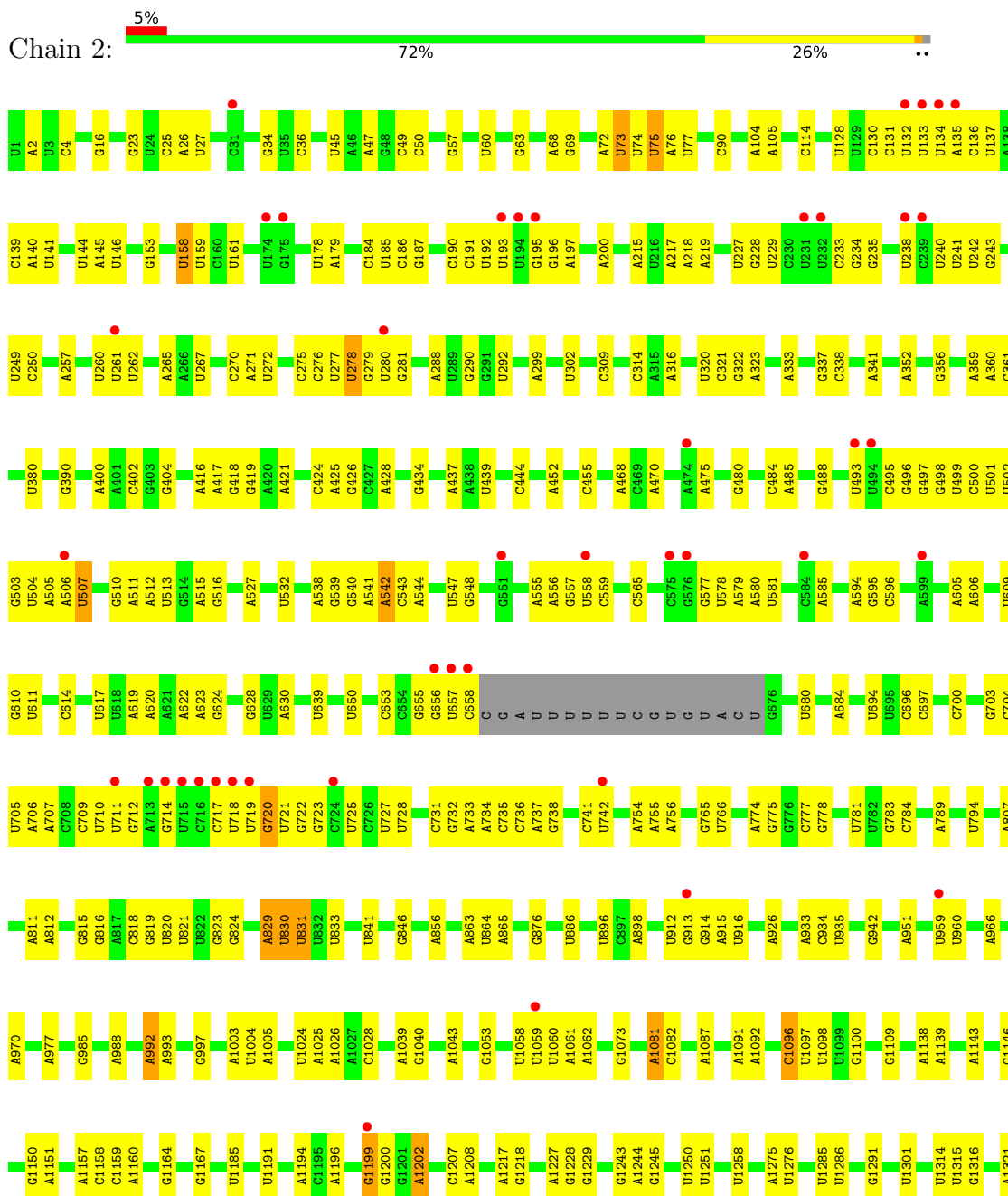
- Molecule 90 is water.

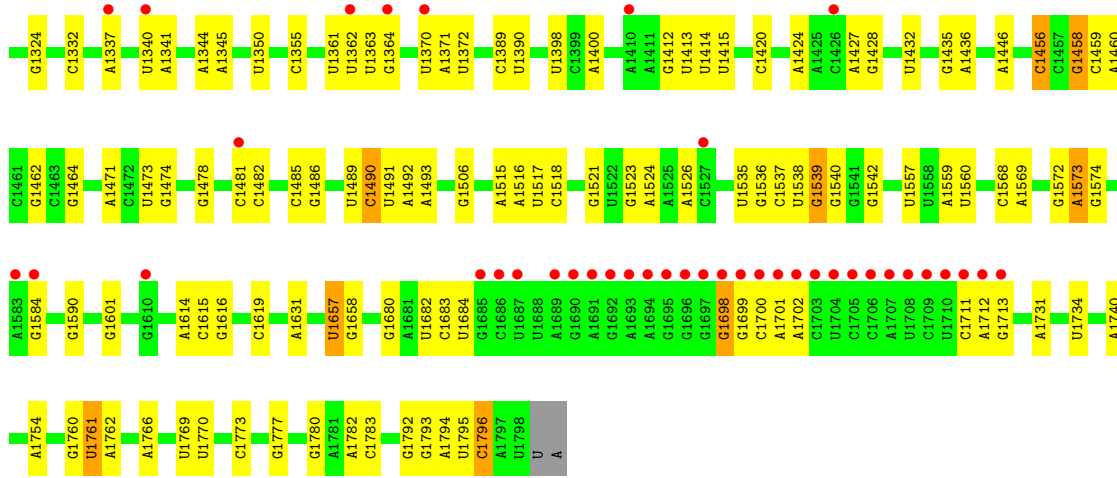
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
90	5	6	Total	O	0	0
			6	6		
90	f	6	Total	O	0	0
			6	6		

3 Residue-property plots

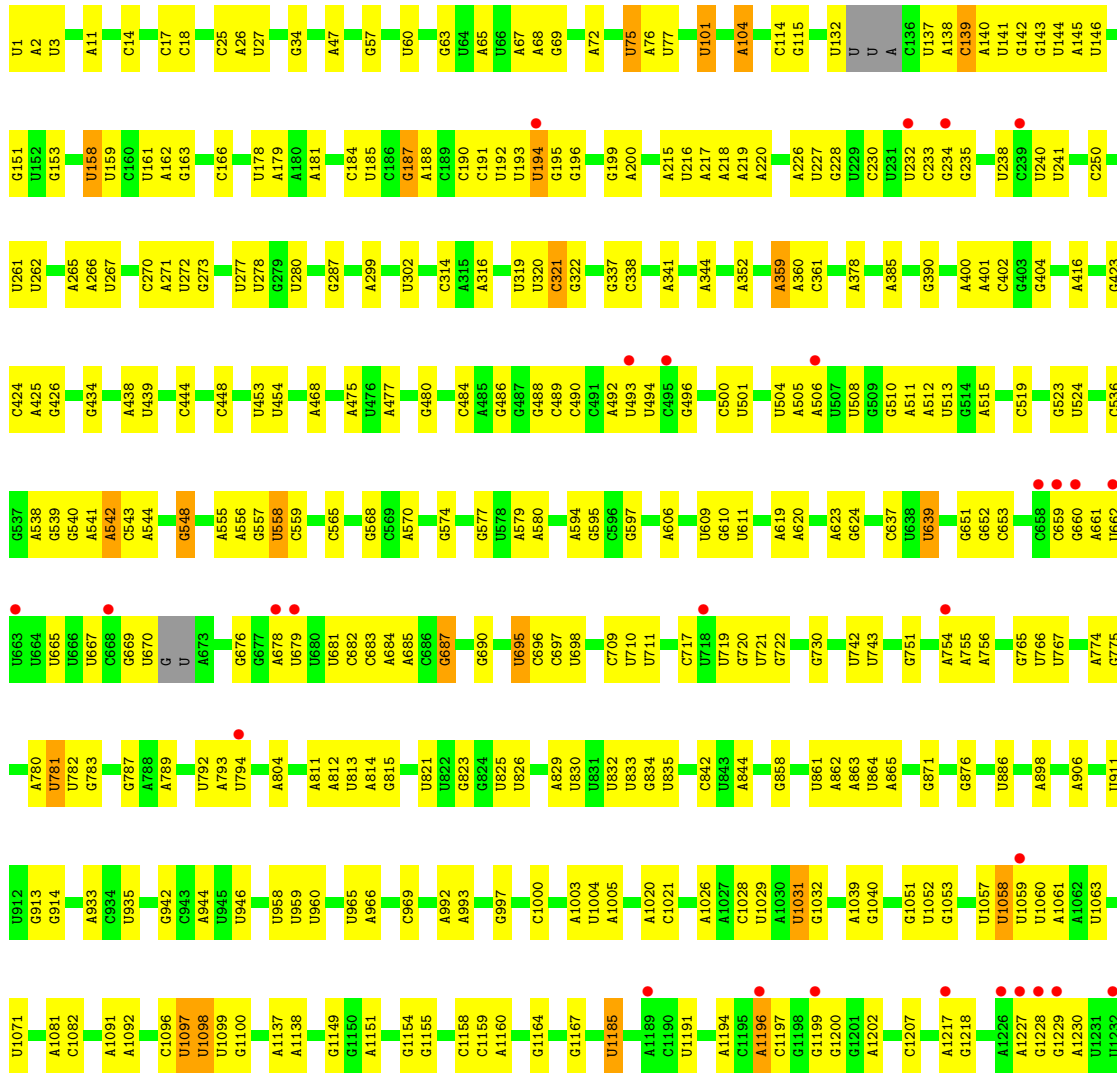
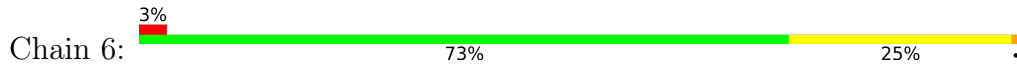
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 18S ribosomal RNA



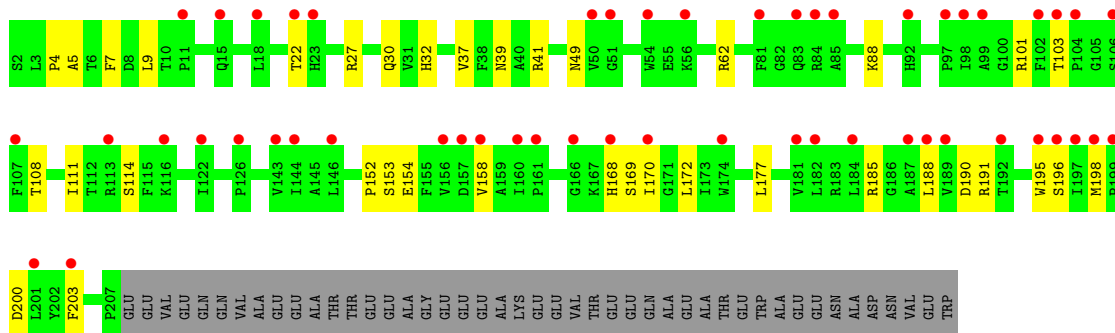


• Molecule 1: 18S ribosomal RNA

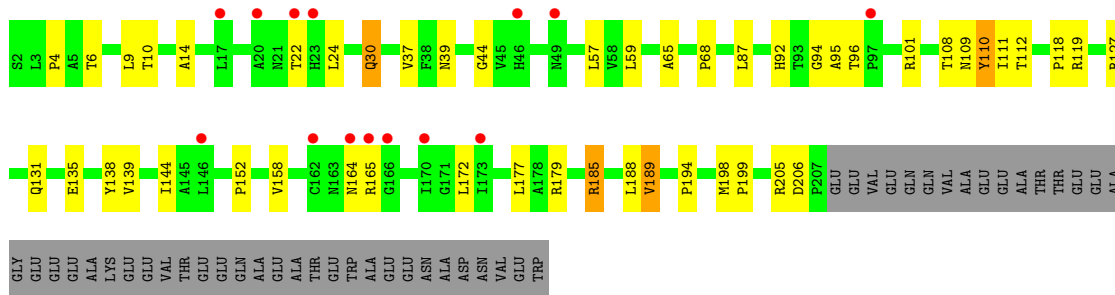




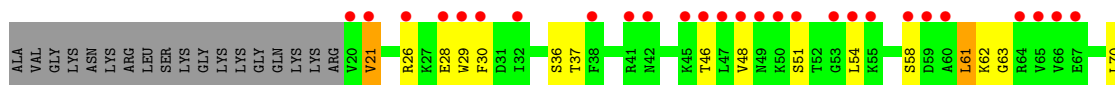
• Molecule 2: 40S ribosomal protein S0-A

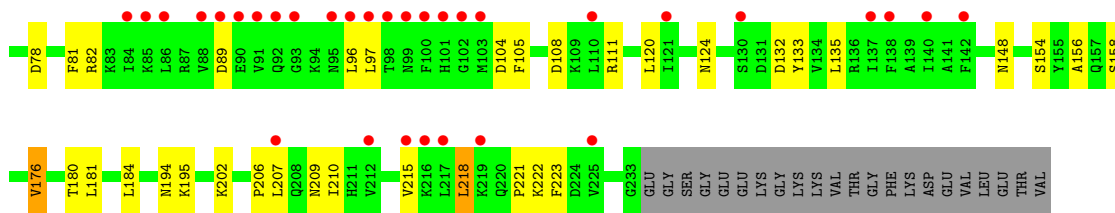


• Molecule 2: 40S ribosomal protein S0-A

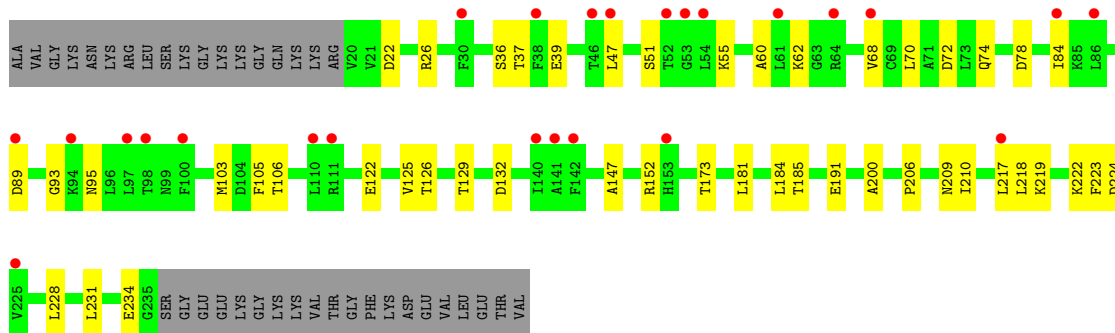


• Molecule 3: 40S ribosomal protein S1-A

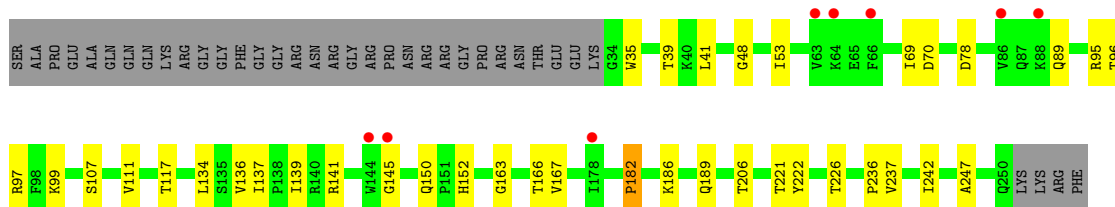
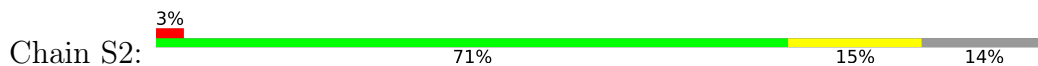




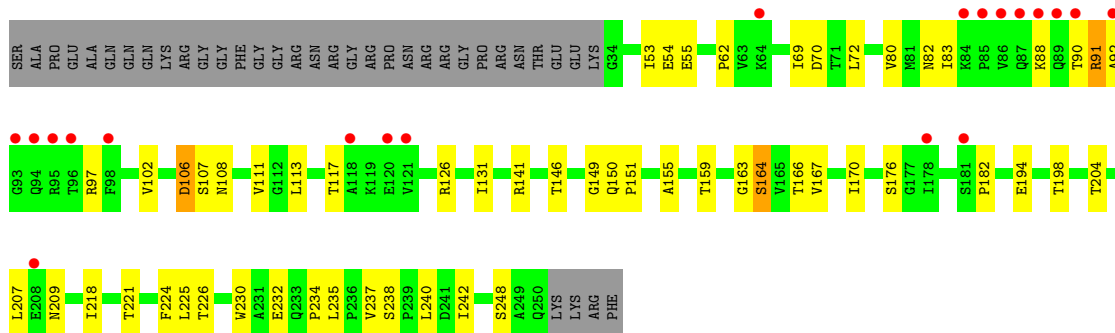
• Molecule 3: 40S ribosomal protein S1-A



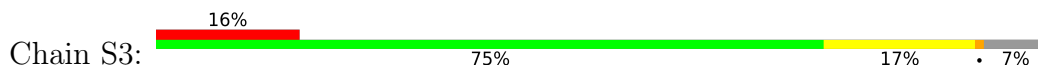
• Molecule 4: 40S ribosomal protein S2

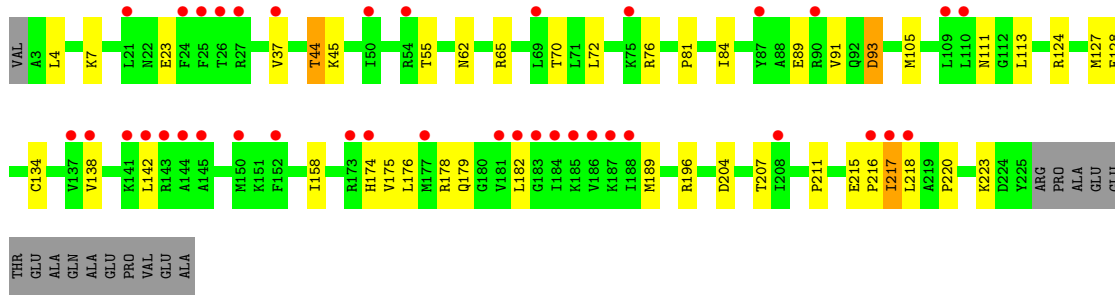


• Molecule 4: 40S ribosomal protein S2

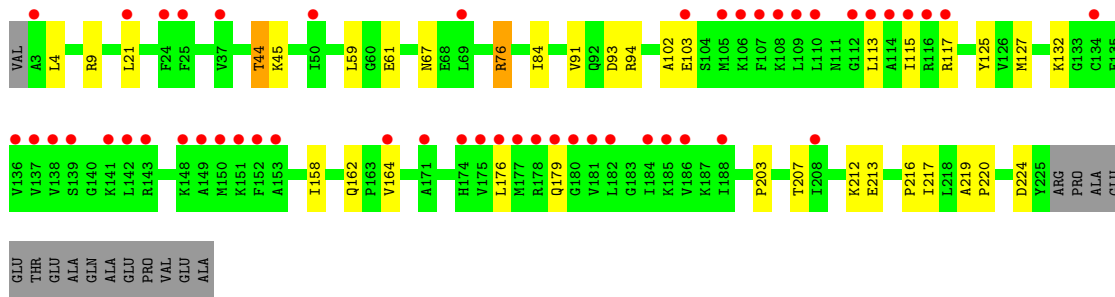
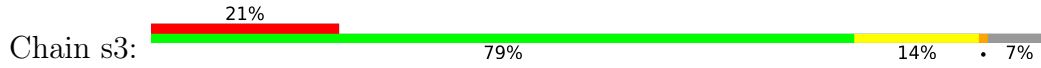


• Molecule 5: 40S ribosomal protein S3

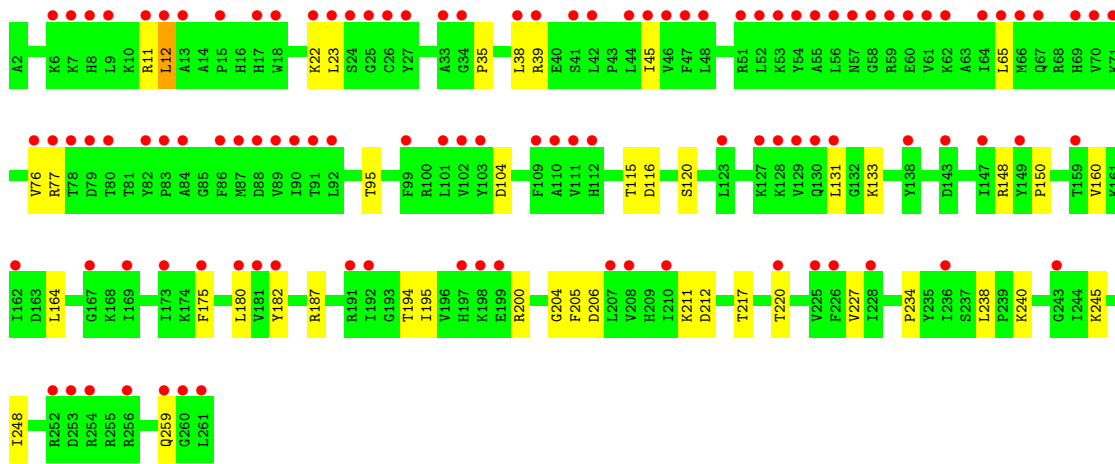
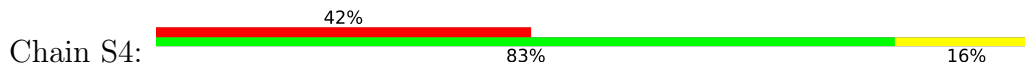




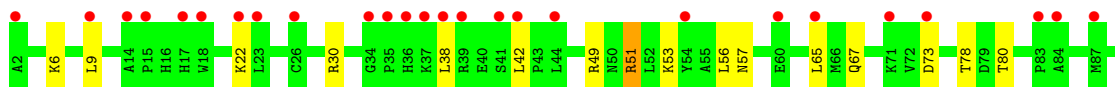
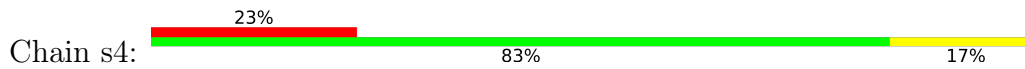
• Molecule 5: 40S ribosomal protein S3

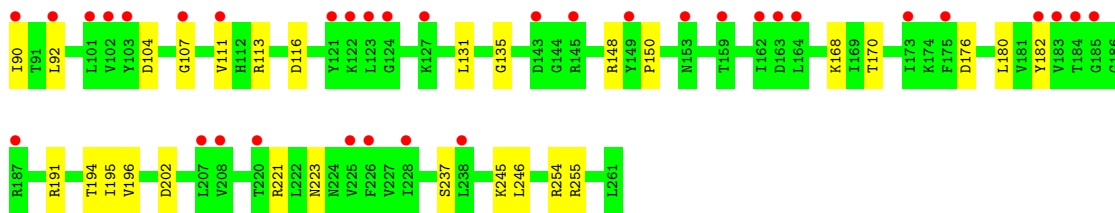


• Molecule 6: 40S ribosomal protein S4-A

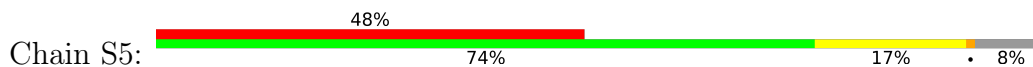


• Molecule 6: 40S ribosomal protein S4-A





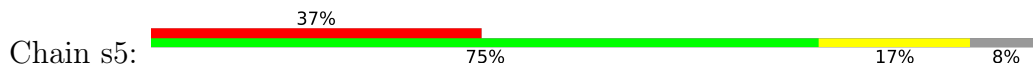
• Molecule 7: 40S ribosomal protein S5



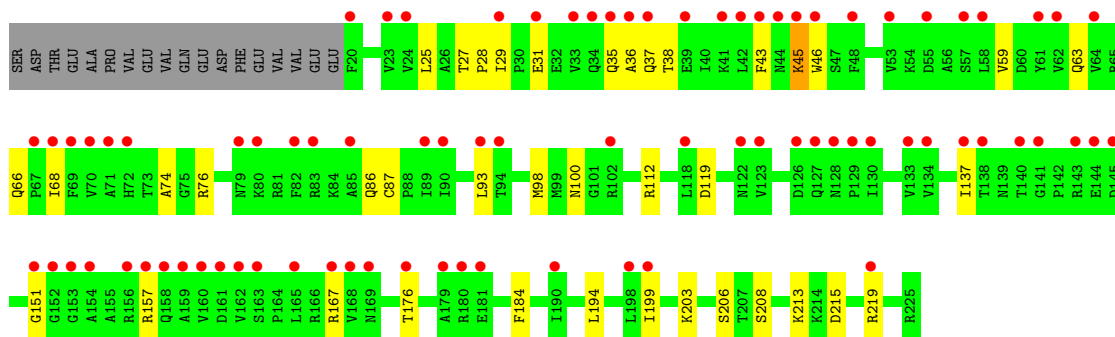
Chain S5:



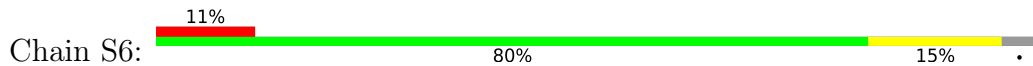
• Molecule 7: 40S ribosomal protein S5



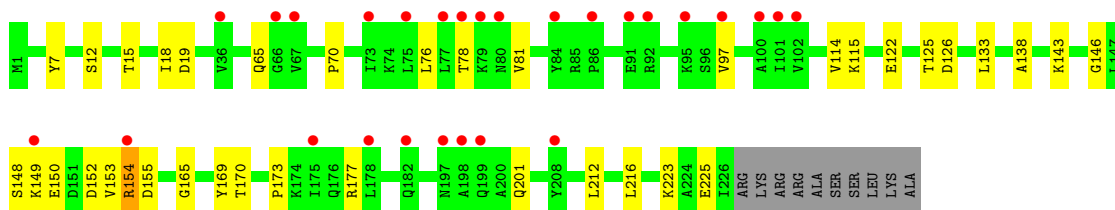
Chain s5:



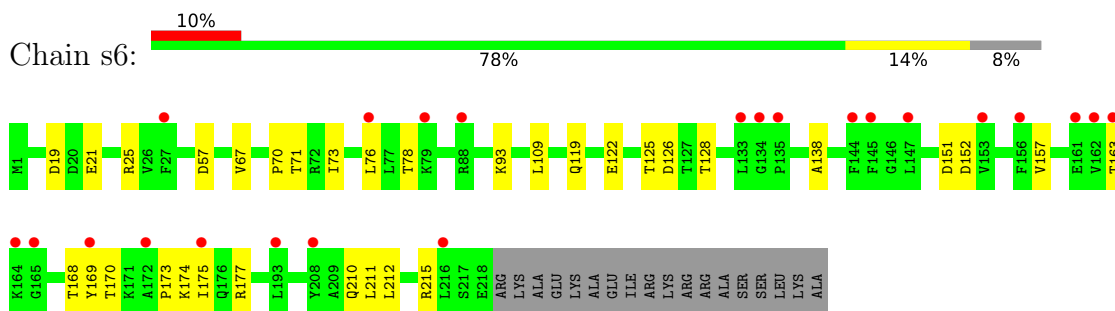
• Molecule 8: 40S ribosomal protein S6-A



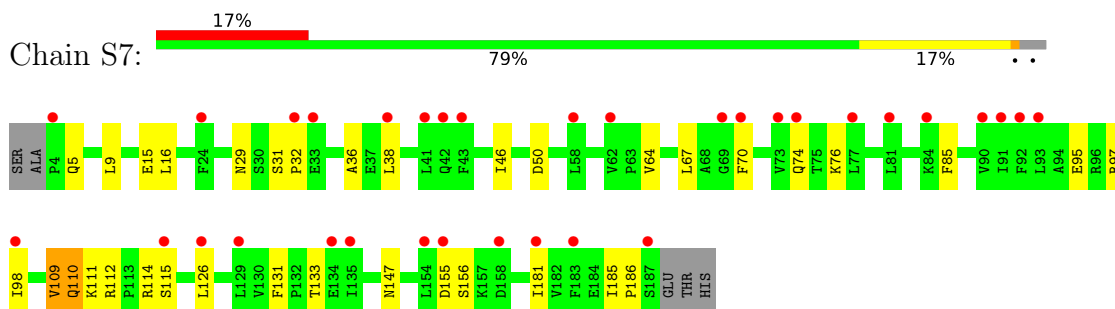
Chain S6:



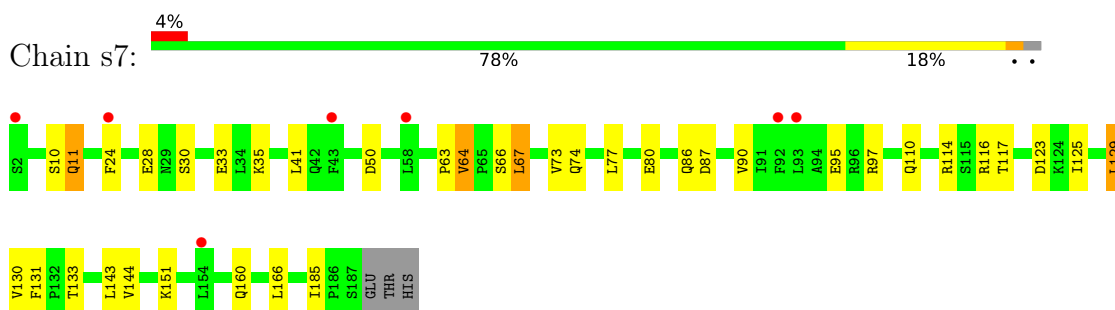
- Molecule 8: 40S ribosomal protein S6-A



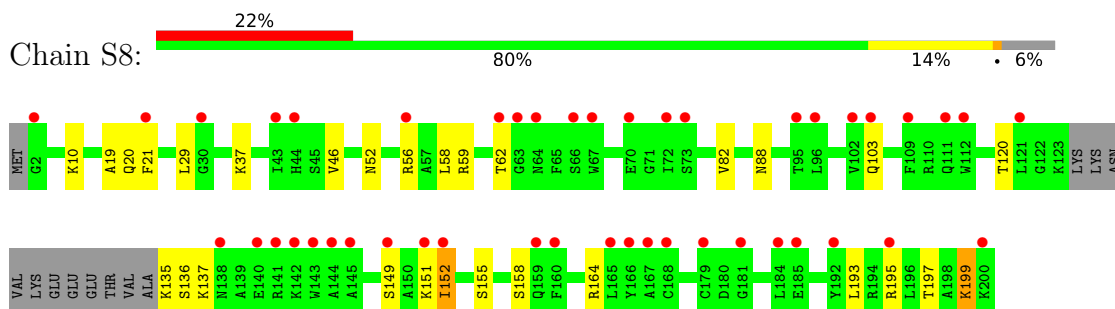
- Molecule 9: 40S ribosomal protein S7-A



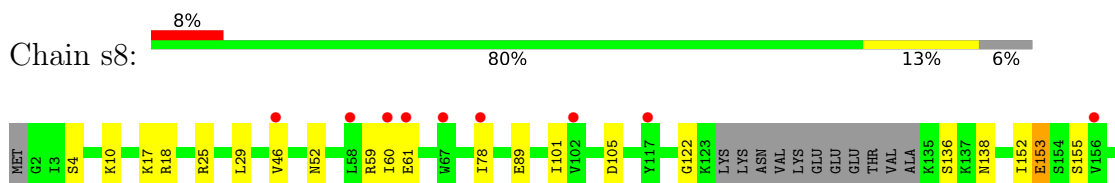
- Molecule 9: 40S ribosomal protein S7-A

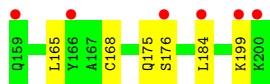


- Molecule 10: 40S ribosomal protein S8-A

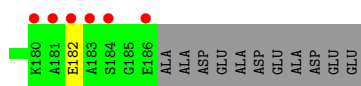
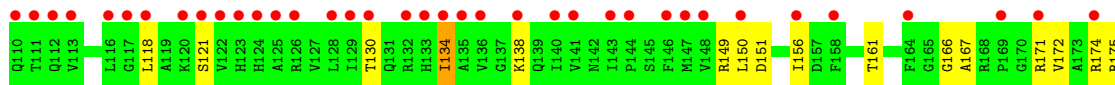
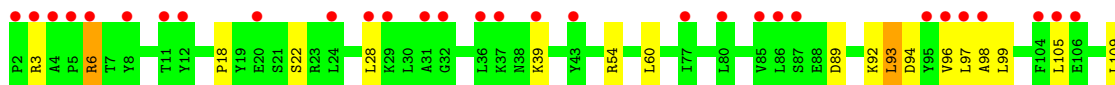
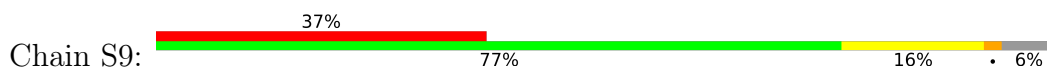


- Molecule 10: 40S ribosomal protein S8-A

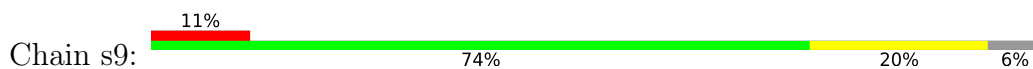




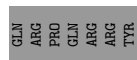
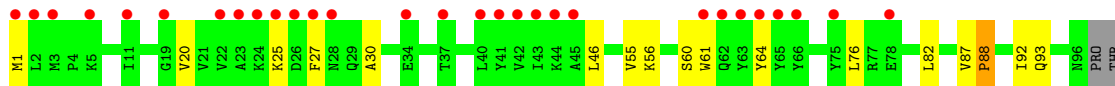
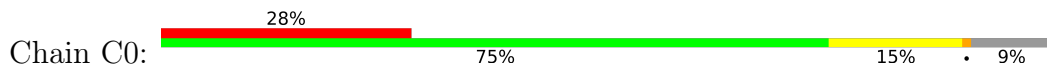
- Molecule 11: 40S ribosomal protein S9-A



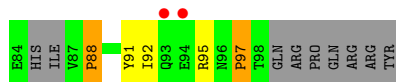
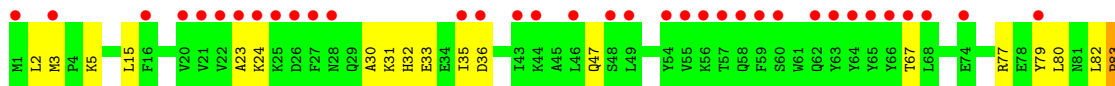
- Molecule 11: 40S ribosomal protein S9-A



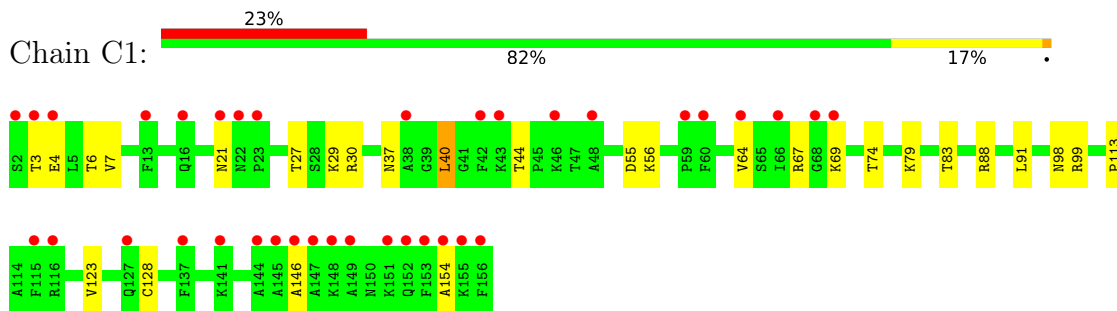
- Molecule 12: 40S ribosomal protein S10-A



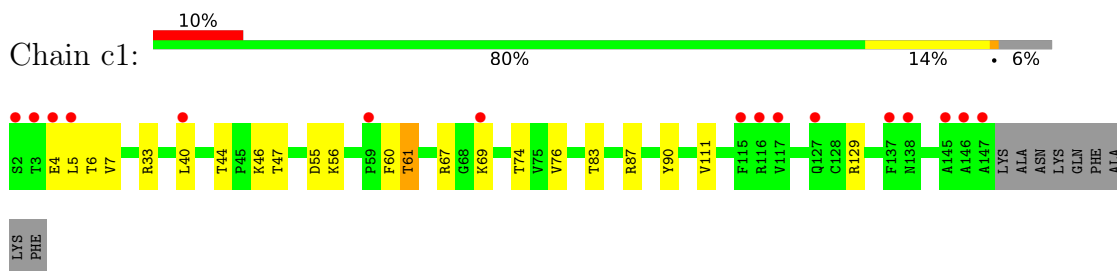
- Molecule 12: 40S ribosomal protein S10-A



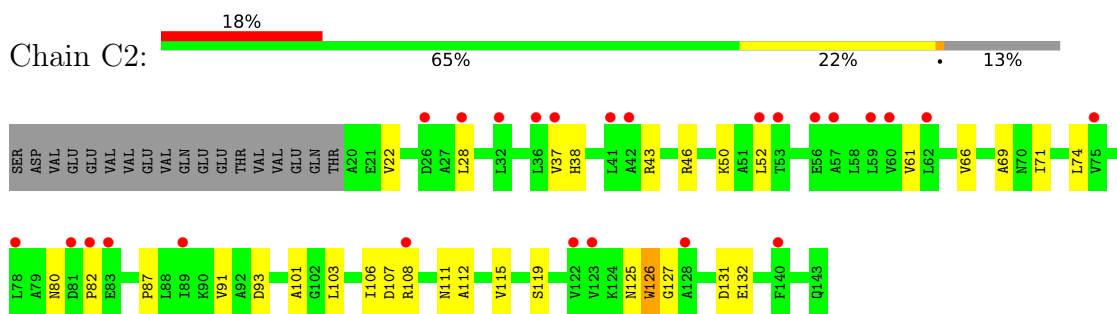
• Molecule 13: 40S ribosomal protein S11-A



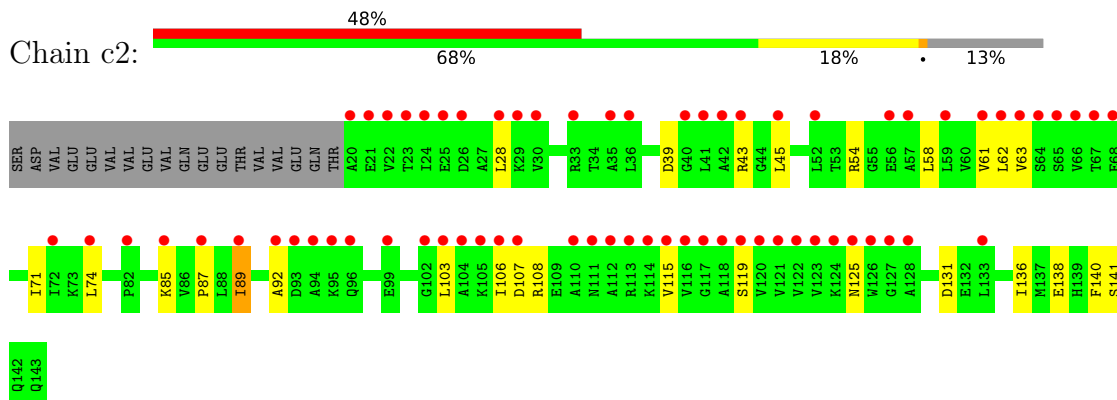
• Molecule 13: 40S ribosomal protein S11-A



• Molecule 14: 40S ribosomal protein S12

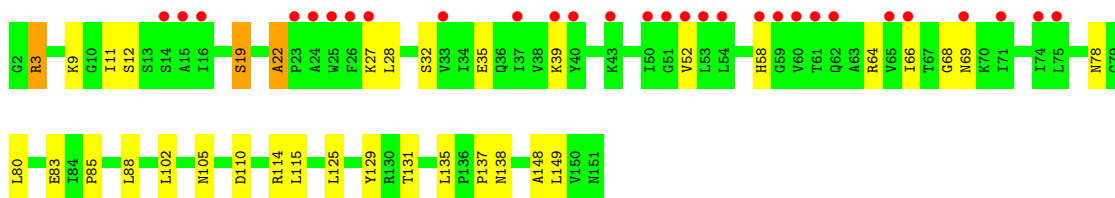


• Molecule 14: 40S ribosomal protein S12

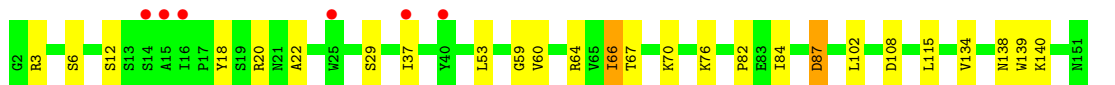
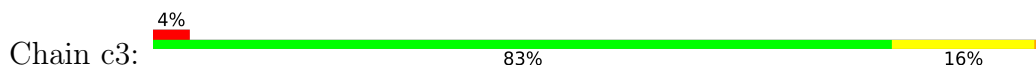


• Molecule 15: 40S ribosomal protein S13

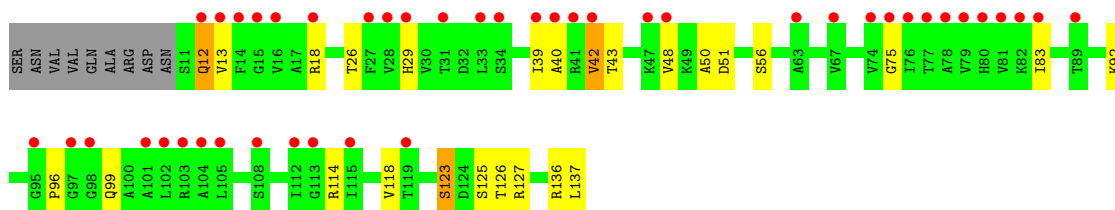
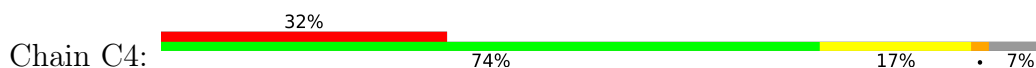




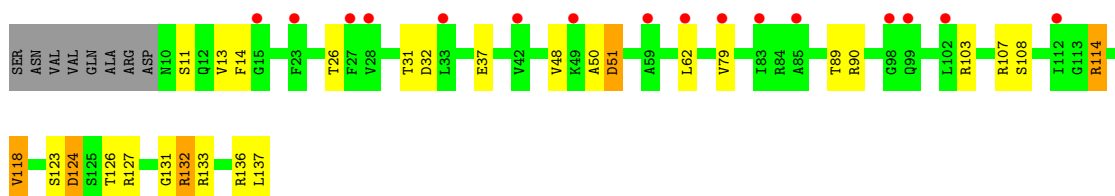
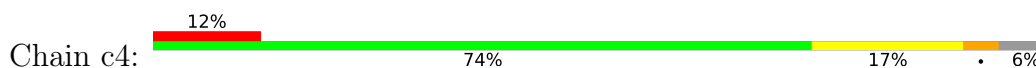
- Molecule 15: 40S ribosomal protein S13



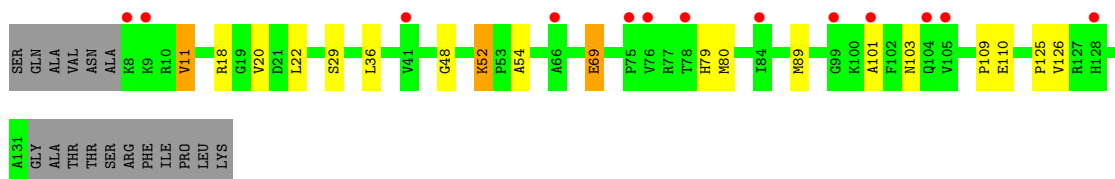
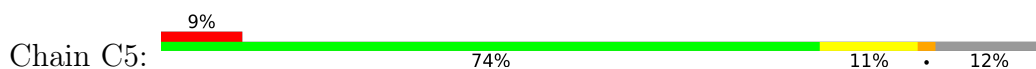
- Molecule 16: 40S ribosomal protein S14-A



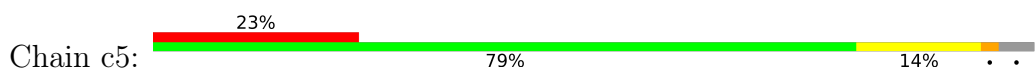
- Molecule 16: 40S ribosomal protein S14-A

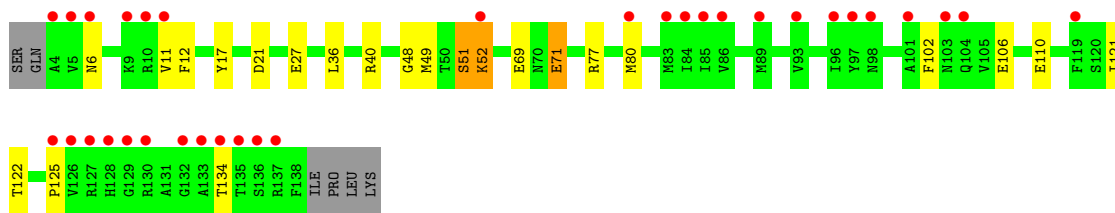


- Molecule 17: 40S ribosomal protein S15

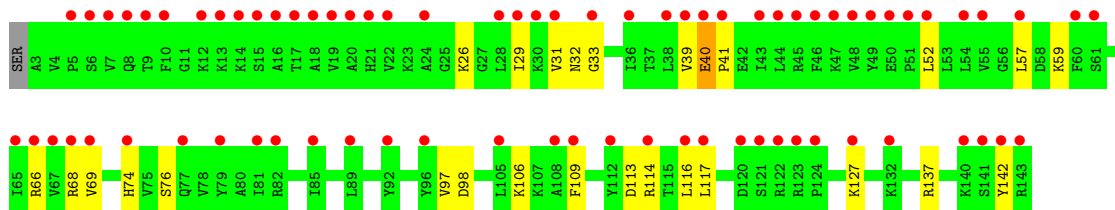
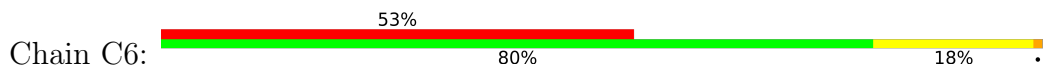


- Molecule 17: 40S ribosomal protein S15

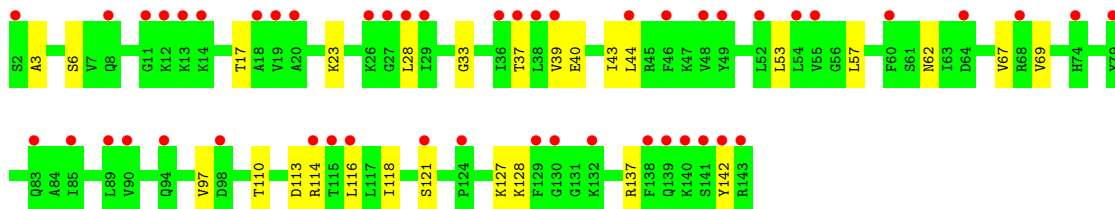
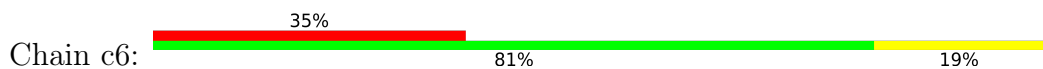




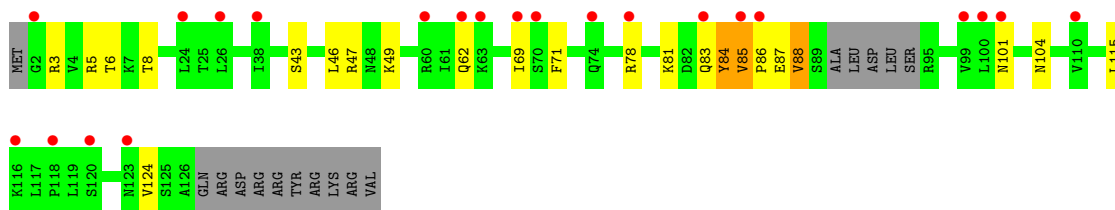
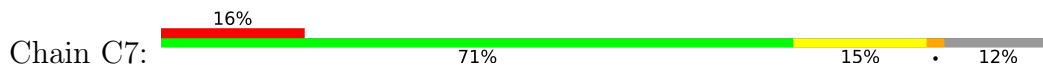
- Molecule 18: 40S ribosomal protein S16-A



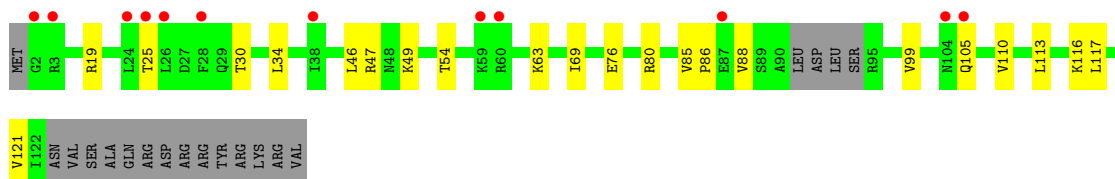
- Molecule 18: 40S ribosomal protein S16-A



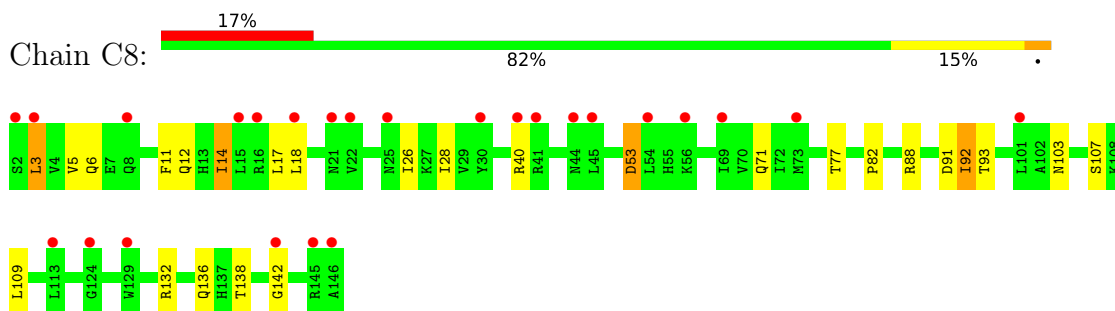
- Molecule 19: 40S ribosomal protein S17-A



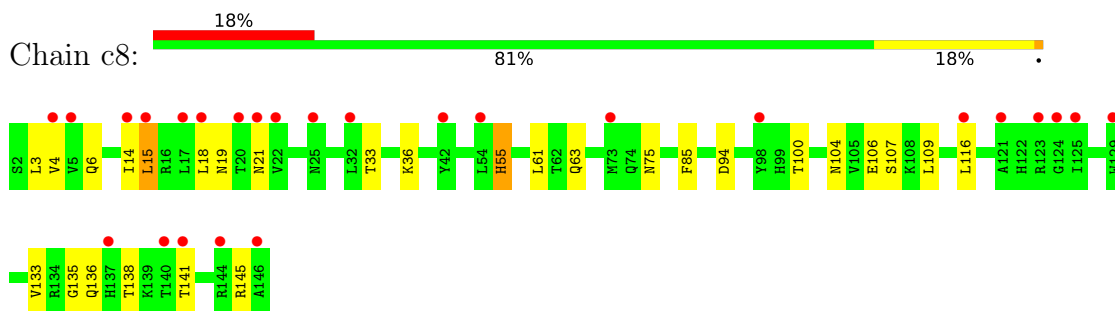
- Molecule 19: 40S ribosomal protein S17-A



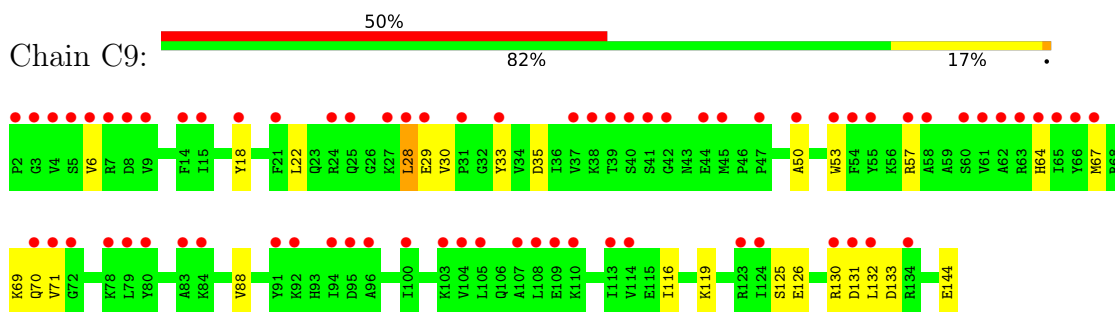
- Molecule 20: 40S ribosomal protein S18-A



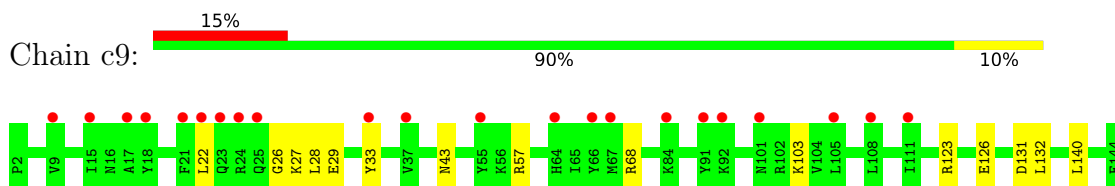
- Molecule 20: 40S ribosomal protein S18-A



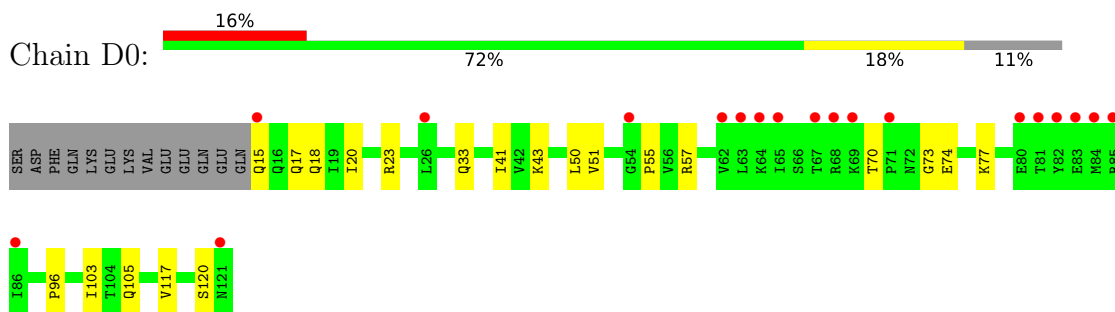
- Molecule 21: 40S ribosomal protein S19-A



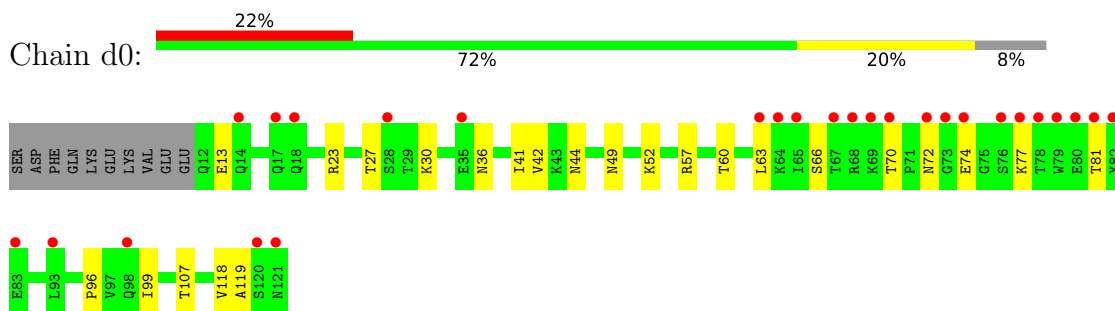
- Molecule 21: 40S ribosomal protein S19-A



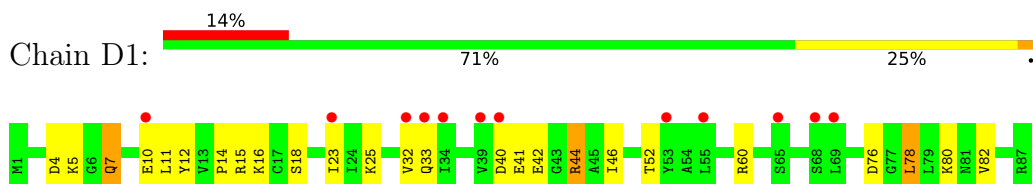
- Molecule 22: 40S ribosomal protein S20



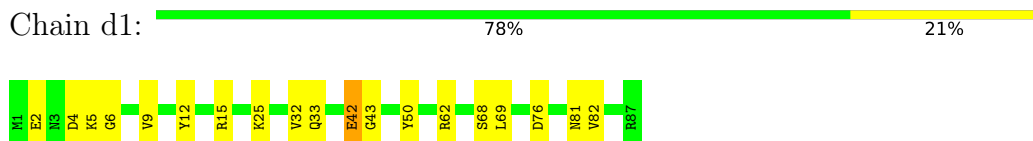
- Molecule 22: 40S ribosomal protein S20



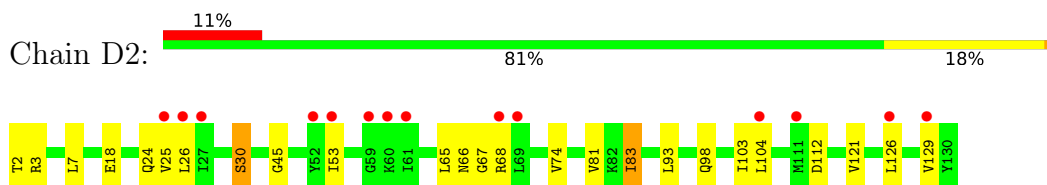
- Molecule 23: 40S ribosomal protein S21-A



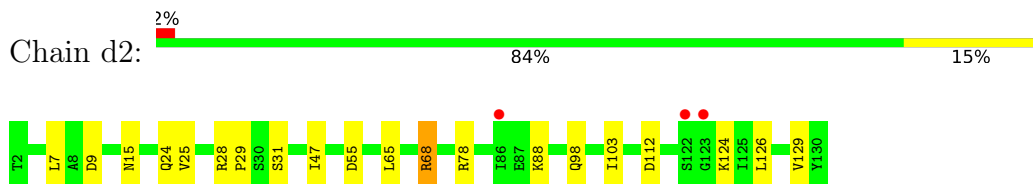
- Molecule 23: 40S ribosomal protein S21-A



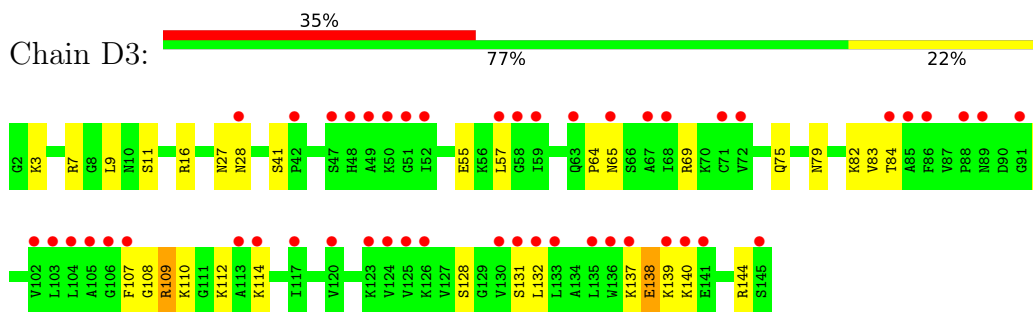
- Molecule 24: 40S ribosomal protein S22-A



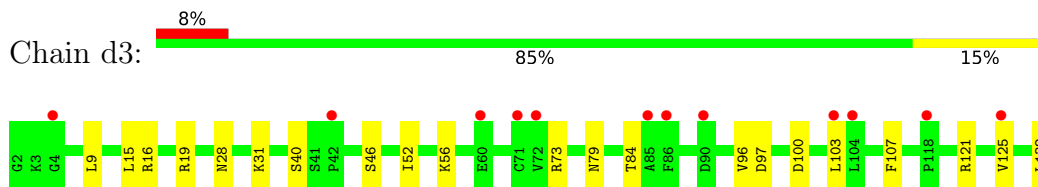
- Molecule 24: 40S ribosomal protein S22-A



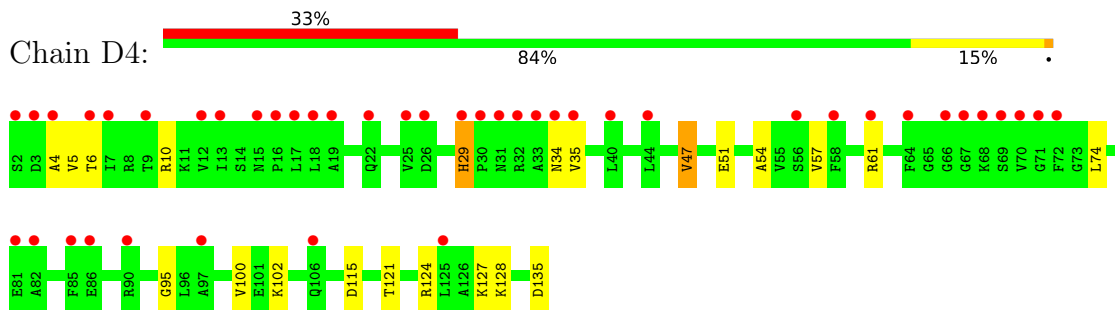
- Molecule 25: 40S ribosomal protein S23-A



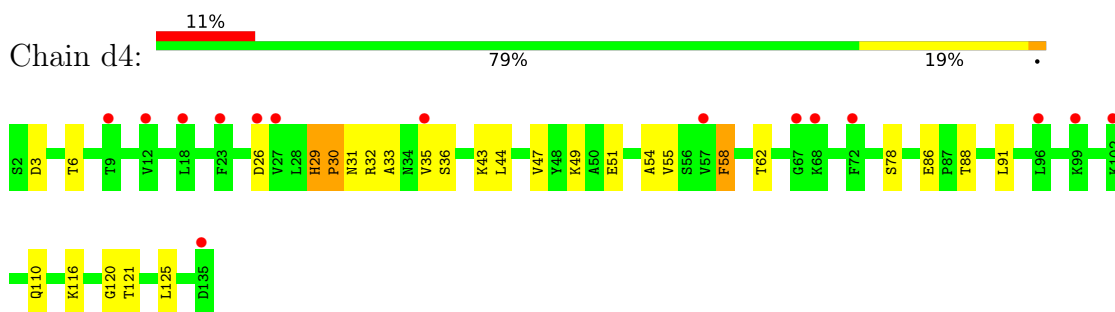
• Molecule 25: 40S ribosomal protein S23-A



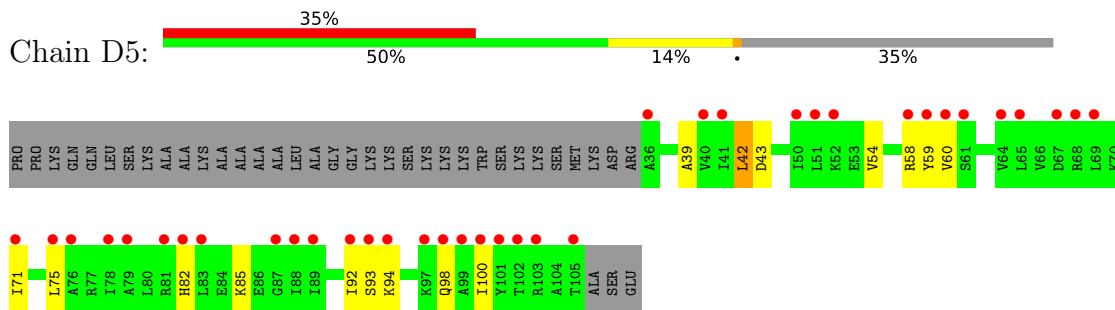
• Molecule 26: 40S ribosomal protein S24-A



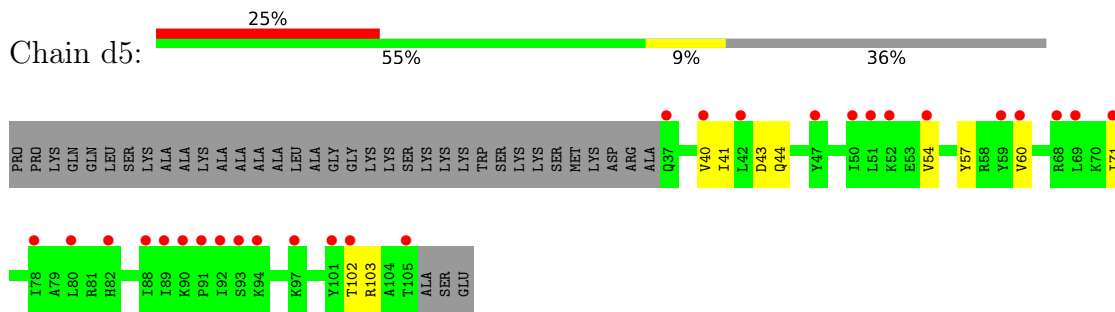
• Molecule 26: 40S ribosomal protein S24-A



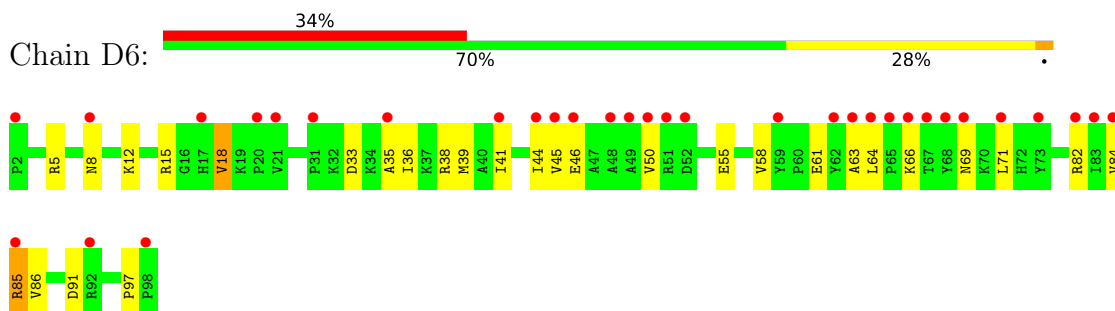
• Molecule 27: 40S ribosomal protein S25-A



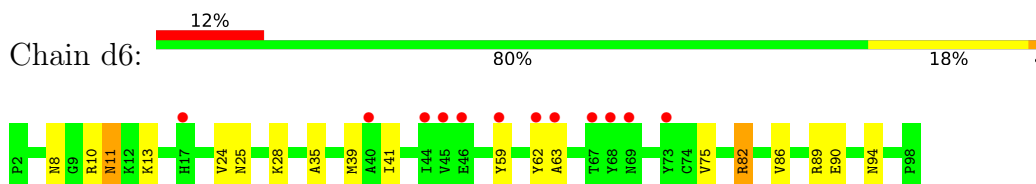
• Molecule 27: 40S ribosomal protein S25-A



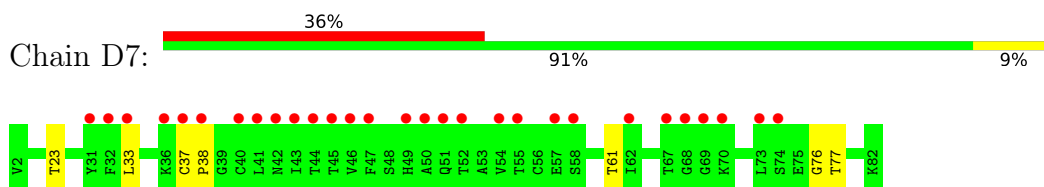
- Molecule 28: 40S ribosomal protein S26-A



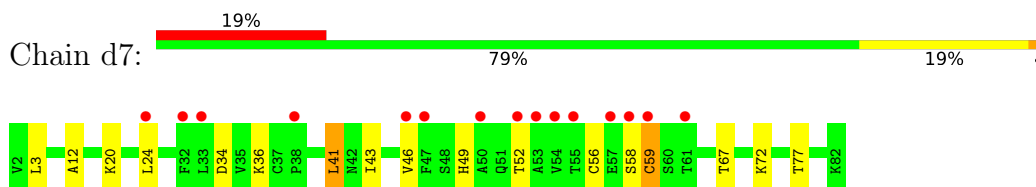
- Molecule 28: 40S ribosomal protein S26-A



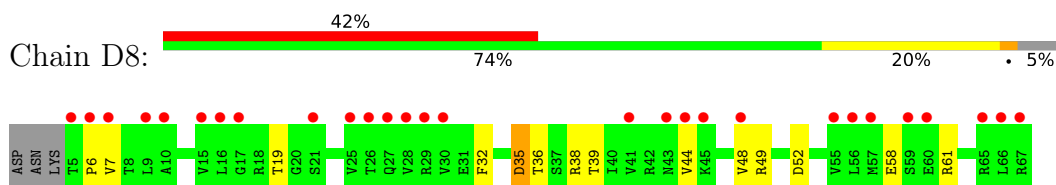
- Molecule 29: 40S ribosomal protein S27-A



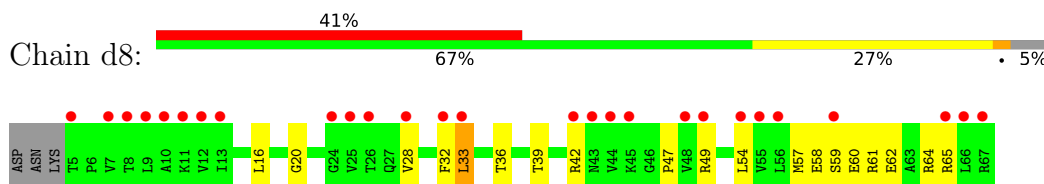
- Molecule 29: 40S ribosomal protein S27-A



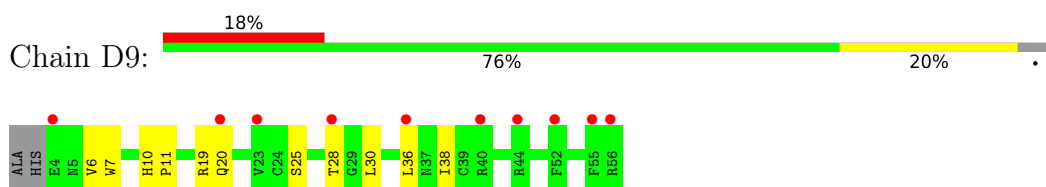
- Molecule 30: 40S ribosomal protein S28-A



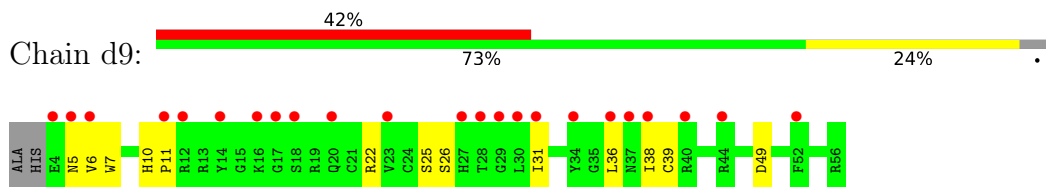
- Molecule 30: 40S ribosomal protein S28-A



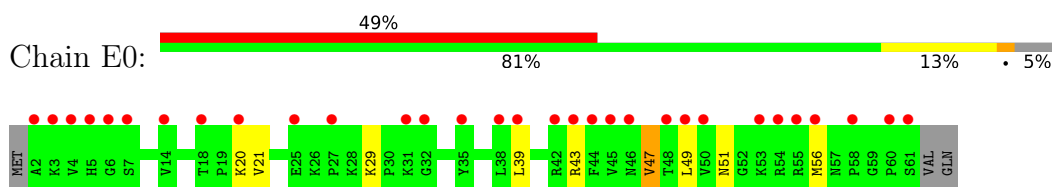
- Molecule 31: 40S ribosomal protein S29-A



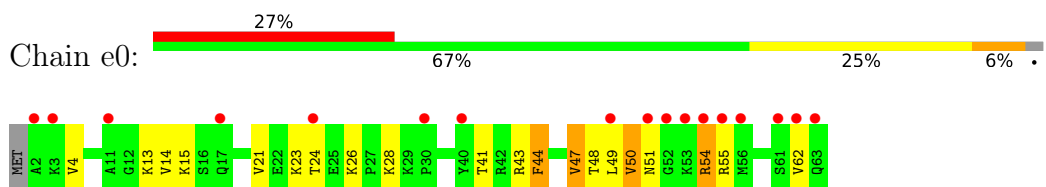
- Molecule 31: 40S ribosomal protein S29-A



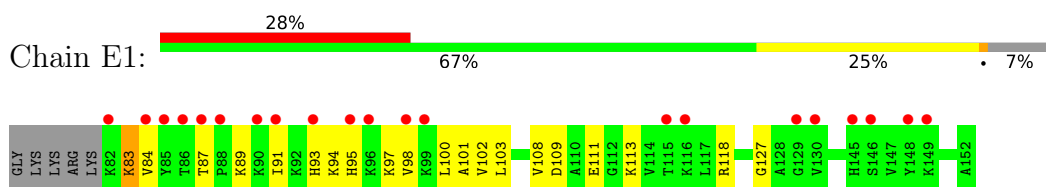
- Molecule 32: 40S ribosomal protein S30-A



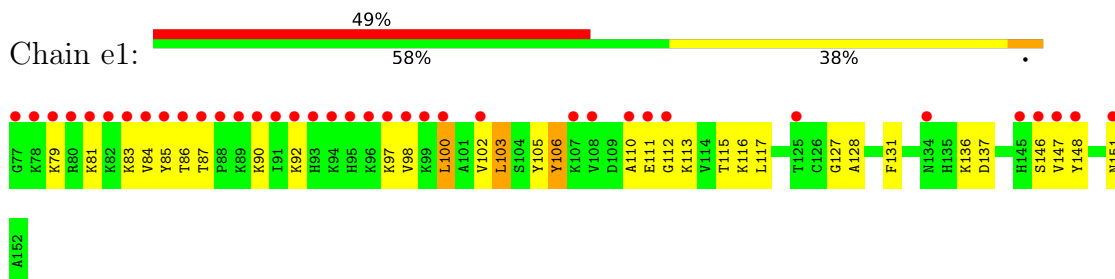
- Molecule 32: 40S ribosomal protein S30-A



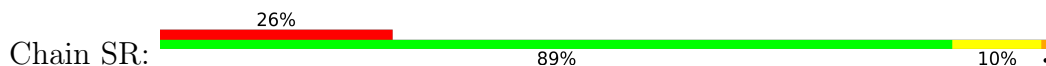
- Molecule 33: Ubiquitin-40S ribosomal protein S31

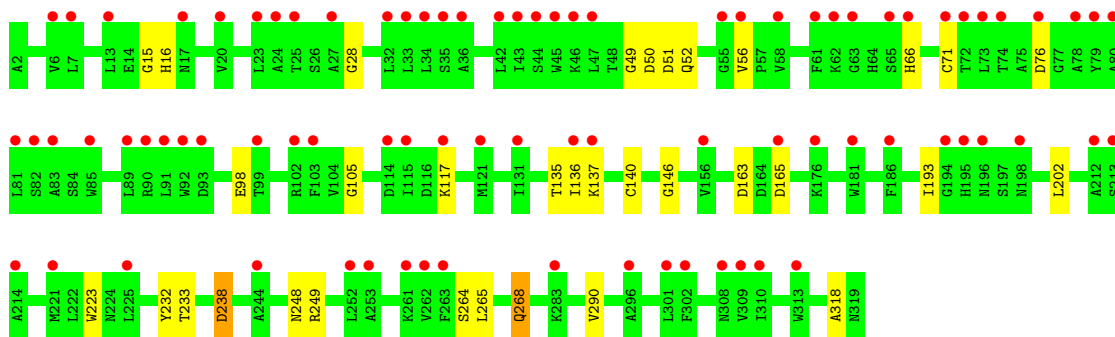


- Molecule 33: Ubiquitin-40S ribosomal protein S31

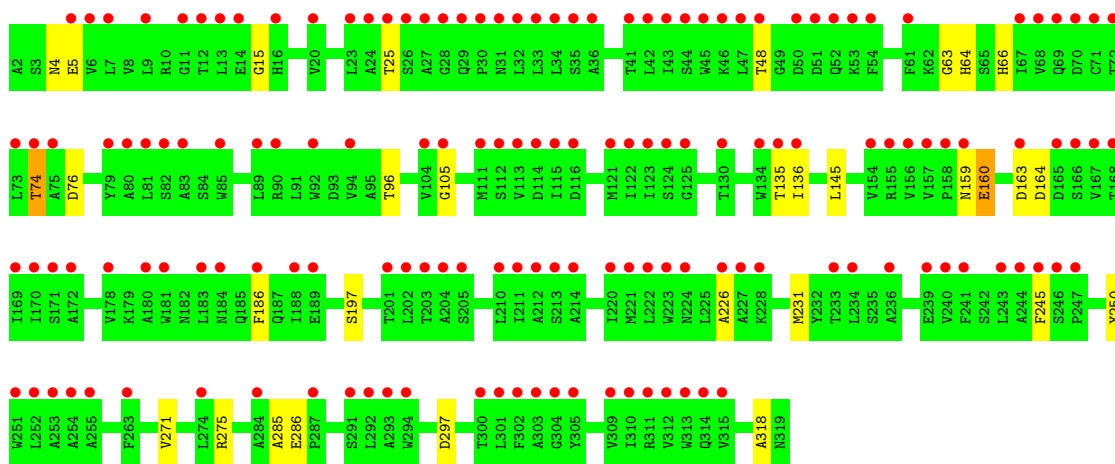
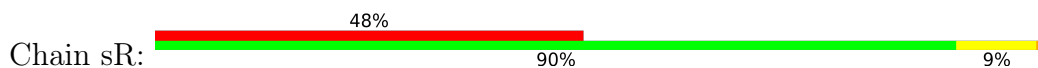


- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

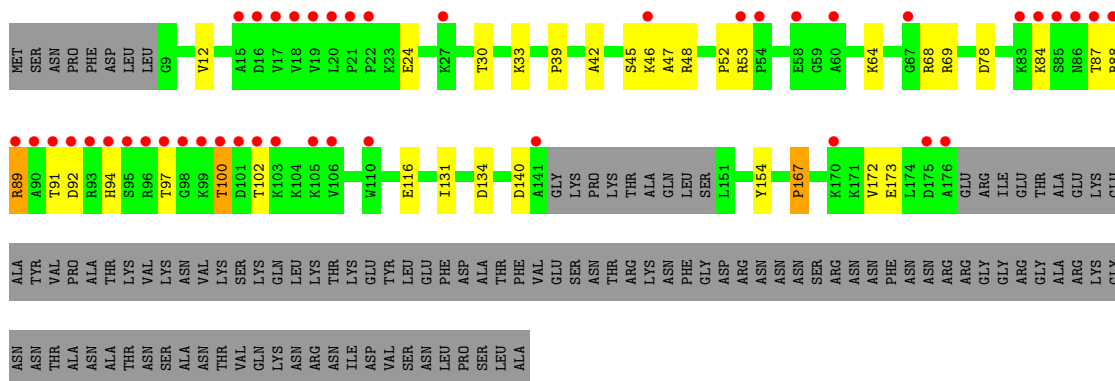




• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

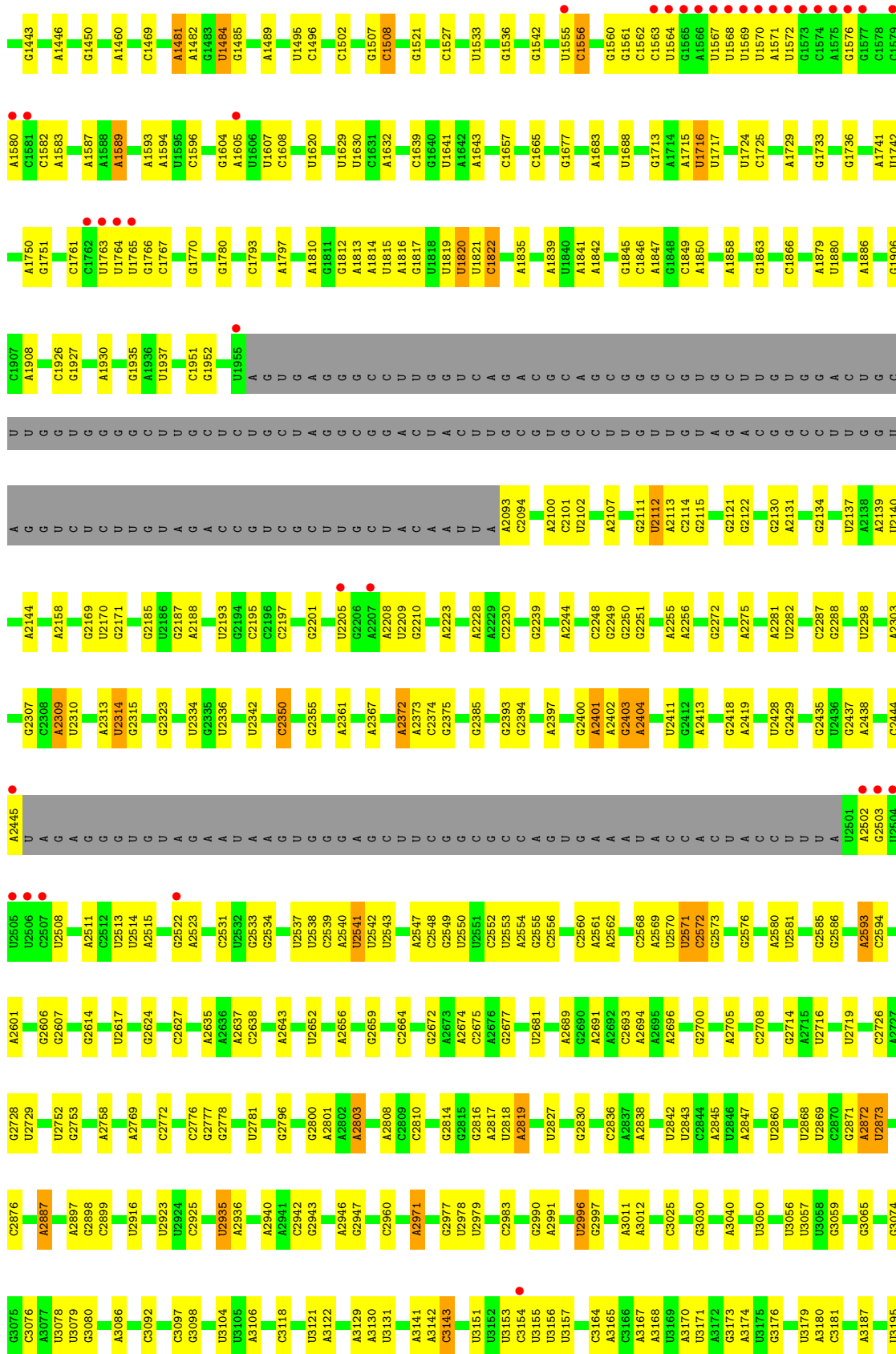


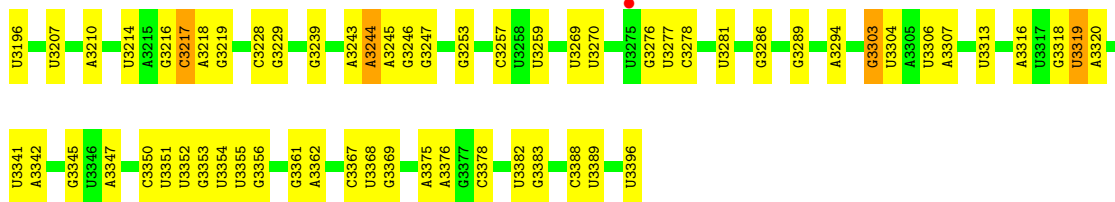
• Molecule 35: Suppressor protein STM1



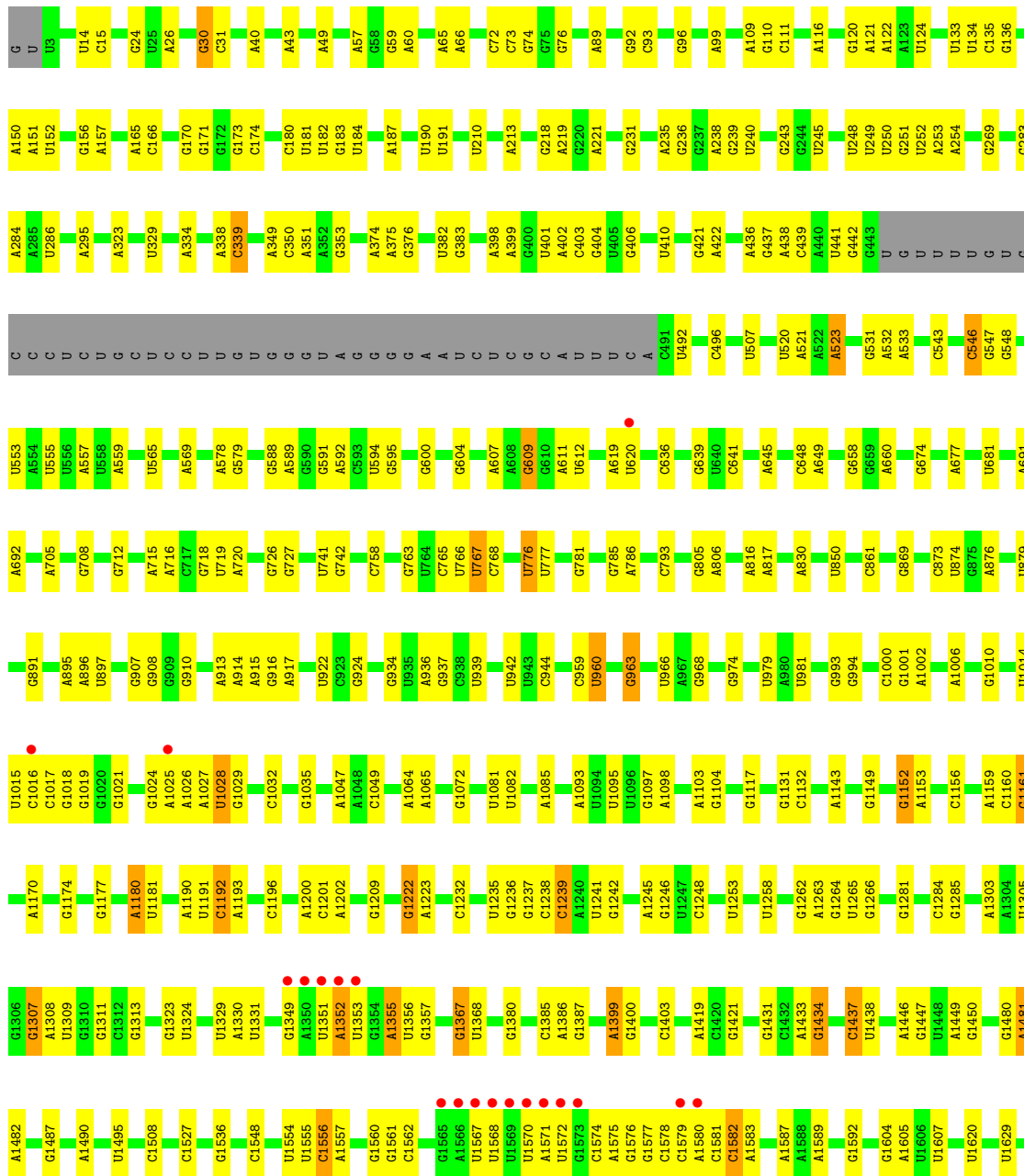
• Molecule 35: Suppressor protein STM1

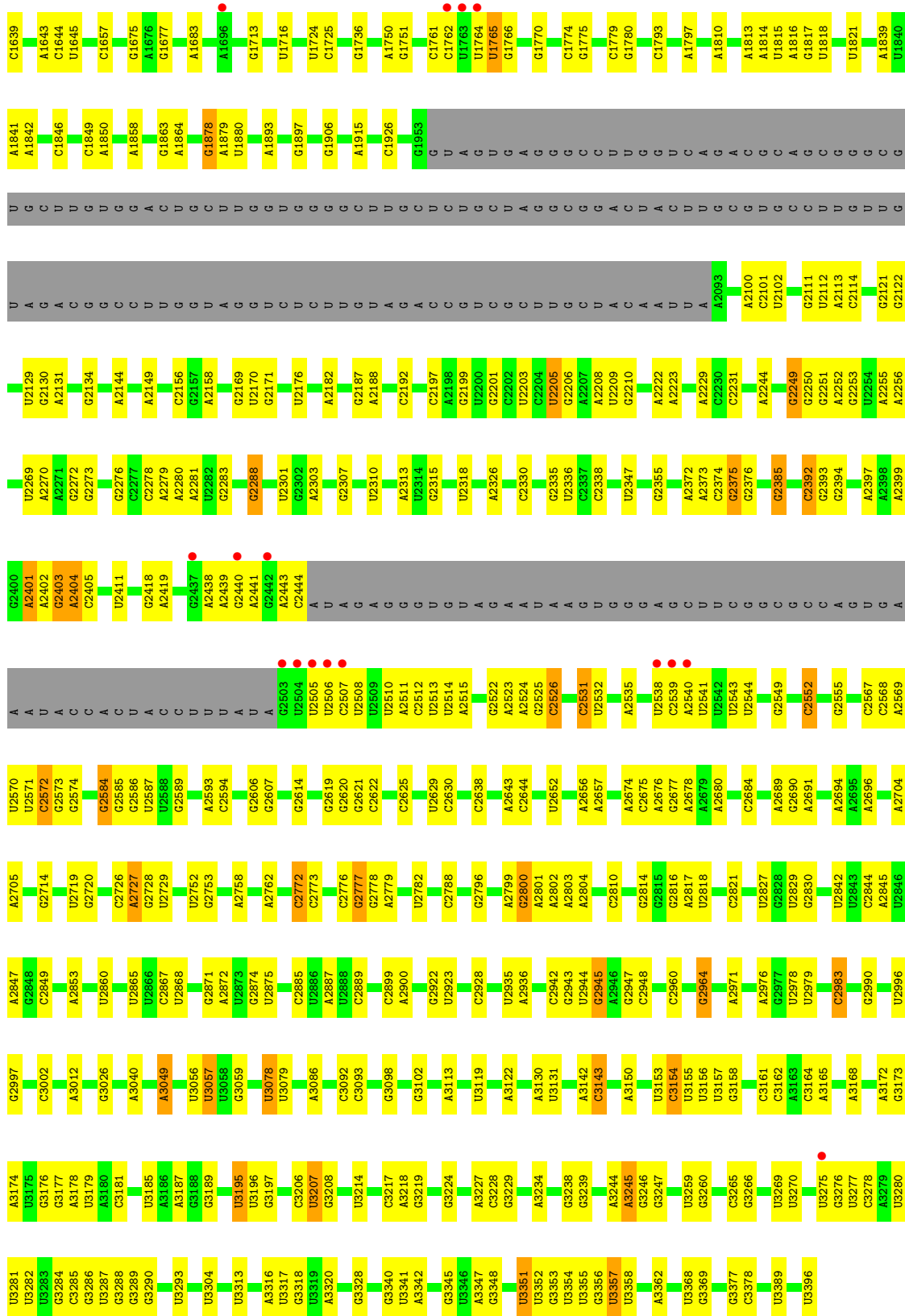






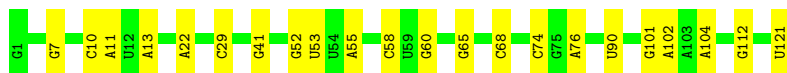
• Molecule 36: 25S ribosomal RNA



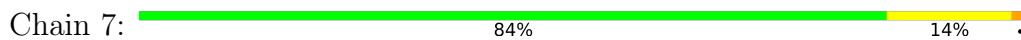


• Molecule 37: 5S ribosomal RNA

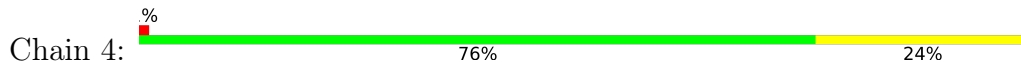
Chain 3: 82% 18%



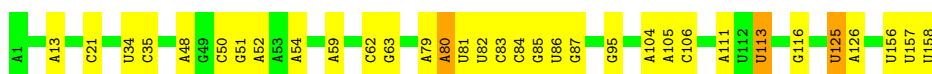
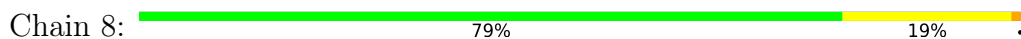
- Molecule 37: 5S ribosomal RNA



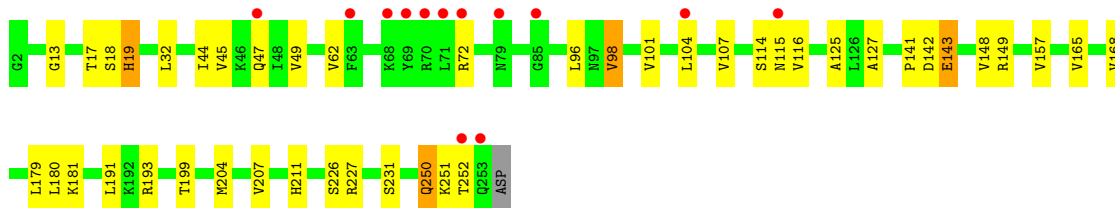
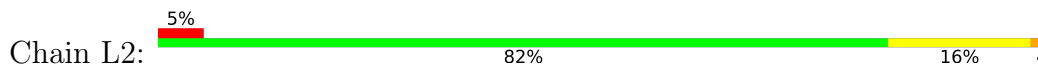
- Molecule 38: 5.8S ribosomal RNA



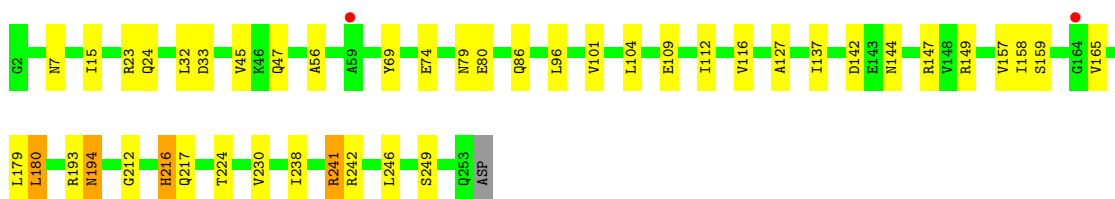
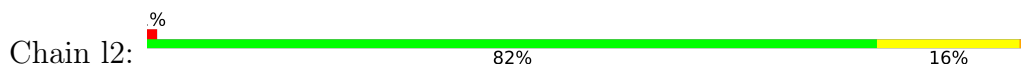
- Molecule 38: 5.8S ribosomal RNA



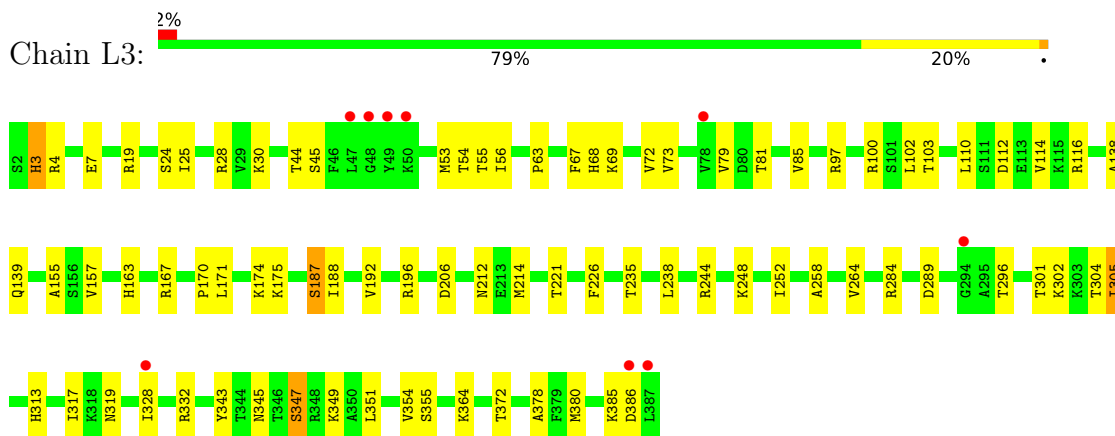
- Molecule 39: 60S ribosomal protein L2-A



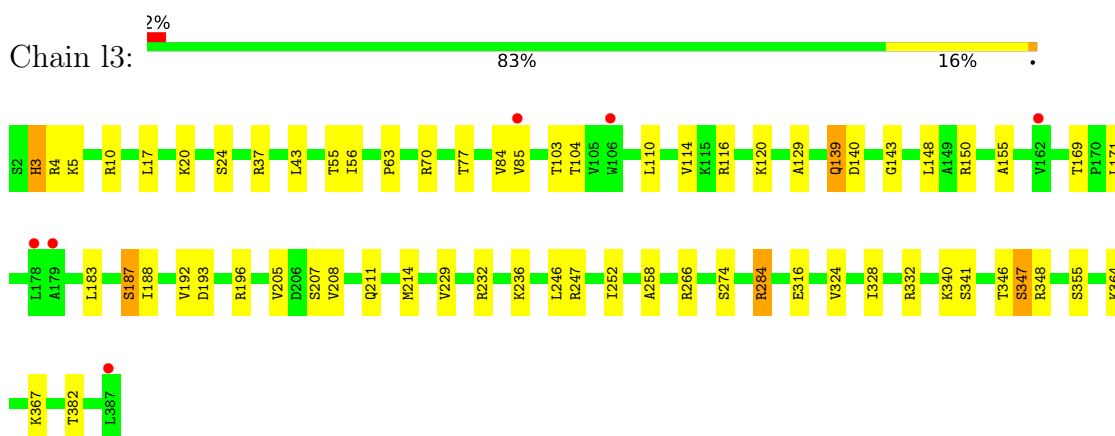
- Molecule 39: 60S ribosomal protein L2-A



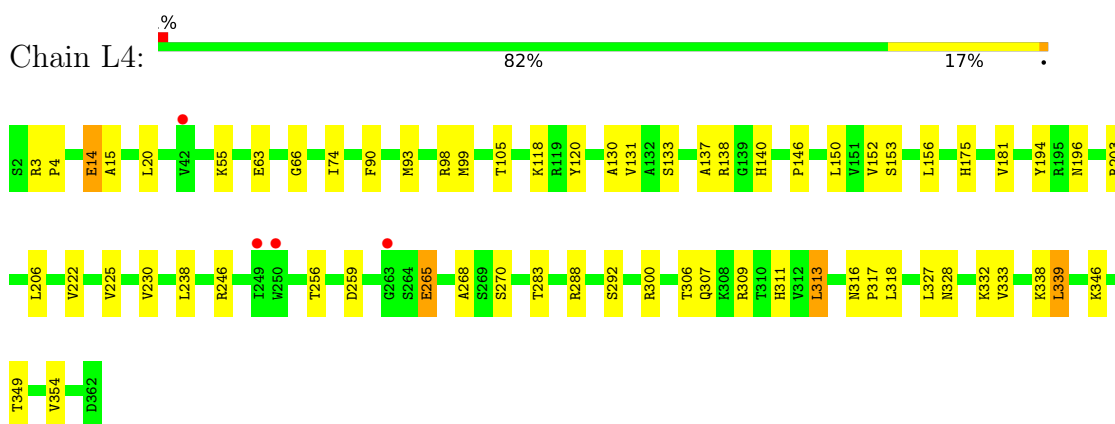
- Molecule 40: 60S ribosomal protein L3



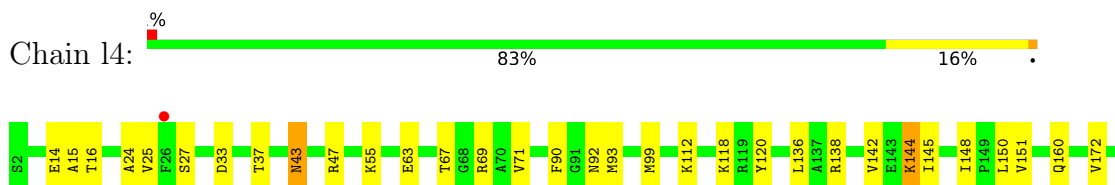
• Molecule 40: 60S ribosomal protein L3



• Molecule 41: 60S ribosomal protein L4-A



• Molecule 41: 60S ribosomal protein L4-A





- Molecule 44: 60S ribosomal protein L7-A

Chain L7: 79% 11% 9%



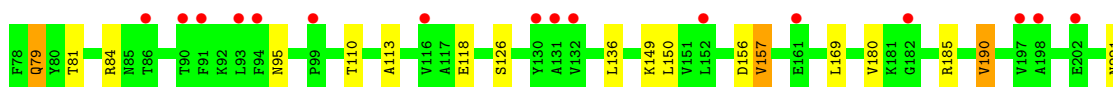
- Molecule 44: 60S ribosomal protein L7-A

Chain L7: 80% 10% 8%



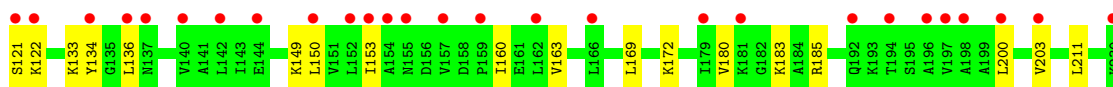
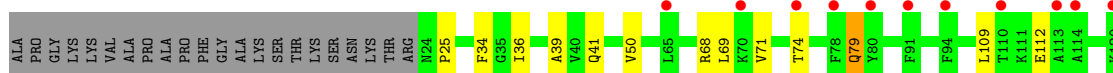
- Molecule 45: 60S ribosomal protein L8-A

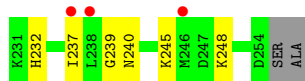
Chain L8: 13% 78% 12% 9%



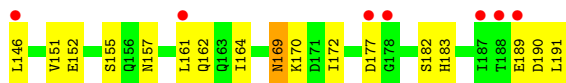
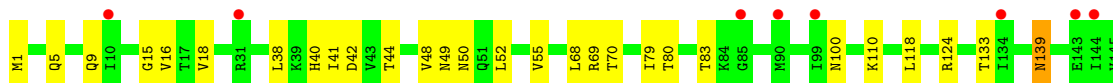
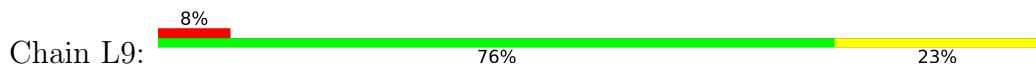
- Molecule 45: 60S ribosomal protein L8-A

Chain L8: 16% 76% 14% 9%

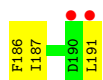
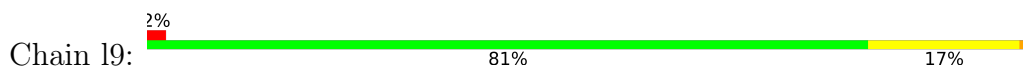




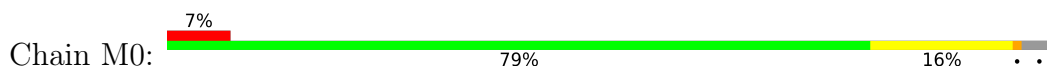
- Molecule 46: 60S ribosomal protein L9-A



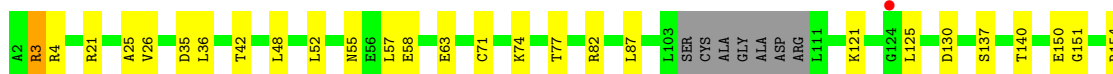
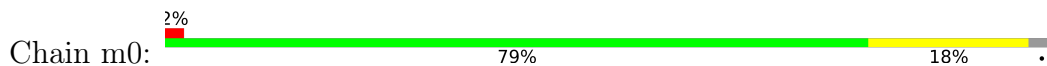
- Molecule 46: 60S ribosomal protein L9-A



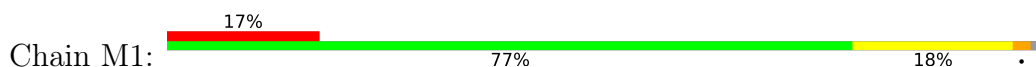
- Molecule 47: 60S ribosomal protein L10

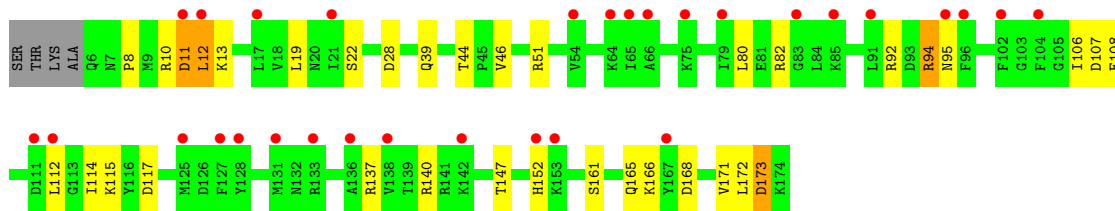


- Molecule 47: 60S ribosomal protein L10

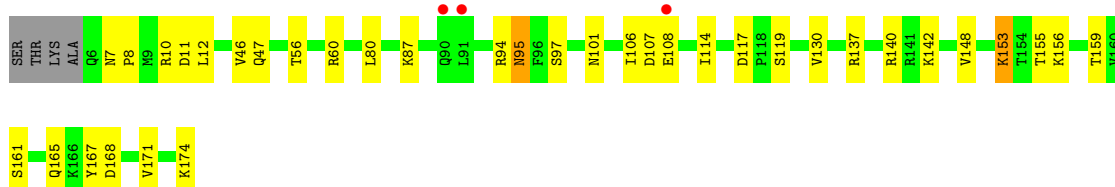
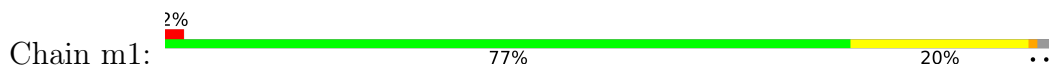


- Molecule 48: 60S ribosomal protein L11-A

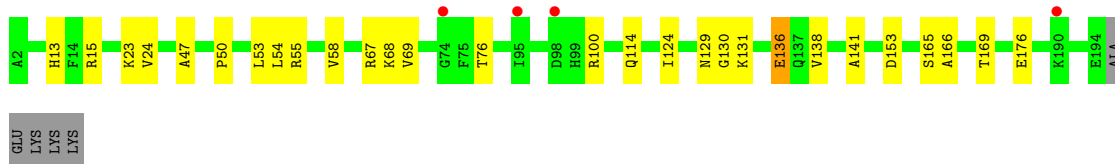
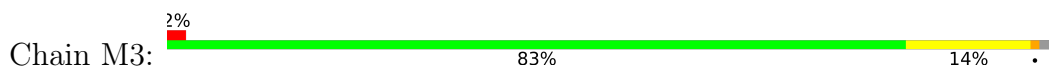




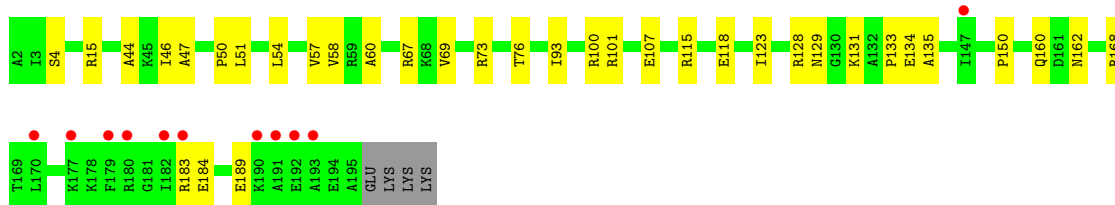
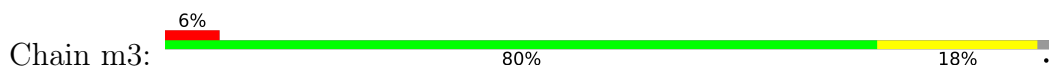
• Molecule 48: 60S ribosomal protein L11-A



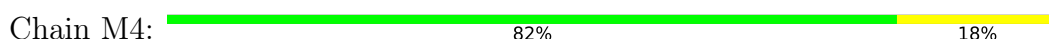
• Molecule 49: 60S ribosomal protein L13-A



• Molecule 49: 60S ribosomal protein L13-A



• Molecule 50: 60S ribosomal protein L14-A

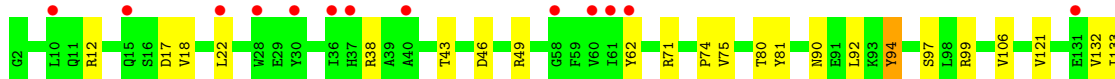
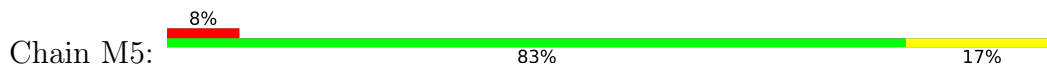


• Molecule 50: 60S ribosomal protein L14-A

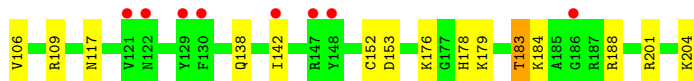
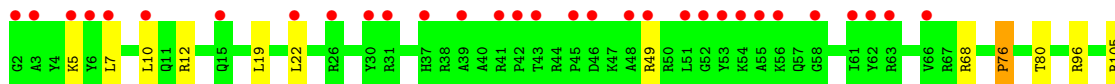
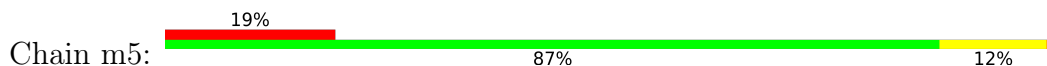




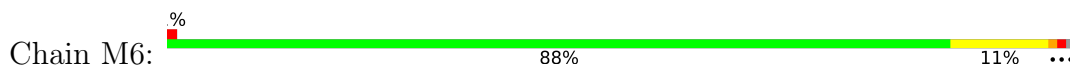
- Molecule 51: 60S ribosomal protein L15-A



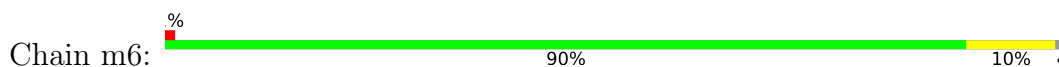
- Molecule 51: 60S ribosomal protein L15-A



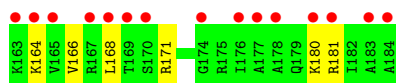
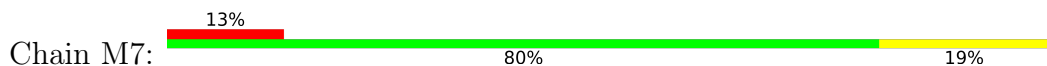
- Molecule 52: 60S ribosomal protein L16-A



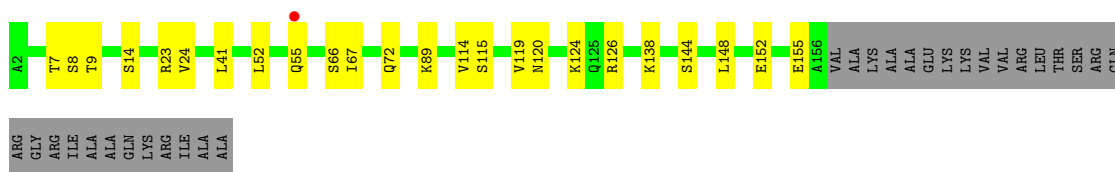
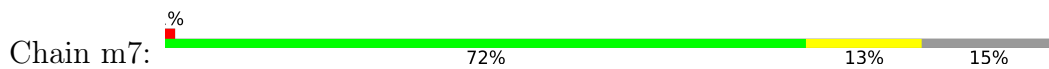
- Molecule 52: 60S ribosomal protein L16-A



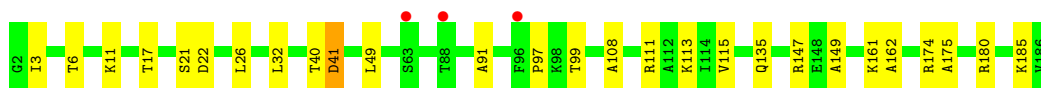
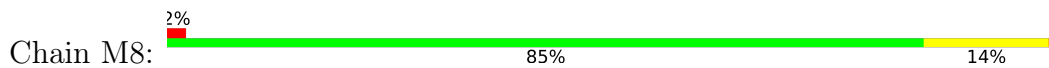
- Molecule 53: 60S ribosomal protein L17-A



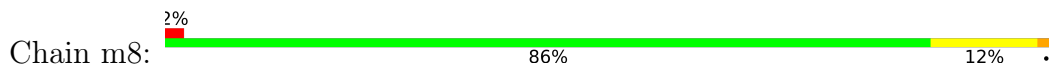
• Molecule 53: 60S ribosomal protein L17-A



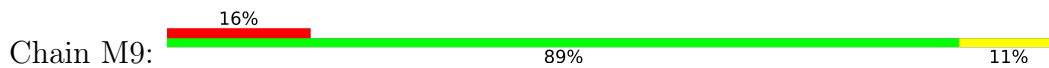
• Molecule 54: 60S ribosomal protein L18-A



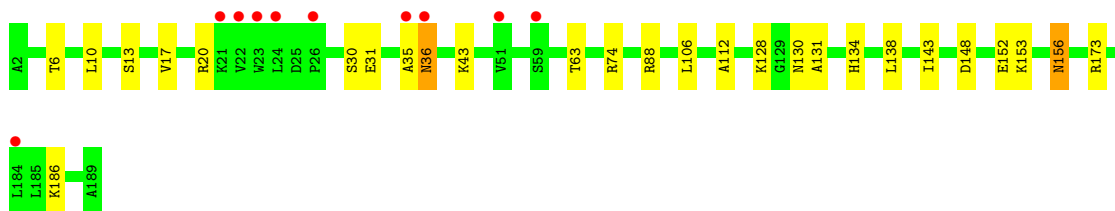
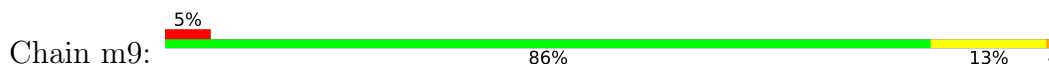
• Molecule 54: 60S ribosomal protein L18-A



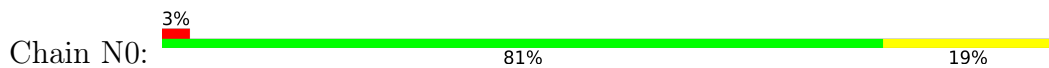
• Molecule 55: 60S ribosomal protein L19-A

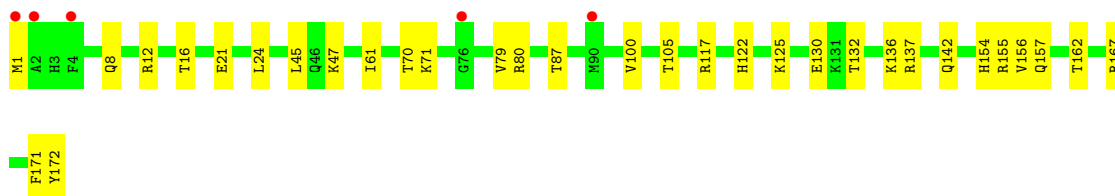


• Molecule 55: 60S ribosomal protein L19-A

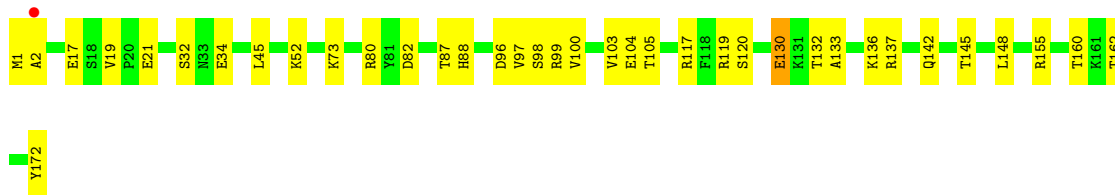
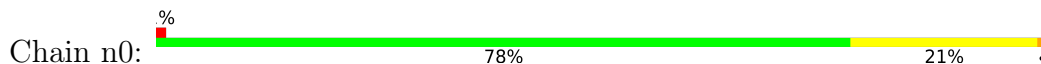


• Molecule 56: 60S ribosomal protein L20-A

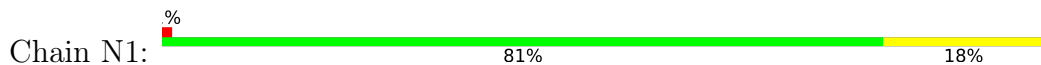




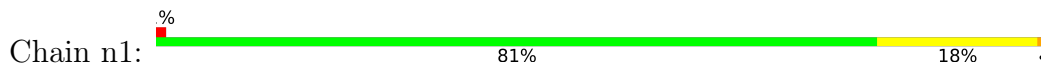
• Molecule 56: 60S ribosomal protein L20-A



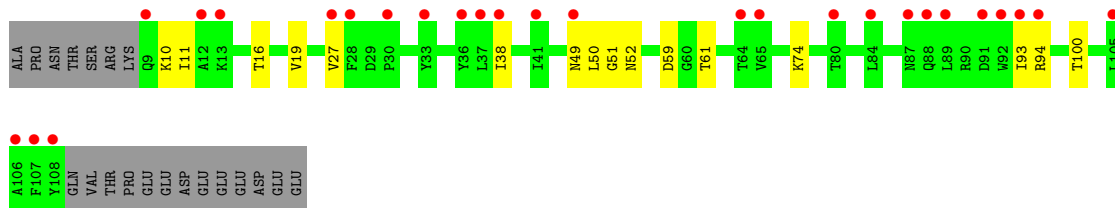
• Molecule 57: 60S ribosomal protein L21-A



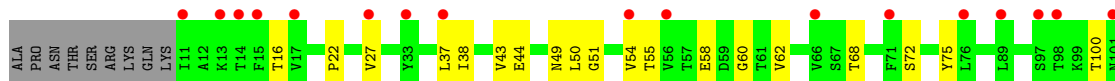
• Molecule 57: 60S ribosomal protein L21-A

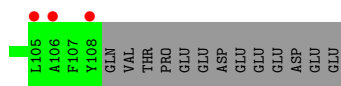


• Molecule 58: 60S ribosomal protein L22-A

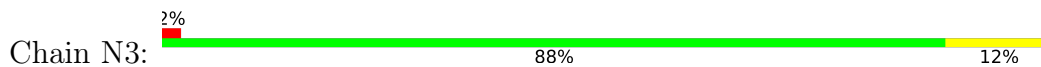


• Molecule 58: 60S ribosomal protein L22-A

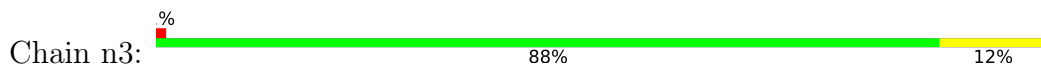




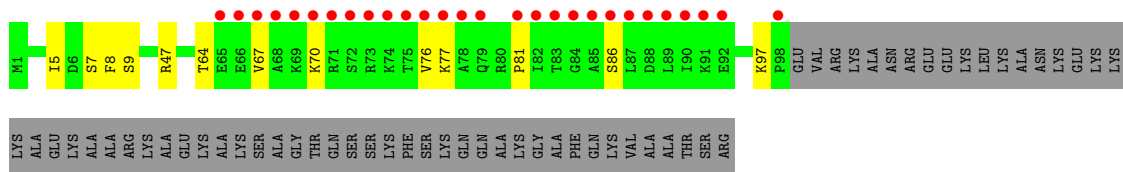
• Molecule 59: 60S ribosomal protein L23-A



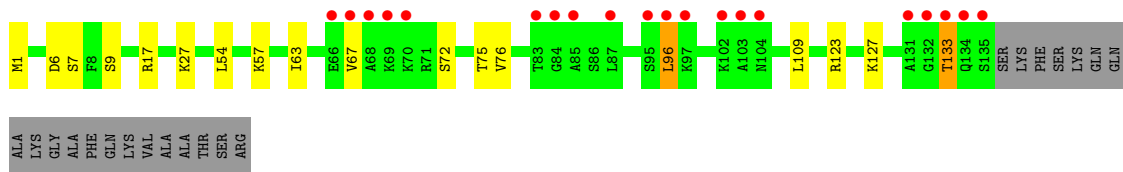
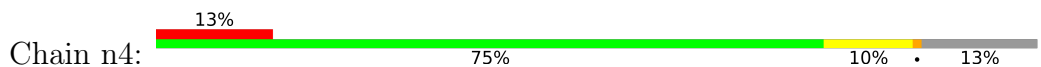
• Molecule 59: 60S ribosomal protein L23-A



• Molecule 60: 60S ribosomal protein L24-A



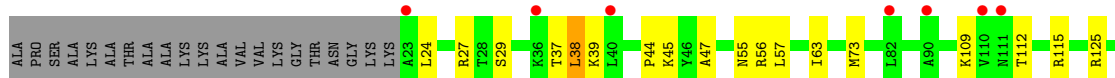
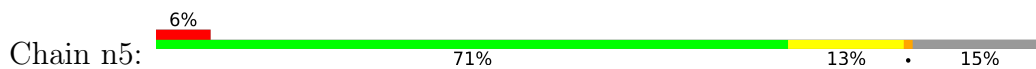
• Molecule 60: 60S ribosomal protein L24-A



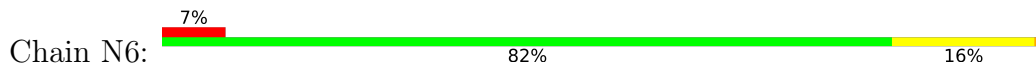
• Molecule 61: 60S ribosomal protein L25



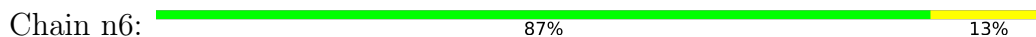
• Molecule 61: 60S ribosomal protein L25



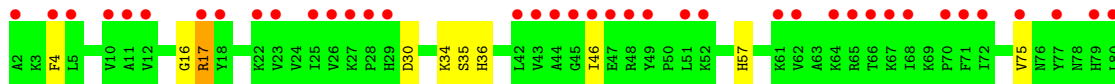
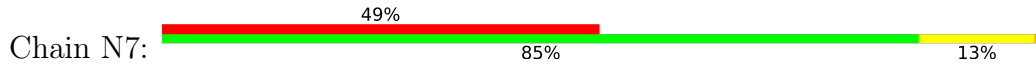
- Molecule 62: 60S ribosomal protein L26-A



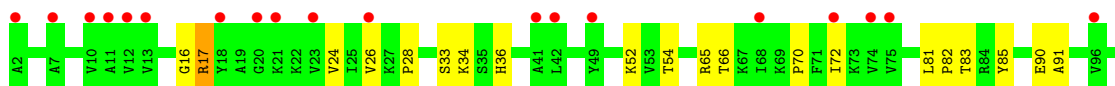
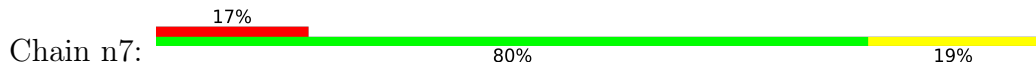
- Molecule 62: 60S ribosomal protein L26-A



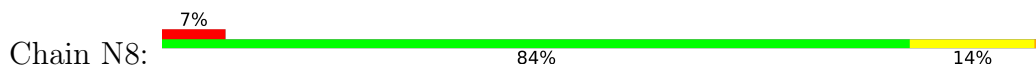
- Molecule 63: 60S ribosomal protein L27-A

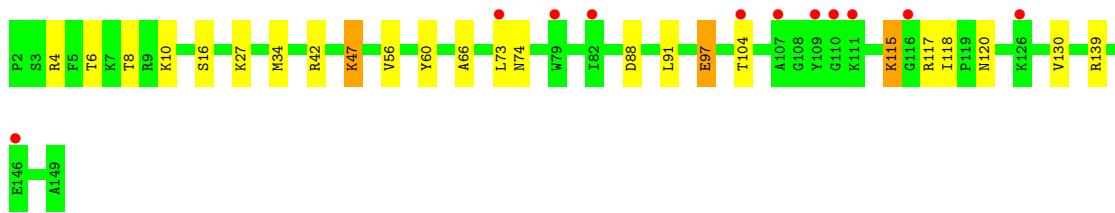


- Molecule 63: 60S ribosomal protein L27-A

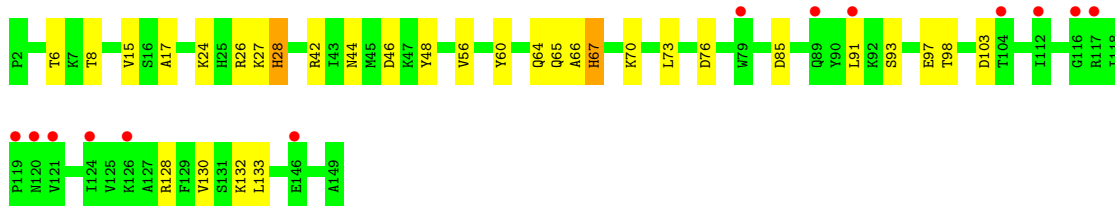
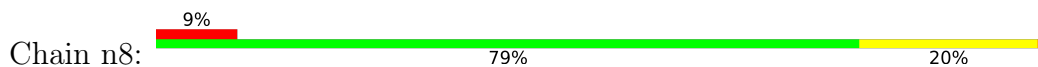


- Molecule 64: 60S ribosomal protein L28

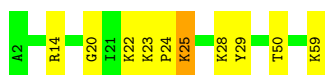
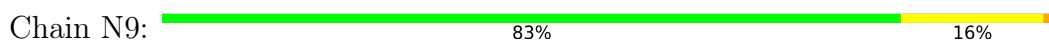




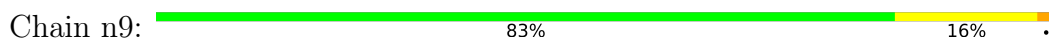
• Molecule 64: 60S ribosomal protein L28



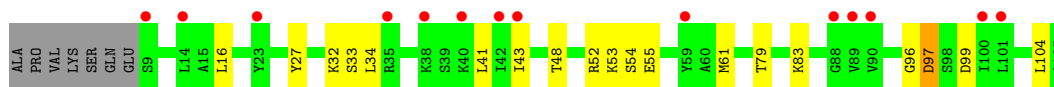
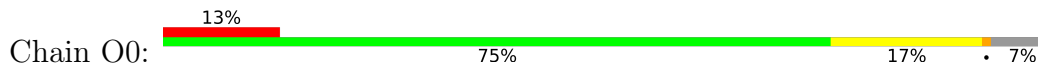
• Molecule 65: 60S ribosomal protein L29



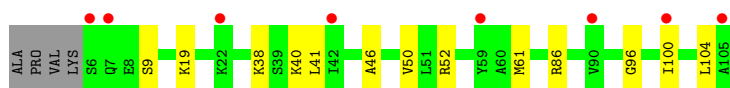
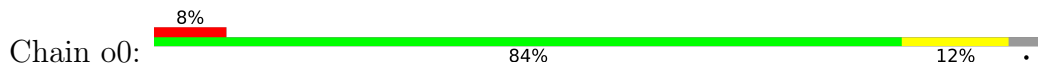
• Molecule 65: 60S ribosomal protein L29



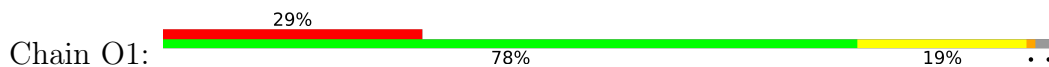
• Molecule 66: 60S ribosomal protein L30

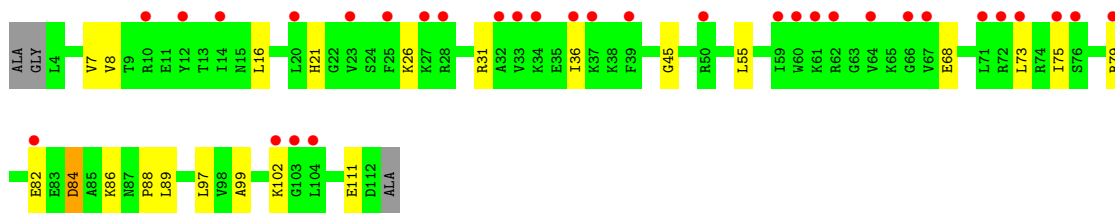


• Molecule 66: 60S ribosomal protein L30

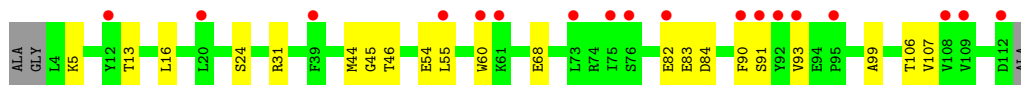
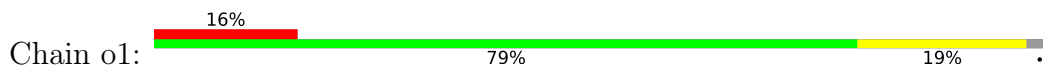


• Molecule 67: 60S ribosomal protein L31-A

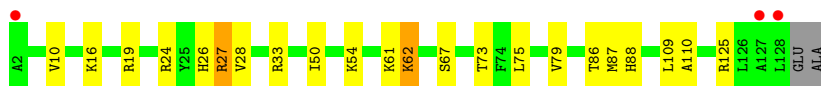
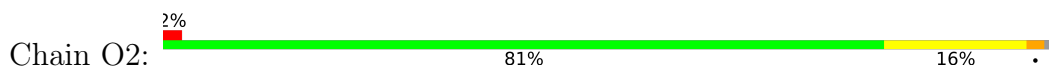




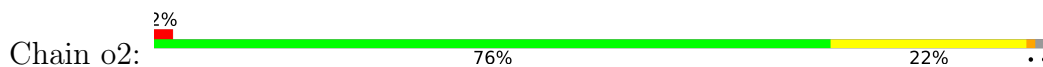
• Molecule 67: 60S ribosomal protein L31-A



• Molecule 68: 60S ribosomal protein L32



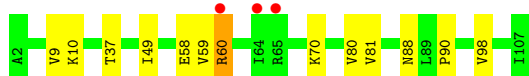
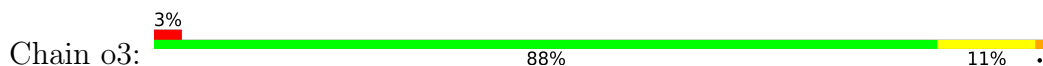
• Molecule 68: 60S ribosomal protein L32



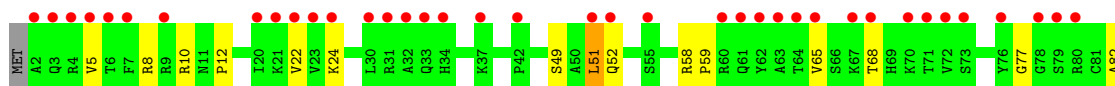
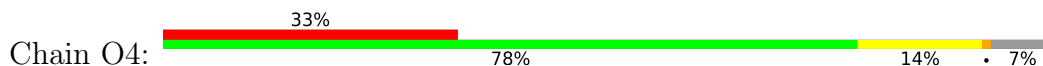
• Molecule 69: 60S ribosomal protein L33-A

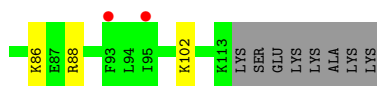


• Molecule 69: 60S ribosomal protein L33-A

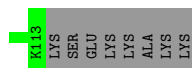
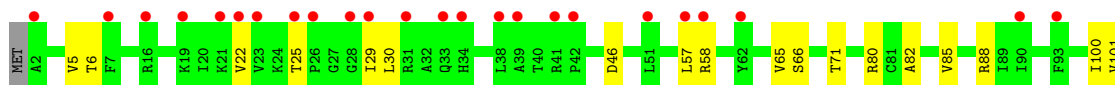
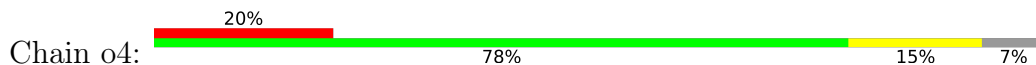


• Molecule 70: 60S ribosomal protein L34-A

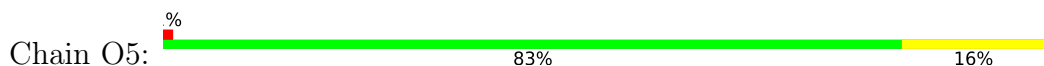




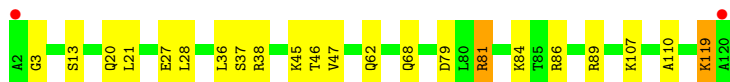
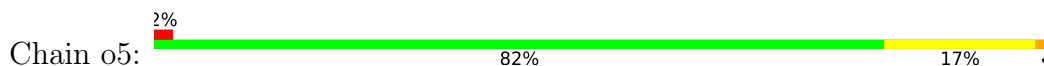
- Molecule 70: 60S ribosomal protein L34-A



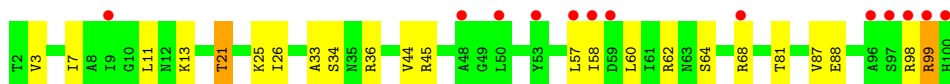
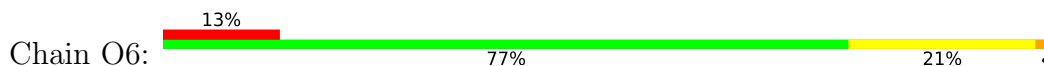
- Molecule 71: 60S ribosomal protein L35-A



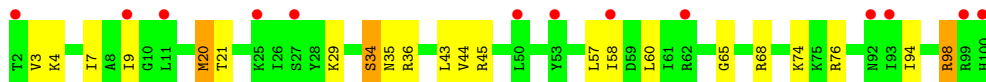
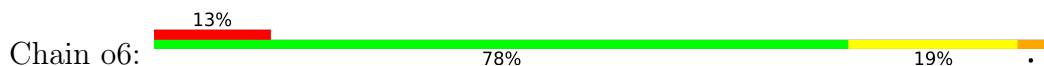
- Molecule 71: 60S ribosomal protein L35-A



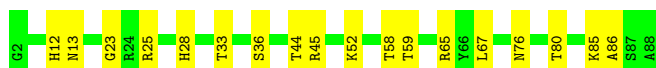
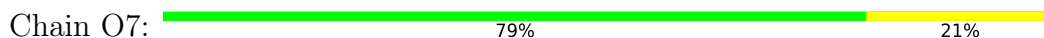
- Molecule 72: 60S ribosomal protein L36-A




- Molecule 72: 60S ribosomal protein L36-A

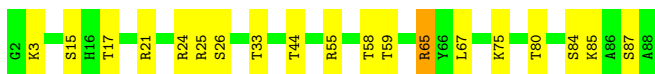


- Molecule 73: 60S ribosomal protein L37-A




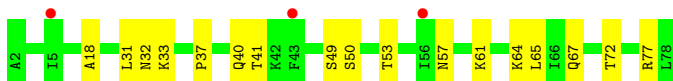
- Molecule 73: 60S ribosomal protein L37-A

Chain o7:  78% 21%




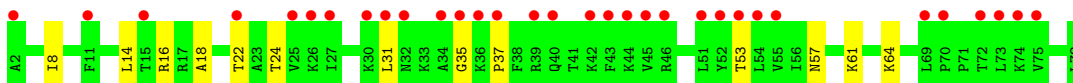
- Molecule 74: 60S ribosomal protein L38

Chain O8:  4% 78% 22%




- Molecule 74: 60S ribosomal protein L38

Chain o8:  42% 83% 17%

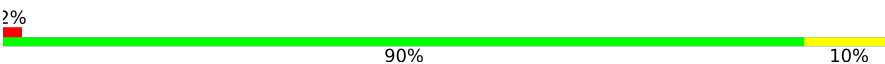


- Molecule 75: 60S ribosomal protein L39

Chain O9:  82% 16%




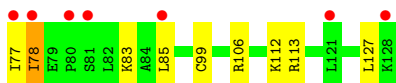
- Molecule 75: 60S ribosomal protein L39

Chain o9:  2% 90% 10%




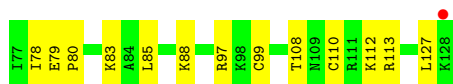
- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:  13% 83% 15%

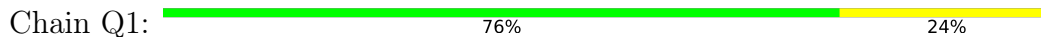


- Molecule 76: Ubiquitin-60S ribosomal protein L40

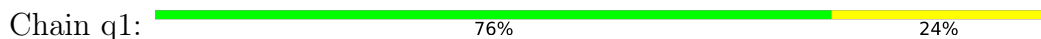
Chain q0:  2% 75% 25%



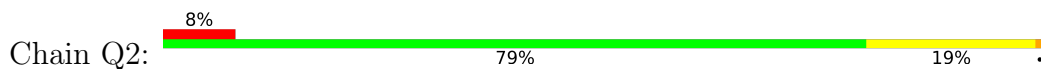
- Molecule 77: 60S ribosomal protein L41-A



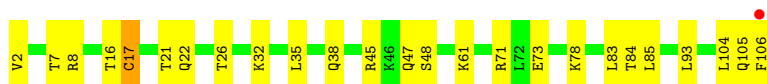
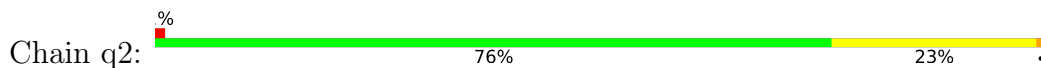
- Molecule 77: 60S ribosomal protein L41-A



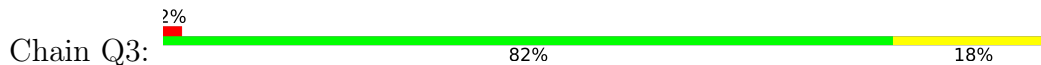
- Molecule 78: 60S ribosomal protein L42-A



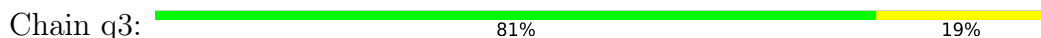
- Molecule 78: 60S ribosomal protein L42-A



- Molecule 79: 60S ribosomal protein L43-A

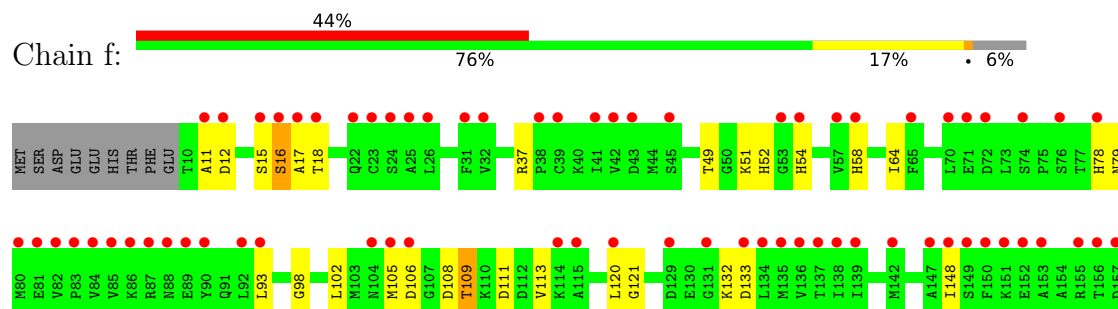


- Molecule 79: 60S ribosomal protein L43-A



- Molecule 80: 60S ribosomal protein L12-A

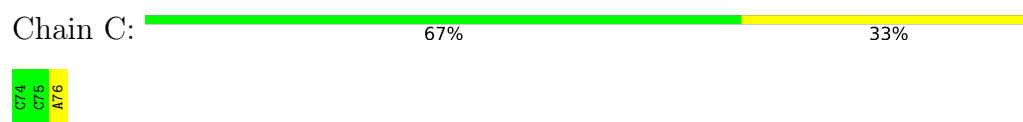
- Molecule 83: Eukaryotic translation initiation factor 5A-1



- Molecule 84: DNA (5'-R(*CP*CP*(NA))-3')



- Molecule 84: DNA (5'-R(*CP*CP*(NA))-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	438.00Å 289.05Å 305.26Å 90.00° 98.95° 90.00°	Depositor
Resolution (Å)	122.88 – 3.45 123.03 – 3.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (122.88-3.45) 99.9 (123.03-3.45)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 3.49Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.207 , 0.263 0.208 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	90.1	Xtrriage
Anisotropy	0.105	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 92.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	413121	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OHX, SPS, 8AN, ZN, 5CT

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	0.44	0/42467	0.98	58/66169 (0.1%)
1	6	0.53	0/42790	1.04	77/66673 (0.1%)
2	S0	0.33	0/1617	0.55	0/2215
2	s0	0.36	0/1623	0.58	0/2222
3	S1	0.30	0/1735	0.53	1/2335 (0.0%)
3	s1	0.34	0/1748	0.56	0/2352
4	S2	0.34	0/1665	0.56	0/2263
4	s2	0.41	0/1665	0.63	0/2263
5	S3	0.33	0/1759	0.53	0/2368
5	s3	0.33	0/1759	0.50	0/2368
6	S4	0.34	0/2109	0.57	0/2839
6	s4	0.39	0/2109	0.62	0/2839
7	S5	0.31	0/1629	0.52	0/2202
7	s5	0.30	0/1629	0.51	0/2202
8	S6	0.34	0/1823	0.52	0/2439
8	s6	0.39	0/1779	0.61	0/2379
9	S7	0.32	0/1506	0.54	0/2028
9	s7	0.34	0/1516	0.57	0/2043
10	S8	0.36	0/1514	0.53	0/2021
10	s8	0.41	0/1514	0.58	0/2021
11	S9	0.33	0/1519	0.49	0/2035
11	s9	0.38	0/1519	0.57	0/2035
12	C0	0.31	0/790	0.54	1/1069 (0.1%)
12	c0	0.30	0/777	0.59	3/1049 (0.3%)
13	C1	0.38	0/1240	0.56	0/1675
13	c1	0.44	0/1194	0.61	0/1610
14	C2	0.29	0/900	0.51	0/1224
14	c2	0.25	0/900	0.48	0/1224
15	C3	0.35	0/1215	0.56	1/1638 (0.1%)
15	c3	0.37	0/1215	0.58	0/1638
16	C4	0.30	0/901	0.56	0/1217
16	c4	0.35	0/960	0.56	0/1290

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	C5	0.34	0/998	0.56	0/1341
17	c5	0.36	0/1060	0.57	0/1426
18	C6	0.32	0/1125	0.57	2/1510 (0.1%)
18	c6	0.34	0/1131	0.54	0/1518
19	C7	0.36	0/935	0.59	0/1254
19	c7	0.32	0/914	0.54	0/1224
20	C8	0.35	0/1211	0.54	1/1628 (0.1%)
20	c8	0.34	0/1211	0.57	1/1628 (0.1%)
21	C9	0.32	0/1130	0.52	0/1517
21	c9	0.33	0/1130	0.51	0/1517
22	D0	0.32	0/865	0.55	0/1169
22	d0	0.35	0/892	0.54	0/1205
23	D1	0.34	0/693	0.53	0/935
23	d1	0.37	0/693	0.61	0/935
24	D2	0.34	0/1038	0.61	1/1395 (0.1%)
24	d2	0.41	0/1038	0.62	0/1395
25	D3	0.39	0/1139	0.59	0/1518
25	d3	0.45	0/1139	0.62	0/1518
26	D4	0.34	0/1087	0.50	0/1449
26	d4	0.39	0/1087	0.62	0/1449
27	D5	0.32	0/571	0.57	0/768
27	d5	0.33	0/566	0.53	0/761
28	D6	0.33	0/782	0.54	0/1047
28	d6	0.38	0/782	0.58	0/1047
29	D7	0.32	0/620	0.52	0/838
29	d7	0.36	0/620	0.57	0/838
30	D8	0.29	0/499	0.51	0/670
30	d8	0.32	0/499	0.57	0/670
31	D9	0.40	0/452	0.57	0/600
31	d9	0.35	0/452	0.52	0/600
32	E0	0.32	0/483	0.49	0/643
32	e0	0.38	0/499	0.62	0/665
33	E1	0.35	0/577	0.61	0/770
33	e1	0.34	0/619	0.61	0/822
34	SR	0.29	0/2489	0.51	0/3389
34	sR	0.28	0/2494	0.49	0/3395
35	SM	0.38	0/1113	0.57	2/1502 (0.1%)
35	sM	0.34	0/683	0.55	1/923 (0.1%)
36	1	0.66	6/75394 (0.0%)	1.15	212/117545 (0.2%)
36	5	0.71	8/75414 (0.0%)	1.18	277/117575 (0.2%)
37	3	0.57	0/2883	1.03	1/4491 (0.0%)
37	7	0.69	0/2883	1.15	7/4491 (0.2%)
38	4	0.60	0/3746	1.07	5/5832 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	8	0.60	0/3746	1.08	7/5832 (0.1%)
39	L2	0.43	0/1948	0.62	0/2617
39	l2	0.45	0/1946	0.65	0/2614
40	L3	0.46	0/3146	0.63	0/4228
40	l3	0.53	0/3146	0.63	0/4228
41	L4	0.49	0/2800	0.67	0/3790
41	l4	0.47	0/2800	0.66	0/3790
42	L5	0.41	0/2425	0.57	0/3271
42	l5	0.51	0/2408	0.64	1/3248 (0.0%)
43	L6	0.45	0/1260	0.61	0/1694
43	l6	0.47	0/1269	0.61	0/1705
44	L7	0.49	0/1821	0.64	1/2451 (0.0%)
44	l7	0.52	0/1828	0.65	1/2461 (0.0%)
45	L8	0.36	0/1836	0.54	0/2481
45	l8	0.38	0/1796	0.57	0/2431
46	L9	0.43	0/1539	0.60	0/2073
46	l9	0.51	0/1539	0.64	0/2073
47	M0	0.45	0/1741	0.58	0/2335
47	m0	0.51	0/1758	0.65	0/2358
48	M1	0.37	0/1374	0.57	0/1842
48	m1	0.45	0/1374	0.60	0/1842
49	M3	0.44	0/1568	0.65	0/2106
49	m3	0.46	0/1573	0.61	0/2113
50	M4	0.44	0/1068	0.59	0/1438
50	m4	0.49	0/1074	0.64	0/1446
51	M5	0.46	0/1757	0.59	0/2354
51	m5	0.44	0/1757	0.58	0/2354
52	M6	0.53	0/1585	0.54	0/2128
52	m6	0.62	0/1585	0.57	0/2128
53	M7	0.48	0/1443	0.62	0/1944
53	m7	0.54	0/1250	0.63	0/1683
54	M8	0.48	0/1465	0.65	0/1965
54	m8	0.47	0/1465	0.67	0/1965
55	M9	0.37	0/1538	0.54	0/2050
55	m9	0.40	0/1538	0.55	0/2050
56	N0	0.46	0/1481	0.61	1/1990 (0.1%)
56	n0	0.54	0/1481	0.65	0/1990
57	N1	0.45	0/1300	0.60	0/1743
57	n1	0.53	0/1300	0.59	0/1743
58	N2	0.35	0/812	0.55	0/1099
58	n2	0.39	0/794	0.58	0/1076
59	N3	0.46	0/1018	0.59	0/1369
59	n3	0.54	0/1018	0.69	1/1369 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	N4	0.37	0/712	0.55	0/958
60	n4	0.44	0/1052	0.60	0/1398
61	N5	0.40	0/979	0.59	0/1321
61	n5	0.41	0/974	0.62	0/1314
62	N6	0.43	0/1004	0.63	1/1341 (0.1%)
62	n6	0.42	0/1004	0.60	0/1341
63	N7	0.36	0/1118	0.56	0/1497
63	n7	0.38	0/1118	0.52	0/1497
64	N8	0.47	0/1204	0.68	0/1612
64	n8	0.49	0/1204	0.66	1/1612 (0.1%)
65	N9	0.45	0/473	0.67	0/629
65	n9	0.53	0/473	0.74	0/629
66	O0	0.33	0/750	0.54	0/1008
66	o0	0.38	0/774	0.59	0/1040
67	O1	0.41	0/890	0.57	0/1196
67	o1	0.49	0/897	0.67	0/1205
68	O2	0.51	0/1041	0.62	0/1394
68	o2	0.52	0/1041	0.66	0/1394
69	O3	0.55	0/868	0.63	0/1168
69	o3	0.54	0/868	0.63	0/1168
70	O4	0.39	0/890	0.60	1/1189 (0.1%)
70	o4	0.44	0/890	0.59	0/1189
71	O5	0.43	0/978	0.61	0/1301
71	o5	0.41	0/974	0.59	0/1297
72	O6	0.40	0/778	0.59	0/1034
72	o6	0.42	0/777	0.61	0/1033
73	O7	0.48	0/696	0.70	0/923
73	o7	0.46	0/696	0.65	1/923 (0.1%)
74	O8	0.34	0/618	0.52	0/826
74	o8	0.38	0/614	0.60	0/822
75	O9	0.48	0/443	0.64	0/588
75	o9	0.45	0/443	0.63	0/588
76	Q0	0.48	0/423	0.72	0/562
76	q0	0.55	0/423	0.65	0/562
77	Q1	0.43	0/234	0.55	0/300
77	q1	0.50	0/234	0.65	0/300
78	Q2	0.61	1/860 (0.1%)	0.72	1/1136 (0.1%)
78	q2	0.58	1/860 (0.1%)	0.67	1/1136 (0.1%)
79	Q3	0.46	0/701	0.65	0/934
79	q3	0.50	0/701	0.61	0/934
80	m2	0.34	0/736	0.76	10/1019 (1.0%)
81	p0	0.30	0/1092	0.52	0/1474
82	p1	0.29	0/234	0.49	1/326 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
82	p2	0.31	0/229	0.46	1/319 (0.3%)
83	f	0.40	0/1121	0.61	0/1508
84	B	0.71	0/40	1.67	0/60
84	C	0.62	0/43	1.18	0/64
All	All	0.54	16/433264 (0.0%)	0.94	681/635894 (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
9	s7	0	1
16	C4	0	1
17	c5	0	1
18	c6	0	1
19	C7	0	1
39	L2	0	2
40	l3	0	1
52	M6	0	1
53	m7	0	1
56	n0	0	1
65	N9	0	1
83	f	1	0
All	All	1	12

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	Q2	17	CYS	CB-SG	9.97	1.99	1.82
78	q2	17	CYS	CB-SG	8.34	1.96	1.82
36	5	1152	G	N9-C4	-6.27	1.32	1.38
36	5	2401	A	N9-C4	6.26	1.41	1.37
36	5	2860	U	N1-C2	5.96	1.44	1.38
36	5	2401	A	N3-C4	5.91	1.38	1.34
36	1	2401	A	N3-C4	5.75	1.38	1.34
36	1	2401	A	C5-C4	5.70	1.42	1.38
36	1	48	A	N9-C4	-5.56	1.34	1.37
36	5	2401	A	C5-C4	5.55	1.42	1.38
36	5	2326	A	N9-C4	-5.39	1.34	1.37
36	5	1915	A	N9-C4	-5.39	1.34	1.37
36	1	2401	A	N9-C4	5.34	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	1	1369	A	N9-C4	-5.17	1.34	1.37
36	1	1192	C	N3-C4	5.14	1.37	1.33
36	5	1303	A	N9-C4	-5.04	1.34	1.37

All (681) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-N9	-11.84	118.90	126.00
36	5	2355	G	N1-C6-O6	11.18	126.61	119.90
1	6	321	C	N1-C2-O2	11.14	125.58	118.90
36	5	1152	G	N3-C4-C5	11.03	134.11	128.60
36	5	1897	G	N1-C6-O6	10.10	125.96	119.90
36	5	1152	G	C2-N3-C4	-10.07	106.87	111.90
36	1	3278	C	N1-C2-O2	9.98	124.89	118.90
36	5	1307	G	P-O3'-C3'	9.97	131.66	119.70
1	6	321	C	C2-N1-C1'	9.85	129.64	118.80
36	1	3217	C	C2-N1-C1'	9.42	129.16	118.80
38	8	80	A	C8-N9-C4	-9.32	102.07	105.80
36	1	2572	C	N1-C2-O2	8.85	124.21	118.90
36	5	3207	U	C2-N1-C1'	-8.83	107.11	117.70
1	2	75	U	C2-N1-C1'	8.70	128.14	117.70
1	6	321	C	N3-C2-O2	-8.69	115.82	121.90
36	1	2617	U	C5-C4-O4	8.54	131.03	125.90
36	5	2943	G	C6-C5-N7	-8.52	125.29	130.40
36	5	2572	C	N1-C2-O2	8.49	123.99	118.90
36	5	2572	C	C2-N1-C1'	8.34	127.97	118.80
1	2	75	U	N1-C2-O2	8.33	128.63	122.80
36	5	2403	G	N1-C6-O6	8.32	124.89	119.90
36	5	2964	G	N1-C6-O6	-8.28	114.93	119.90
38	8	80	A	N7-C8-N9	8.16	117.88	113.80
36	5	3154	C	C2-N1-C1'	8.06	127.66	118.80
36	5	3154	C	N1-C2-O2	8.06	123.73	118.90
36	1	1604	G	C4-N9-C1'	8.02	136.93	126.50
1	2	1096	C	N1-C2-O2	8.00	123.70	118.90
36	1	2572	C	C2-N1-C1'	7.97	127.56	118.80
36	5	2355	G	C6-C5-N7	-7.93	125.64	130.40
36	5	3245	A	C2-N3-C4	-7.93	106.64	110.60
36	5	2403	G	C5-C6-N1	-7.88	107.56	111.50
1	6	1637	C	N1-C2-O2	7.86	123.61	118.90
1	6	453	U	C2-N1-C1'	7.73	126.97	117.70
36	5	2403	G	C4-C5-C6	7.67	123.41	118.80
36	1	3278	C	N3-C2-O2	-7.65	116.54	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2943	G	N1-C6-O6	7.64	124.48	119.90
36	5	1028	U	C2-N1-C1'	7.64	126.86	117.70
36	1	3278	C	C2-N1-C1'	7.62	127.18	118.80
36	1	672	A	C8-N9-C4	7.61	108.84	105.80
36	5	1152	G	C8-N9-C1'	7.55	136.81	127.00
36	5	609	G	C5-C6-O6	-7.54	124.07	128.60
36	5	1200	A	N1-C6-N6	7.54	123.12	118.60
36	1	2572	C	N3-C2-O2	-7.53	116.63	121.90
36	5	2943	G	C4-C5-N7	7.53	113.81	110.80
36	1	780	A	N1-C6-N6	-7.53	114.08	118.60
36	5	1152	G	N3-C2-N2	-7.48	114.66	119.90
1	2	1096	C	C2-N1-C1'	7.47	127.02	118.80
1	6	194	U	C2-N1-C1'	7.47	126.66	117.70
36	1	2838	A	C8-N9-C4	7.45	108.78	105.80
36	5	1152	G	C5-N7-C8	-7.43	100.58	104.30
36	5	3197	G	N3-C4-C5	7.43	132.31	128.60
36	5	2355	G	C5-C6-N1	-7.40	107.80	111.50
36	5	3245	A	N1-C6-N6	7.38	123.03	118.60
36	5	2943	G	C5-C6-O6	-7.38	124.17	128.60
36	5	2964	G	C5-C6-O6	7.37	133.02	128.60
1	6	14	C	C6-N1-C2	-7.37	117.35	120.30
36	1	2314	U	C5-C6-N1	7.37	126.39	122.70
36	1	3217	C	C6-N1-C1'	-7.36	111.97	120.80
36	1	637	C	P-O3'-C3'	7.34	128.51	119.70
36	1	2617	U	N1-C2-N3	7.34	119.31	114.90
1	6	1637	C	C2-N1-C1'	7.30	126.83	118.80
1	6	321	C	C6-N1-C1'	-7.26	112.09	120.80
36	1	2617	U	C4-C5-C6	7.22	124.03	119.70
36	1	2197	C	C6-N1-C2	7.21	123.19	120.30
36	1	1308	A	C8-N9-C4	-7.19	102.92	105.80
36	1	2726	C	N3-C4-N4	-7.16	112.99	118.00
36	5	3207	U	C6-N1-C1'	7.16	131.22	121.20
36	5	648	C	O5'-P-OP1	-7.15	99.27	105.70
1	6	453	U	N1-C2-O2	7.14	127.80	122.80
36	5	2842	U	N3-C2-O2	-7.13	117.20	122.20
1	6	1473	U	N1-C2-O2	7.10	127.77	122.80
36	1	2403	G	N1-C6-O6	7.10	124.16	119.90
36	1	1269	U	C2-N1-C1'	7.06	126.17	117.70
36	1	2617	U	N3-C2-O2	-7.06	117.26	122.20
36	5	2726	C	C5-C4-N4	7.05	125.14	120.20
1	6	453	U	N3-C2-O2	-7.05	117.26	122.20
1	2	507	U	C2-N1-C1'	7.03	126.13	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1000	C	C2-N1-C1'	7.03	126.53	118.80
62	N6	57	LEU	CA-CB-CG	7.02	131.44	115.30
36	1	1484	U	P-O3'-C3'	7.02	128.12	119.70
36	5	2964	G	C4-C5-N7	-6.95	108.02	110.80
36	1	1604	G	N3-C4-C5	-6.94	125.13	128.60
36	1	2726	C	N3-C2-O2	-6.93	117.05	121.90
36	5	1481	A	C8-N9-C4	-6.92	103.03	105.80
18	C6	40	GLU	C-N-CD	-6.91	105.40	120.60
1	2	831	U	C2-N1-C1'	6.91	125.99	117.70
1	2	75	U	N3-C2-O2	-6.89	117.38	122.20
36	5	1152	G	N1-C6-O6	6.88	124.03	119.90
36	1	1131	G	N1-C6-O6	6.84	124.01	119.90
36	5	658	G	C8-N9-C4	-6.84	103.66	106.40
1	6	101	U	N3-C2-O2	-6.82	117.42	122.20
36	5	339	C	C6-N1-C2	-6.80	117.58	120.30
1	2	1657	U	N1-C2-O2	6.80	127.56	122.80
36	1	2403	G	C6-C5-N7	-6.79	126.33	130.40
1	2	507	U	N1-C2-O2	6.78	127.55	122.80
36	1	2816	G	N1-C6-O6	6.76	123.96	119.90
36	5	2726	C	C6-N1-C2	-6.74	117.61	120.30
36	5	2199	G	N1-C6-O6	6.73	123.94	119.90
1	2	1096	C	C6-N1-C1'	-6.72	112.73	120.80
36	1	3143	C	N1-C2-O2	-6.72	114.87	118.90
36	5	1897	G	C5-C6-O6	-6.71	124.57	128.60
36	5	2404	A	N1-C6-N6	6.71	122.63	118.60
36	5	2964	G	N9-C4-C5	6.69	108.08	105.40
36	5	942	U	N3-C4-C5	-6.69	110.59	114.60
36	5	3245	A	C5-N7-C8	-6.67	100.57	103.90
37	7	49	G	N1-C6-O6	6.66	123.90	119.90
36	5	1367	G	N1-C6-O6	6.64	123.89	119.90
38	4	137	C	C6-N1-C2	6.64	122.95	120.30
38	8	125	U	N1-C2-O2	6.64	127.45	122.80
36	5	3362	A	N1-C6-N6	6.63	122.58	118.60
1	2	1039	A	O4'-C1'-N9	6.63	113.50	108.20
36	1	3277	U	N3-C2-O2	-6.62	117.56	122.20
36	5	2629	U	N3-C2-O2	6.61	126.83	122.20
36	1	1604	G	N3-C4-N9	6.60	129.96	126.00
36	1	1594	A	N1-C6-N6	-6.59	114.64	118.60
36	1	1604	G	C8-N9-C1'	-6.58	118.44	127.00
36	1	648	C	C6-N1-C2	-6.58	117.67	120.30
36	1	2627	C	N1-C2-O2	-6.57	114.96	118.90
36	5	1177	G	C6-C5-N7	-6.56	126.46	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	2193	U	N1-C2-O2	6.55	127.39	122.80
36	5	3208	G	N1-C6-O6	6.54	123.83	119.90
36	1	1119	C	C6-N1-C2	6.54	122.92	120.30
36	5	645	A	N1-C6-N6	-6.54	114.68	118.60
37	7	73	C	N1-C2-O2	6.51	122.81	118.90
73	o7	65	ARG	NE-CZ-NH1	6.51	123.56	120.30
36	5	1556	C	N1-C2-O2	6.49	122.79	118.90
1	2	1773	C	C6-N1-C2	-6.47	117.71	120.30
37	7	87	G	C5-C6-O6	-6.47	124.72	128.60
36	5	2199	G	C6-C5-N7	-6.46	126.52	130.40
36	1	1296	C	C6-N1-C2	-6.44	117.72	120.30
36	1	2193	U	N3-C2-O2	-6.43	117.70	122.20
1	6	101	U	N1-C2-O2	6.43	127.30	122.80
36	5	1897	G	C6-C5-N7	-6.43	126.54	130.40
36	5	641	C	N1-C2-N3	-6.43	114.70	119.20
36	5	1487	G	C8-N9-C4	-6.43	103.83	106.40
12	c0	97	PRO	N-CA-CB	6.42	111.01	103.30
36	1	3217	C	N1-C2-O2	6.42	122.75	118.90
1	6	1473	U	N3-C2-O2	-6.41	117.71	122.20
36	1	1495	U	C5-C6-N1	-6.41	119.50	122.70
36	5	639	G	N1-C6-O6	6.41	123.74	119.90
36	5	3207	U	C5-C4-O4	6.40	129.74	125.90
12	C0	88	PRO	N-CA-CB	6.39	110.97	103.30
1	6	194	U	N1-C2-O2	6.39	127.27	122.80
36	1	676	G	C6-C5-N7	-6.38	126.57	130.40
36	5	2684	C	C6-N1-C2	-6.38	117.75	120.30
36	5	3245	A	N7-C8-N9	6.37	116.98	113.80
36	5	2572	C	N3-C2-O2	-6.37	117.44	121.90
36	5	1481	A	N7-C8-N9	6.36	116.98	113.80
36	5	2197	C	C6-N1-C2	6.34	122.83	120.30
36	5	2777	G	C4-N9-C1'	-6.33	118.27	126.50
36	1	2996	U	N1-C2-O2	6.33	127.23	122.80
36	5	2800	G	C8-N9-C4	-6.33	103.87	106.40
36	5	3362	A	C6-C5-N7	-6.33	127.87	132.30
36	1	406	G	O4'-C1'-N9	6.32	113.26	108.20
1	6	1473	U	C2-N1-C1'	6.32	125.28	117.70
1	6	1698	G	P-O3'-C3'	6.32	127.28	119.70
1	6	1637	C	N3-C2-O2	-6.31	117.48	121.90
36	5	2552	C	C2-N1-C1'	6.31	125.74	118.80
36	5	3245	A	C6-C5-N7	-6.31	127.89	132.30
36	5	3197	G	N3-C4-N9	-6.31	122.22	126.00
1	6	687	G	N3-C2-N2	-6.30	115.49	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	963	G	N1-C6-O6	-6.29	116.12	119.90
1	2	507	U	N3-C2-O2	-6.29	117.79	122.20
36	5	3351	U	C2-N1-C1'	6.29	125.25	117.70
1	2	1389	C	C6-N1-C2	-6.28	117.79	120.30
78	Q2	93	LEU	CA-CB-CG	6.28	129.75	115.30
36	1	2617	U	N3-C4-C5	-6.28	110.83	114.60
1	2	75	U	C6-N1-C1'	-6.28	112.41	121.20
36	1	672	A	N1-C6-N6	6.28	122.37	118.60
36	5	939	U	O5'-P-OP1	6.28	118.23	110.70
36	5	3093	C	C6-N1-C2	6.28	122.81	120.30
36	1	2819	A	O5'-P-OP2	-6.27	100.06	105.70
35	sM	167	PRO	N-CA-CB	6.27	110.83	103.30
80	m2	42	PRO	N-CA-CB	6.27	110.83	103.30
36	1	1604	G	C6-C5-N7	-6.27	126.64	130.40
36	5	2978	U	O4'-C1'-N1	6.27	113.21	108.20
36	5	942	U	N3-C4-O4	6.26	123.78	119.40
36	1	676	G	C8-N9-C4	-6.26	103.89	106.40
36	1	2803	A	O5'-P-OP1	-6.26	100.06	105.70
36	1	2726	C	C5-C4-N4	6.26	124.58	120.20
1	2	1389	C	N1-C2-O2	6.25	122.65	118.90
36	5	1481	A	P-O3'-C3'	6.24	127.19	119.70
36	5	1399	A	N1-C6-N6	6.24	122.34	118.60
36	5	2842	U	N1-C2-O2	6.23	127.16	122.80
36	1	2946	A	N1-C6-N6	6.23	122.34	118.60
36	5	2376	G	C4-C5-N7	6.23	113.29	110.80
36	1	59	G	N1-C6-O6	6.22	123.63	119.90
80	m2	46	PRO	N-CA-CB	6.22	110.77	103.30
36	5	1190	A	C4-N9-C1'	6.22	137.49	126.30
36	5	2827	U	C2-N1-C1'	6.22	125.16	117.70
1	6	194	U	N3-C2-O2	-6.21	117.85	122.20
36	5	283	G	C4-C5-N7	6.21	113.28	110.80
36	5	2376	G	C5-C6-O6	-6.21	124.88	128.60
36	1	2978	U	O4'-C1'-N1	6.20	113.16	108.20
36	5	2403	G	C6-C5-N7	-6.19	126.69	130.40
1	2	831	U	C5-C6-N1	6.19	125.79	122.70
36	5	2355	G	C4-C5-C6	6.19	122.51	118.80
36	1	1269	U	N1-C2-O2	6.18	127.13	122.80
36	5	2572	C	C6-N1-C1'	-6.18	113.38	120.80
36	5	2272	G	O4'-C1'-N9	6.18	113.14	108.20
36	5	1190	A	C4-C5-C6	6.17	120.08	117.00
1	2	1698	G	P-O3'-C3'	6.17	127.10	119.70
1	6	1097	U	P-O3'-C3'	6.17	127.10	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	c0	83	PRO	N-CA-CB	6.17	110.70	103.30
36	1	3180	A	C2-N3-C4	-6.16	107.52	110.60
36	5	1170	A	C8-N9-C4	6.15	108.26	105.80
80	m2	101	PRO	N-CA-CB	6.15	110.67	103.30
36	1	1820	U	P-O3'-C3'	6.14	127.07	119.70
36	5	922	U	C5-C6-N1	-6.14	119.63	122.70
36	1	3362	A	O4'-C1'-N9	6.12	113.10	108.20
36	1	3118	C	C6-N1-C2	-6.11	117.86	120.30
36	1	2571	U	C2-N1-C1'	6.11	125.03	117.70
36	5	2288	G	C4-N9-C1'	6.10	134.43	126.50
82	p1	36	PRO	N-CA-CB	6.10	110.62	103.30
36	5	2156	C	C6-N1-C2	6.10	122.74	120.30
35	SM	167	PRO	N-CA-CB	6.10	110.62	103.30
36	5	410	U	N1-C2-O2	-6.09	118.53	122.80
36	1	2355	G	N1-C6-O6	6.09	123.55	119.90
1	6	858	G	O4'-C1'-N9	6.08	113.07	108.20
36	5	2777	G	C6-C5-N7	6.08	134.04	130.40
1	6	75	U	P-O3'-C3'	6.07	126.99	119.70
36	1	65	A	P-O3'-C3'	6.06	126.97	119.70
36	5	3154	C	N3-C2-O2	-6.06	117.66	121.90
1	6	804	A	C8-N9-C4	-6.05	103.38	105.80
36	5	2199	G	N7-C8-N9	6.04	116.12	113.10
36	5	3040	A	C8-N9-C4	6.04	108.22	105.80
36	1	3277	U	C2-N1-C1'	6.04	124.94	117.70
36	5	1556	C	C2-N1-C1'	6.03	125.43	118.80
36	5	523	A	N1-C6-N6	-6.02	114.99	118.60
80	m2	88	PRO	N-CA-CB	6.02	110.53	103.30
36	5	934	G	C4-N9-C1'	6.01	134.32	126.50
1	2	934	C	C2-N1-C1'	6.01	125.41	118.80
36	1	2571	U	N1-C2-O2	6.00	127.00	122.80
36	5	3245	A	N1-C2-N3	6.00	132.30	129.30
36	1	1369	A	C2-N3-C4	-6.00	107.60	110.60
36	1	2350	C	N3-C2-O2	-6.00	117.70	121.90
36	5	1156	C	C6-N1-C2	-6.00	117.90	120.30
36	1	2404	A	N1-C6-N6	5.99	122.19	118.60
36	5	1143	A	C2-N3-C4	-5.99	107.61	110.60
36	5	1028	U	N1-C2-O2	5.98	126.98	122.80
1	2	1389	C	C2-N1-C1'	5.98	125.37	118.80
36	5	876	A	C8-N9-C4	5.96	108.19	105.80
36	5	1152	G	C4-N9-C1'	-5.96	118.76	126.50
36	1	1306	G	N1-C6-O6	5.95	123.47	119.90
36	5	2288	G	C8-N9-C1'	-5.95	119.27	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	m2	51	PRO	N-CA-CB	5.94	110.43	103.30
36	1	2700	G	C6-C5-N7	-5.94	126.84	130.40
36	5	2130	G	C4-N9-C1'	-5.94	118.78	126.50
36	5	2619	G	N3-C4-N9	5.93	129.56	126.00
1	2	1796	C	C6-N1-C2	-5.93	117.93	120.30
36	5	3195	U	C2-N1-C1'	5.92	124.80	117.70
36	5	641	C	C2-N3-C4	5.92	122.86	119.90
80	m2	161	PRO	N-CA-CB	5.91	110.40	103.30
36	1	435	C	C6-N1-C2	5.91	122.66	120.30
36	1	917	A	N1-C6-N6	-5.91	115.06	118.60
1	2	581	U	C2-N1-C1'	5.90	124.78	117.70
36	5	1437	C	C2-N1-C1'	5.90	125.29	118.80
1	2	1539	G	N7-C8-N9	5.90	116.05	113.10
1	2	720	G	OP1-P-O3'	5.89	118.16	105.20
1	6	163	G	N3-C4-N9	-5.89	122.47	126.00
36	5	1878	G	C4-N9-C1'	5.89	134.16	126.50
1	2	992	A	O4'-C1'-N9	5.89	112.91	108.20
36	1	2827	U	N3-C4-O4	-5.89	115.28	119.40
1	2	16	G	N3-C4-C5	-5.88	125.66	128.60
36	1	2664	C	C6-N1-C2	-5.88	117.95	120.30
82	p2	36	PRO	N-CA-CB	5.88	110.36	103.30
38	4	94	C	C6-N1-C2	5.88	122.65	120.30
1	6	151	G	N3-C2-N2	-5.87	115.79	119.90
36	5	776	U	N1-C2-N3	5.87	118.42	114.90
36	1	1001	G	N1-C6-O6	5.87	123.42	119.90
12	c0	88	PRO	N-CA-CB	5.87	110.34	103.30
36	5	2727	A	N1-C6-N6	-5.87	115.08	118.60
36	5	1490	A	C8-N9-C4	-5.86	103.46	105.80
36	5	2621	G	N1-C6-O6	5.85	123.41	119.90
1	2	1291	G	N3-C4-N9	-5.85	122.49	126.00
36	5	2199	G	C8-N9-C4	-5.85	104.06	106.40
1	6	524	U	N3-C2-O2	-5.85	118.11	122.20
80	m2	10	PRO	N-CA-CB	5.85	110.32	103.30
36	5	1765	U	O5'-P-OP1	5.85	117.72	110.70
36	1	1858	A	C2-N3-C4	5.84	113.52	110.60
36	5	2944	U	N1-C2-O2	5.84	126.89	122.80
36	5	2620	G	C4-N9-C1'	-5.84	118.91	126.50
38	8	125	U	N3-C2-O2	-5.84	118.11	122.20
36	1	2553	U	C2-N1-C1'	5.83	124.70	117.70
36	1	1489	A	N1-C6-N6	5.83	122.10	118.60
36	1	2887	A	C2-N3-C4	5.82	113.51	110.60
1	6	104	A	O4'-C1'-N9	5.82	112.85	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1480	G	C8-N9-C4	5.81	108.72	106.40
36	5	2283	G	N1-C6-O6	5.80	123.38	119.90
36	1	1305	U	N1-C2-O2	5.80	126.86	122.80
36	1	981	U	C5-C6-N1	5.79	125.60	122.70
36	5	2777	G	N3-C4-N9	-5.79	122.52	126.00
1	2	1389	C	N3-C2-O2	-5.79	117.85	121.90
1	6	781	U	N1-C2-O2	5.77	126.84	122.80
36	5	776	U	C4-C5-C6	5.77	123.16	119.70
36	5	1161	G	C2-N3-C4	5.77	114.78	111.90
36	5	2584	G	C4-N9-C1'	5.76	134.00	126.50
36	5	383	G	C8-N9-C4	5.76	108.70	106.40
36	1	1307	G	O4'-C1'-N9	5.76	112.81	108.20
1	6	548	G	N1-C6-O6	5.75	123.35	119.90
44	L7	179	LEU	CA-CB-CG	5.75	128.52	115.30
36	1	361	A	N1-C6-N6	-5.74	115.16	118.60
36	1	637	C	C2-N1-C1'	5.74	125.12	118.80
36	1	3367	C	C6-N1-C2	5.74	122.60	120.30
36	5	793	C	C6-N1-C2	-5.74	118.00	120.30
36	5	3078	U	N3-C2-O2	-5.74	118.18	122.20
36	5	1177	G	N1-C6-O6	5.73	123.34	119.90
1	6	542	A	P-O3'-C3'	5.73	126.58	119.70
1	2	1456	C	C2-N1-C1'	5.73	125.10	118.80
36	5	2176	U	N3-C2-O2	-5.72	118.19	122.20
36	5	3154	C	C6-N1-C1'	-5.72	113.94	120.80
36	1	3303	G	C8-N9-C4	5.72	108.69	106.40
36	5	719	U	C5-C6-N1	5.72	125.56	122.70
36	1	780	A	N9-C4-C5	5.71	108.09	105.80
36	5	2392	C	N3-C4-C5	5.71	124.18	121.90
80	m2	15	PRO	N-CA-CB	5.71	110.15	103.30
36	5	2821	C	N1-C2-O2	-5.71	115.48	118.90
38	4	39	G	N1-C6-O6	-5.70	116.48	119.90
36	1	3319	U	P-O3'-C3'	5.70	126.53	119.70
80	m2	102	PRO	N-CA-CB	5.70	110.13	103.30
36	1	922	U	C2-N1-C1'	5.69	124.53	117.70
36	5	2788	C	C6-N1-C2	5.69	122.58	120.30
36	1	1000	C	C6-N1-C2	5.69	122.58	120.30
36	1	2309	A	N1-C6-N6	5.69	122.02	118.60
70	O4	51	LEU	CA-CB-CG	5.69	128.39	115.30
36	1	1160	C	N1-C2-O2	-5.69	115.49	118.90
36	5	2860	U	N3-C2-O2	-5.69	118.22	122.20
36	5	3197	G	C4-N9-C1'	-5.69	119.11	126.50
36	1	2298	U	O4'-C1'-N1	5.68	112.75	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	901	G	N1-C6-O6	5.68	123.31	119.90
36	5	1434	G	C5-C6-O6	-5.68	125.19	128.60
36	5	1495	U	C2-N1-C1'	5.68	124.51	117.70
36	5	2205	U	O4'-C1'-N1	5.67	112.74	108.20
36	1	640	U	N3-C4-O4	5.67	123.37	119.40
78	q2	17	CYS	CA-CB-SG	5.67	124.20	114.00
36	5	2278	C	N1-C2-O2	5.66	122.30	118.90
36	5	2945	G	C5-C6-O6	-5.66	125.20	128.60
36	5	3328	G	N1-C6-O6	-5.66	116.50	119.90
1	6	18	C	C6-N1-C2	-5.66	118.03	120.30
36	1	3106	A	N1-C6-N6	-5.66	115.20	118.60
36	1	1269	U	N3-C2-O2	-5.65	118.24	122.20
36	5	2860	U	O4'-C1'-N1	5.65	112.72	108.20
36	5	2885	C	C6-N1-C2	5.65	122.56	120.30
1	6	1098	U	C2-N1-C1'	5.64	124.47	117.70
36	1	2601	A	C8-N9-C4	5.64	108.06	105.80
36	5	1303	A	C8-N9-C4	5.64	108.06	105.80
36	5	1556	C	N3-C2-O2	-5.64	117.95	121.90
36	5	3078	U	N1-C2-O2	5.64	126.75	122.80
36	1	2827	U	C5-C4-O4	5.63	129.28	125.90
36	5	1495	U	C5-C6-N1	5.63	125.52	122.70
1	6	1000	C	C6-N1-C2	-5.63	118.05	120.30
36	5	3362	A	C5-N7-C8	-5.63	101.09	103.90
36	5	410	U	N3-C4-C5	-5.62	111.23	114.60
3	S1	218	LEU	CA-CB-CG	5.62	128.23	115.30
36	1	2572	C	C6-N1-C1'	-5.62	114.05	120.80
36	5	2625	C	C6-N1-C2	5.62	122.55	120.30
36	1	1716	U	P-O3'-C3'	5.61	126.44	119.70
36	5	934	G	N3-C4-C5	-5.61	125.80	128.60
36	1	2808	A	O5'-P-OP1	-5.60	100.66	105.70
36	5	3057	U	C2-N1-C1'	5.60	124.42	117.70
37	7	73	C	N3-C2-O2	-5.60	117.98	121.90
1	2	1456	C	N1-C2-O2	5.59	122.26	118.90
1	6	1274	C	C2-N1-C1'	5.59	124.95	118.80
36	5	3026	G	N1-C6-O6	5.59	123.25	119.90
37	7	73	C	C6-N1-C2	-5.58	118.07	120.30
36	5	2205	U	C5-C6-N1	5.58	125.49	122.70
18	C6	40	GLU	C-N-CA	5.57	145.41	122.00
36	5	406	G	N3-C4-N9	-5.57	122.66	126.00
36	5	2303	A	C8-N9-C4	5.57	108.03	105.80
36	5	1447	G	O4'-C1'-N9	5.57	112.65	108.20
36	5	2622	C	C6-N1-C2	-5.56	118.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	577	G	C4-C5-N7	5.56	113.03	110.80
36	1	3277	U	N1-C2-O2	5.56	126.69	122.80
36	5	1192	C	N1-C2-O2	5.56	122.24	118.90
1	2	1324	G	N3-C4-N9	-5.56	122.67	126.00
1	6	1058	U	OP1-P-O3'	5.56	117.42	105.20
36	5	2978	U	C5-C6-N1	-5.55	119.92	122.70
1	6	1773	C	N3-C4-C5	-5.55	119.68	121.90
37	7	10	C	C2-N1-C1'	5.55	124.90	118.80
36	1	676	G	N7-C8-N9	5.55	115.87	113.10
1	6	151	G	N3-C4-N9	-5.54	122.67	126.00
36	5	2943	G	C5-N7-C8	-5.54	101.53	104.30
36	5	1311	G	O5'-P-OP2	-5.54	100.72	105.70
38	8	125	U	C2-N1-C1'	5.53	124.34	117.70
36	1	2617	U	C6-N1-C2	-5.53	117.68	121.00
36	5	1403	C	C6-N1-C2	5.53	122.51	120.30
36	5	1177	G	C4-N9-C1'	5.53	133.69	126.50
36	5	2943	G	N3-C4-N9	5.53	129.32	126.00
36	5	3351	U	N1-C2-O2	5.52	126.67	122.80
1	6	163	G	C2-N3-C4	-5.52	109.14	111.90
1	6	163	G	C8-N9-C4	-5.52	104.19	106.40
36	5	1132	C	C6-N1-C2	5.52	122.51	120.30
36	5	2288	G	N3-C4-N9	5.52	129.31	126.00
36	1	2314	U	C2-N1-C1'	5.51	124.31	117.70
1	2	959	U	N1-C2-O2	5.51	126.65	122.80
36	1	2719	U	N1-C2-O2	-5.50	118.95	122.80
36	1	3306	U	C5-C4-O4	5.50	129.20	125.90
36	5	546	C	N1-C2-O2	5.50	122.20	118.90
1	6	558	U	P-O3'-C3'	5.50	126.30	119.70
1	2	542	A	O4'-C1'-N9	5.50	112.60	108.20
24	D2	93	LEU	CA-CB-CG	5.49	127.92	115.30
36	5	915	A	C2-N3-C4	5.49	113.34	110.60
1	6	139	C	P-O3'-C3'	5.48	126.28	119.70
36	5	2330	C	N1-C2-O2	-5.48	115.61	118.90
36	1	2185	G	C8-N9-C4	-5.48	104.21	106.40
1	2	728	U	C2-N1-C1'	5.47	124.27	117.70
36	1	496	C	C5-C6-N1	5.47	123.74	121.00
36	5	1307	G	OP2-P-O3'	5.47	117.24	105.20
36	5	2777	G	C8-N9-C1'	5.47	134.11	127.00
36	1	1367	G	N1-C6-O6	5.47	123.18	119.90
36	5	2704	A	O5'-P-OP1	-5.47	100.78	105.70
36	5	2867	C	C6-N1-C2	5.47	122.49	120.30
36	1	1296	C	C5-C6-N1	5.46	123.73	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1657	U	N3-C2-O2	-5.46	118.38	122.20
36	1	3076	C	C6-N1-C2	-5.45	118.12	120.30
1	6	1	U	N3-C2-O2	-5.45	118.39	122.20
36	1	934	G	C4-C5-N7	5.44	112.98	110.80
36	1	3216	G	N1-C6-O6	5.44	123.16	119.90
1	6	965	U	N3-C2-O2	-5.43	118.40	122.20
36	1	637	C	N1-C2-O2	5.43	122.16	118.90
36	1	89	A	N1-C6-N6	-5.43	115.34	118.60
36	5	639	G	C6-C5-N7	-5.43	127.14	130.40
36	5	1152	G	N7-C8-N9	5.43	115.81	113.10
36	5	353	G	C4-N9-C1'	-5.43	119.44	126.50
1	2	959	U	N3-C2-O2	-5.42	118.40	122.20
36	5	609	G	N1-C6-O6	5.42	123.15	119.90
36	1	2275	A	C8-N9-C4	-5.42	103.63	105.80
36	5	1028	U	N3-C2-O2	-5.42	118.41	122.20
42	l5	110	LEU	CA-CB-CG	5.42	127.76	115.30
36	1	851	C	C2-N1-C1'	5.42	124.76	118.80
80	m2	11	PRO	N-CA-CB	5.42	109.80	103.30
36	5	2758	A	O4'-C1'-N9	5.41	112.53	108.20
36	1	2693	C	C6-N1-C2	5.40	122.46	120.30
36	1	216	G	O5'-P-OP1	-5.39	100.84	105.70
36	5	2842	U	C2-N1-C1'	5.39	124.17	117.70
36	5	2376	G	C6-C5-N7	-5.39	127.17	130.40
36	5	1000	C	C6-N1-C2	5.39	122.45	120.30
1	2	830	U	N3-C2-O2	-5.38	118.43	122.20
36	1	1733	G	N3-C4-C5	-5.38	125.91	128.60
36	5	24	G	N1-C6-O6	5.38	123.13	119.90
36	1	1822	C	C6-N1-C2	-5.38	118.15	120.30
36	1	2624	G	C8-N9-C4	-5.38	104.25	106.40
36	5	2288	G	C6-C5-N7	-5.38	127.17	130.40
1	2	1199	G	C4-N9-C1'	5.38	133.49	126.50
36	1	2550	U	N3-C2-O2	-5.38	118.43	122.20
38	4	11	C	N1-C2-O2	-5.38	115.67	118.90
36	5	1604	G	C4-N9-C1'	5.38	133.49	126.50
36	1	213	A	C8-N9-C4	5.38	107.95	105.80
36	1	2112	U	P-O3'-C3'	5.38	126.15	119.70
36	5	1192	C	C2-N1-C1'	5.38	124.72	118.80
36	1	2776	C	C6-N1-C2	5.38	122.45	120.30
20	c8	15	LEU	CA-CB-CG	5.37	127.66	115.30
36	1	2314	U	C5-C4-O4	-5.37	122.68	125.90
1	6	813	U	C2-N1-C1'	5.37	124.14	117.70
36	1	1481	A	P-O3'-C3'	5.37	126.14	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	344	A	N1-C6-N6	-5.36	115.38	118.60
36	5	1897	G	C4-C5-N7	5.36	112.94	110.80
36	1	851	C	C5-C6-N1	5.36	123.68	121.00
36	1	1368	U	C2-N1-C1'	5.36	124.13	117.70
36	1	2991	A	N1-C6-N6	5.36	121.81	118.60
1	2	1458	G	C4-N9-C1'	5.35	133.46	126.50
36	1	1820	U	OP2-P-O3'	5.35	116.97	105.20
36	1	2137	U	C2-N1-C1'	5.35	124.12	117.70
36	1	2719	U	C2-N1-C1'	-5.35	111.28	117.70
36	1	1495	U	C4-C5-C6	5.35	122.91	119.70
36	5	591	G	N1-C6-O6	5.35	123.11	119.90
1	2	36	C	C5-C4-N4	-5.35	116.46	120.20
36	1	1351	U	N1-C2-O2	5.35	126.54	122.80
36	5	1152	G	C8-N9-C4	-5.35	104.26	106.40
36	5	1858	A	C8-N9-C4	-5.34	103.66	105.80
36	1	2700	G	C5-C6-O6	-5.34	125.39	128.60
36	1	648	C	O5'-P-OP1	-5.34	100.89	105.70
36	1	1355	A	P-O3'-C3'	5.34	126.11	119.70
36	1	984	G	N3-C4-C5	-5.34	125.93	128.60
36	1	2309	A	C4-C5-N7	5.34	113.37	110.70
36	5	1222	G	P-O3'-C3'	5.34	126.11	119.70
1	6	1642	G	N1-C6-O6	5.33	123.10	119.90
36	1	2643	A	C8-N9-C4	5.33	107.93	105.80
36	1	2868	U	N3-C2-O2	-5.33	118.47	122.20
1	6	695	U	N3-C2-O2	-5.33	118.47	122.20
36	5	1180	A	O4'-C1'-N9	-5.33	103.94	108.20
1	6	1747	G	C8-N9-C4	5.32	108.53	106.40
36	5	3377	G	C5-C6-O6	-5.32	125.41	128.60
36	1	1306	G	C5-C6-O6	-5.32	125.41	128.60
36	1	1847	A	N1-C6-N6	-5.32	115.41	118.60
1	2	158	U	P-O3'-C3'	5.32	126.08	119.70
36	1	2935	U	C2-N1-C1'	5.32	124.08	117.70
36	5	718	G	C4-N9-C1'	5.31	133.41	126.50
36	1	1930	A	C8-N9-C4	5.31	107.92	105.80
1	6	639	U	C2-N1-C1'	5.30	124.07	117.70
36	5	3195	U	O4'-C1'-N1	5.30	112.44	108.20
44	17	83	LEU	CA-CB-CG	5.30	127.50	115.30
36	1	913	A	C8-N9-C4	-5.30	103.68	105.80
36	1	2869	U	O5'-P-OP1	-5.30	100.93	105.70
36	1	1160	C	N3-C2-O2	5.30	125.61	121.90
38	4	103	G	N3-C4-C5	-5.30	125.95	128.60
36	5	2171	G	N1-C6-O6	-5.29	116.72	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2249	G	C8-N9-C4	-5.29	104.28	106.40
36	1	831	G	C8-N9-C4	5.29	108.52	106.40
1	2	1560	U	N3-C2-O2	-5.29	118.50	122.20
36	1	2303	A	N1-C6-N6	5.29	121.77	118.60
36	1	979	U	P-O3'-C3'	5.29	126.04	119.70
36	5	1190	A	C8-N9-C1'	-5.28	118.19	127.70
64	n8	28	HIS	N-CA-C	5.28	125.27	111.00
36	1	2572	C	C6-N1-C2	-5.28	118.19	120.30
36	1	2873	U	C5-C4-O4	5.28	129.07	125.90
36	1	2971	A	O4'-C1'-N9	5.28	112.42	108.20
1	6	1389	C	C2-N1-C1'	5.28	124.61	118.80
36	1	3306	U	N3-C2-O2	-5.28	118.51	122.20
36	1	880	G	O4'-C1'-N9	5.27	112.42	108.20
1	6	1340	U	N1-C2-O2	5.27	126.49	122.80
36	1	2541	U	P-O3'-C3'	5.27	126.02	119.70
36	1	992	A	C8-N9-C4	-5.27	103.69	105.80
1	2	1291	G	N3-C4-C5	5.26	131.23	128.60
36	5	1582	C	C6-N1-C2	-5.26	118.19	120.30
36	1	641	C	C6-N1-C2	5.26	122.41	120.30
36	5	2868	U	N1-C2-O2	5.26	126.48	122.80
36	1	672	A	N9-C4-C5	-5.26	103.70	105.80
36	1	799	G	C8-N9-C4	5.26	108.50	106.40
36	1	1352	A	P-O3'-C3'	5.26	126.01	119.70
36	5	641	C	C5-C6-N1	5.26	123.63	121.00
1	6	359	A	C8-N9-C4	5.25	107.90	105.80
36	5	3362	A	N7-C8-N9	5.25	116.43	113.80
1	6	523	G	N3-C4-N9	5.25	129.15	126.00
36	5	2620	G	C6-C5-N7	5.25	133.55	130.40
36	1	3244	A	O5'-P-OP2	-5.25	100.98	105.70
36	5	2983	C	O5'-P-OP1	-5.25	100.98	105.70
36	1	3361	G	N3-C4-N9	5.25	129.15	126.00
36	5	1149	G	N3-C4-C5	-5.25	125.98	128.60
1	2	728	U	N1-C2-O2	5.25	126.47	122.80
36	1	3278	C	C6-N1-C1'	-5.24	114.51	120.80
36	5	718	G	O4'-C1'-N9	5.24	112.39	108.20
36	5	3143	C	N3-C4-C5	-5.24	119.80	121.90
36	1	1508	C	C6-N1-C2	-5.24	118.20	120.30
36	1	2413	A	C4-C5-C6	-5.24	114.38	117.00
36	5	2403	G	C8-N9-C1'	-5.24	120.19	127.00
38	8	113	U	C2-N1-C1'	5.24	123.98	117.70
36	5	3049	A	N1-C6-N6	5.23	121.74	118.60
1	6	1097	U	N3-C2-O2	-5.23	118.54	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1239	C	C5-C6-N1	5.23	123.62	121.00
36	5	1434	G	N1-C6-O6	5.23	123.04	119.90
1	2	720	G	P-O3'-C3'	5.23	125.98	119.70
1	2	1761	U	P-O3'-C3'	5.23	125.98	119.70
36	5	404	G	O5'-P-OP2	-5.23	100.99	105.70
15	C3	22	ALA	C-N-CD	-5.23	109.10	120.60
1	2	1539	G	C8-N9-C4	-5.22	104.31	106.40
36	1	2836	C	N3-C2-O2	-5.22	118.25	121.90
36	5	406	G	C4-N9-C1'	-5.22	119.72	126.50
1	2	1490	C	C6-N1-C2	-5.22	118.21	120.30
36	5	3362	A	O4'-C1'-N9	5.21	112.37	108.20
36	1	3216	G	C5-C6-O6	-5.21	125.47	128.60
36	5	1156	C	C2-N1-C1'	5.21	124.53	118.80
36	1	1422	G	N1-C6-O6	5.21	123.02	119.90
36	5	2976	A	N1-C2-N3	5.21	131.90	129.30
35	SM	134	ASP	CB-CG-OD2	5.20	122.98	118.30
36	1	1296	C	C2-N1-C1'	5.19	124.51	118.80
1	6	639	U	N1-C2-O2	5.19	126.43	122.80
36	5	2231	C	C2-N1-C1'	5.19	124.51	118.80
36	5	2945	G	O5'-P-OP1	-5.19	101.03	105.70
37	3	58	C	C6-N1-C2	-5.19	118.22	120.30
36	1	1469	C	N1-C2-O2	5.19	122.01	118.90
36	5	942	U	C6-N1-C2	-5.18	117.89	121.00
36	5	2182	A	N1-C6-N6	5.18	121.71	118.60
36	5	1449	A	C8-N9-C4	5.18	107.87	105.80
36	5	3362	A	C4-C5-N7	5.18	113.29	110.70
36	1	59	G	C5-C6-O6	-5.17	125.50	128.60
36	5	641	C	C4-C5-C6	-5.17	114.81	117.40
36	5	2772	C	P-O3'-C3'	5.17	125.91	119.70
36	1	1000	C	N1-C2-N3	-5.17	115.58	119.20
1	2	1332	C	C6-N1-C2	-5.17	118.23	120.30
36	1	650	C	N1-C2-O2	-5.17	115.80	118.90
1	2	1573	A	P-O3'-C3'	5.17	125.90	119.70
36	1	1556	C	C2-N1-C1'	5.17	124.48	118.80
1	6	1196	A	P-O3'-C3'	5.17	125.90	119.70
36	5	3161	C	C6-N1-C2	-5.16	118.23	120.30
36	5	3214	U	N3-C2-O2	-5.16	118.58	122.20
36	1	1149	G	N3-C4-N9	-5.16	122.90	126.00
1	6	194	U	C5-C6-N1	5.16	125.28	122.70
1	6	781	U	N3-C2-O2	-5.16	118.59	122.20
1	6	1274	C	N1-C2-O2	5.16	122.00	118.90
36	5	1323	G	N3-C4-C5	-5.16	126.02	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1657	C	N1-C2-O2	5.15	121.99	118.90
36	1	3217	C	N3-C2-O2	-5.14	118.30	121.90
36	5	2385	G	N3-C4-C5	5.14	131.17	128.60
1	6	321	C	C6-N1-C2	-5.14	118.24	120.30
1	2	829	A	P-O3'-C3'	5.14	125.86	119.70
1	2	73	U	O4'-C1'-N1	5.13	112.31	108.20
1	2	278	U	P-O3'-C3'	5.13	125.86	119.70
36	5	2630	C	C2-N1-C1'	5.13	124.45	118.80
1	2	1081	A	O4'-C1'-N9	5.13	112.31	108.20
36	5	2726	C	N3-C4-N4	-5.13	114.41	118.00
36	1	620	U	C2-N1-C1'	-5.13	111.55	117.70
1	6	1537	C	C5-C6-N1	5.13	123.56	121.00
1	6	158	U	P-O3'-C3'	5.12	125.85	119.70
37	7	92	A	N1-C6-N6	5.12	121.67	118.60
1	2	728	U	N3-C2-O2	-5.12	118.61	122.20
36	5	966	U	N3-C2-O2	-5.12	118.62	122.20
36	5	1352	A	P-O3'-C3'	5.12	125.84	119.70
36	1	2193	U	C2-N1-C1'	5.11	123.83	117.70
36	5	2399	A	C8-N9-C4	5.11	107.84	105.80
36	5	2948	C	N1-C2-O2	5.10	121.96	118.90
36	1	890	C	N1-C2-O2	5.10	121.96	118.90
1	6	687	G	N1-C2-N2	5.10	120.79	116.20
1	6	858	G	C4-N9-C1'	5.10	133.13	126.50
36	5	2531	C	N1-C2-O2	5.10	121.96	118.90
36	5	1355	A	P-O3'-C3'	5.10	125.82	119.70
38	8	54	A	C8-N9-C4	-5.10	103.76	105.80
36	1	2403	G	C4-C5-C6	5.10	121.86	118.80
36	1	2847	A	C8-N9-C4	5.10	107.84	105.80
36	1	1362	G	C8-N9-C4	5.09	108.44	106.40
1	6	1098	U	N1-C2-O2	5.09	126.37	122.80
1	6	1751	C	O5'-P-OP2	-5.09	101.11	105.70
36	1	881	C	N1-C2-O2	5.09	121.96	118.90
36	5	2156	C	C5-C6-N1	-5.09	118.45	121.00
36	5	3347	A	C8-N9-C4	5.09	107.84	105.80
36	1	347	G	C4-C5-N7	5.09	112.84	110.80
36	5	960	U	N1-C2-O2	5.09	126.36	122.80
36	5	2403	G	C4-N9-C1'	5.09	133.12	126.50
36	1	1429	G	O4'-C1'-N9	-5.09	104.13	108.20
36	1	2230	C	C6-N1-C2	-5.09	118.27	120.30
36	5	2526	C	N1-C2-O2	5.09	121.95	118.90
1	2	1324	G	N3-C2-N2	-5.08	116.34	119.90
36	5	180	C	N3-C2-O2	-5.08	118.34	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2643	A	C8-N9-C4	5.08	107.83	105.80
1	6	1031	U	OP2-P-O3'	5.08	116.37	105.20
36	1	2808	A	N1-C6-N6	5.08	121.64	118.60
36	5	2288	G	N1-C2-N3	5.08	126.94	123.90
36	5	406	G	C6-C5-N7	5.07	133.44	130.40
59	n3	48	ARG	NE-CZ-NH1	5.07	122.83	120.30
36	5	406	G	N1-C6-O6	-5.07	116.86	119.90
36	5	546	C	C2-N1-C1'	5.07	124.38	118.80
36	1	1716	U	OP1-P-O3'	5.07	116.35	105.20
36	1	1589	A	N1-C6-N6	-5.07	115.56	118.60
56	N0	24	LEU	CA-CB-CG	5.06	126.95	115.30
36	1	2593	A	P-O3'-C3'	5.06	125.77	119.70
1	2	1202	A	C8-N9-C4	-5.06	103.78	105.80
36	5	2376	G	N1-C6-O6	5.06	122.94	119.90
36	5	2644	C	C6-N1-C2	5.06	122.32	120.30
36	5	30	G	C8-N9-C4	5.06	108.42	106.40
36	1	3214	U	O4'-C1'-N1	5.06	112.25	108.20
1	6	1637	C	C6-N1-C1'	-5.05	114.74	120.80
36	5	2375	G	O4'-C1'-N9	5.05	112.24	108.20
36	1	94	G	C8-N9-C4	5.05	108.42	106.40
36	1	2872	A	C2-N3-C4	5.05	113.13	110.60
36	5	674	G	N3-C4-C5	5.05	131.12	128.60
36	1	2624	G	N7-C8-N9	5.05	115.62	113.10
36	1	14	U	O5'-P-OP2	-5.04	101.16	105.70
36	1	2093	A	C2-N3-C4	5.04	113.12	110.60
1	6	14	C	C5-C6-N1	5.04	123.52	121.00
36	5	767	U	O4'-C1'-N1	5.04	112.23	108.20
36	1	979	U	C6-N1-C2	-5.04	117.98	121.00
36	5	2943	G	N7-C8-N9	5.04	115.62	113.10
36	1	1437	C	C2-N1-C1'	5.04	124.34	118.80
1	6	187	G	OP1-P-O3'	5.04	116.28	105.20
36	1	2372	A	N3-C4-C5	-5.04	123.27	126.80
36	5	2827	U	N1-C2-O2	5.04	126.33	122.80
36	5	3189	G	C5-C6-N1	-5.04	108.98	111.50
36	1	2413	A	C8-N9-C4	5.03	107.81	105.80
36	1	3057	U	N1-C2-N3	5.03	117.92	114.90
36	5	3245	A	C4-C5-N7	5.03	113.21	110.70
1	6	3	U	C6-N1-C2	5.02	124.01	121.00
1	6	1549	C	C6-N1-C2	-5.02	118.29	120.30
36	5	1779	C	C6-N1-C2	5.02	122.31	120.30
36	5	3002	C	C6-N1-C2	5.02	122.31	120.30
36	5	3195	U	C6-N1-C1'	-5.02	114.17	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1129	A	N1-C6-N6	5.02	121.61	118.60
36	1	3278	C	C6-N1-C2	-5.02	118.29	120.30
1	6	151	G	N1-C2-N2	5.02	120.72	116.20
1	6	151	G	N9-C4-C5	5.02	107.41	105.40
1	6	1185	U	N1-C2-O2	5.02	126.31	122.80
36	5	805	G	C8-N9-C4	5.02	108.41	106.40
36	1	1417	G	C8-N9-C4	5.02	108.41	106.40
36	5	1177	G	C8-N9-C1'	-5.02	120.48	127.00
36	5	1592	G	N1-C6-O6	5.01	122.91	119.90
36	5	406	G	C8-N9-C1'	5.01	133.52	127.00
36	5	2355	G	C5-C6-O6	-5.01	125.59	128.60
36	5	942	U	C5-C6-N1	5.01	125.20	122.70
36	5	3357	U	P-O3'-C3'	5.01	125.71	119.70
36	1	1151	U	N3-C4-C5	-5.00	111.60	114.60
36	5	2830	G	N1-C2-N3	5.00	126.90	123.90
20	C8	3	LEU	CA-CB-CG	5.00	126.80	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
83	f	51	5CT	C2

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	C4	123	SER	Peptide
19	C7	85	VAL	Peptide
39	L2	142	ASP	Peptide
39	L2	19	HIS	Peptide
52	M6	110	PRO	Peptide
65	N9	20	GLY	Peptide
17	c5	52	LYS	Peptide
18	c6	40	GLU	Peptide
40	l3	346	THR	Peptide
53	m7	66	SER	Peptide
56	n0	133	ALA	Peptide
9	s7	130	VAL	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S0	204/251 (81%)	157 (77%)	34 (17%)	13 (6%)	1	13
2	s0	204/251 (81%)	148 (72%)	31 (15%)	25 (12%)	0	4
3	S1	212/254 (84%)	154 (73%)	38 (18%)	20 (9%)	0	7
3	s1	214/254 (84%)	169 (79%)	30 (14%)	15 (7%)	1	11
4	S2	215/253 (85%)	169 (79%)	36 (17%)	10 (5%)	2	19
4	s2	215/253 (85%)	172 (80%)	25 (12%)	18 (8%)	1	8
5	S3	221/239 (92%)	186 (84%)	24 (11%)	11 (5%)	2	18
5	s3	221/239 (92%)	172 (78%)	36 (16%)	13 (6%)	1	14
6	S4	258/260 (99%)	197 (76%)	44 (17%)	17 (7%)	1	12
6	s4	258/260 (99%)	200 (78%)	42 (16%)	16 (6%)	1	13
7	S5	204/224 (91%)	153 (75%)	35 (17%)	16 (8%)	1	9
7	s5	204/224 (91%)	150 (74%)	41 (20%)	13 (6%)	1	13
8	S6	224/236 (95%)	189 (84%)	23 (10%)	12 (5%)	2	16
8	s6	216/236 (92%)	176 (82%)	32 (15%)	8 (4%)	3	25
9	S7	182/189 (96%)	127 (70%)	39 (21%)	16 (9%)	1	7
9	s7	184/189 (97%)	141 (77%)	29 (16%)	14 (8%)	1	9
10	S8	184/200 (92%)	150 (82%)	25 (14%)	9 (5%)	2	18
10	s8	184/200 (92%)	151 (82%)	27 (15%)	6 (3%)	4	27
11	S9	183/196 (93%)	148 (81%)	27 (15%)	8 (4%)	2	21
11	s9	183/196 (93%)	141 (77%)	33 (18%)	9 (5%)	2	18
12	C0	94/105 (90%)	69 (73%)	16 (17%)	9 (10%)	0	7
12	c0	92/105 (88%)	63 (68%)	14 (15%)	15 (16%)	0	2
13	C1	153/155 (99%)	122 (80%)	21 (14%)	10 (6%)	1	12
13	c1	144/155 (93%)	120 (83%)	19 (13%)	5 (4%)	3	26
14	C2	122/142 (86%)	71 (58%)	33 (27%)	18 (15%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	c2	122/142 (86%)	78 (64%)	30 (25%)	14 (12%)	0	5
15	C3	148/150 (99%)	120 (81%)	17 (12%)	11 (7%)	1	10
15	c3	148/150 (99%)	116 (78%)	20 (14%)	12 (8%)	1	9
16	C4	125/136 (92%)	89 (71%)	24 (19%)	12 (10%)	0	7
16	c4	126/136 (93%)	96 (76%)	16 (13%)	14 (11%)	0	5
17	C5	122/141 (86%)	99 (81%)	13 (11%)	10 (8%)	1	8
17	c5	133/141 (94%)	86 (65%)	38 (29%)	9 (7%)	1	12
18	C6	139/142 (98%)	118 (85%)	13 (9%)	8 (6%)	1	15
18	c6	140/142 (99%)	118 (84%)	13 (9%)	9 (6%)	1	13
19	C7	116/136 (85%)	90 (78%)	18 (16%)	8 (7%)	1	11
19	c7	113/136 (83%)	86 (76%)	18 (16%)	9 (8%)	1	9
20	C8	143/145 (99%)	111 (78%)	25 (18%)	7 (5%)	2	18
20	c8	143/145 (99%)	117 (82%)	19 (13%)	7 (5%)	2	18
21	C9	141/143 (99%)	116 (82%)	18 (13%)	7 (5%)	2	18
21	c9	141/143 (99%)	116 (82%)	21 (15%)	4 (3%)	5	31
22	D0	105/120 (88%)	89 (85%)	12 (11%)	4 (4%)	3	24
22	d0	108/120 (90%)	90 (83%)	13 (12%)	5 (5%)	2	20
23	D1	85/87 (98%)	64 (75%)	8 (9%)	13 (15%)	0	2
23	d1	85/87 (98%)	61 (72%)	17 (20%)	7 (8%)	1	8
24	D2	127/129 (98%)	106 (84%)	16 (13%)	5 (4%)	3	24
24	d2	127/129 (98%)	107 (84%)	17 (13%)	3 (2%)	6	34
25	D3	142/144 (99%)	104 (73%)	22 (16%)	16 (11%)	0	5
25	d3	142/144 (99%)	117 (82%)	24 (17%)	1 (1%)	22	60
26	D4	132/134 (98%)	106 (80%)	16 (12%)	10 (8%)	1	9
26	d4	132/134 (98%)	101 (76%)	20 (15%)	11 (8%)	1	8
27	D5	68/107 (64%)	50 (74%)	12 (18%)	6 (9%)	1	7
27	d5	67/107 (63%)	49 (73%)	16 (24%)	2 (3%)	4	29
28	D6	95/97 (98%)	57 (60%)	24 (25%)	14 (15%)	0	2
28	d6	95/97 (98%)	69 (73%)	14 (15%)	12 (13%)	0	4
29	D7	79/81 (98%)	69 (87%)	7 (9%)	3 (4%)	3	24
29	d7	79/81 (98%)	57 (72%)	16 (20%)	6 (8%)	1	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	D8	61/66 (92%)	47 (77%)	10 (16%)	4 (7%)	1	12
30	d8	61/66 (92%)	41 (67%)	11 (18%)	9 (15%)	0	2
31	D9	51/55 (93%)	37 (72%)	11 (22%)	3 (6%)	1	14
31	d9	51/55 (93%)	40 (78%)	8 (16%)	3 (6%)	1	14
32	E0	58/63 (92%)	41 (71%)	15 (26%)	2 (3%)	3	27
32	e0	60/63 (95%)	38 (63%)	15 (25%)	7 (12%)	0	4
33	E1	69/76 (91%)	38 (55%)	19 (28%)	12 (17%)	0	2
33	e1	74/76 (97%)	39 (53%)	12 (16%)	23 (31%)	0	0
34	SR	316/318 (99%)	260 (82%)	43 (14%)	13 (4%)	3	23
34	sR	316/318 (99%)	264 (84%)	38 (12%)	14 (4%)	2	21
35	SM	155/273 (57%)	107 (69%)	32 (21%)	16 (10%)	0	6
35	sM	98/273 (36%)	66 (67%)	23 (24%)	9 (9%)	1	7
39	L2	250/253 (99%)	217 (87%)	23 (9%)	10 (4%)	3	23
39	l2	250/253 (99%)	204 (82%)	33 (13%)	13 (5%)	2	17
40	L3	384/386 (100%)	315 (82%)	46 (12%)	23 (6%)	1	14
40	l3	384/386 (100%)	337 (88%)	35 (9%)	12 (3%)	4	29
41	L4	359/361 (99%)	285 (79%)	52 (14%)	22 (6%)	1	13
41	l4	359/361 (99%)	288 (80%)	53 (15%)	18 (5%)	2	18
42	L5	294/296 (99%)	229 (78%)	42 (14%)	23 (8%)	1	9
42	l5	292/296 (99%)	250 (86%)	35 (12%)	7 (2%)	6	34
43	L6	152/175 (87%)	132 (87%)	17 (11%)	3 (2%)	7	37
43	l6	153/175 (87%)	123 (80%)	25 (16%)	5 (3%)	4	27
44	L7	220/243 (90%)	173 (79%)	39 (18%)	8 (4%)	3	25
44	l7	221/243 (91%)	193 (87%)	23 (10%)	5 (2%)	6	34
45	L8	231/255 (91%)	184 (80%)	38 (16%)	9 (4%)	3	24
45	l8	229/255 (90%)	167 (73%)	48 (21%)	14 (6%)	1	13
46	L9	189/191 (99%)	159 (84%)	19 (10%)	11 (6%)	1	15
46	l9	189/191 (99%)	163 (86%)	21 (11%)	5 (3%)	5	32
47	M0	207/220 (94%)	167 (81%)	31 (15%)	9 (4%)	2	21
47	m0	209/220 (95%)	165 (79%)	33 (16%)	11 (5%)	2	16
48	M1	167/173 (96%)	134 (80%)	19 (11%)	14 (8%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	m1	167/173 (96%)	137 (82%)	19 (11%)	11 (7%)	1	12
49	M3	191/198 (96%)	153 (80%)	27 (14%)	11 (6%)	1	15
49	m3	192/198 (97%)	153 (80%)	24 (12%)	15 (8%)	1	9
50	M4	134/137 (98%)	114 (85%)	15 (11%)	5 (4%)	3	25
50	m4	135/137 (98%)	115 (85%)	16 (12%)	4 (3%)	4	29
51	M5	201/203 (99%)	176 (88%)	19 (10%)	6 (3%)	4	29
51	m5	201/203 (99%)	174 (87%)	23 (11%)	4 (2%)	7	37
52	M6	195/198 (98%)	173 (89%)	16 (8%)	6 (3%)	4	29
52	m6	195/198 (98%)	182 (93%)	9 (5%)	4 (2%)	7	36
53	M7	181/183 (99%)	150 (83%)	25 (14%)	6 (3%)	4	27
53	m7	153/183 (84%)	127 (83%)	25 (16%)	1 (1%)	22	60
54	M8	183/185 (99%)	151 (82%)	24 (13%)	8 (4%)	2	21
54	m8	183/185 (99%)	154 (84%)	20 (11%)	9 (5%)	2	18
55	M9	186/188 (99%)	160 (86%)	23 (12%)	3 (2%)	9	42
55	m9	186/188 (99%)	166 (89%)	13 (7%)	7 (4%)	3	24
56	N0	170/172 (99%)	155 (91%)	12 (7%)	3 (2%)	8	39
56	n0	170/172 (99%)	152 (89%)	15 (9%)	3 (2%)	8	39
57	N1	157/159 (99%)	137 (87%)	15 (10%)	5 (3%)	4	28
57	n1	157/159 (99%)	131 (83%)	24 (15%)	2 (1%)	12	46
58	N2	98/120 (82%)	72 (74%)	23 (24%)	3 (3%)	4	29
58	n2	96/120 (80%)	80 (83%)	11 (12%)	5 (5%)	2	17
59	N3	134/136 (98%)	117 (87%)	15 (11%)	2 (2%)	10	43
59	n3	134/136 (98%)	122 (91%)	7 (5%)	5 (4%)	3	25
60	N4	96/155 (62%)	68 (71%)	18 (19%)	10 (10%)	0	6
60	n4	133/155 (86%)	102 (77%)	22 (16%)	9 (7%)	1	12
61	N5	119/141 (84%)	99 (83%)	14 (12%)	6 (5%)	2	18
61	n5	118/141 (84%)	94 (80%)	19 (16%)	5 (4%)	3	22
62	N6	124/126 (98%)	107 (86%)	13 (10%)	4 (3%)	4	28
62	n6	124/126 (98%)	102 (82%)	21 (17%)	1 (1%)	19	57
63	N7	133/135 (98%)	114 (86%)	10 (8%)	9 (7%)	1	12
63	n7	133/135 (98%)	112 (84%)	12 (9%)	9 (7%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
64	N8	146/148 (99%)	118 (81%)	22 (15%)	6 (4%)	3	23
64	n8	146/148 (99%)	111 (76%)	24 (16%)	11 (8%)	1	10
65	N9	56/58 (97%)	41 (73%)	12 (21%)	3 (5%)	2	16
65	n9	56/58 (97%)	39 (70%)	12 (21%)	5 (9%)	1	7
66	O0	95/104 (91%)	80 (84%)	11 (12%)	4 (4%)	3	22
66	o0	98/104 (94%)	84 (86%)	11 (11%)	3 (3%)	4	29
67	O1	107/112 (96%)	89 (83%)	8 (8%)	10 (9%)	0	7
67	o1	107/112 (96%)	83 (78%)	18 (17%)	6 (6%)	2	15
68	O2	125/129 (97%)	104 (83%)	18 (14%)	3 (2%)	6	34
68	o2	125/129 (97%)	103 (82%)	16 (13%)	6 (5%)	2	19
69	O3	104/106 (98%)	96 (92%)	7 (7%)	1 (1%)	15	52
69	o3	104/106 (98%)	92 (88%)	9 (9%)	3 (3%)	4	30
70	O4	110/121 (91%)	88 (80%)	17 (16%)	5 (4%)	2	20
70	o4	110/121 (91%)	98 (89%)	11 (10%)	1 (1%)	17	54
71	O5	117/119 (98%)	93 (80%)	22 (19%)	2 (2%)	9	40
71	o5	117/119 (98%)	98 (84%)	14 (12%)	5 (4%)	2	21
72	O6	97/99 (98%)	78 (80%)	13 (13%)	6 (6%)	1	13
72	o6	97/99 (98%)	78 (80%)	14 (14%)	5 (5%)	2	17
73	O7	85/87 (98%)	64 (75%)	16 (19%)	5 (6%)	1	14
73	o7	85/87 (98%)	72 (85%)	11 (13%)	2 (2%)	6	34
74	O8	75/77 (97%)	62 (83%)	9 (12%)	4 (5%)	2	16
74	o8	75/77 (97%)	60 (80%)	12 (16%)	3 (4%)	3	23
75	O9	48/50 (96%)	40 (83%)	7 (15%)	1 (2%)	7	36
75	o9	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
76	Q0	50/52 (96%)	42 (84%)	7 (14%)	1 (2%)	7	37
76	q0	50/52 (96%)	46 (92%)	2 (4%)	2 (4%)	3	23
77	Q1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
77	q1	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
78	Q2	103/105 (98%)	80 (78%)	17 (16%)	6 (6%)	1	15
78	q2	103/105 (98%)	95 (92%)	7 (7%)	1 (1%)	15	52
79	Q3	89/91 (98%)	71 (80%)	10 (11%)	8 (9%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
79	q3	89/91 (98%)	74 (83%)	12 (14%)	3 (3%)	3	27
80	m2	144/165 (87%)	67 (46%)	48 (33%)	29 (20%)	0	1
81	p0	139/311 (45%)	110 (79%)	20 (14%)	9 (6%)	1	12
82	p1	45/106 (42%)	26 (58%)	17 (38%)	2 (4%)	2	21
82	p2	44/106 (42%)	33 (75%)	6 (14%)	5 (11%)	0	5
83	f	145/157 (92%)	97 (67%)	34 (23%)	14 (10%)	0	6
All	All	22711/24683 (92%)	18197 (80%)	3231 (14%)	1283 (6%)	2	15

All (1283) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	158	VAL
2	S0	169	SER
2	S0	191	ARG
3	S1	82	ARG
3	S1	132	ASP
3	S1	206	PRO
4	S2	48	GLY
5	S3	62	ASN
5	S3	211	PRO
5	S3	220	PRO
6	S4	104	ASP
7	S5	39	GLU
7	S5	43	PHE
7	S5	153	GLY
8	S6	149	LYS
8	S6	153	VAL
8	S6	154	ARG
8	S6	225	GLU
9	S7	29	ASN
9	S7	31	SER
9	S7	64	VAL
9	S7	74	GLN
9	S7	155	ASP
10	S8	149	SER
11	S9	93	LEU
11	S9	98	ALA
11	S9	134	ILE
12	C0	60	SER

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Mol	Chain	Res	Type
12	C0	61	TRP
12	C0	87	VAL
12	C0	88	PRO
13	C1	3	THR
13	C1	7	VAL
13	C1	40	LEU
13	C1	154	ALA
14	C2	22	VAL
14	C2	91	VAL
15	C3	12	SER
15	C3	68	GLY
15	C3	138	ASN
15	C3	149	LEU
16	C4	42	VAL
17	C5	54	ALA
17	C5	125	PRO
17	C5	126	VAL
18	C6	41	PRO
19	C7	85	VAL
19	C7	86	PRO
19	C7	88	VAL
20	C8	14	ILE
20	C8	82	PRO
20	C8	92	ILE
21	C9	53	TRP
21	C9	69	LYS
21	C9	116	ILE
23	D1	7	GLN
23	D1	82	VAL
25	D3	3	LYS
25	D3	92	CYS
25	D3	138	GLU
27	D5	93	SER
28	D6	82	ARG
28	D6	84	VAL
28	D6	86	VAL
32	E0	47	VAL
33	E1	84	VAL
33	E1	94	LYS
33	E1	98	VAL
34	SR	318	ALA
35	SM	42	ALA

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Mol	Chain	Res	Type
35	SM	47	ALA
35	SM	52	PRO
35	SM	167	PRO
35	SM	172	VAL
39	L2	98	VAL
39	L2	115	ASN
39	L2	141	PRO
40	L3	3	HIS
40	L3	4	ARG
40	L3	69	LYS
40	L3	139	GLN
40	L3	187	SER
40	L3	347	SER
41	L4	4	PRO
41	L4	131	VAL
41	L4	175	HIS
41	L4	270	SER
41	L4	311	HIS
41	L4	339	LEU
42	L5	85	ARG
42	L5	178	ASN
42	L5	228	ALA
42	L5	233	ALA
42	L5	234	ASP
42	L5	296	GLN
43	L6	97	ASN
44	L7	25	GLN
44	L7	163	LEU
45	L8	25	PRO
45	L8	31	PRO
46	L9	50	ASN
46	L9	169	ASN
48	M1	11	ASP
48	M1	115	LYS
48	M1	165	GLN
49	M3	129	ASN
50	M4	9	ALA
50	M4	36	VAL
51	M5	74	PRO
51	M5	75	VAL
51	M5	94	TYR
52	M6	66	LYS

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Mol	Chain	Res	Type
52	M6	110	PRO
52	M6	111	PRO
56	N0	167	ARG
60	N4	8	PHE
60	N4	64	THR
60	N4	81	PRO
61	N5	44	PRO
61	N5	50	ALA
62	N6	37	LYS
63	N7	17	ARG
63	N7	35	SER
63	N7	125	GLY
67	O1	7	VAL
67	O1	84	ASP
68	O2	27	ARG
70	O4	10	ARG
73	O7	59	THR
74	O8	33	LYS
75	O9	4	GLN
76	Q0	78	ILE
78	Q2	30	ALA
78	Q2	34	SER
78	Q2	100	LYS
79	Q3	58	SER
2	s0	4	PRO
2	s0	111	ILE
2	s0	158	VAL
2	s0	164	ASN
2	s0	189	VAL
2	s0	206	ASP
3	s1	106	THR
3	s1	132	ASP
4	s2	92	ALA
4	s2	164	SER
4	s2	176	SER
4	s2	248	SER
5	s3	61	GLU
5	s3	216	PRO
5	s3	220	PRO
6	s4	53	LYS
6	s4	104	ASP
6	s4	196	VAL

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Mol	Chain	Res	Type
7	s5	28	PRO
7	s5	184	PHE
8	s6	122	GLU
8	s6	173	PRO
8	s6	174	LYS
9	s7	63	PRO
9	s7	64	VAL
9	s7	66	SER
9	s7	74	GLN
9	s7	131	PHE
10	s8	153	GLU
11	s9	118	LEU
11	s9	144	PRO
12	c0	32	HIS
12	c0	83	PRO
12	c0	88	PRO
12	c0	97	PRO
13	c1	61	THR
15	c3	12	SER
15	c3	18	TYR
15	c3	66	ILE
15	c3	87	ASP
16	c4	126	THR
16	c4	132	ARG
17	c5	11	VAL
17	c5	51	SER
17	c5	52	LYS
17	c5	125	PRO
18	c6	116	LEU
19	c7	99	VAL
20	c8	14	ILE
23	d1	4	ASP
23	d1	6	GLY
24	d2	68	ARG
26	d4	30	PRO
26	d4	32	ARG
29	d7	12	ALA
29	d7	20	LYS
30	d8	32	PHE
30	d8	59	SER
31	d9	6	VAL
31	d9	7	TRP

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Mol	Chain	Res	Type
32	e0	43	ARG
32	e0	47	VAL
33	e1	83	LYS
33	e1	87	THR
33	e1	92	LYS
33	e1	98	VAL
33	e1	103	LEU
33	e1	110	ALA
34	sR	4	ASN
34	sR	160	GLU
35	sM	50	ASN
35	sM	120	GLU
35	sM	172	VAL
39	l2	144	ASN
39	l2	212	GLY
39	l2	238	ILE
40	l3	140	ASP
40	l3	143	GLY
40	l3	155	ALA
41	l4	14	GLU
41	l4	25	VAL
41	l4	142	VAL
41	l4	145	ILE
41	l4	301	PRO
41	l4	313	LEU
41	l4	353	ALA
42	l5	178	ASN
42	l5	258	LYS
43	l6	98	VAL
44	l7	193	PRO
44	l7	229	PHE
45	l8	25	PRO
45	l8	34	PHE
45	l8	133	LYS
46	l9	62	ARG
47	m0	74	LYS
48	m1	8	PRO
80	m2	11	PRO
80	m2	15	PRO
80	m2	18	VAL
80	m2	87	VAL
80	m2	88	PRO

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Mol	Chain	Res	Type
80	m2	101	PRO
80	m2	102	PRO
80	m2	121	GLU
80	m2	123	ILE
49	m3	47	ALA
49	m3	93	ILE
49	m3	100	ARG
49	m3	101	ARG
49	m3	134	GLU
49	m3	150	PRO
49	m3	162	ASN
51	m5	76	PRO
54	m8	99	THR
55	m9	112	ALA
58	n2	44	GLU
59	n3	42	SER
61	n5	38	LEU
61	n5	44	PRO
61	n5	45	LYS
61	n5	55	ASN
62	n6	84	LYS
63	n7	17	ARG
64	n8	76	ASP
65	n9	21	ILE
65	n9	23	LYS
65	n9	24	PRO
66	o0	38	LYS
67	o1	5	LYS
67	o1	45	GLY
68	o2	6	HIS
69	o3	60	ARG
72	o6	4	LYS
72	o6	98	ARG
73	o7	87	SER
76	q0	78	ILE
78	q2	17	CYS
81	p0	93	LEU
82	p1	35	VAL
82	p2	36	PRO
83	f	18	THR
83	f	64	ILE
83	f	109	THR

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Mol	Chain	Res	Type
83	f	111	ASP
2	S0	39	ASN
2	S0	111	ILE
2	S0	190	ASP
3	S1	21	VAL
3	S1	37	THR
3	S1	63	GLY
3	S1	158	SER
3	S1	176	VAL
3	S1	209	ASN
4	S2	163	GLY
4	S2	182	PRO
5	S3	93	ASP
5	S3	218	LEU
6	S4	11	ARG
6	S4	12	LEU
6	S4	195	ILE
6	S4	200	ARG
7	S5	26	ALA
7	S5	47	SER
7	S5	58	LEU
7	S5	63	GLN
7	S5	71	ALA
7	S5	150	GLY
8	S6	70	PRO
8	S6	122	GLU
8	S6	138	ALA
8	S6	152	ASP
8	S6	165	GLY
8	S6	173	PRO
9	S7	32	PRO
9	S7	36	ALA
9	S7	186	PRO
10	S8	52	ASN
10	S8	152	ILE
11	S9	6	ARG
11	S9	166	GLY
12	C0	30	ALA
12	C0	92	ILE
12	C0	93	GLN
13	C1	6	THR
13	C1	30	ARG

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Mol	Chain	Res	Type
14	C2	69	ALA
14	C2	107	ASP
14	C2	126	TRP
14	C2	127	GLY
15	C3	22	ALA
15	C3	148	ALA
16	C4	48	VAL
16	C4	114	ARG
17	C5	11	VAL
17	C5	48	GLY
17	C5	52	LYS
18	C6	32	ASN
18	C6	39	VAL
18	C6	97	VAL
19	C7	115	LEU
19	C7	124	VAL
20	C8	103	ASN
22	D0	96	PRO
23	D1	4	ASP
23	D1	15	ARG
23	D1	44	ARG
23	D1	78	LEU
25	D3	11	SER
25	D3	112	LYS
25	D3	114	LYS
25	D3	137	LYS
26	D4	4	ALA
26	D4	35	VAL
26	D4	47	VAL
27	D5	42	LEU
27	D5	71	ILE
28	D6	5	ARG
28	D6	35	ALA
28	D6	36	ILE
28	D6	45	VAL
28	D6	46	GLU
28	D6	63	ALA
33	E1	118	ARG
34	SR	98	GLU
34	SR	146	GLY
34	SR	238	ASP
35	SM	69	ARG

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Mol	Chain	Res	Type
35	SM	154	TYR
39	L2	13	GLY
39	L2	143	GLU
39	L2	250	GLN
40	L3	138	ALA
40	L3	155	ALA
40	L3	170	PRO
40	L3	171	LEU
40	L3	175	LYS
40	L3	221	THR
40	L3	351	LEU
40	L3	385	LYS
41	L4	14	GLU
41	L4	15	ALA
41	L4	265	GLU
41	L4	292	SER
41	L4	309	ARG
41	L4	313	LEU
41	L4	317	PRO
42	L5	148	ILE
42	L5	153	THR
42	L5	202	GLY
43	L6	98	VAL
44	L7	55	TYR
44	L7	159	GLN
45	L8	36	ILE
45	L8	39	ALA
45	L8	76	ALA
45	L8	157	VAL
45	L8	190	VAL
46	L9	80	THR
46	L9	139	ASN
47	M0	78	THR
47	M0	117	GLY
47	M0	189	GLU
47	M0	194	GLY
47	M0	207	GLU
48	M1	8	PRO
48	M1	12	LEU
48	M1	94	ARG
48	M1	95	ASN
48	M1	114	ILE

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Mol	Chain	Res	Type
49	M3	47	ALA
49	M3	67	ARG
49	M3	136	GLU
49	M3	141	ALA
49	M3	166	ALA
51	M5	81	TYR
51	M5	158	HIS
52	M6	16	VAL
53	M7	36	ILE
53	M7	157	VAL
53	M7	159	LYS
54	M8	91	ALA
55	M9	130	ASN
56	N0	130	GLU
56	N0	154	HIS
57	N1	22	HIS
57	N1	124	VAL
57	N1	159	PHE
58	N2	11	ILE
58	N2	51	GLY
59	N3	134	GLY
60	N4	76	VAL
60	N4	97	LYS
61	N5	45	LYS
63	N7	4	PHE
63	N7	16	GLY
63	N7	30	ASP
64	N8	27	LYS
64	N8	66	ALA
64	N8	97	GLU
66	O0	27	TYR
66	O0	96	GLY
67	O1	111	GLU
71	O5	119	LYS
74	O8	37	PRO
74	O8	49	SER
79	Q3	3	LYS
79	Q3	9	GLY
79	Q3	59	CYS
2	s0	30	GLN
2	s0	44	GLY
2	s0	68	PRO

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Mol	Chain	Res	Type
2	s0	94	GLY
2	s0	95	ALA
2	s0	110	TYR
3	s1	72	ASP
3	s1	93	GLY
3	s1	200	ALA
3	s1	206	PRO
4	s2	106	ASP
4	s2	149	GLY
5	s3	203	PRO
5	s3	217	ILE
6	s4	194	THR
7	s5	36	ALA
7	s5	43	PHE
8	s6	25	ARG
9	s7	67	LEU
9	s7	73	VAL
10	s8	122	GLY
11	s9	169	PRO
12	c0	23	ALA
12	c0	80	LEU
12	c0	92	ILE
13	c1	6	THR
13	c1	7	VAL
13	c1	55	ASP
14	c2	63	VAL
15	c3	3	ARG
15	c3	108	ASP
16	c4	48	VAL
16	c4	90	ARG
16	c4	124	ASP
17	c5	17	TYR
18	c6	39	VAL
19	c7	88	VAL
21	c9	26	GLY
21	c9	33	TYR
22	d0	96	PRO
23	d1	43	GLY
24	d2	78	ARG
25	d3	46	SER
26	d4	33	ALA
26	d4	35	VAL

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Mol	Chain	Res	Type
26	d4	54	ALA
26	d4	121	THR
27	d5	103	ARG
28	d6	28	LYS
28	d6	63	ALA
29	d7	24	LEU
30	d8	16	LEU
30	d8	33	LEU
30	d8	61	ARG
32	e0	51	ASN
33	e1	79	LYS
33	e1	84	VAL
33	e1	102	VAL
33	e1	105	TYR
33	e1	127	GLY
34	sR	96	THR
34	sR	163	ASP
34	sR	226	ALA
34	sR	271	VAL
35	sM	31	SER
35	sM	47	ALA
39	l2	24	GLN
39	l2	142	ASP
39	l2	194	ASN
39	l2	216	HIS
40	l3	129	ALA
40	l3	139	GLN
40	l3	187	SER
40	l3	258	ALA
40	l3	347	SER
41	l4	15	ALA
41	l4	43	ASN
41	l4	144	LYS
42	l5	127	GLY
42	l5	260	PHE
42	l5	296	GLN
43	l6	140	VAL
44	l7	178	ILE
45	l8	79	GLN
45	l8	121	SER
45	l8	122	LYS
45	l8	203	VAL

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Mol	Chain	Res	Type
45	l8	239	GLY
46	l9	144	ILE
46	l9	167	VAL
47	m0	3	ARG
47	m0	82	ARG
47	m0	204	GLY
48	m1	94	ARG
48	m1	165	GLN
80	m2	22	TYR
80	m2	30	VAL
80	m2	67	LYS
80	m2	97	ALA
80	m2	125	ILE
80	m2	148	THR
50	m4	41	GLN
50	m4	136	ALA
51	m5	183	THR
51	m5	184	LYS
54	m8	112	ALA
54	m8	113	LYS
54	m8	147	ARG
55	m9	131	ALA
56	n0	45	LEU
58	n2	50	LEU
58	n2	51	GLY
60	n4	63	ILE
60	n4	75	THR
60	n4	76	VAL
60	n4	133	THR
63	n7	134	LEU
64	n8	24	LYS
64	n8	65	GLN
64	n8	67	HIS
65	n9	39	PHE
66	o0	46	ALA
67	o1	82	GLU
67	o1	84	ASP
68	o2	62	LYS
68	o2	125	ARG
69	o3	59	VAL
71	o5	37	SER
72	o6	20	MET

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Mol	Chain	Res	Type
81	p0	68	SER
82	p2	16	ASP
82	p2	17	SER
2	S0	30	GLN
3	S1	26	ARG
3	S1	48	VAL
3	S1	54	LEU
3	S1	58	SER
3	S1	62	LYS
3	S1	221	PRO
4	S2	35	TRP
4	S2	136	VAL
5	S3	44	THR
5	S3	216	PRO
5	S3	217	ILE
6	S4	120	SER
6	S4	175	PHE
6	S4	204	GLY
7	S5	50	GLU
7	S5	99	MET
8	S6	148	SER
9	S7	110	GLN
9	S7	112	ARG
9	S7	131	PHE
10	S8	10	LYS
10	S8	19	ALA
11	S9	18	PRO
11	S9	167	ALA
12	C0	64	TYR
13	C1	4	GLU
13	C1	55	ASP
13	C1	146	ALA
14	C2	93	ASP
14	C2	101	ALA
14	C2	106	ILE
14	C2	111	ASN
14	C2	125	ASN
14	C2	131	ASP
15	C3	3	ARG
15	C3	28	LEU
15	C3	137	PRO
16	C4	12	GLN

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Mol	Chain	Res	Type
16	C4	50	ALA
16	C4	75	GLY
17	C5	69	GLU
19	C7	101	ASN
20	C8	91	ASP
21	C9	28	LEU
22	D0	17	GLN
22	D0	73	GLY
23	D1	10	GLU
23	D1	42	GLU
24	D2	83	ILE
25	D3	41	SER
25	D3	110	LYS
25	D3	139	LYS
26	D4	5	VAL
26	D4	54	ALA
27	D5	39	ALA
27	D5	43	ASP
27	D5	94	LYS
28	D6	8	ASN
28	D6	58	VAL
28	D6	97	PRO
29	D7	76	GLY
31	D9	11	PRO
31	D9	20	GLN
33	E1	102	VAL
33	E1	109	ASP
34	SR	49	GLY
34	SR	163	ASP
35	SM	68	ARG
39	L2	125	ALA
39	L2	251	LYS
40	L3	63	PRO
40	L3	174	LYS
40	L3	258	ALA
40	L3	302	LYS
40	L3	378	ALA
40	L3	386	ASP
41	L4	90	PHE
41	L4	140	HIS
42	L5	72	ASP
42	L5	93	THR

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Mol	Chain	Res	Type
42	L5	111	GLN
42	L5	163	LEU
42	L5	253	PHE
42	L5	259	LYS
44	L7	91	GLY
45	L8	79	GLN
46	L9	40	HIS
46	L9	49	ASN
46	L9	79	ILE
46	L9	110	LYS
46	L9	190	ASP
47	M0	82	ARG
48	M1	117	ASP
48	M1	152	HIS
49	M3	130	GLY
49	M3	165	SER
49	M3	176	GLU
50	M4	113	THR
52	M6	89	SER
53	M7	109	ALA
54	M8	41	ASP
54	M8	97	PRO
54	M8	99	THR
55	M9	53	LYS
57	N1	122	GLN
57	N1	146	ASN
58	N2	27	VAL
60	N4	9	SER
60	N4	70	LYS
60	N4	86	SER
61	N5	36	LYS
61	N5	117	ASN
62	N6	125	LYS
63	N7	102	GLU
66	O0	53	LYS
67	O1	21	HIS
67	O1	99	ALA
67	O1	102	LYS
68	O2	62	LYS
69	O3	59	VAL
71	O5	35	LYS
72	O6	21	THR

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Mol	Chain	Res	Type
72	O6	33	ALA
72	O6	64	SER
72	O6	98	ARG
72	O6	99	ARG
78	Q2	95	GLY
2	s0	10	THR
2	s0	65	ALA
2	s0	194	PRO
2	s0	205	ARG
3	s1	60	ALA
3	s1	129	THR
3	s1	147	ALA
3	s1	209	ASN
3	s1	224	ASP
4	s2	88	LYS
4	s2	163	GLY
4	s2	182	PRO
5	s3	76	ARG
5	s3	93	ASP
5	s3	219	ALA
6	s4	51	ARG
6	s4	135	GLY
6	s4	245	LYS
7	s5	74	ALA
7	s5	176	THR
8	s6	70	PRO
8	s6	126	ASP
8	s6	138	ALA
9	s7	10	SER
9	s7	30	SER
11	s9	88	GLU
11	s9	147	MET
12	c0	30	ALA
12	c0	31	LYS
12	c0	82	LEU
12	c0	95	ARG
14	c2	39	ASP
14	c2	54	ARG
15	c3	29	SER
15	c3	139	TRP
15	c3	140	LYS
16	c4	11	SER

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Mol	Chain	Res	Type
16	c4	50	ALA
16	c4	108	SER
16	c4	131	GLY
17	c5	80	MET
18	c6	3	ALA
18	c6	142	TYR
19	c7	63	LYS
19	c7	86	PRO
19	c7	116	LYS
20	c8	55	HIS
20	c8	61	LEU
20	c8	107	SER
21	c9	29	GLU
22	d0	49	ASN
22	d0	52	LYS
22	d0	119	ALA
23	d1	15	ARG
23	d1	42	GLU
26	d4	58	PHE
28	d6	62	TYR
28	d6	94	ASN
29	d7	41	LEU
29	d7	59	CYS
30	d8	60	GLU
30	d8	62	GLU
31	d9	11	PRO
33	e1	85	TYR
33	e1	100	LEU
33	e1	111	GLU
33	e1	131	PHE
33	e1	136	LYS
33	e1	146	SER
34	sR	15	GLY
34	sR	63	GLY
34	sR	105	GLY
35	sM	168	GLU
39	l2	69	TYR
39	l2	80	GLU
41	l4	90	PHE
41	l4	233	LEU
41	l4	311	HIS
41	l4	345	GLU

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Mol	Chain	Res	Type
43	l6	10	TYR
43	l6	138	GLN
44	l7	191	VAL
44	l7	228	SER
45	l8	39	ALA
45	l8	112	GLU
45	l8	237	ILE
47	m0	25	ALA
47	m0	151	GLY
47	m0	220	GLN
48	m1	95	ASN
80	m2	10	PRO
80	m2	58	ASP
80	m2	89	SER
80	m2	119	LEU
49	m3	76	THR
49	m3	129	ASN
49	m3	133	PRO
49	m3	135	ALA
50	m4	60	LEU
50	m4	135	LEU
52	m6	12	LYS
54	m8	8	LYS
54	m8	84	VAL
55	m9	35	ALA
55	m9	36	ASN
55	m9	156	ASN
56	n0	130	GLU
57	n1	117	ALA
59	n3	68	GLU
60	n4	6	ASP
61	n5	47	ALA
63	n7	91	ALA
64	n8	17	ALA
64	n8	48	TYR
64	n8	66	ALA
67	o1	99	ALA
69	o3	90	PRO
70	o4	82	ALA
71	o5	81	ARG
71	o5	110	ALA
74	o8	35	GLY

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Mol	Chain	Res	Type
79	q3	51	ALA
81	p0	21	GLU
81	p0	33	VAL
81	p0	94	THR
82	p1	16	ASP
83	f	15	SER
83	f	16	SER
83	f	17	ALA
2	S0	185	ARG
3	S1	207	LEU
4	S2	145	GLY
4	S2	150	GLN
5	S3	196	ARG
6	S4	22	LYS
6	S4	23	LEU
6	S4	194	THR
6	S4	245	LYS
7	S5	31	GLU
7	S5	45	LYS
7	S5	51	VAL
7	S5	64	VAL
7	S5	65	ARG
8	S6	146	GLY
9	S7	98	ILE
9	S7	111	LYS
9	S7	156	SER
10	S8	120	THR
14	C2	87	PRO
15	C3	19	SER
16	C4	40	ALA
17	C5	80	MET
17	C5	101	ALA
18	C6	40	GLU
18	C6	142	TYR
19	C7	84	TYR
19	C7	87	GLU
21	C9	29	GLU
21	C9	50	ALA
21	C9	119	LYS
22	D0	55	PRO
24	D2	30	SER
24	D2	66	ASN

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Mol	Chain	Res	Type
25	D3	64	PRO
25	D3	109	ARG
25	D3	131	SER
26	D4	34	ASN
29	D7	23	THR
30	D8	36	THR
31	D9	6	VAL
32	E0	51	ASN
33	E1	83	LYS
33	E1	87	THR
33	E1	100	LEU
33	E1	127	GLY
34	SR	51	ASP
34	SR	249	ARG
34	SR	268	GLN
35	SM	12	VAL
35	SM	39	PRO
35	SM	48	ARG
35	SM	88	ARG
35	SM	173	GLU
41	L4	137	ALA
41	L4	268	ALA
42	L5	7	ALA
42	L5	125	VAL
42	L5	177	GLU
42	L5	258	LYS
44	L7	72	ALA
45	L8	113	ALA
46	L9	15	GLY
47	M0	77	THR
48	M1	108	GLU
48	M1	168	ASP
48	M1	172	LEU
49	M3	50	PRO
49	M3	76	THR
51	M5	183	THR
53	M7	164	LYS
54	M8	108	ALA
60	N4	67	VAL
64	N8	47	LYS
64	N8	115	LYS
65	N9	24	PRO

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Mol	Chain	Res	Type
66	O0	97	ASP
67	O1	82	GLU
67	O1	97	LEU
68	O2	110	ALA
70	O4	82	ALA
73	O7	12	HIS
73	O7	85	LYS
73	O7	86	ALA
74	O8	18	ALA
78	Q2	15	LYS
78	Q2	17	CYS
79	Q3	7	LYS
79	Q3	84	ARG
2	s0	14	ALA
2	s0	92	HIS
2	s0	109	ASN
2	s0	127	ARG
2	s0	152	PRO
2	s0	185	ARG
3	s1	55	LYS
3	s1	210	ILE
4	s2	62	PRO
4	s2	155	ALA
4	s2	235	LEU
4	s2	238	SER
5	s3	94	ARG
5	s3	113	LEU
6	s4	30	ARG
6	s4	90	ILE
6	s4	168	LYS
6	s4	195	ILE
6	s4	202	ASP
7	s5	35	GLN
7	s5	37	GLN
7	s5	45	LYS
7	s5	100	ASN
9	s7	11	GLN
9	s7	133	THR
9	s7	151	LYS
10	s8	52	ASN
10	s8	136	SER
11	s9	162	SER

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Mol	Chain	Res	Type
11	s9	167	ALA
12	c0	3	MET
12	c0	35	ILE
12	c0	91	TYR
14	c2	58	LEU
14	c2	87	PRO
14	c2	89	ILE
14	c2	106	ILE
14	c2	131	ASP
14	c2	141	SER
16	c4	37	GLU
16	c4	114	ARG
18	c6	33	GLY
18	c6	97	VAL
18	c6	113	ASP
18	c6	121	SER
26	d4	36	SER
26	d4	51	GLU
28	d6	11	ASN
28	d6	35	ALA
28	d6	82	ARG
33	e1	81	LYS
33	e1	106	TYR
33	e1	112	GLY
33	e1	128	ALA
33	e1	148	TYR
34	sR	231	MET
34	sR	285	ALA
35	sM	43	ASP
39	l2	56	ALA
39	l2	127	ALA
39	l2	180	LEU
40	l3	3	HIS
40	l3	63	PRO
40	l3	236	LYS
40	l3	284	ARG
43	l6	97	ASN
45	l8	69	LEU
45	l8	240	ASN
46	l9	2	LYS
47	m0	173	PHE
47	m0	196	PHE

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Mol	Chain	Res	Type
48	m1	114	ILE
48	m1	167	TYR
48	m1	168	ASP
80	m2	36	ALA
80	m2	55	VAL
80	m2	99	LYS
80	m2	159	LYS
49	m3	44	ALA
49	m3	50	PRO
49	m3	60	ALA
52	m6	65	ASN
56	n0	2	ALA
60	n4	72	SER
63	n7	103	GLN
67	o1	60	TRP
71	o5	3	GLY
71	o5	119	LYS
72	o6	34	SER
72	o6	65	GLY
74	o8	18	ALA
79	q3	10	ILE
79	q3	45	LYS
81	p0	48	ARG
82	p2	35	VAL
83	f	11	ALA
83	f	98	GLY
83	f	113	VAL
83	f	132	LYS
2	S0	103	THR
2	S0	195	TRP
3	S1	61	LEU
3	S1	156	ALA
3	S1	210	ILE
4	S2	39	THR
4	S2	247	ALA
6	S4	45	ILE
9	S7	5	GLN
10	S8	136	SER
11	S9	118	LEU
12	C0	25	LYS
14	C2	112	ALA
16	C4	18	ARG

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Mol	Chain	Res	Type
16	C4	51	ASP
17	C5	109	PRO
20	C8	53	ASP
24	D2	45	GLY
25	D3	27	ASN
25	D3	128	SER
26	D4	6	THR
26	D4	100	VAL
30	D8	35	ASP
33	E1	101	ALA
33	E1	111	GLU
34	SR	15	GLY
34	SR	28	GLY
34	SR	105	GLY
34	SR	135	THR
35	SM	100	THR
39	L2	47	GLN
39	L2	127	ALA
40	L3	68	HIS
40	L3	317	ILE
41	L4	130	ALA
41	L4	146	PRO
41	L4	181	VAL
42	L5	119	TYR
42	L5	260	PHE
42	L5	295	GLY
46	L9	83	THR
47	M0	47	PRO
48	M1	173	ASP
50	M4	10	SER
53	M7	160	ALA
54	M8	149	ALA
54	M8	162	ALA
54	M8	175	ALA
55	M9	129	GLY
59	N3	46	LEU
60	N4	77	LYS
62	N6	49	PRO
63	N7	36	HIS
63	N7	103	GLN
64	N8	117	ARG
65	N9	25	LYS

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Mol	Chain	Res	Type
70	O4	12	PRO
72	O6	3	VAL
3	s1	218	LEU
4	s2	91	ARG
4	s2	150	GLN
4	s2	204	THR
4	s2	234	PRO
5	s3	44	THR
5	s3	45	LYS
6	s4	80	THR
6	s4	150	PRO
7	s5	98	MET
7	s5	151	GLY
9	s7	41	LEU
10	s8	101	ILE
11	s9	5	PRO
14	c2	92	ALA
14	c2	107	ASP
14	c2	108	ARG
14	c2	115	VAL
14	c2	119	SER
16	c4	32	ASP
16	c4	51	ASP
17	c5	6	ASN
17	c5	71	GLU
18	c6	44	LEU
19	c7	19	ARG
19	c7	117	LEU
21	c9	43	ASN
28	d6	8	ASN
29	d7	58	SER
30	d8	20	GLY
32	e0	44	PHE
34	sR	74	THR
34	sR	186	PHE
34	sR	318	ALA
35	sM	36	ASP
39	l2	241	ARG
41	l4	24	ALA
41	l4	272	VAL
41	l4	342	LYS
47	m0	77	THR

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Mol	Chain	Res	Type
48	m1	108	GLU
80	m2	51	PRO
80	m2	105	ARG
49	m3	51	LEU
51	m5	68	ARG
52	m6	16	VAL
54	m8	155	MET
55	m9	130	ASN
60	n4	7	SER
60	n4	96	LEU
63	n7	16	GLY
63	n7	28	PRO
63	n7	36	HIS
64	n8	93	SER
68	o2	5	PRO
68	o2	124	GLY
81	p0	47	GLY
83	f	93	LEU
83	f	121	GLY
83	f	148	ILE
2	S0	5	ALA
2	S0	152	PRO
3	S1	51	SER
5	S3	72	LEU
5	S3	81	PRO
6	S4	35	PRO
6	S4	205	PHE
6	S4	234	PRO
9	S7	109	VAL
10	S8	59	ARG
10	S8	199	LYS
14	C2	108	ARG
14	C2	119	SER
16	C4	125	SER
16	C4	126	THR
18	C6	33	GLY
18	C6	113	ASP
23	D1	12	TYR
23	D1	14	PRO
23	D1	16	LYS
24	D2	67	GLY
28	D6	85	ARG

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Mol	Chain	Res	Type
35	SM	87	THR
35	SM	89	ARG
42	L5	213	ASP
44	L7	158	LYS
50	M4	6	ILE
52	M6	112	TYR
65	N9	29	TYR
67	O1	45	GLY
70	O4	59	PRO
70	O4	77	GLY
79	Q3	51	ALA
2	s0	139	VAL
3	s1	22	ASP
4	s2	151	PRO
5	s3	102	ALA
7	s5	29	ILE
8	s6	152	ASP
9	s7	129	LEU
10	s8	78	ILE
12	c0	24	LYS
16	c4	118	VAL
19	c7	105	GLN
20	c8	145	ARG
22	d0	118	VAL
23	d1	2	GLU
27	d5	44	GLN
28	d6	13	LYS
28	d6	59	TYR
28	d6	86	VAL
32	e0	54	ARG
33	e1	137	ASP
41	l4	302	ALA
42	l5	139	PRO
46	l9	110	LYS
47	m0	176	LEU
48	m1	11	ASP
48	m1	117	ASP
48	m1	153	LYS
80	m2	103	ARG
52	m6	5	PRO
54	m8	91	ALA
54	m8	171	LYS

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Mol	Chain	Res	Type
64	n8	28	HIS
68	o2	127	ALA
73	o7	85	LYS
82	p2	22	SER
4	S2	236	PRO
6	S4	150	PRO
44	L7	26	VAL
6	s4	107	GLY
11	s9	168	ARG
19	c7	121	VAL
23	d1	9	VAL
35	sM	51	ARG
80	m2	86	VAL
55	m9	143	ILE
57	n1	124	VAL
58	n2	60	GLY
59	n3	16	GLY
66	o0	96	GLY
13	C1	113	PRO
14	C2	82	PRO
14	C2	115	VAL
16	C4	96	PRO
23	D1	23	ILE
26	D4	95	GLY
41	L4	66	GLY
41	L4	328	ASN
47	M0	16	PRO
2	s0	199	PRO
6	s4	111	VAL
28	d6	75	VAL
32	e0	50	VAL
45	l8	36	ILE
80	m2	141	VAL
76	q0	80	PRO
20	C8	142	GLY
23	D1	46	ILE
26	D4	29	HIS
40	L3	305	ILE
43	L6	6	ALA
61	N5	35	PRO
62	N6	92	GLY
67	O1	88	PRO

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Mol	Chain	Res	Type
2	s0	118	PRO
13	c1	76	VAL
15	c3	59	GLY
15	c3	82	PRO
20	c8	4	VAL
20	c8	135	GLY
26	d4	29	HIS
32	e0	14	VAL
42	l5	255	PRO
80	m2	59	ILE
53	m7	67	ILE
59	n3	3	GLY
60	n4	67	VAL
63	n7	82	PRO
65	n9	29	TYR
74	o8	37	PRO
81	p0	214	VAL
25	D3	108	GLY
28	D6	18	VAL
30	D8	44	VAL
73	O7	23	GLY
79	Q3	8	VAL
15	c3	22	ALA
17	c5	48	GLY
26	d4	120	GLY
30	d8	47	PRO
59	n3	107	GLY
64	n8	56	VAL
64	n8	70	LYS
15	C3	85	PRO
29	D7	38	PRO
30	D8	6	PRO
58	n2	22	PRO
63	n7	70	PRO
81	p0	80	VAL
24	d2	29	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S0	164/209 (78%)	140 (85%)	24 (15%)	3	16
2	s0	165/209 (79%)	137 (83%)	28 (17%)	2	10
3	S1	191/223 (86%)	157 (82%)	34 (18%)	2	8
3	s1	192/223 (86%)	160 (83%)	32 (17%)	2	11
4	S2	176/204 (86%)	147 (84%)	29 (16%)	2	12
4	s2	176/204 (86%)	134 (76%)	42 (24%)	0	3
5	S3	182/194 (94%)	146 (80%)	36 (20%)	1	5
5	s3	182/194 (94%)	158 (87%)	24 (13%)	4	19
6	S4	221/221 (100%)	194 (88%)	27 (12%)	5	22
6	s4	221/221 (100%)	192 (87%)	29 (13%)	4	20
7	S5	173/190 (91%)	146 (84%)	27 (16%)	2	14
7	s5	173/190 (91%)	146 (84%)	27 (16%)	2	14
8	S6	188/201 (94%)	162 (86%)	26 (14%)	3	18
8	s6	187/201 (93%)	162 (87%)	25 (13%)	4	19
9	S7	165/169 (98%)	144 (87%)	21 (13%)	4	20
9	s7	165/169 (98%)	138 (84%)	27 (16%)	2	12
10	S8	150/161 (93%)	128 (85%)	22 (15%)	3	16
10	s8	150/161 (93%)	128 (85%)	22 (15%)	3	16
11	S9	158/165 (96%)	128 (81%)	30 (19%)	1	7
11	s9	158/165 (96%)	128 (81%)	30 (19%)	1	7
12	C0	77/98 (79%)	69 (90%)	8 (10%)	7	29
12	c0	73/98 (74%)	64 (88%)	9 (12%)	4	22
13	C1	129/136 (95%)	110 (85%)	19 (15%)	3	16
13	c1	129/136 (95%)	111 (86%)	18 (14%)	3	17
14	C2	88/118 (75%)	73 (83%)	15 (17%)	2	10
14	c2	88/118 (75%)	74 (84%)	14 (16%)	2	13
15	C3	127/127 (100%)	101 (80%)	26 (20%)	1	5
15	c3	127/127 (100%)	111 (87%)	16 (13%)	4	21
16	C4	81/104 (78%)	65 (80%)	16 (20%)	1	5
16	c4	97/104 (93%)	78 (80%)	19 (20%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	C5	101/117 (86%)	89 (88%)	12 (12%)	5	23
17	c5	103/117 (88%)	87 (84%)	16 (16%)	2	14
18	C6	117/118 (99%)	98 (84%)	19 (16%)	2	12
18	c6	118/118 (100%)	101 (86%)	17 (14%)	3	16
19	C7	94/124 (76%)	77 (82%)	17 (18%)	1	8
19	c7	92/124 (74%)	79 (86%)	13 (14%)	3	17
20	C8	128/128 (100%)	106 (83%)	22 (17%)	2	10
20	c8	128/128 (100%)	106 (83%)	22 (17%)	2	10
21	C9	115/115 (100%)	95 (83%)	20 (17%)	2	9
21	c9	115/115 (100%)	104 (90%)	11 (10%)	8	32
22	D0	100/113 (88%)	83 (83%)	17 (17%)	2	10
22	d0	103/113 (91%)	84 (82%)	19 (18%)	1	7
23	D1	74/74 (100%)	59 (80%)	15 (20%)	1	5
23	d1	74/74 (100%)	61 (82%)	13 (18%)	2	9
24	D2	110/110 (100%)	89 (81%)	21 (19%)	1	6
24	d2	110/110 (100%)	92 (84%)	18 (16%)	2	12
25	D3	119/119 (100%)	100 (84%)	19 (16%)	2	13
25	d3	119/119 (100%)	98 (82%)	21 (18%)	2	9
26	D4	112/112 (100%)	98 (88%)	14 (12%)	4	21
26	d4	112/112 (100%)	92 (82%)	20 (18%)	2	8
27	D5	61/88 (69%)	50 (82%)	11 (18%)	1	8
27	d5	61/88 (69%)	53 (87%)	8 (13%)	4	20
28	D6	83/83 (100%)	66 (80%)	17 (20%)	1	5
28	d6	83/83 (100%)	74 (89%)	9 (11%)	6	27
29	D7	70/70 (100%)	66 (94%)	4 (6%)	20	52
29	d7	70/70 (100%)	57 (81%)	13 (19%)	1	7
30	D8	56/59 (95%)	45 (80%)	11 (20%)	1	6
30	d8	56/59 (95%)	45 (80%)	11 (20%)	1	6
31	D9	47/48 (98%)	39 (83%)	8 (17%)	2	10
31	d9	47/48 (98%)	37 (79%)	10 (21%)	1	4
32	E0	51/54 (94%)	43 (84%)	8 (16%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	e0	53/54 (98%)	36 (68%)	17 (32%)	0	1
33	E1	62/66 (94%)	53 (86%)	9 (14%)	3	16
33	e1	66/66 (100%)	54 (82%)	12 (18%)	1	8
34	SR	259/261 (99%)	236 (91%)	23 (9%)	9	36
34	sR	260/261 (100%)	241 (93%)	19 (7%)	14	45
35	SM	97/228 (42%)	78 (80%)	19 (20%)	1	6
35	sM	54/228 (24%)	44 (82%)	10 (18%)	1	7
39	L2	193/195 (99%)	157 (81%)	36 (19%)	1	7
39	l2	192/195 (98%)	157 (82%)	35 (18%)	1	8
40	L3	319/322 (99%)	256 (80%)	63 (20%)	1	6
40	l3	320/322 (99%)	263 (82%)	57 (18%)	2	8
41	L4	288/288 (100%)	242 (84%)	46 (16%)	2	13
41	l4	288/288 (100%)	242 (84%)	46 (16%)	2	13
42	L5	244/244 (100%)	206 (84%)	38 (16%)	2	14
42	l5	243/244 (100%)	193 (79%)	50 (21%)	1	5
43	L6	134/152 (88%)	116 (87%)	18 (13%)	4	19
43	l6	135/152 (89%)	112 (83%)	23 (17%)	2	10
44	L7	186/204 (91%)	162 (87%)	24 (13%)	4	20
44	l7	187/204 (92%)	162 (87%)	25 (13%)	4	19
45	L8	187/207 (90%)	160 (86%)	27 (14%)	3	16
45	l8	177/207 (86%)	153 (86%)	24 (14%)	3	18
46	L9	171/171 (100%)	135 (79%)	36 (21%)	1	4
46	l9	171/171 (100%)	137 (80%)	34 (20%)	1	5
47	M0	177/186 (95%)	146 (82%)	31 (18%)	2	9
47	m0	179/186 (96%)	149 (83%)	30 (17%)	2	11
48	M1	147/150 (98%)	122 (83%)	25 (17%)	2	10
48	m1	147/150 (98%)	120 (82%)	27 (18%)	1	7
49	M3	154/158 (98%)	136 (88%)	18 (12%)	5	24
49	m3	154/158 (98%)	134 (87%)	20 (13%)	4	20
50	M4	107/108 (99%)	88 (82%)	19 (18%)	2	8
50	m4	108/108 (100%)	88 (82%)	20 (18%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	M5	175/175 (100%)	145 (83%)	30 (17%)	2	10
51	m5	175/175 (100%)	150 (86%)	25 (14%)	3	17
52	M6	160/161 (99%)	141 (88%)	19 (12%)	5	23
52	m6	160/161 (99%)	145 (91%)	15 (9%)	8	33
53	M7	140/145 (97%)	108 (77%)	32 (23%)	1	3
53	m7	125/145 (86%)	103 (82%)	22 (18%)	2	9
54	M8	150/150 (100%)	130 (87%)	20 (13%)	4	19
54	m8	150/150 (100%)	130 (87%)	20 (13%)	4	19
55	M9	153/153 (100%)	135 (88%)	18 (12%)	5	23
55	m9	153/153 (100%)	131 (86%)	22 (14%)	3	16
56	N0	156/156 (100%)	128 (82%)	28 (18%)	2	8
56	n0	156/156 (100%)	122 (78%)	34 (22%)	1	4
57	N1	136/136 (100%)	109 (80%)	27 (20%)	1	5
57	n1	136/136 (100%)	107 (79%)	29 (21%)	1	4
58	N2	87/106 (82%)	74 (85%)	13 (15%)	3	16
58	n2	85/106 (80%)	71 (84%)	14 (16%)	2	12
59	N3	104/104 (100%)	90 (86%)	14 (14%)	4	19
59	n3	104/104 (100%)	92 (88%)	12 (12%)	5	24
60	N4	57/129 (44%)	54 (95%)	3 (5%)	22	54
60	n4	100/129 (78%)	89 (89%)	11 (11%)	6	27
61	N5	104/117 (89%)	82 (79%)	22 (21%)	1	4
61	n5	104/117 (89%)	88 (85%)	16 (15%)	2	14
62	N6	109/109 (100%)	88 (81%)	21 (19%)	1	6
62	n6	109/109 (100%)	94 (86%)	15 (14%)	3	18
63	N7	115/115 (100%)	102 (89%)	13 (11%)	6	25
63	n7	115/115 (100%)	95 (83%)	20 (17%)	2	9
64	N8	118/118 (100%)	97 (82%)	21 (18%)	2	8
64	n8	118/118 (100%)	97 (82%)	21 (18%)	2	8
65	N9	46/46 (100%)	39 (85%)	7 (15%)	3	15
65	n9	46/46 (100%)	40 (87%)	6 (13%)	4	20
66	O0	81/87 (93%)	65 (80%)	16 (20%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
66	o0	84/87 (97%)	74 (88%)	10 (12%)	5	23
67	O1	92/96 (96%)	79 (86%)	13 (14%)	3	17
67	o1	94/96 (98%)	79 (84%)	15 (16%)	2	13
68	O2	109/110 (99%)	88 (81%)	21 (19%)	1	6
68	o2	109/110 (99%)	85 (78%)	24 (22%)	1	4
69	O3	90/90 (100%)	80 (89%)	10 (11%)	6	26
69	o3	90/90 (100%)	79 (88%)	11 (12%)	5	22
70	O4	95/103 (92%)	82 (86%)	13 (14%)	3	18
70	o4	95/103 (92%)	78 (82%)	17 (18%)	2	8
71	O5	104/104 (100%)	85 (82%)	19 (18%)	1	7
71	o5	103/104 (99%)	84 (82%)	19 (18%)	1	7
72	O6	81/81 (100%)	62 (76%)	19 (24%)	1	3
72	o6	80/81 (99%)	60 (75%)	20 (25%)	0	3
73	O7	70/70 (100%)	57 (81%)	13 (19%)	1	7
73	o7	70/70 (100%)	53 (76%)	17 (24%)	0	3
74	O8	68/68 (100%)	55 (81%)	13 (19%)	1	6
74	o8	67/68 (98%)	57 (85%)	10 (15%)	3	16
75	O9	45/45 (100%)	36 (80%)	9 (20%)	1	5
75	o9	45/45 (100%)	40 (89%)	5 (11%)	6	26
76	Q0	47/47 (100%)	38 (81%)	9 (19%)	1	6
76	q0	47/47 (100%)	36 (77%)	11 (23%)	1	3
77	Q1	23/23 (100%)	17 (74%)	6 (26%)	0	2
77	q1	23/23 (100%)	17 (74%)	6 (26%)	0	2
78	Q2	90/90 (100%)	73 (81%)	17 (19%)	1	6
78	q2	90/90 (100%)	66 (73%)	24 (27%)	0	2
79	Q3	71/71 (100%)	63 (89%)	8 (11%)	6	25
79	q3	71/71 (100%)	57 (80%)	14 (20%)	1	6
81	p0	105/253 (42%)	86 (82%)	19 (18%)	1	8
83	f	123/132 (93%)	107 (87%)	16 (13%)	4	20
All	All	18849/20379 (92%)	15796 (84%)	3053 (16%)	2	12

All (3053) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S0	7	PHE
2	S0	9	LEU
2	S0	22	THR
2	S0	27	ARG
2	S0	32	HIS
2	S0	37	VAL
2	S0	41	ARG
2	S0	49	ASN
2	S0	62	ARG
2	S0	88	LYS
2	S0	101	ARG
2	S0	108	THR
2	S0	114	SER
2	S0	153	SER
2	S0	154	GLU
2	S0	168	HIS
2	S0	170	ILE
2	S0	172	LEU
2	S0	177	LEU
2	S0	188	LEU
2	S0	196	SER
2	S0	198	MET
2	S0	200	ASP
2	S0	203	PHE
3	S1	21	VAL
3	S1	28	GLU
3	S1	29	TRP
3	S1	30	PHE
3	S1	36	SER
3	S1	46	THR
3	S1	61	LEU
3	S1	70	LEU
3	S1	78	ASP
3	S1	81	PHE
3	S1	89	ASP
3	S1	96	LEU
3	S1	97	LEU
3	S1	104	ASP
3	S1	105	PHE
3	S1	108	ASP
3	S1	111	ARG
3	S1	120	LEU
3	S1	124	ASN

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Mol	Chain	Res	Type
3	S1	133	TYR
3	S1	135	LEU
3	S1	148	ASN
3	S1	154	SER
3	S1	176	VAL
3	S1	180	THR
3	S1	181	LEU
3	S1	184	LEU
3	S1	194	ASN
3	S1	195	LYS
3	S1	202	LYS
3	S1	215	VAL
3	S1	218	LEU
3	S1	222	LYS
3	S1	223	PHE
4	S2	41	LEU
4	S2	53	ILE
4	S2	69	ILE
4	S2	70	ASP
4	S2	78	ASP
4	S2	89	GLN
4	S2	95	ARG
4	S2	96	THR
4	S2	97	ARG
4	S2	99	LYS
4	S2	107	SER
4	S2	111	VAL
4	S2	117	THR
4	S2	134	LEU
4	S2	137	ILE
4	S2	139	ILE
4	S2	141	ARG
4	S2	152	HIS
4	S2	166	THR
4	S2	167	VAL
4	S2	182	PRO
4	S2	186	LYS
4	S2	189	GLN
4	S2	206	THR
4	S2	221	THR
4	S2	222	TYR
4	S2	226	THR

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Mol	Chain	Res	Type
4	S2	237	VAL
4	S2	242	ILE
5	S3	4	LEU
5	S3	7	LYS
5	S3	23	GLU
5	S3	37	VAL
5	S3	44	THR
5	S3	45	LYS
5	S3	55	THR
5	S3	65	ARG
5	S3	70	THR
5	S3	76	ARG
5	S3	84	ILE
5	S3	89	GLU
5	S3	91	VAL
5	S3	93	ASP
5	S3	105	MET
5	S3	111	ASN
5	S3	113	LEU
5	S3	124	ARG
5	S3	127	MET
5	S3	128	GLU
5	S3	134	CYS
5	S3	138	VAL
5	S3	142	LEU
5	S3	158	ILE
5	S3	174	HIS
5	S3	175	VAL
5	S3	176	LEU
5	S3	178	ARG
5	S3	179	GLN
5	S3	182	LEU
5	S3	189	MET
5	S3	204	ASP
5	S3	207	THR
5	S3	215	GLU
5	S3	217	ILE
5	S3	223	LYS
6	S4	12	LEU
6	S4	38	LEU
6	S4	39	ARG
6	S4	65	LEU

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Mol	Chain	Res	Type
6	S4	76	VAL
6	S4	77	ARG
6	S4	95	THR
6	S4	115	THR
6	S4	116	ASP
6	S4	131	LEU
6	S4	133	LYS
6	S4	148	ARG
6	S4	160	VAL
6	S4	164	LEU
6	S4	180	LEU
6	S4	182	TYR
6	S4	187	ARG
6	S4	206	ASP
6	S4	211	LYS
6	S4	212	ASP
6	S4	217	THR
6	S4	220	THR
6	S4	227	VAL
6	S4	238	LEU
6	S4	240	LYS
6	S4	248	ILE
6	S4	259	GLN
7	S5	24	VAL
7	S5	25	LEU
7	S5	27	THR
7	S5	32	GLU
7	S5	38	THR
7	S5	41	LYS
7	S5	45	LYS
7	S5	46	TRP
7	S5	48	PHE
7	S5	53	VAL
7	S5	65	ARG
7	S5	70	VAL
7	S5	76	ARG
7	S5	84	LYS
7	S5	89	ILE
7	S5	93	LEU
7	S5	94	THR
7	S5	97	LEU
7	S5	98	MET

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Mol	Chain	Res	Type
7	S5	109	LYS
7	S5	119	ASP
7	S5	128	ASN
7	S5	147	THR
7	S5	156	ARG
7	S5	157	ARG
7	S5	166	ARG
7	S5	219	ARG
8	S6	7	TYR
8	S6	12	SER
8	S6	15	THR
8	S6	18	ILE
8	S6	19	ASP
8	S6	65	GLN
8	S6	76	LEU
8	S6	78	THR
8	S6	81	VAL
8	S6	97	VAL
8	S6	114	VAL
8	S6	115	LYS
8	S6	125	THR
8	S6	126	ASP
8	S6	133	LEU
8	S6	143	LYS
8	S6	150	GLU
8	S6	154	ARG
8	S6	155	ASP
8	S6	169	TYR
8	S6	170	THR
8	S6	177	ARG
8	S6	201	GLN
8	S6	212	LEU
8	S6	216	LEU
8	S6	223	LYS
9	S7	9	LEU
9	S7	15	GLU
9	S7	16	LEU
9	S7	38	LEU
9	S7	46	ILE
9	S7	50	ASP
9	S7	67	LEU
9	S7	70	PHE

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Mol	Chain	Res	Type
9	S7	76	LYS
9	S7	85	PHE
9	S7	95	GLU
9	S7	97	ARG
9	S7	109	VAL
9	S7	110	GLN
9	S7	114	ARG
9	S7	115	SER
9	S7	126	LEU
9	S7	133	THR
9	S7	147	ASN
9	S7	181	ILE
9	S7	185	ILE
10	S8	20	GLN
10	S8	21	PHE
10	S8	29	LEU
10	S8	37	LYS
10	S8	46	VAL
10	S8	56	ARG
10	S8	58	LEU
10	S8	62	THR
10	S8	82	VAL
10	S8	88	ASN
10	S8	103	GLN
10	S8	135	LYS
10	S8	137	LYS
10	S8	151	LYS
10	S8	152	ILE
10	S8	155	SER
10	S8	158	SER
10	S8	164	ARG
10	S8	193	LEU
10	S8	195	ARG
10	S8	197	THR
10	S8	199	LYS
11	S9	3	ARG
11	S9	6	ARG
11	S9	22	SER
11	S9	28	LEU
11	S9	39	LYS
11	S9	54	ARG
11	S9	60	LEU

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Mol	Chain	Res	Type
11	S9	89	ASP
11	S9	92	LYS
11	S9	93	LEU
11	S9	94	ASP
11	S9	96	VAL
11	S9	97	LEU
11	S9	99	LEU
11	S9	105	LEU
11	S9	109	LEU
11	S9	121	SER
11	S9	130	THR
11	S9	134	ILE
11	S9	138	LYS
11	S9	149	ARG
11	S9	150	LEU
11	S9	151	ASP
11	S9	156	ILE
11	S9	161	THR
11	S9	171	ARG
11	S9	172	VAL
11	S9	174	ARG
11	S9	175	ARG
11	S9	182	GLU
12	C0	1	MET
12	C0	20	VAL
12	C0	27	PHE
12	C0	46	LEU
12	C0	55	VAL
12	C0	56	LYS
12	C0	76	LEU
12	C0	82	LEU
13	C1	21	ASN
13	C1	27	THR
13	C1	29	LYS
13	C1	37	ASN
13	C1	40	LEU
13	C1	44	THR
13	C1	56	LYS
13	C1	64	VAL
13	C1	67	ARG
13	C1	69	LYS
13	C1	74	THR

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Mol	Chain	Res	Type
13	C1	79	LYS
13	C1	83	THR
13	C1	88	ARG
13	C1	91	LEU
13	C1	98	ASN
13	C1	99	ARG
13	C1	123	VAL
13	C1	128	CYS
14	C2	28	LEU
14	C2	37	VAL
14	C2	38	HIS
14	C2	43	ARG
14	C2	46	ARG
14	C2	50	LYS
14	C2	52	LEU
14	C2	61	VAL
14	C2	66	VAL
14	C2	71	ILE
14	C2	74	LEU
14	C2	80	ASN
14	C2	103	LEU
14	C2	126	TRP
14	C2	132	GLU
15	C3	3	ARG
15	C3	9	LYS
15	C3	11	ILE
15	C3	19	SER
15	C3	27	LYS
15	C3	32	SER
15	C3	35	GLU
15	C3	39	LYS
15	C3	52	VAL
15	C3	58	HIS
15	C3	64	ARG
15	C3	66	ILE
15	C3	69	ASN
15	C3	78	ASN
15	C3	80	LEU
15	C3	83	GLU
15	C3	88	LEU
15	C3	102	LEU
15	C3	105	ASN

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Mol	Chain	Res	Type
15	C3	110	ASP
15	C3	114	ARG
15	C3	115	LEU
15	C3	125	LEU
15	C3	129	TYR
15	C3	131	THR
15	C3	135	LEU
16	C4	12	GLN
16	C4	13	VAL
16	C4	26	THR
16	C4	29	HIS
16	C4	39	ILE
16	C4	42	VAL
16	C4	43	THR
16	C4	56	SER
16	C4	83	ILE
16	C4	92	LYS
16	C4	99	GLN
16	C4	118	VAL
16	C4	123	SER
16	C4	127	ARG
16	C4	136	ARG
16	C4	137	LEU
17	C5	11	VAL
17	C5	18	ARG
17	C5	20	VAL
17	C5	22	LEU
17	C5	29	SER
17	C5	36	LEU
17	C5	52	LYS
17	C5	69	GLU
17	C5	79	HIS
17	C5	89	MET
17	C5	103	ASN
17	C5	110	GLU
18	C6	26	LYS
18	C6	29	ILE
18	C6	31	VAL
18	C6	52	LEU
18	C6	57	LEU
18	C6	59	LYS
18	C6	66	ARG

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Mol	Chain	Res	Type
18	C6	68	ARG
18	C6	69	VAL
18	C6	74	HIS
18	C6	76	SER
18	C6	98	ASP
18	C6	106	LYS
18	C6	109	PHE
18	C6	114	ARG
18	C6	116	LEU
18	C6	117	LEU
18	C6	127	LYS
18	C6	137	ARG
19	C7	3	ARG
19	C7	5	ARG
19	C7	6	THR
19	C7	8	THR
19	C7	43	SER
19	C7	46	LEU
19	C7	47	ARG
19	C7	49	LYS
19	C7	62	GLN
19	C7	69	ILE
19	C7	71	PHE
19	C7	78	ARG
19	C7	81	LYS
19	C7	83	GLN
19	C7	84	TYR
19	C7	88	VAL
19	C7	104	ASN
20	C8	3	LEU
20	C8	5	VAL
20	C8	6	GLN
20	C8	11	PHE
20	C8	12	GLN
20	C8	14	ILE
20	C8	17	LEU
20	C8	18	LEU
20	C8	26	ILE
20	C8	28	ILE
20	C8	40	ARG
20	C8	53	ASP
20	C8	71	GLN

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Mol	Chain	Res	Type
20	C8	77	THR
20	C8	88	ARG
20	C8	92	ILE
20	C8	93	THR
20	C8	107	SER
20	C8	109	LEU
20	C8	132	ARG
20	C8	136	GLN
20	C8	138	THR
21	C9	6	VAL
21	C9	18	TYR
21	C9	22	LEU
21	C9	28	LEU
21	C9	30	VAL
21	C9	33	TYR
21	C9	35	ASP
21	C9	57	ARG
21	C9	64	HIS
21	C9	67	MET
21	C9	70	GLN
21	C9	71	VAL
21	C9	88	VAL
21	C9	125	SER
21	C9	126	GLU
21	C9	130	ARG
21	C9	131	ASP
21	C9	132	LEU
21	C9	133	ASP
21	C9	144	GLU
22	D0	15	GLN
22	D0	18	GLN
22	D0	20	ILE
22	D0	23	ARG
22	D0	33	GLN
22	D0	41	ILE
22	D0	43	LYS
22	D0	50	LEU
22	D0	51	VAL
22	D0	57	ARG
22	D0	70	THR
22	D0	74	GLU
22	D0	77	LYS

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Mol	Chain	Res	Type
22	D0	103	ILE
22	D0	105	GLN
22	D0	117	VAL
22	D0	120	SER
23	D1	5	LYS
23	D1	7	GLN
23	D1	11	LEU
23	D1	18	SER
23	D1	25	LYS
23	D1	32	VAL
23	D1	33	GLN
23	D1	40	ASP
23	D1	41	GLU
23	D1	44	ARG
23	D1	52	THR
23	D1	60	ARG
23	D1	76	ASP
23	D1	78	LEU
23	D1	80	LYS
24	D2	2	THR
24	D2	3	ARG
24	D2	7	LEU
24	D2	18	GLU
24	D2	24	GLN
24	D2	25	VAL
24	D2	26	LEU
24	D2	30	SER
24	D2	53	ILE
24	D2	65	LEU
24	D2	68	ARG
24	D2	74	VAL
24	D2	81	VAL
24	D2	83	ILE
24	D2	98	GLN
24	D2	103	ILE
24	D2	104	LEU
24	D2	112	ASP
24	D2	121	VAL
24	D2	126	LEU
24	D2	129	VAL
25	D3	7	ARG
25	D3	9	LEU

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Mol	Chain	Res	Type
25	D3	16	ARG
25	D3	28	ASN
25	D3	55	GLU
25	D3	57	LEU
25	D3	65	ASN
25	D3	69	ARG
25	D3	75	GLN
25	D3	79	ASN
25	D3	82	LYS
25	D3	83	VAL
25	D3	84	THR
25	D3	107	PHE
25	D3	109	ARG
25	D3	132	LEU
25	D3	138	GLU
25	D3	140	LYS
25	D3	144	ARG
26	D4	10	ARG
26	D4	29	HIS
26	D4	47	VAL
26	D4	51	GLU
26	D4	57	VAL
26	D4	61	ARG
26	D4	74	LEU
26	D4	102	LYS
26	D4	115	ASP
26	D4	121	THR
26	D4	124	ARG
26	D4	127	LYS
26	D4	128	LYS
26	D4	135	ASP
27	D5	42	LEU
27	D5	54	VAL
27	D5	58	ARG
27	D5	59	TYR
27	D5	60	VAL
27	D5	75	LEU
27	D5	82	HIS
27	D5	85	LYS
27	D5	92	ILE
27	D5	98	GLN
27	D5	100	ILE

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Mol	Chain	Res	Type
28	D6	12	LYS
28	D6	15	ARG
28	D6	18	VAL
28	D6	33	ASP
28	D6	38	ARG
28	D6	39	MET
28	D6	41	ILE
28	D6	44	ILE
28	D6	50	VAL
28	D6	55	GLU
28	D6	61	GLU
28	D6	64	LEU
28	D6	66	LYS
28	D6	69	ASN
28	D6	71	LEU
28	D6	85	ARG
28	D6	91	ASP
29	D7	33	LEU
29	D7	37	CYS
29	D7	61	THR
29	D7	77	THR
30	D8	7	VAL
30	D8	19	THR
30	D8	32	PHE
30	D8	35	ASP
30	D8	38	ARG
30	D8	39	THR
30	D8	48	VAL
30	D8	49	ARG
30	D8	52	ASP
30	D8	58	GLU
30	D8	61	ARG
31	D9	7	TRP
31	D9	10	HIS
31	D9	19	ARG
31	D9	25	SER
31	D9	28	THR
31	D9	30	LEU
31	D9	36	LEU
31	D9	38	ILE
32	E0	20	LYS
32	E0	21	VAL

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Mol	Chain	Res	Type
32	E0	29	LYS
32	E0	39	LEU
32	E0	43	ARG
32	E0	47	VAL
32	E0	49	LEU
32	E0	56	MET
33	E1	83	LYS
33	E1	89	LYS
33	E1	91	ILE
33	E1	93	HIS
33	E1	95	HIS
33	E1	97	LYS
33	E1	103	LEU
33	E1	108	VAL
33	E1	113	LYS
34	SR	16	HIS
34	SR	50	ASP
34	SR	52	GLN
34	SR	56	VAL
34	SR	66	HIS
34	SR	71	CYS
34	SR	76	ASP
34	SR	117	LYS
34	SR	136	ILE
34	SR	137	LYS
34	SR	140	CYS
34	SR	165	ASP
34	SR	193	ILE
34	SR	202	LEU
34	SR	223	TRP
34	SR	232	TYR
34	SR	233	THR
34	SR	238	ASP
34	SR	248	ASN
34	SR	264	SER
34	SR	265	LEU
34	SR	268	GLN
34	SR	290	VAL
35	SM	24	GLU
35	SM	30	THR
35	SM	33	LYS
35	SM	45	SER

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Mol	Chain	Res	Type
35	SM	46	LYS
35	SM	53	ARG
35	SM	64	LYS
35	SM	78	ASP
35	SM	84	LYS
35	SM	89	ARG
35	SM	91	THR
35	SM	92	ASP
35	SM	94	HIS
35	SM	97	THR
35	SM	100	THR
35	SM	102	THR
35	SM	116	GLU
35	SM	131	ILE
35	SM	140	ASP
39	L2	17	THR
39	L2	18	SER
39	L2	19	HIS
39	L2	32	LEU
39	L2	44	ILE
39	L2	45	VAL
39	L2	49	VAL
39	L2	62	VAL
39	L2	72	ARG
39	L2	96	LEU
39	L2	98	VAL
39	L2	101	VAL
39	L2	104	LEU
39	L2	107	VAL
39	L2	114	SER
39	L2	116	VAL
39	L2	143	GLU
39	L2	148	VAL
39	L2	149	ARG
39	L2	157	VAL
39	L2	165	VAL
39	L2	168	VAL
39	L2	179	LEU
39	L2	180	LEU
39	L2	181	LYS
39	L2	191	LEU
39	L2	193	ARG

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Mol	Chain	Res	Type
39	L2	199	THR
39	L2	204	MET
39	L2	207	VAL
39	L2	211	HIS
39	L2	226	SER
39	L2	227	ARG
39	L2	231	SER
39	L2	250	GLN
39	L2	252	THR
40	L3	3	HIS
40	L3	7	GLU
40	L3	19	ARG
40	L3	24	SER
40	L3	25	ILE
40	L3	28	ARG
40	L3	30	LYS
40	L3	44	THR
40	L3	45	SER
40	L3	53	MET
40	L3	54	THR
40	L3	55	THR
40	L3	56	ILE
40	L3	67	PHE
40	L3	72	VAL
40	L3	73	VAL
40	L3	79	VAL
40	L3	81	THR
40	L3	85	VAL
40	L3	97	ARG
40	L3	100	ARG
40	L3	102	LEU
40	L3	103	THR
40	L3	110	LEU
40	L3	112	ASP
40	L3	114	VAL
40	L3	116	ARG
40	L3	157	VAL
40	L3	163	HIS
40	L3	167	ARG
40	L3	187	SER
40	L3	188	ILE
40	L3	192	VAL

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Mol	Chain	Res	Type
40	L3	196	ARG
40	L3	206	ASP
40	L3	212	ASN
40	L3	214	MET
40	L3	226	PHE
40	L3	235	THR
40	L3	238	LEU
40	L3	244	ARG
40	L3	248	LYS
40	L3	252	ILE
40	L3	264	VAL
40	L3	284	ARG
40	L3	289	ASP
40	L3	296	THR
40	L3	301	THR
40	L3	304	THR
40	L3	305	ILE
40	L3	313	HIS
40	L3	319	ASN
40	L3	328	ILE
40	L3	332	ARG
40	L3	343	TYR
40	L3	345	ASN
40	L3	347	SER
40	L3	349	LYS
40	L3	354	VAL
40	L3	355	SER
40	L3	364	LYS
40	L3	372	THR
40	L3	380	MET
41	L4	3	ARG
41	L4	14	GLU
41	L4	20	LEU
41	L4	55	LYS
41	L4	63	GLU
41	L4	74	ILE
41	L4	93	MET
41	L4	98	ARG
41	L4	99	MET
41	L4	105	THR
41	L4	118	LYS
41	L4	120	TYR

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Mol	Chain	Res	Type
41	L4	133	SER
41	L4	138	ARG
41	L4	150	LEU
41	L4	152	VAL
41	L4	153	SER
41	L4	156	LEU
41	L4	194	TYR
41	L4	196	ASN
41	L4	203	ARG
41	L4	206	LEU
41	L4	222	VAL
41	L4	225	VAL
41	L4	230	VAL
41	L4	238	LEU
41	L4	246	ARG
41	L4	256	THR
41	L4	259	ASP
41	L4	265	GLU
41	L4	283	THR
41	L4	288	ARG
41	L4	300	ARG
41	L4	306	THR
41	L4	307	GLN
41	L4	313	LEU
41	L4	316	ASN
41	L4	318	LEU
41	L4	327	LEU
41	L4	332	LYS
41	L4	333	VAL
41	L4	338	LYS
41	L4	339	LEU
41	L4	346	LYS
41	L4	349	THR
41	L4	354	VAL
42	L5	4	GLN
42	L5	9	SER
42	L5	15	ARG
42	L5	22	ARG
42	L5	23	ARG
42	L5	35	ARG
42	L5	41	LYS
42	L5	50	ARG

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Mol	Chain	Res	Type
42	L5	67	SER
42	L5	69	ILE
42	L5	70	THR
42	L5	81	HIS
42	L5	92	LEU
42	L5	105	ILE
42	L5	107	ARG
42	L5	115	LEU
42	L5	131	LEU
42	L5	140	ARG
42	L5	144	VAL
42	L5	146	LEU
42	L5	155	THR
42	L5	159	VAL
42	L5	163	LEU
42	L5	185	PHE
42	L5	187	THR
42	L5	188	GLU
42	L5	189	GLU
42	L5	193	GLU
42	L5	231	ILE
42	L5	236	LEU
42	L5	245	GLU
42	L5	257	GLU
42	L5	259	LYS
42	L5	263	GLU
42	L5	273	ARG
42	L5	278	SER
42	L5	279	LYS
42	L5	293	LEU
43	L6	5	LYS
43	L6	18	LEU
43	L6	21	THR
43	L6	31	ARG
43	L6	52	VAL
43	L6	65	ILE
43	L6	78	ARG
43	L6	79	VAL
43	L6	84	VAL
43	L6	89	THR
43	L6	90	LYS
43	L6	102	ASN

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Mol	Chain	Res	Type
43	L6	129	GLU
43	L6	134	ARG
43	L6	146	ILE
43	L6	154	LEU
43	L6	164	SER
43	L6	173	MET
44	L7	24	GLU
44	L7	25	GLN
44	L7	26	VAL
44	L7	38	LYS
44	L7	46	GLU
44	L7	77	VAL
44	L7	82	LYS
44	L7	83	LEU
44	L7	92	ILE
44	L7	93	ASN
44	L7	100	ARG
44	L7	121	LYS
44	L7	124	LEU
44	L7	128	LYS
44	L7	129	LEU
44	L7	140	SER
44	L7	143	THR
44	L7	157	ASN
44	L7	161	VAL
44	L7	179	LEU
44	L7	181	ILE
44	L7	182	ASP
44	L7	184	LEU
44	L7	239	LEU
45	L8	26	LEU
45	L8	27	THR
45	L8	41	GLN
45	L8	43	LYS
45	L8	71	VAL
45	L8	74	THR
45	L8	77	GLN
45	L8	79	GLN
45	L8	81	THR
45	L8	84	ARG
45	L8	95	ASN
45	L8	110	THR

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Mol	Chain	Res	Type
45	L8	118	GLU
45	L8	126	SER
45	L8	136	LEU
45	L8	149	LYS
45	L8	150	LEU
45	L8	156	ASP
45	L8	157	VAL
45	L8	169	LEU
45	L8	180	VAL
45	L8	185	ARG
45	L8	190	VAL
45	L8	221	ASN
45	L8	229	VAL
45	L8	246	MET
45	L8	248	LYS
46	L9	1	MET
46	L9	5	GLN
46	L9	9	GLN
46	L9	16	VAL
46	L9	18	VAL
46	L9	38	LEU
46	L9	41	ILE
46	L9	42	ASP
46	L9	44	THR
46	L9	48	VAL
46	L9	52	LEU
46	L9	55	VAL
46	L9	68	LEU
46	L9	69	ARG
46	L9	70	THR
46	L9	100	ASN
46	L9	118	LEU
46	L9	124	ARG
46	L9	133	THR
46	L9	139	ASN
46	L9	146	LEU
46	L9	151	VAL
46	L9	152	GLU
46	L9	155	SER
46	L9	157	ASN
46	L9	161	LEU
46	L9	162	GLN

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Mol	Chain	Res	Type
46	L9	164	ILE
46	L9	169	ASN
46	L9	170	LYS
46	L9	172	ILE
46	L9	177	ASP
46	L9	182	SER
46	L9	183	HIS
46	L9	189	GLU
46	L9	191	LEU
47	M0	3	ARG
47	M0	4	ARG
47	M0	7	ARG
47	M0	32	ARG
47	M0	33	ILE
47	M0	42	THR
47	M0	48	LEU
47	M0	52	LEU
47	M0	55	ASN
47	M0	57	LEU
47	M0	63	GLU
47	M0	82	ARG
47	M0	83	ASP
47	M0	87	LEU
47	M0	91	VAL
47	M0	116	ARG
47	M0	121	LYS
47	M0	128	ARG
47	M0	129	VAL
47	M0	133	GLN
47	M0	138	VAL
47	M0	156	ARG
47	M0	163	GLN
47	M0	165	ILE
47	M0	174	THR
47	M0	175	ASN
47	M0	177	ASP
47	M0	197	VAL
47	M0	203	LYS
47	M0	207	GLU
47	M0	209	ASN
48	M1	10	ARG
48	M1	11	ASP

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Mol	Chain	Res	Type
48	M1	12	LEU
48	M1	13	LYS
48	M1	19	LEU
48	M1	22	SER
48	M1	28	ASP
48	M1	39	GLN
48	M1	44	THR
48	M1	46	VAL
48	M1	51	ARG
48	M1	80	LEU
48	M1	82	ARG
48	M1	92	ARG
48	M1	94	ARG
48	M1	106	ILE
48	M1	107	ASP
48	M1	112	LEU
48	M1	137	ARG
48	M1	140	ARG
48	M1	147	THR
48	M1	161	SER
48	M1	166	LYS
48	M1	171	VAL
48	M1	173	ASP
49	M3	13	HIS
49	M3	15	ARG
49	M3	23	LYS
49	M3	24	VAL
49	M3	53	LEU
49	M3	54	LEU
49	M3	55	ARG
49	M3	58	VAL
49	M3	68	LYS
49	M3	69	VAL
49	M3	100	ARG
49	M3	114	GLN
49	M3	124	ILE
49	M3	131	LYS
49	M3	136	GLU
49	M3	138	VAL
49	M3	153	ASP
49	M3	169	THR
50	M4	8	LYS

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Mol	Chain	Res	Type
50	M4	27	GLN
50	M4	28	SER
50	M4	38	ILE
50	M4	50	LYS
50	M4	53	VAL
50	M4	55	ARG
50	M4	58	ILE
50	M4	72	LEU
50	M4	83	LYS
50	M4	90	VAL
50	M4	102	LYS
50	M4	105	GLN
50	M4	108	ARG
50	M4	120	VAL
50	M4	124	ARG
50	M4	128	ARG
50	M4	133	LYS
50	M4	135	LEU
51	M5	12	ARG
51	M5	17	ASP
51	M5	18	VAL
51	M5	22	LEU
51	M5	38	ARG
51	M5	43	THR
51	M5	46	ASP
51	M5	49	ARG
51	M5	62	TYR
51	M5	71	ARG
51	M5	80	THR
51	M5	90	ASN
51	M5	92	LEU
51	M5	94	TYR
51	M5	97	SER
51	M5	99	ARG
51	M5	106	VAL
51	M5	121	VAL
51	M5	132	VAL
51	M5	133	ILE
51	M5	138	GLN
51	M5	151	ILE
51	M5	159	ARG
51	M5	171	SER

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Mol	Chain	Res	Type
51	M5	178	HIS
51	M5	182	ASN
51	M5	187	ARG
51	M5	188	ARG
51	M5	196	THR
51	M5	204	LYS
52	M6	33	ILE
52	M6	34	VAL
52	M6	42	ASN
52	M6	66	LYS
52	M6	67	THR
52	M6	77	SER
52	M6	78	ARG
52	M6	79	ILE
52	M6	85	ARG
52	M6	110	PRO
52	M6	116	LYS
52	M6	124	LEU
52	M6	128	ARG
52	M6	143	THR
52	M6	160	ARG
52	M6	184	THR
52	M6	188	SER
52	M6	189	ASP
52	M6	190	VAL
53	M7	7	THR
53	M7	10	ASN
53	M7	23	ARG
53	M7	24	VAL
53	M7	29	THR
53	M7	36	ILE
53	M7	41	LEU
53	M7	52	LEU
53	M7	55	GLN
53	M7	56	ARG
53	M7	67	ILE
53	M7	69	ARG
53	M7	72	GLN
53	M7	90	PHE
53	M7	95	LEU
53	M7	114	VAL
53	M7	118	GLN

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Mol	Chain	Res	Type
53	M7	119	VAL
53	M7	127	ARG
53	M7	128	ARG
53	M7	129	THR
53	M7	135	ARG
53	M7	137	ASN
53	M7	142	SER
53	M7	144	SER
53	M7	148	LEU
53	M7	157	VAL
53	M7	166	VAL
53	M7	168	LEU
53	M7	171	ARG
53	M7	180	LYS
53	M7	181	ARG
54	M8	3	ILE
54	M8	6	THR
54	M8	11	LYS
54	M8	17	THR
54	M8	21	SER
54	M8	22	ASP
54	M8	26	LEU
54	M8	32	LEU
54	M8	40	THR
54	M8	41	ASP
54	M8	49	LEU
54	M8	111	ARG
54	M8	113	LYS
54	M8	115	VAL
54	M8	135	GLN
54	M8	147	ARG
54	M8	161	LYS
54	M8	174	ARG
54	M8	180	ARG
54	M8	185	LYS
55	M9	5	ARG
55	M9	17	VAL
55	M9	31	GLU
55	M9	44	LEU
55	M9	49	THR
55	M9	51	VAL
55	M9	59	SER

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Mol	Chain	Res	Type
55	M9	74	ARG
55	M9	81	ARG
55	M9	92	GLN
55	M9	104	ARG
55	M9	116	ASP
55	M9	123	LEU
55	M9	134	HIS
55	M9	139	VAL
55	M9	143	ILE
55	M9	164	LEU
55	M9	173	ARG
56	N0	1	MET
56	N0	8	GLN
56	N0	12	ARG
56	N0	16	THR
56	N0	21	GLU
56	N0	45	LEU
56	N0	47	LYS
56	N0	61	ILE
56	N0	70	THR
56	N0	71	LYS
56	N0	79	VAL
56	N0	80	ARG
56	N0	87	THR
56	N0	100	VAL
56	N0	105	THR
56	N0	117	ARG
56	N0	122	HIS
56	N0	125	LYS
56	N0	132	THR
56	N0	136	LYS
56	N0	137	ARG
56	N0	142	GLN
56	N0	155	ARG
56	N0	156	VAL
56	N0	157	GLN
56	N0	162	THR
56	N0	171	PHE
56	N0	172	TYR
57	N1	11	THR
57	N1	26	HIS
57	N1	27	LEU

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Mol	Chain	Res	Type
57	N1	29	THR
57	N1	32	LYS
57	N1	47	SER
57	N1	75	ILE
57	N1	78	LYS
57	N1	79	MET
57	N1	80	VAL
57	N1	88	ARG
57	N1	89	LEU
57	N1	92	ARG
57	N1	93	VAL
57	N1	96	ILE
57	N1	102	ARG
57	N1	104	GLU
57	N1	106	LEU
57	N1	122	GLN
57	N1	126	VAL
57	N1	127	GLN
57	N1	128	LEU
57	N1	131	GLN
57	N1	139	ARG
57	N1	146	ASN
57	N1	149	GLN
57	N1	158	THR
58	N2	10	LYS
58	N2	16	THR
58	N2	19	VAL
58	N2	38	ILE
58	N2	49	ASN
58	N2	50	LEU
58	N2	52	ASN
58	N2	59	ASP
58	N2	61	THR
58	N2	74	LYS
58	N2	93	ILE
58	N2	94	ARG
58	N2	100	THR
59	N3	13	ILE
59	N3	36	ILE
59	N3	48	ARG
59	N3	54	LEU
59	N3	69	LEU

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Mol	Chain	Res	Type
59	N3	83	LYS
59	N3	98	ASN
59	N3	102	ILE
59	N3	104	ASN
59	N3	120	LYS
59	N3	124	ASP
59	N3	132	ASN
59	N3	133	SER
59	N3	135	VAL
60	N4	5	ILE
60	N4	7	SER
60	N4	47	ARG
61	N5	25	LYS
61	N5	26	VAL
61	N5	27	ARG
61	N5	29	SER
61	N5	31	THR
61	N5	34	LEU
61	N5	38	LEU
61	N5	39	LYS
61	N5	59	SER
61	N5	63	ILE
61	N5	73	MET
61	N5	87	SER
61	N5	92	LYS
61	N5	105	VAL
61	N5	112	THR
61	N5	113	LEU
61	N5	115	ARG
61	N5	125	ARG
61	N5	133	LEU
61	N5	135	ILE
61	N5	139	ILE
61	N5	142	ILE
62	N6	3	LYS
62	N6	8	VAL
62	N6	10	SER
62	N6	13	ARG
62	N6	28	ARG
62	N6	37	LYS
62	N6	39	LEU
62	N6	48	LEU

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Mol	Chain	Res	Type
62	N6	57	LEU
62	N6	72	SER
62	N6	74	TYR
62	N6	76	LEU
62	N6	78	PHE
62	N6	87	LYS
62	N6	88	GLU
62	N6	90	VAL
62	N6	105	VAL
62	N6	110	HIS
62	N6	115	ARG
62	N6	125	LYS
62	N6	126	LEU
63	N7	17	ARG
63	N7	34	LYS
63	N7	46	ILE
63	N7	57	HIS
63	N7	75	VAL
63	N7	81	LEU
63	N7	86	THR
63	N7	87	LEU
63	N7	90	GLU
63	N7	92	PHE
63	N7	103	GLN
63	N7	132	SER
63	N7	134	LEU
64	N8	4	ARG
64	N8	6	THR
64	N8	8	THR
64	N8	10	LYS
64	N8	16	SER
64	N8	34	MET
64	N8	42	ARG
64	N8	47	LYS
64	N8	56	VAL
64	N8	60	TYR
64	N8	73	LEU
64	N8	74	ASN
64	N8	88	ASP
64	N8	91	LEU
64	N8	97	GLU
64	N8	104	THR

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Mol	Chain	Res	Type
64	N8	115	LYS
64	N8	118	ILE
64	N8	120	ASN
64	N8	130	VAL
64	N8	139	ARG
65	N9	14	ARG
65	N9	22	LYS
65	N9	23	LYS
65	N9	25	LYS
65	N9	28	LYS
65	N9	50	THR
65	N9	59	LYS
66	O0	16	LEU
66	O0	32	LYS
66	O0	33	SER
66	O0	34	LEU
66	O0	41	LEU
66	O0	43	ILE
66	O0	48	THR
66	O0	52	ARG
66	O0	54	SER
66	O0	55	GLU
66	O0	61	MET
66	O0	79	THR
66	O0	83	LYS
66	O0	97	ASP
66	O0	99	ASP
66	O0	104	LEU
67	O1	8	VAL
67	O1	16	LEU
67	O1	26	LYS
67	O1	31	ARG
67	O1	36	ILE
67	O1	55	LEU
67	O1	68	GLU
67	O1	73	LEU
67	O1	75	ILE
67	O1	79	ARG
67	O1	84	ASP
67	O1	86	LYS
67	O1	89	LEU
68	O2	10	VAL

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Mol	Chain	Res	Type
68	O2	16	LYS
68	O2	19	ARG
68	O2	24	ARG
68	O2	26	HIS
68	O2	27	ARG
68	O2	28	VAL
68	O2	33	ARG
68	O2	50	ILE
68	O2	54	LYS
68	O2	61	LYS
68	O2	62	LYS
68	O2	67	SER
68	O2	73	THR
68	O2	75	LEU
68	O2	79	VAL
68	O2	86	THR
68	O2	87	MET
68	O2	88	HIS
68	O2	109	LEU
68	O2	125	ARG
69	O3	4	SER
69	O3	15	SER
69	O3	22	VAL
69	O3	28	SER
69	O3	37	THR
69	O3	45	LEU
69	O3	59	VAL
69	O3	70	LYS
69	O3	80	VAL
69	O3	98	VAL
70	O4	5	VAL
70	O4	8	ARG
70	O4	22	VAL
70	O4	24	LYS
70	O4	49	SER
70	O4	51	LEU
70	O4	52	GLN
70	O4	58	ARG
70	O4	65	VAL
70	O4	68	THR
70	O4	86	LYS
70	O4	88	ARG

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Mol	Chain	Res	Type
70	O4	102	LYS
71	O5	13	SER
71	O5	15	GLU
71	O5	22	VAL
71	O5	27	GLU
71	O5	28	LEU
71	O5	30	GLU
71	O5	31	LEU
71	O5	43	LYS
71	O5	45	LYS
71	O5	47	VAL
71	O5	49	LYS
71	O5	71	LYS
71	O5	85	THR
71	O5	89	ARG
71	O5	101	THR
71	O5	102	GLU
71	O5	104	GLN
71	O5	111	PHE
71	O5	119	LYS
72	O6	7	ILE
72	O6	11	LEU
72	O6	13	LYS
72	O6	21	THR
72	O6	25	LYS
72	O6	26	ILE
72	O6	34	SER
72	O6	36	ARG
72	O6	44	VAL
72	O6	45	ARG
72	O6	57	LEU
72	O6	58	ILE
72	O6	60	LEU
72	O6	62	ARG
72	O6	68	ARG
72	O6	81	THR
72	O6	87	VAL
72	O6	88	GLU
72	O6	99	ARG
73	O7	13	ASN
73	O7	25	ARG
73	O7	28	HIS

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Mol	Chain	Res	Type
73	O7	33	THR
73	O7	36	SER
73	O7	44	THR
73	O7	45	ARG
73	O7	52	LYS
73	O7	58	THR
73	O7	65	ARG
73	O7	67	LEU
73	O7	76	ASN
73	O7	80	THR
74	O8	31	LEU
74	O8	32	ASN
74	O8	40	GLN
74	O8	41	THR
74	O8	50	SER
74	O8	53	THR
74	O8	57	ASN
74	O8	61	LYS
74	O8	64	LYS
74	O8	65	LEU
74	O8	67	GLN
74	O8	72	THR
74	O8	77	ARG
75	O9	4	GLN
75	O9	9	ILE
75	O9	19	GLN
75	O9	21	ARG
75	O9	23	LEU
75	O9	34	THR
75	O9	37	TYR
75	O9	45	ARG
75	O9	51	ILE
76	Q0	77	ILE
76	Q0	78	ILE
76	Q0	83	LYS
76	Q0	85	LEU
76	Q0	99	CYS
76	Q0	106	ARG
76	Q0	112	LYS
76	Q0	113	ARG
76	Q0	127	LEU
77	Q1	2	ARG

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Mol	Chain	Res	Type
77	Q1	11	ARG
77	Q1	13	LEU
77	Q1	17	ARG
77	Q1	19	LYS
77	Q1	21	ARG
78	Q2	3	ASN
78	Q2	8	ARG
78	Q2	16	THR
78	Q2	17	CYS
78	Q2	24	LYS
78	Q2	26	THR
78	Q2	35	LEU
78	Q2	45	ARG
78	Q2	54	THR
78	Q2	60	LYS
78	Q2	61	LYS
78	Q2	64	THR
78	Q2	78	LYS
78	Q2	83	LEU
78	Q2	84	THR
78	Q2	85	LEU
78	Q2	93	LEU
79	Q3	11	THR
79	Q3	16	VAL
79	Q3	45	LYS
79	Q3	49	ARG
79	Q3	57	CYS
79	Q3	71	VAL
79	Q3	73	THR
79	Q3	91	GLU
2	s0	6	THR
2	s0	9	LEU
2	s0	22	THR
2	s0	24	LEU
2	s0	30	GLN
2	s0	37	VAL
2	s0	39	ASN
2	s0	57	LEU
2	s0	59	LEU
2	s0	87	LEU
2	s0	96	THR
2	s0	101	ARG

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Mol	Chain	Res	Type
2	s0	108	THR
2	s0	110	TYR
2	s0	112	THR
2	s0	119	ARG
2	s0	131	GLN
2	s0	135	GLU
2	s0	138	TYR
2	s0	144	ILE
2	s0	165	ARG
2	s0	172	LEU
2	s0	177	LEU
2	s0	179	ARG
2	s0	185	ARG
2	s0	188	LEU
2	s0	189	VAL
2	s0	198	MET
3	s1	26	ARG
3	s1	36	SER
3	s1	37	THR
3	s1	39	GLU
3	s1	47	LEU
3	s1	51	SER
3	s1	62	LYS
3	s1	68	VAL
3	s1	70	LEU
3	s1	74	GLN
3	s1	78	ASP
3	s1	84	ILE
3	s1	89	ASP
3	s1	95	ASN
3	s1	103	MET
3	s1	105	PHE
3	s1	122	GLU
3	s1	125	VAL
3	s1	126	THR
3	s1	152	ARG
3	s1	173	THR
3	s1	181	LEU
3	s1	184	LEU
3	s1	185	THR
3	s1	191	GLU
3	s1	217	LEU

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Mol	Chain	Res	Type
3	s1	219	LYS
3	s1	222	LYS
3	s1	223	PHE
3	s1	228	LEU
3	s1	231	LEU
3	s1	234	GLU
4	s2	53	ILE
4	s2	54	GLU
4	s2	55	GLU
4	s2	69	ILE
4	s2	70	ASP
4	s2	72	LEU
4	s2	80	VAL
4	s2	82	ASN
4	s2	83	ILE
4	s2	90	THR
4	s2	91	ARG
4	s2	97	ARG
4	s2	102	VAL
4	s2	106	ASP
4	s2	107	SER
4	s2	108	ASN
4	s2	111	VAL
4	s2	113	LEU
4	s2	117	THR
4	s2	126	ARG
4	s2	131	ILE
4	s2	141	ARG
4	s2	146	THR
4	s2	159	THR
4	s2	164	SER
4	s2	166	THR
4	s2	167	VAL
4	s2	170	ILE
4	s2	194	GLU
4	s2	198	THR
4	s2	207	LEU
4	s2	209	ASN
4	s2	218	ILE
4	s2	221	THR
4	s2	224	PHE
4	s2	225	LEU

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Mol	Chain	Res	Type
4	s2	226	THR
4	s2	230	TRP
4	s2	232	GLU
4	s2	237	VAL
4	s2	240	LEU
4	s2	242	ILE
5	s3	4	LEU
5	s3	9	ARG
5	s3	21	LEU
5	s3	44	THR
5	s3	59	LEU
5	s3	67	ASN
5	s3	76	ARG
5	s3	84	ILE
5	s3	91	VAL
5	s3	103	GLU
5	s3	115	ILE
5	s3	117	ARG
5	s3	125	TYR
5	s3	127	MET
5	s3	132	LYS
5	s3	158	ILE
5	s3	162	GLN
5	s3	164	VAL
5	s3	176	LEU
5	s3	179	GLN
5	s3	207	THR
5	s3	212	LYS
5	s3	213	GLU
5	s3	224	ASP
6	s4	6	LYS
6	s4	9	LEU
6	s4	22	LYS
6	s4	38	LEU
6	s4	42	LEU
6	s4	49	ARG
6	s4	51	ARG
6	s4	56	LEU
6	s4	57	ASN
6	s4	65	LEU
6	s4	67	GLN
6	s4	73	ASP

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Mol	Chain	Res	Type
6	s4	78	THR
6	s4	92	LEU
6	s4	113	ARG
6	s4	116	ASP
6	s4	131	LEU
6	s4	148	ARG
6	s4	170	THR
6	s4	176	ASP
6	s4	180	LEU
6	s4	182	TYR
6	s4	191	ARG
6	s4	221	ARG
6	s4	223	ASN
6	s4	237	SER
6	s4	246	LEU
6	s4	254	ARG
6	s4	255	ARG
7	s5	25	LEU
7	s5	27	THR
7	s5	31	GLU
7	s5	38	THR
7	s5	45	LYS
7	s5	46	TRP
7	s5	59	VAL
7	s5	63	GLN
7	s5	66	GLN
7	s5	68	ILE
7	s5	76	ARG
7	s5	86	GLN
7	s5	87	CYS
7	s5	93	LEU
7	s5	112	ARG
7	s5	119	ASP
7	s5	137	ILE
7	s5	157	ARG
7	s5	167	ARG
7	s5	194	LEU
7	s5	199	ILE
7	s5	203	LYS
7	s5	206	SER
7	s5	208	SER
7	s5	213	LYS

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Mol	Chain	Res	Type
7	s5	215	ASP
7	s5	219	ARG
8	s6	19	ASP
8	s6	21	GLU
8	s6	57	ASP
8	s6	67	VAL
8	s6	71	THR
8	s6	73	ILE
8	s6	76	LEU
8	s6	78	THR
8	s6	93	LYS
8	s6	109	LEU
8	s6	119	GLN
8	s6	125	THR
8	s6	128	THR
8	s6	151	ASP
8	s6	157	VAL
8	s6	163	THR
8	s6	168	THR
8	s6	169	TYR
8	s6	170	THR
8	s6	175	ILE
8	s6	177	ARG
8	s6	210	GLN
8	s6	211	LEU
8	s6	212	LEU
8	s6	215	ARG
9	s7	11	GLN
9	s7	24	PHE
9	s7	28	GLU
9	s7	33	GLU
9	s7	35	LYS
9	s7	50	ASP
9	s7	64	VAL
9	s7	67	LEU
9	s7	77	LEU
9	s7	80	GLU
9	s7	86	GLN
9	s7	87	ASP
9	s7	90	VAL
9	s7	95	GLU
9	s7	97	ARG

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Mol	Chain	Res	Type
9	s7	110	GLN
9	s7	114	ARG
9	s7	116	ARG
9	s7	117	THR
9	s7	123	ASP
9	s7	125	ILE
9	s7	129	LEU
9	s7	143	LEU
9	s7	144	VAL
9	s7	160	GLN
9	s7	166	LEU
9	s7	185	ILE
10	s8	4	SER
10	s8	10	LYS
10	s8	17	LYS
10	s8	18	ARG
10	s8	25	ARG
10	s8	29	LEU
10	s8	46	VAL
10	s8	59	ARG
10	s8	60	ILE
10	s8	61	GLU
10	s8	89	GLU
10	s8	105	ASP
10	s8	138	ASN
10	s8	152	ILE
10	s8	153	GLU
10	s8	155	SER
10	s8	165	LEU
10	s8	168	CYS
10	s8	175	GLN
10	s8	176	SER
10	s8	184	LEU
10	s8	199	LYS
11	s9	3	ARG
11	s9	7	THR
11	s9	9	SER
11	s9	14	THR
11	s9	21	SER
11	s9	28	LEU
11	s9	49	LEU
11	s9	53	ARG

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Mol	Chain	Res	Type
11	s9	57	ARG
11	s9	71	PHE
11	s9	78	ARG
11	s9	82	ARG
11	s9	87	SER
11	s9	89	ASP
11	s9	93	LEU
11	s9	101	VAL
11	s9	103	ASP
11	s9	105	LEU
11	s9	109	LEU
11	s9	130	THR
11	s9	133	HIS
11	s9	134	ILE
11	s9	143	ILE
11	s9	149	ARG
11	s9	151	ASP
11	s9	156	ILE
11	s9	172	VAL
11	s9	175	ARG
11	s9	180	LYS
11	s9	182	GLU
12	c0	2	LEU
12	c0	5	LYS
12	c0	15	LEU
12	c0	33	GLU
12	c0	36	ASP
12	c0	47	GLN
12	c0	67	THR
12	c0	77	ARG
12	c0	79	TYR
13	c1	4	GLU
13	c1	5	LEU
13	c1	33	ARG
13	c1	40	LEU
13	c1	44	THR
13	c1	46	LYS
13	c1	47	THR
13	c1	56	LYS
13	c1	60	PHE
13	c1	61	THR
13	c1	67	ARG

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Mol	Chain	Res	Type
13	c1	69	LYS
13	c1	74	THR
13	c1	83	THR
13	c1	87	ARG
13	c1	90	TYR
13	c1	111	VAL
13	c1	129	ARG
14	c2	28	LEU
14	c2	43	ARG
14	c2	45	LEU
14	c2	61	VAL
14	c2	62	LEU
14	c2	71	ILE
14	c2	74	LEU
14	c2	85	LYS
14	c2	89	ILE
14	c2	103	LEU
14	c2	125	ASN
14	c2	136	ILE
14	c2	138	GLU
14	c2	140	PHE
15	c3	6	SER
15	c3	20	ARG
15	c3	37	ILE
15	c3	53	LEU
15	c3	60	VAL
15	c3	64	ARG
15	c3	66	ILE
15	c3	67	THR
15	c3	70	LYS
15	c3	76	LYS
15	c3	84	ILE
15	c3	87	ASP
15	c3	102	LEU
15	c3	115	LEU
15	c3	134	VAL
15	c3	138	ASN
16	c4	13	VAL
16	c4	14	PHE
16	c4	26	THR
16	c4	31	THR
16	c4	51	ASP

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Mol	Chain	Res	Type
16	c4	62	LEU
16	c4	79	VAL
16	c4	89	THR
16	c4	103	ARG
16	c4	107	ARG
16	c4	114	ARG
16	c4	118	VAL
16	c4	123	SER
16	c4	124	ASP
16	c4	127	ARG
16	c4	132	ARG
16	c4	133	ARG
16	c4	136	ARG
16	c4	137	LEU
17	c5	12	PHE
17	c5	21	ASP
17	c5	27	GLU
17	c5	36	LEU
17	c5	40	ARG
17	c5	49	MET
17	c5	51	SER
17	c5	69	GLU
17	c5	71	GLU
17	c5	77	ARG
17	c5	102	PHE
17	c5	106	GLU
17	c5	110	GLU
17	c5	121	ILE
17	c5	122	THR
17	c5	134	THR
18	c6	6	SER
18	c6	17	THR
18	c6	23	LYS
18	c6	28	LEU
18	c6	37	THR
18	c6	43	ILE
18	c6	53	LEU
18	c6	57	LEU
18	c6	62	ASN
18	c6	67	VAL
18	c6	69	VAL
18	c6	110	THR

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Mol	Chain	Res	Type
18	c6	114	ARG
18	c6	118	ILE
18	c6	127	LYS
18	c6	128	LYS
18	c6	137	ARG
19	c7	25	THR
19	c7	30	THR
19	c7	34	LEU
19	c7	46	LEU
19	c7	47	ARG
19	c7	49	LYS
19	c7	54	THR
19	c7	69	ILE
19	c7	76	GLU
19	c7	80	ARG
19	c7	85	VAL
19	c7	110	VAL
19	c7	113	LEU
20	c8	3	LEU
20	c8	6	GLN
20	c8	15	LEU
20	c8	18	LEU
20	c8	19	ASN
20	c8	21	ASN
20	c8	33	THR
20	c8	36	LYS
20	c8	55	HIS
20	c8	63	GLN
20	c8	75	ASN
20	c8	85	PHE
20	c8	94	ASP
20	c8	100	THR
20	c8	104	ASN
20	c8	106	GLU
20	c8	109	LEU
20	c8	116	LEU
20	c8	133	VAL
20	c8	136	GLN
20	c8	138	THR
20	c8	141	THR
21	c9	22	LEU
21	c9	27	LYS

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Mol	Chain	Res	Type
21	c9	28	LEU
21	c9	57	ARG
21	c9	68	ARG
21	c9	103	LYS
21	c9	123	ARG
21	c9	126	GLU
21	c9	131	ASP
21	c9	132	LEU
21	c9	140	LEU
22	d0	13	GLU
22	d0	23	ARG
22	d0	27	THR
22	d0	30	LYS
22	d0	36	ASN
22	d0	41	ILE
22	d0	42	VAL
22	d0	44	ASN
22	d0	57	ARG
22	d0	60	THR
22	d0	63	LEU
22	d0	66	SER
22	d0	70	THR
22	d0	72	ASN
22	d0	74	GLU
22	d0	77	LYS
22	d0	81	THR
22	d0	99	ILE
22	d0	107	THR
23	d1	5	LYS
23	d1	12	TYR
23	d1	25	LYS
23	d1	32	VAL
23	d1	33	GLN
23	d1	42	GLU
23	d1	50	TYR
23	d1	62	ARG
23	d1	68	SER
23	d1	69	LEU
23	d1	76	ASP
23	d1	81	ASN
23	d1	82	VAL
24	d2	7	LEU

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Mol	Chain	Res	Type
24	d2	9	ASP
24	d2	15	ASN
24	d2	24	GLN
24	d2	25	VAL
24	d2	28	ARG
24	d2	31	SER
24	d2	47	ILE
24	d2	55	ASP
24	d2	65	LEU
24	d2	68	ARG
24	d2	88	LYS
24	d2	98	GLN
24	d2	103	ILE
24	d2	112	ASP
24	d2	124	LYS
24	d2	126	LEU
24	d2	129	VAL
25	d3	9	LEU
25	d3	15	LEU
25	d3	16	ARG
25	d3	19	ARG
25	d3	28	ASN
25	d3	31	LYS
25	d3	40	SER
25	d3	52	ILE
25	d3	56	LYS
25	d3	73	ARG
25	d3	79	ASN
25	d3	84	THR
25	d3	96	VAL
25	d3	97	ASP
25	d3	100	ASP
25	d3	103	LEU
25	d3	107	PHE
25	d3	121	ARG
25	d3	125	VAL
25	d3	132	LEU
25	d3	144	ARG
26	d4	3	ASP
26	d4	6	THR
26	d4	26	ASP
26	d4	29	HIS

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Mol	Chain	Res	Type
26	d4	30	PRO
26	d4	31	ASN
26	d4	43	LYS
26	d4	44	LEU
26	d4	47	VAL
26	d4	49	LYS
26	d4	55	VAL
26	d4	58	PHE
26	d4	62	THR
26	d4	78	SER
26	d4	86	GLU
26	d4	88	THR
26	d4	91	LEU
26	d4	110	GLN
26	d4	116	LYS
26	d4	125	LEU
27	d5	40	VAL
27	d5	41	ILE
27	d5	43	ASP
27	d5	54	VAL
27	d5	57	TYR
27	d5	60	VAL
27	d5	71	ILE
27	d5	102	THR
28	d6	10	ARG
28	d6	11	ASN
28	d6	24	VAL
28	d6	25	ASN
28	d6	39	MET
28	d6	41	ILE
28	d6	82	ARG
28	d6	89	ARG
28	d6	90	GLU
29	d7	3	LEU
29	d7	34	ASP
29	d7	36	LYS
29	d7	41	LEU
29	d7	43	ILE
29	d7	46	VAL
29	d7	49	HIS
29	d7	52	THR
29	d7	56	CYS

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Mol	Chain	Res	Type
29	d7	59	CYS
29	d7	67	THR
29	d7	72	LYS
29	d7	77	THR
30	d8	28	VAL
30	d8	33	LEU
30	d8	36	THR
30	d8	39	THR
30	d8	42	ARG
30	d8	49	ARG
30	d8	54	LEU
30	d8	57	MET
30	d8	58	GLU
30	d8	64	ARG
30	d8	65	ARG
31	d9	5	ASN
31	d9	10	HIS
31	d9	22	ARG
31	d9	25	SER
31	d9	26	SER
31	d9	31	ILE
31	d9	36	LEU
31	d9	38	ILE
31	d9	39	CYS
31	d9	49	ASP
32	e0	4	VAL
32	e0	13	LYS
32	e0	15	LYS
32	e0	21	VAL
32	e0	23	LYS
32	e0	24	THR
32	e0	26	LYS
32	e0	28	LYS
32	e0	41	THR
32	e0	44	PHE
32	e0	47	VAL
32	e0	48	THR
32	e0	49	LEU
32	e0	50	VAL
32	e0	54	ARG
32	e0	55	ARG
32	e0	62	VAL

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Mol	Chain	Res	Type
33	e1	86	THR
33	e1	90	LYS
33	e1	97	LYS
33	e1	100	LEU
33	e1	103	LEU
33	e1	106	TYR
33	e1	113	LYS
33	e1	115	THR
33	e1	116	LYS
33	e1	117	LEU
33	e1	147	VAL
33	e1	151	ASN
34	sR	5	GLU
34	sR	25	THR
34	sR	48	THR
34	sR	64	HIS
34	sR	66	HIS
34	sR	74	THR
34	sR	76	ASP
34	sR	135	THR
34	sR	136	ILE
34	sR	145	LEU
34	sR	159	ASN
34	sR	160	GLU
34	sR	164	ASP
34	sR	197	SER
34	sR	245	PHE
34	sR	250	TYR
34	sR	275	ARG
34	sR	286	GLU
34	sR	297	ASP
35	sM	34	LYS
35	sM	37	VAL
35	sM	41	SER
35	sM	48	ARG
35	sM	49	LYS
35	sM	50	ASN
35	sM	68	ARG
35	sM	69	ARG
35	sM	74	LYS
35	sM	75	ASP
39	l2	7	ASN

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Mol	Chain	Res	Type
39	l2	15	ILE
39	l2	23	ARG
39	l2	32	LEU
39	l2	33	ASP
39	l2	45	VAL
39	l2	47	GLN
39	l2	74	GLU
39	l2	79	ASN
39	l2	86	GLN
39	l2	96	LEU
39	l2	101	VAL
39	l2	104	LEU
39	l2	109	GLU
39	l2	112	ILE
39	l2	116	VAL
39	l2	137	ILE
39	l2	147	ARG
39	l2	149	ARG
39	l2	157	VAL
39	l2	158	ILE
39	l2	159	SER
39	l2	165	VAL
39	l2	179	LEU
39	l2	180	LEU
39	l2	193	ARG
39	l2	194	ASN
39	l2	216	HIS
39	l2	217	GLN
39	l2	224	THR
39	l2	230	VAL
39	l2	241	ARG
39	l2	242	ARG
39	l2	246	LEU
39	l2	249	SER
40	l3	3	HIS
40	l3	4	ARG
40	l3	5	LYS
40	l3	10	ARG
40	l3	17	LEU
40	l3	20	LYS
40	l3	24	SER
40	l3	37	ARG

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Mol	Chain	Res	Type
40	l3	43	LEU
40	l3	55	THR
40	l3	56	ILE
40	l3	70	ARG
40	l3	77	THR
40	l3	84	VAL
40	l3	85	VAL
40	l3	103	THR
40	l3	104	THR
40	l3	110	LEU
40	l3	114	VAL
40	l3	116	ARG
40	l3	120	LYS
40	l3	139	GLN
40	l3	148	LEU
40	l3	150	ARG
40	l3	169	THR
40	l3	171	LEU
40	l3	183	LEU
40	l3	187	SER
40	l3	188	ILE
40	l3	192	VAL
40	l3	193	ASP
40	l3	196	ARG
40	l3	205	VAL
40	l3	207	SER
40	l3	208	VAL
40	l3	211	GLN
40	l3	214	MET
40	l3	229	VAL
40	l3	232	ARG
40	l3	246	LEU
40	l3	247	ARG
40	l3	252	ILE
40	l3	266	ARG
40	l3	274	SER
40	l3	284	ARG
40	l3	316	GLU
40	l3	324	VAL
40	l3	328	ILE
40	l3	332	ARG
40	l3	340	LYS

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Mol	Chain	Res	Type
40	13	341	SER
40	13	347	SER
40	13	348	ARG
40	13	355	SER
40	13	364	LYS
40	13	367	LYS
40	13	382	THR
41	14	16	THR
41	14	27	SER
41	14	33	ASP
41	14	37	THR
41	14	43	ASN
41	14	47	ARG
41	14	55	LYS
41	14	63	GLU
41	14	67	THR
41	14	69	ARG
41	14	71	VAL
41	14	92	ASN
41	14	93	MET
41	14	99	MET
41	14	112	LYS
41	14	118	LYS
41	14	120	TYR
41	14	136	LEU
41	14	138	ARG
41	14	144	LYS
41	14	148	ILE
41	14	150	LEU
41	14	151	VAL
41	14	160	GLN
41	14	172	VAL
41	14	179	LEU
41	14	187	LEU
41	14	193	LYS
41	14	200	THR
41	14	203	ARG
41	14	206	LEU
41	14	217	LYS
41	14	220	ARG
41	14	222	VAL
41	14	227	THR

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Mol	Chain	Res	Type
41	14	230	VAL
41	14	258	LEU
41	14	283	THR
41	14	313	LEU
41	14	319	LYS
41	14	327	LEU
41	14	333	VAL
41	14	339	LEU
41	14	345	GLU
41	14	347	THR
41	14	359	LEU
42	15	5	LYS
42	15	9	SER
42	15	34	LYS
42	15	38	THR
42	15	41	LYS
42	15	51	LEU
42	15	52	VAL
42	15	61	ILE
42	15	65	ILE
42	15	70	THR
42	15	73	VAL
42	15	75	LEU
42	15	81	HIS
42	15	89	THR
42	15	110	LEU
42	15	111	GLN
42	15	112	LYS
42	15	113	LEU
42	15	118	THR
42	15	122	VAL
42	15	128	GLU
42	15	132	THR
42	15	133	GLU
42	15	135	VAL
42	15	137	ASP
42	15	140	ARG
42	15	146	LEU
42	15	148	ILE
42	15	155	THR
42	15	171	LEU
42	15	185	PHE

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Mol	Chain	Res	Type
42	15	187	THR
42	15	189	GLU
42	15	203	HIS
42	15	206	GLN
42	15	208	MET
42	15	211	LEU
42	15	227	LEU
42	15	230	ASP
42	15	241	THR
42	15	242	SER
42	15	258	LYS
42	15	259	LYS
42	15	260	PHE
42	15	265	TYR
42	15	268	GLU
42	15	273	ARG
42	15	275	THR
42	15	293	LEU
42	15	297	GLN
43	16	4	GLN
43	16	5	LYS
43	16	12	SER
43	16	15	VAL
43	16	21	THR
43	16	31	ARG
43	16	46	ARG
43	16	48	ARG
43	16	50	LYS
43	16	57	HIS
43	16	64	LEU
43	16	65	ILE
43	16	78	ARG
43	16	88	SER
43	16	91	VAL
43	16	94	GLU
43	16	98	VAL
43	16	105	TYR
43	16	109	GLU
43	16	131	LYS
43	16	152	THR
43	16	154	LEU
43	16	155	LEU

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Mol	Chain	Res	Type
44	17	33	ARG
44	17	41	ARG
44	17	83	LEU
44	17	88	ARG
44	17	93	ASN
44	17	110	ARG
44	17	121	LYS
44	17	124	LEU
44	17	130	ILE
44	17	153	PHE
44	17	156	ILE
44	17	158	LYS
44	17	165	ASP
44	17	173	LEU
44	17	175	LYS
44	17	176	TYR
44	17	179	LEU
44	17	184	LEU
44	17	189	ILE
44	17	194	HIS
44	17	196	LYS
44	17	225	GLN
44	17	228	SER
44	17	229	PHE
44	17	239	LEU
45	18	41	GLN
45	18	50	VAL
45	18	68	ARG
45	18	71	VAL
45	18	74	THR
45	18	79	GLN
45	18	109	LEU
45	18	134	TYR
45	18	136	LEU
45	18	149	LYS
45	18	150	LEU
45	18	153	ILE
45	18	160	ILE
45	18	163	VAL
45	18	169	LEU
45	18	172	LYS
45	18	180	VAL

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Mol	Chain	Res	Type
45	18	183	LYS
45	18	185	ARG
45	18	200	LEU
45	18	211	LEU
45	18	232	HIS
45	18	245	LYS
45	18	248	LYS
46	19	1	MET
46	19	5	GLN
46	19	6	THR
46	19	17	THR
46	19	18	VAL
46	19	40	HIS
46	19	44	THR
46	19	52	LEU
46	19	55	VAL
46	19	62	ARG
46	19	68	LEU
46	19	69	ARG
46	19	73	SER
46	19	80	THR
46	19	106	LYS
46	19	107	ASP
46	19	118	LEU
46	19	120	ASP
46	19	122	LYS
46	19	132	VAL
46	19	133	THR
46	19	143	GLU
46	19	144	ILE
46	19	146	LEU
46	19	151	VAL
46	19	157	ASN
46	19	161	LEU
46	19	167	VAL
46	19	173	ARG
46	19	179	ILE
46	19	184	LYS
46	19	186	PHE
46	19	187	ILE
46	19	191	LEU
47	m0	3	ARG

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Mol	Chain	Res	Type
47	m0	4	ARG
47	m0	21	ARG
47	m0	26	VAL
47	m0	35	ASP
47	m0	36	LEU
47	m0	42	THR
47	m0	48	LEU
47	m0	52	LEU
47	m0	55	ASN
47	m0	57	LEU
47	m0	58	GLU
47	m0	63	GLU
47	m0	71	CYS
47	m0	87	LEU
47	m0	121	LYS
47	m0	125	LEU
47	m0	130	ASP
47	m0	137	SER
47	m0	140	THR
47	m0	150	GLU
47	m0	154	ARG
47	m0	156	ARG
47	m0	163	GLN
47	m0	167	LEU
47	m0	169	LYS
47	m0	177	ASP
47	m0	185	ARG
47	m0	205	SER
47	m0	212	GLU
48	m1	7	ASN
48	m1	10	ARG
48	m1	12	LEU
48	m1	46	VAL
48	m1	47	GLN
48	m1	56	THR
48	m1	60	ARG
48	m1	80	LEU
48	m1	87	LYS
48	m1	95	ASN
48	m1	97	SER
48	m1	101	ASN
48	m1	106	ILE

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Mol	Chain	Res	Type
48	m1	107	ASP
48	m1	119	SER
48	m1	130	VAL
48	m1	137	ARG
48	m1	140	ARG
48	m1	142	LYS
48	m1	148	VAL
48	m1	153	LYS
48	m1	155	THR
48	m1	156	LYS
48	m1	159	THR
48	m1	161	SER
48	m1	171	VAL
48	m1	174	LYS
49	m3	4	SER
49	m3	15	ARG
49	m3	46	ILE
49	m3	54	LEU
49	m3	57	VAL
49	m3	58	VAL
49	m3	67	ARG
49	m3	69	VAL
49	m3	73	ARG
49	m3	107	GLU
49	m3	115	ARG
49	m3	118	GLU
49	m3	123	ILE
49	m3	128	ARG
49	m3	131	LYS
49	m3	160	GLN
49	m3	168	ARG
49	m3	183	ARG
49	m3	184	GLU
49	m3	189	GLU
50	m4	4	ASP
50	m4	12	TRP
50	m4	15	VAL
50	m4	25	LYS
50	m4	28	SER
50	m4	37	GLU
50	m4	53	VAL
50	m4	58	ILE

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Mol	Chain	Res	Type
50	m4	62	GLN
50	m4	63	VAL
50	m4	64	VAL
50	m4	70	PHE
50	m4	72	LEU
50	m4	91	CYS
50	m4	107	GLU
50	m4	115	PHE
50	m4	123	LEU
50	m4	126	GLN
50	m4	130	THR
50	m4	135	LEU
51	m5	5	LYS
51	m5	7	LEU
51	m5	10	LEU
51	m5	12	ARG
51	m5	19	LEU
51	m5	22	LEU
51	m5	49	ARG
51	m5	76	PRO
51	m5	80	THR
51	m5	96	ARG
51	m5	105	ARG
51	m5	106	VAL
51	m5	109	ARG
51	m5	117	ASN
51	m5	138	GLN
51	m5	142	ILE
51	m5	152	CYS
51	m5	153	ASP
51	m5	176	LYS
51	m5	178	HIS
51	m5	179	LYS
51	m5	183	THR
51	m5	188	ARG
51	m5	201	ARG
51	m5	204	LYS
52	m6	22	VAL
52	m6	34	VAL
52	m6	43	ILE
52	m6	67	THR
52	m6	78	ARG

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Mol	Chain	Res	Type
52	m6	85	ARG
52	m6	100	GLU
52	m6	106	GLU
52	m6	115	LYS
52	m6	126	VAL
52	m6	130	LYS
52	m6	142	SER
52	m6	143	THR
52	m6	175	THR
52	m6	188	SER
53	m7	7	THR
53	m7	8	SER
53	m7	9	THR
53	m7	14	SER
53	m7	23	ARG
53	m7	24	VAL
53	m7	41	LEU
53	m7	52	LEU
53	m7	55	GLN
53	m7	72	GLN
53	m7	89	LYS
53	m7	114	VAL
53	m7	115	SER
53	m7	119	VAL
53	m7	120	ASN
53	m7	124	LYS
53	m7	126	ARG
53	m7	138	LYS
53	m7	144	SER
53	m7	148	LEU
53	m7	152	GLU
53	m7	155	GLU
54	m8	7	SER
54	m8	17	THR
54	m8	23	ASN
54	m8	24	VAL
54	m8	26	LEU
54	m8	32	LEU
54	m8	57	ILE
54	m8	63	SER
54	m8	69	ARG
54	m8	80	THR

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Mol	Chain	Res	Type
54	m8	111	ARG
54	m8	113	LYS
54	m8	135	GLN
54	m8	147	ARG
54	m8	155	MET
54	m8	161	LYS
54	m8	165	ILE
54	m8	178	ARG
54	m8	180	ARG
54	m8	181	SER
55	m9	6	THR
55	m9	10	LEU
55	m9	13	SER
55	m9	17	VAL
55	m9	20	ARG
55	m9	30	SER
55	m9	31	GLU
55	m9	36	ASN
55	m9	43	LYS
55	m9	63	THR
55	m9	74	ARG
55	m9	88	ARG
55	m9	106	LEU
55	m9	128	LYS
55	m9	134	HIS
55	m9	138	LEU
55	m9	148	ASP
55	m9	152	GLU
55	m9	153	LYS
55	m9	156	ASN
55	m9	173	ARG
55	m9	186	LYS
56	n0	1	MET
56	n0	17	GLU
56	n0	19	VAL
56	n0	21	GLU
56	n0	32	SER
56	n0	34	GLU
56	n0	52	LYS
56	n0	73	LYS
56	n0	80	ARG
56	n0	82	ASP

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Mol	Chain	Res	Type
56	n0	87	THR
56	n0	88	HIS
56	n0	96	ASP
56	n0	97	VAL
56	n0	98	SER
56	n0	99	ARG
56	n0	100	VAL
56	n0	103	VAL
56	n0	104	GLU
56	n0	105	THR
56	n0	117	ARG
56	n0	119	ARG
56	n0	120	SER
56	n0	130	GLU
56	n0	132	THR
56	n0	136	LYS
56	n0	137	ARG
56	n0	142	GLN
56	n0	145	THR
56	n0	148	LEU
56	n0	155	ARG
56	n0	160	THR
56	n0	162	THR
56	n0	172	TYR
57	n1	12	ARG
57	n1	18	ASP
57	n1	25	VAL
57	n1	27	LEU
57	n1	35	LYS
57	n1	71	SER
57	n1	76	ILE
57	n1	78	LYS
57	n1	80	VAL
57	n1	83	ARG
57	n1	86	GLU
57	n1	88	ARG
57	n1	89	LEU
57	n1	93	VAL
57	n1	103	GLN
57	n1	104	GLU
57	n1	112	ASN
57	n1	124	VAL

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Mol	Chain	Res	Type
57	n1	126	VAL
57	n1	127	GLN
57	n1	131	GLN
57	n1	139	ARG
57	n1	141	VAL
57	n1	143	THR
57	n1	144	GLU
57	n1	149	GLN
57	n1	150	THR
57	n1	151	LEU
57	n1	154	VAL
58	n2	16	THR
58	n2	27	VAL
58	n2	37	LEU
58	n2	38	ILE
58	n2	43	VAL
58	n2	49	ASN
58	n2	54	VAL
58	n2	55	THR
58	n2	58	GLU
58	n2	62	VAL
58	n2	68	THR
58	n2	72	SER
58	n2	75	TYR
58	n2	100	THR
59	n3	4	ASN
59	n3	7	GLN
59	n3	9	THR
59	n3	13	ILE
59	n3	14	SER
59	n3	22	ILE
59	n3	48	ARG
59	n3	72	LYS
59	n3	88	ARG
59	n3	98	ASN
59	n3	101	VAL
59	n3	124	ASP
60	n4	1	MET
60	n4	9	SER
60	n4	17	ARG
60	n4	27	LYS
60	n4	54	LEU

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Mol	Chain	Res	Type
60	n4	57	LYS
60	n4	96	LEU
60	n4	109	LEU
60	n4	123	ARG
60	n4	127	LYS
60	n4	133	THR
61	n5	24	LEU
61	n5	27	ARG
61	n5	29	SER
61	n5	37	THR
61	n5	38	LEU
61	n5	39	LYS
61	n5	56	ARG
61	n5	57	LEU
61	n5	63	ILE
61	n5	73	MET
61	n5	109	LYS
61	n5	112	THR
61	n5	115	ARG
61	n5	125	ARG
61	n5	134	ASP
61	n5	135	ILE
62	n6	7	ASP
62	n6	12	ARG
62	n6	13	ARG
62	n6	32	SER
62	n6	37	LYS
62	n6	40	ARG
62	n6	45	ILE
62	n6	50	ILE
62	n6	51	ARG
62	n6	56	VAL
62	n6	59	VAL
62	n6	66	GLN
62	n6	67	GLU
62	n6	74	TYR
62	n6	120	GLN
63	n7	17	ARG
63	n7	24	VAL
63	n7	26	VAL
63	n7	33	SER
63	n7	34	LYS

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Mol	Chain	Res	Type
63	n7	52	LYS
63	n7	54	THR
63	n7	65	ARG
63	n7	66	THR
63	n7	72	ILE
63	n7	81	LEU
63	n7	83	THR
63	n7	85	TYR
63	n7	90	GLU
63	n7	99	GLU
63	n7	100	THR
63	n7	103	GLN
63	n7	114	VAL
63	n7	126	LYS
63	n7	128	GLN
64	n8	6	THR
64	n8	8	THR
64	n8	15	VAL
64	n8	26	ARG
64	n8	27	LYS
64	n8	42	ARG
64	n8	44	ASN
64	n8	46	ASP
64	n8	60	TYR
64	n8	64	GLN
64	n8	67	HIS
64	n8	73	LEU
64	n8	85	ASP
64	n8	91	LEU
64	n8	97	GLU
64	n8	98	THR
64	n8	103	ASP
64	n8	128	ARG
64	n8	130	VAL
64	n8	132	LYS
64	n8	133	LEU
65	n9	19	ASN
65	n9	21	ILE
65	n9	26	THR
65	n9	33	LYS
65	n9	40	ARG
65	n9	59	LYS

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Mol	Chain	Res	Type
66	o0	9	SER
66	o0	19	LYS
66	o0	40	LYS
66	o0	41	LEU
66	o0	50	VAL
66	o0	52	ARG
66	o0	61	MET
66	o0	86	ARG
66	o0	100	ILE
66	o0	104	LEU
67	o1	13	THR
67	o1	16	LEU
67	o1	24	SER
67	o1	31	ARG
67	o1	44	MET
67	o1	46	THR
67	o1	54	GLU
67	o1	55	LEU
67	o1	68	GLU
67	o1	83	GLU
67	o1	90	PHE
67	o1	91	SER
67	o1	93	VAL
67	o1	106	THR
67	o1	107	VAL
68	o2	4	LEU
68	o2	14	THR
68	o2	15	LYS
68	o2	19	ARG
68	o2	24	ARG
68	o2	27	ARG
68	o2	33	ARG
68	o2	35	GLN
68	o2	41	VAL
68	o2	50	ILE
68	o2	61	LYS
68	o2	71	HIS
68	o2	72	LYS
68	o2	73	THR
68	o2	75	LEU
68	o2	81	ASP
68	o2	82	LEU

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Mol	Chain	Res	Type
68	o2	86	THR
68	o2	87	MET
68	o2	109	LEU
68	o2	113	LYS
68	o2	119	VAL
68	o2	125	ARG
68	o2	126	LEU
69	o3	9	VAL
69	o3	10	LYS
69	o3	37	THR
69	o3	49	ILE
69	o3	58	GLU
69	o3	60	ARG
69	o3	70	LYS
69	o3	80	VAL
69	o3	81	VAL
69	o3	88	ASN
69	o3	98	VAL
70	o4	5	VAL
70	o4	6	THR
70	o4	22	VAL
70	o4	25	THR
70	o4	29	ILE
70	o4	30	LEU
70	o4	46	ASP
70	o4	57	LEU
70	o4	58	ARG
70	o4	65	VAL
70	o4	66	SER
70	o4	71	THR
70	o4	80	ARG
70	o4	85	VAL
70	o4	88	ARG
70	o4	100	ILE
70	o4	101	VAL
71	o5	13	SER
71	o5	20	GLN
71	o5	21	LEU
71	o5	27	GLU
71	o5	28	LEU
71	o5	36	LEU
71	o5	38	ARG

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Mol	Chain	Res	Type
71	o5	45	LYS
71	o5	46	THR
71	o5	47	VAL
71	o5	62	GLN
71	o5	68	GLN
71	o5	79	ASP
71	o5	81	ARG
71	o5	84	LYS
71	o5	86	ARG
71	o5	89	ARG
71	o5	107	LYS
71	o5	119	LYS
72	o6	3	VAL
72	o6	7	ILE
72	o6	9	ILE
72	o6	20	MET
72	o6	21	THR
72	o6	29	LYS
72	o6	34	SER
72	o6	35	ASN
72	o6	36	ARG
72	o6	43	LEU
72	o6	44	VAL
72	o6	45	ARG
72	o6	57	LEU
72	o6	58	ILE
72	o6	60	LEU
72	o6	68	ARG
72	o6	74	LYS
72	o6	76	ARG
72	o6	94	ILE
72	o6	98	ARG
73	o7	3	LYS
73	o7	15	SER
73	o7	17	THR
73	o7	21	ARG
73	o7	24	ARG
73	o7	25	ARG
73	o7	26	SER
73	o7	33	THR
73	o7	44	THR
73	o7	55	ARG

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Mol	Chain	Res	Type
73	o7	58	THR
73	o7	59	THR
73	o7	65	ARG
73	o7	67	LEU
73	o7	75	LYS
73	o7	80	THR
73	o7	84	SER
74	o8	8	ILE
74	o8	14	LEU
74	o8	16	ARG
74	o8	22	THR
74	o8	24	THR
74	o8	31	LEU
74	o8	53	THR
74	o8	57	ASN
74	o8	61	LYS
74	o8	64	LYS
75	o9	5	LYS
75	o9	15	LYS
75	o9	21	ARG
75	o9	23	LEU
75	o9	45	ARG
76	q0	79	GLU
76	q0	83	LYS
76	q0	85	LEU
76	q0	88	LYS
76	q0	97	ARG
76	q0	99	CYS
76	q0	108	THR
76	q0	110	CYS
76	q0	112	LYS
76	q0	113	ARG
76	q0	127	LEU
77	q1	2	ARG
77	q1	13	LEU
77	q1	14	LYS
77	q1	17	ARG
77	q1	21	ARG
77	q1	23	ARG
78	q2	2	VAL
78	q2	7	THR
78	q2	8	ARG

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Mol	Chain	Res	Type
78	q2	16	THR
78	q2	21	THR
78	q2	22	GLN
78	q2	26	THR
78	q2	32	LYS
78	q2	35	LEU
78	q2	38	GLN
78	q2	45	ARG
78	q2	47	GLN
78	q2	48	SER
78	q2	61	LYS
78	q2	71	ARG
78	q2	73	GLU
78	q2	78	LYS
78	q2	83	LEU
78	q2	84	THR
78	q2	85	LEU
78	q2	93	LEU
78	q2	104	LEU
78	q2	105	GLN
78	q2	106	PHE
79	q3	3	LYS
79	q3	4	ARG
79	q3	13	LYS
79	q3	16	VAL
79	q3	24	ARG
79	q3	38	ASP
79	q3	42	CYS
79	q3	54	ILE
79	q3	56	THR
79	q3	58	SER
79	q3	64	VAL
79	q3	79	VAL
79	q3	82	THR
79	q3	89	MET
81	p0	4	ILE
81	p0	5	ARG
81	p0	6	GLU
81	p0	39	HIS
81	p0	42	ARG
81	p0	43	LYS
81	p0	48	ARG

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Mol	Chain	Res	Type
81	p0	51	VAL
81	p0	52	LEU
81	p0	66	PHE
81	p0	67	LEU
81	p0	69	ASP
81	p0	70	LEU
81	p0	72	ASP
81	p0	76	LEU
81	p0	81	LYS
81	p0	91	GLU
81	p0	93	LEU
81	p0	97	LYS
83	f	12	ASP
83	f	16	SER
83	f	37	ARG
83	f	49	THR
83	f	52	HIS
83	f	54	HIS
83	f	58	HIS
83	f	78	HIS
83	f	79	ASN
83	f	102	LEU
83	f	105	MET
83	f	106	ASP
83	f	108	ASP
83	f	109	THR
83	f	120	LEU
83	f	133	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
2	S0	23	HIS
3	S1	79	HIS
3	S1	95	ASN
5	S3	159	HIS
7	S5	103	ASN
9	S7	71	HIS
9	S7	180	GLN
12	C0	39	ASN
23	D1	75	ASN
34	SR	52	GLN

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Mol	Chain	Res	Type
34	SR	184	ASN
35	SM	108	GLN
39	L2	132	ASN
40	L3	371	GLN
41	L4	59	GLN
41	L4	328	ASN
41	L4	361	HIS
43	L6	28	GLN
43	L6	57	HIS
44	L7	37	ASN
44	L7	48	ASN
44	L7	159	GLN
46	L9	50	ASN
47	M0	59	GLN
48	M1	109	HIS
51	M5	194	GLN
53	M7	101	ASN
56	N0	138	GLN
57	N1	146	ASN
65	N9	19	ASN
70	O4	18	ASN
73	O7	76	ASN
75	O9	11	GLN
75	O9	19	GLN
7	s5	72	HIS
9	s7	71	HIS
9	s7	74	GLN
10	s8	138	ASN
12	c0	32	HIS
20	c8	89	GLN
23	d1	3	ASN
24	d2	56	HIS
27	d5	44	GLN
28	d6	69	ASN
29	d7	19	HIS
34	sR	237	GLN
40	l3	211	GLN
40	l3	231	HIS
42	l5	81	HIS
44	l7	172	ASN
46	l9	8	GLN
47	m0	12	GLN

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Mol	Chain	Res	Type
51	m5	11	GLN
52	m6	42	ASN
54	m8	5	HIS
56	n0	157	GLN
61	n5	65	GLN
63	n7	57	HIS
64	n8	49	HIS
70	o4	18	ASN
75	o9	4	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1776/1800 (98%)	463 (26%)	42 (2%)
1	6	1791/1800 (99%)	450 (25%)	35 (1%)
36	1	3145/3396 (92%)	683 (21%)	65 (2%)
36	5	3145/3396 (92%)	661 (21%)	65 (2%)
37	3	120/121 (99%)	20 (16%)	1 (0%)
37	7	120/121 (99%)	15 (12%)	1 (0%)
38	4	157/158 (99%)	33 (21%)	3 (1%)
38	8	157/158 (99%)	32 (20%)	1 (0%)
84	B	1/3 (33%)	1 (100%)	0
84	C	1/3 (33%)	0	0
All	All	10413/10956 (95%)	2358 (22%)	213 (2%)

All (2358) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	23	G
1	2	25	C
1	2	26	A
1	2	27	U
1	2	34	G
1	2	45	U
1	2	47	A
1	2	49	C
1	2	50	C
1	2	57	G
1	2	60	U

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Mol	Chain	Res	Type
1	2	63	G
1	2	68	A
1	2	69	G
1	2	72	A
1	2	73	U
1	2	74	U
1	2	75	U
1	2	76	A
1	2	77	U
1	2	90	C
1	2	104	A
1	2	105	A
1	2	114	C
1	2	128	U
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U
1	2	135	A
1	2	136	C
1	2	137	U
1	2	140	A
1	2	141	U
1	2	144	U
1	2	145	A
1	2	146	U
1	2	153	G
1	2	158	U
1	2	159	U
1	2	161	U
1	2	178	U
1	2	179	A
1	2	184	C
1	2	185	U
1	2	186	C
1	2	187	G
1	2	190	C
1	2	191	C
1	2	192	U
1	2	193	U
1	2	195	G
1	2	196	G

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Mol	Chain	Res	Type
1	2	197	A
1	2	200	A
1	2	215	A
1	2	217	A
1	2	219	A
1	2	227	U
1	2	228	G
1	2	229	U
1	2	233	C
1	2	234	G
1	2	235	G
1	2	238	U
1	2	240	U
1	2	241	U
1	2	243	G
1	2	249	U
1	2	250	C
1	2	257	A
1	2	260	U
1	2	261	U
1	2	262	U
1	2	265	A
1	2	267	U
1	2	270	C
1	2	271	A
1	2	272	U
1	2	275	C
1	2	276	C
1	2	277	U
1	2	278	U
1	2	279	G
1	2	280	U
1	2	281	G
1	2	288	A
1	2	290	G
1	2	292	U
1	2	299	A
1	2	302	U
1	2	309	C
1	2	314	C
1	2	316	A
1	2	320	U

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Mol	Chain	Res	Type
1	2	321	C
1	2	322	G
1	2	323	A
1	2	333	A
1	2	337	G
1	2	338	C
1	2	341	A
1	2	352	A
1	2	356	G
1	2	359	A
1	2	360	A
1	2	361	C
1	2	380	U
1	2	390	G
1	2	400	A
1	2	402	C
1	2	404	G
1	2	416	A
1	2	418	G
1	2	419	G
1	2	421	A
1	2	424	C
1	2	425	A
1	2	426	G
1	2	428	A
1	2	434	G
1	2	437	A
1	2	439	U
1	2	444	C
1	2	452	A
1	2	455	C
1	2	468	A
1	2	470	A
1	2	475	A
1	2	480	G
1	2	484	C
1	2	485	A
1	2	488	G
1	2	493	U
1	2	495	C
1	2	496	G
1	2	497	G

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Mol	Chain	Res	Type
1	2	498	G
1	2	499	U
1	2	500	C
1	2	502	U
1	2	503	G
1	2	504	U
1	2	505	A
1	2	506	A
1	2	507	U
1	2	510	G
1	2	511	A
1	2	513	U
1	2	515	A
1	2	516	G
1	2	527	A
1	2	532	U
1	2	538	A
1	2	539	G
1	2	540	G
1	2	541	A
1	2	542	A
1	2	543	C
1	2	544	A
1	2	547	U
1	2	548	G
1	2	555	A
1	2	556	A
1	2	557	G
1	2	558	U
1	2	559	C
1	2	565	C
1	2	578	U
1	2	579	A
1	2	580	A
1	2	585	A
1	2	594	A
1	2	595	G
1	2	596	C
1	2	605	A
1	2	606	A
1	2	609	U
1	2	610	G

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Mol	Chain	Res	Type
1	2	611	U
1	2	614	C
1	2	617	U
1	2	619	A
1	2	620	A
1	2	622	A
1	2	623	A
1	2	624	G
1	2	628	G
1	2	630	A
1	2	639	U
1	2	650	U
1	2	653	C
1	2	655	G
1	2	656	G
1	2	657	U
1	2	658	C
1	2	680	U
1	2	684	A
1	2	694	U
1	2	696	C
1	2	697	C
1	2	700	C
1	2	703	G
1	2	704	C
1	2	705	U
1	2	706	A
1	2	707	A
1	2	709	C
1	2	710	U
1	2	711	U
1	2	712	G
1	2	714	G
1	2	717	C
1	2	718	U
1	2	719	U
1	2	720	G
1	2	721	U
1	2	722	G
1	2	723	G
1	2	725	U
1	2	727	U

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Mol	Chain	Res	Type
1	2	731	C
1	2	732	G
1	2	733	A
1	2	734	A
1	2	735	C
1	2	736	C
1	2	737	A
1	2	738	G
1	2	741	C
1	2	742	U
1	2	754	A
1	2	755	A
1	2	756	A
1	2	765	G
1	2	766	U
1	2	774	A
1	2	775	G
1	2	777	C
1	2	778	G
1	2	781	U
1	2	783	G
1	2	784	C
1	2	789	A
1	2	794	U
1	2	807	A
1	2	812	A
1	2	815	G
1	2	816	G
1	2	818	C
1	2	819	G
1	2	820	U
1	2	821	U
1	2	823	G
1	2	824	G
1	2	829	A
1	2	830	U
1	2	831	U
1	2	833	U
1	2	841	U
1	2	846	G
1	2	856	A
1	2	863	A

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Mol	Chain	Res	Type
1	2	864	U
1	2	865	A
1	2	876	G
1	2	886	U
1	2	896	U
1	2	898	A
1	2	912	U
1	2	913	G
1	2	914	G
1	2	915	A
1	2	916	U
1	2	926	A
1	2	933	A
1	2	935	U
1	2	942	G
1	2	951	A
1	2	960	U
1	2	966	A
1	2	970	A
1	2	977	A
1	2	985	G
1	2	988	A
1	2	992	A
1	2	993	A
1	2	997	G
1	2	1003	A
1	2	1004	U
1	2	1005	A
1	2	1024	U
1	2	1025	A
1	2	1026	A
1	2	1028	C
1	2	1040	G
1	2	1043	A
1	2	1053	G
1	2	1058	U
1	2	1059	U
1	2	1060	U
1	2	1061	A
1	2	1062	A
1	2	1073	G
1	2	1081	A

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Mol	Chain	Res	Type
1	2	1082	C
1	2	1087	A
1	2	1091	A
1	2	1092	A
1	2	1096	C
1	2	1097	U
1	2	1098	U
1	2	1100	G
1	2	1109	G
1	2	1138	A
1	2	1139	A
1	2	1143	A
1	2	1146	G
1	2	1150	G
1	2	1151	A
1	2	1157	A
1	2	1158	C
1	2	1159	C
1	2	1160	A
1	2	1164	G
1	2	1167	G
1	2	1185	U
1	2	1191	U
1	2	1194	A
1	2	1196	A
1	2	1199	G
1	2	1200	G
1	2	1202	A
1	2	1207	C
1	2	1208	A
1	2	1217	A
1	2	1218	G
1	2	1227	A
1	2	1228	G
1	2	1229	G
1	2	1243	G
1	2	1244	A
1	2	1245	G
1	2	1251	U
1	2	1258	U
1	2	1275	A
1	2	1276	U

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Mol	Chain	Res	Type
1	2	1285	U
1	2	1286	U
1	2	1301	U
1	2	1314	U
1	2	1315	U
1	2	1316	G
1	2	1321	A
1	2	1337	A
1	2	1340	U
1	2	1341	A
1	2	1344	A
1	2	1345	A
1	2	1350	U
1	2	1355	C
1	2	1361	U
1	2	1362	U
1	2	1363	U
1	2	1364	G
1	2	1370	U
1	2	1371	A
1	2	1372	U
1	2	1390	U
1	2	1398	U
1	2	1400	A
1	2	1412	G
1	2	1413	U
1	2	1414	U
1	2	1415	U
1	2	1420	C
1	2	1424	A
1	2	1427	A
1	2	1428	G
1	2	1432	U
1	2	1435	G
1	2	1436	A
1	2	1446	A
1	2	1456	C
1	2	1458	G
1	2	1459	C
1	2	1460	A
1	2	1462	G
1	2	1464	G

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Mol	Chain	Res	Type
1	2	1471	A
1	2	1473	U
1	2	1474	G
1	2	1478	G
1	2	1482	C
1	2	1485	C
1	2	1486	G
1	2	1489	U
1	2	1490	C
1	2	1491	U
1	2	1492	A
1	2	1493	A
1	2	1506	G
1	2	1515	A
1	2	1516	A
1	2	1517	U
1	2	1518	C
1	2	1521	G
1	2	1523	G
1	2	1524	A
1	2	1526	A
1	2	1535	U
1	2	1536	G
1	2	1537	C
1	2	1538	U
1	2	1539	G
1	2	1540	G
1	2	1542	G
1	2	1557	U
1	2	1559	A
1	2	1569	A
1	2	1572	G
1	2	1573	A
1	2	1574	G
1	2	1584	G
1	2	1590	G
1	2	1601	G
1	2	1614	A
1	2	1616	G
1	2	1619	C
1	2	1631	A
1	2	1657	U

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Mol	Chain	Res	Type
1	2	1658	G
1	2	1680	G
1	2	1682	U
1	2	1683	C
1	2	1684	U
1	2	1698	G
1	2	1699	G
1	2	1700	C
1	2	1701	A
1	2	1702	A
1	2	1712	A
1	2	1713	G
1	2	1731	A
1	2	1734	U
1	2	1740	A
1	2	1754	A
1	2	1760	G
1	2	1762	A
1	2	1766	A
1	2	1769	U
1	2	1770	U
1	2	1777	G
1	2	1780	G
1	2	1782	A
1	2	1783	C
1	2	1792	G
1	2	1793	G
1	2	1794	A
1	2	1795	U
1	2	1796	C
36	1	13	A
36	1	14	U
36	1	16	A
36	1	26	A
36	1	40	A
36	1	43	A
36	1	45	A
36	1	49	A
36	1	59	G
36	1	60	A
36	1	65	A
36	1	66	A

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Mol	Chain	Res	Type
36	1	74	G
36	1	75	G
36	1	92	G
36	1	93	C
36	1	94	G
36	1	99	A
36	1	109	A
36	1	110	G
36	1	111	C
36	1	113	C
36	1	116	A
36	1	117	U
36	1	121	A
36	1	122	A
36	1	130	A
36	1	131	C
36	1	133	U
36	1	136	G
36	1	146	U
36	1	147	U
36	1	156	G
36	1	157	A
36	1	161	G
36	1	166	C
36	1	176	G
36	1	187	A
36	1	190	U
36	1	191	U
36	1	192	C
36	1	205	C
36	1	206	G
36	1	210	U
36	1	213	A
36	1	218	G
36	1	219	A
36	1	240	U
36	1	241	G
36	1	243	G
36	1	249	U
36	1	250	U
36	1	251	G
36	1	252	U

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Mol	Chain	Res	Type
36	1	269	G
36	1	270	U
36	1	286	U
36	1	295	A
36	1	298	U
36	1	315	C
36	1	316	U
36	1	319	A
36	1	323	A
36	1	329	U
36	1	339	C
36	1	349	A
36	1	350	C
36	1	351	A
36	1	376	G
36	1	397	A
36	1	398	A
36	1	399	A
36	1	401	U
36	1	402	A
36	1	403	C
36	1	414	U
36	1	421	G
36	1	422	A
36	1	438	A
36	1	439	C
36	1	440	A
36	1	495	G
36	1	520	U
36	1	521	A
36	1	535	G
36	1	543	C
36	1	544	C
36	1	546	C
36	1	547	G
36	1	548	G
36	1	552	G
36	1	555	U
36	1	556	U
36	1	557	A
36	1	558	U
36	1	559	A

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Mol	Chain	Res	Type
36	1	569	A
36	1	578	A
36	1	579	G
36	1	592	A
36	1	596	C
36	1	597	G
36	1	604	G
36	1	607	A
36	1	609	G
36	1	611	A
36	1	620	U
36	1	621	A
36	1	636	C
36	1	638	C
36	1	649	A
36	1	660	A
36	1	677	A
36	1	681	U
36	1	683	U
36	1	691	A
36	1	705	A
36	1	709	A
36	1	712	G
36	1	715	A
36	1	716	A
36	1	719	U
36	1	720	A
36	1	725	G
36	1	764	U
36	1	765	C
36	1	766	U
36	1	767	U
36	1	776	U
36	1	777	U
36	1	781	G
36	1	785	G
36	1	787	G
36	1	802	C
36	1	806	A
36	1	817	A
36	1	827	A
36	1	830	A

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Mol	Chain	Res	Type
36	1	849	C
36	1	851	C
36	1	861	C
36	1	874	U
36	1	879	U
36	1	890	C
36	1	896	A
36	1	907	G
36	1	908	G
36	1	914	A
36	1	916	G
36	1	917	A
36	1	921	A
36	1	923	C
36	1	924	G
36	1	925	A
36	1	937	G
36	1	944	C
36	1	953	G
36	1	959	C
36	1	960	U
36	1	967	A
36	1	978	G
36	1	979	U
36	1	980	A
36	1	981	U
36	1	982	C
36	1	994	G
36	1	1001	G
36	1	1002	A
36	1	1003	A
36	1	1006	A
36	1	1010	G
36	1	1013	G
36	1	1017	C
36	1	1018	G
36	1	1020	G
36	1	1021	G
36	1	1024	G
36	1	1025	A
36	1	1029	G
36	1	1036	A

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Mol	Chain	Res	Type
36	1	1037	C
36	1	1047	A
36	1	1049	C
36	1	1064	A
36	1	1065	A
36	1	1071	U
36	1	1072	G
36	1	1079	A
36	1	1080	A
36	1	1081	U
36	1	1083	G
36	1	1093	A
36	1	1094	U
36	1	1095	U
36	1	1097	G
36	1	1098	A
36	1	1103	A
36	1	1104	G
36	1	1117	G
36	1	1129	A
36	1	1131	G
36	1	1144	U
36	1	1145	G
36	1	1153	A
36	1	1159	A
36	1	1161	G
36	1	1168	U
36	1	1179	A
36	1	1180	A
36	1	1181	U
36	1	1182	A
36	1	1185	C
36	1	1190	A
36	1	1191	U
36	1	1192	C
36	1	1193	A
36	1	1201	C
36	1	1202	A
36	1	1209	G
36	1	1213	G
36	1	1216	C
36	1	1217	A

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Mol	Chain	Res	Type
36	1	1221	A
36	1	1222	G
36	1	1227	C
36	1	1232	C
36	1	1233	G
36	1	1235	U
36	1	1236	G
36	1	1241	U
36	1	1243	G
36	1	1245	A
36	1	1246	G
36	1	1248	C
36	1	1249	G
36	1	1251	A
36	1	1253	U
36	1	1254	C
36	1	1258	U
36	1	1262	G
36	1	1263	A
36	1	1264	G
36	1	1265	U
36	1	1266	G
36	1	1269	U
36	1	1270	A
36	1	1271	A
36	1	1274	A
36	1	1278	A
36	1	1279	C
36	1	1280	C
36	1	1285	G
36	1	1287	A
36	1	1292	C
36	1	1294	A
36	1	1296	C
36	1	1308	A
36	1	1309	U
36	1	1313	G
36	1	1315	U
36	1	1318	A
36	1	1330	A
36	1	1331	U
36	1	1332	A

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Mol	Chain	Res	Type
36	1	1348	U
36	1	1349	G
36	1	1350	A
36	1	1351	U
36	1	1352	A
36	1	1353	U
36	1	1355	A
36	1	1356	U
36	1	1357	G
36	1	1386	A
36	1	1387	G
36	1	1398	U
36	1	1399	A
36	1	1400	G
36	1	1402	C
36	1	1405	U
36	1	1408	G
36	1	1411	C
36	1	1417	G
36	1	1418	A
36	1	1419	A
36	1	1429	G
36	1	1431	G
36	1	1433	A
36	1	1434	G
36	1	1435	A
36	1	1437	C
36	1	1443	G
36	1	1446	A
36	1	1450	G
36	1	1460	A
36	1	1481	A
36	1	1482	A
36	1	1485	G
36	1	1496	C
36	1	1502	C
36	1	1508	C
36	1	1521	G
36	1	1527	C
36	1	1533	U
36	1	1536	G
36	1	1542	G

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Mol	Chain	Res	Type
36	1	1555	U
36	1	1556	C
36	1	1560	G
36	1	1561	G
36	1	1562	C
36	1	1563	C
36	1	1564	U
36	1	1567	U
36	1	1568	U
36	1	1569	U
36	1	1570	U
36	1	1571	A
36	1	1572	U
36	1	1576	G
36	1	1580	A
36	1	1582	C
36	1	1583	A
36	1	1587	A
36	1	1589	A
36	1	1593	A
36	1	1596	C
36	1	1605	A
36	1	1607	U
36	1	1608	C
36	1	1620	U
36	1	1629	U
36	1	1630	U
36	1	1632	A
36	1	1639	C
36	1	1641	U
36	1	1643	A
36	1	1657	C
36	1	1665	C
36	1	1677	G
36	1	1683	A
36	1	1688	U
36	1	1713	G
36	1	1715	A
36	1	1716	U
36	1	1717	U
36	1	1724	U
36	1	1725	C

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Mol	Chain	Res	Type
36	1	1729	A
36	1	1736	G
36	1	1741	A
36	1	1742	U
36	1	1750	A
36	1	1751	G
36	1	1761	C
36	1	1763	U
36	1	1764	U
36	1	1765	U
36	1	1766	G
36	1	1767	C
36	1	1770	G
36	1	1780	G
36	1	1793	C
36	1	1797	A
36	1	1810	A
36	1	1812	G
36	1	1813	A
36	1	1814	A
36	1	1815	U
36	1	1816	A
36	1	1817	G
36	1	1819	U
36	1	1820	U
36	1	1821	U
36	1	1822	C
36	1	1835	A
36	1	1839	A
36	1	1841	A
36	1	1842	A
36	1	1845	G
36	1	1846	C
36	1	1849	C
36	1	1850	A
36	1	1863	G
36	1	1866	C
36	1	1879	A
36	1	1880	U
36	1	1886	A
36	1	1906	G
36	1	1908	A

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Mol	Chain	Res	Type
36	1	1926	C
36	1	1927	G
36	1	1935	G
36	1	1937	U
36	1	1951	C
36	1	1952	G
36	1	2094	C
36	1	2100	A
36	1	2101	C
36	1	2102	U
36	1	2107	A
36	1	2111	G
36	1	2112	U
36	1	2113	A
36	1	2114	C
36	1	2115	G
36	1	2121	G
36	1	2122	G
36	1	2130	G
36	1	2131	A
36	1	2134	G
36	1	2139	A
36	1	2140	U
36	1	2144	A
36	1	2158	A
36	1	2169	G
36	1	2170	U
36	1	2171	G
36	1	2187	G
36	1	2188	A
36	1	2195	C
36	1	2201	G
36	1	2205	U
36	1	2208	A
36	1	2209	U
36	1	2210	G
36	1	2223	A
36	1	2228	A
36	1	2239	G
36	1	2244	A
36	1	2248	C
36	1	2249	G

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Mol	Chain	Res	Type
36	1	2250	G
36	1	2251	G
36	1	2255	A
36	1	2256	A
36	1	2272	G
36	1	2281	A
36	1	2282	U
36	1	2287	C
36	1	2288	G
36	1	2307	G
36	1	2309	A
36	1	2310	U
36	1	2313	A
36	1	2314	U
36	1	2315	G
36	1	2323	G
36	1	2334	U
36	1	2336	U
36	1	2342	U
36	1	2350	C
36	1	2361	A
36	1	2367	A
36	1	2372	A
36	1	2373	A
36	1	2374	C
36	1	2375	G
36	1	2385	G
36	1	2393	G
36	1	2394	G
36	1	2397	A
36	1	2401	A
36	1	2402	A
36	1	2403	G
36	1	2404	A
36	1	2411	U
36	1	2418	G
36	1	2419	A
36	1	2428	U
36	1	2429	G
36	1	2435	G
36	1	2437	G
36	1	2438	A

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Mol	Chain	Res	Type
36	1	2444	C
36	1	2445	A
36	1	2502	A
36	1	2503	G
36	1	2508	U
36	1	2511	A
36	1	2514	U
36	1	2515	A
36	1	2522	G
36	1	2523	A
36	1	2531	C
36	1	2533	G
36	1	2534	G
36	1	2537	U
36	1	2538	U
36	1	2539	C
36	1	2540	A
36	1	2541	U
36	1	2542	U
36	1	2543	U
36	1	2547	A
36	1	2548	C
36	1	2549	G
36	1	2552	C
36	1	2554	A
36	1	2555	G
36	1	2556	C
36	1	2560	C
36	1	2561	A
36	1	2562	A
36	1	2568	C
36	1	2569	A
36	1	2570	U
36	1	2571	U
36	1	2572	C
36	1	2573	G
36	1	2576	G
36	1	2580	A
36	1	2581	U
36	1	2585	G
36	1	2586	G
36	1	2593	A

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Mol	Chain	Res	Type
36	1	2594	C
36	1	2606	G
36	1	2607	G
36	1	2614	G
36	1	2635	A
36	1	2637	A
36	1	2638	C
36	1	2652	U
36	1	2656	A
36	1	2659	G
36	1	2672	G
36	1	2674	A
36	1	2675	C
36	1	2677	G
36	1	2681	U
36	1	2689	A
36	1	2691	A
36	1	2694	A
36	1	2696	A
36	1	2705	A
36	1	2708	C
36	1	2714	G
36	1	2716	U
36	1	2728	G
36	1	2729	U
36	1	2752	U
36	1	2753	G
36	1	2758	A
36	1	2769	A
36	1	2772	C
36	1	2777	G
36	1	2778	G
36	1	2781	U
36	1	2796	G
36	1	2800	G
36	1	2801	A
36	1	2803	A
36	1	2810	C
36	1	2814	G
36	1	2817	A
36	1	2818	U
36	1	2819	A

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Mol	Chain	Res	Type
36	1	2830	G
36	1	2842	U
36	1	2843	U
36	1	2845	A
36	1	2860	U
36	1	2871	G
36	1	2872	A
36	1	2873	U
36	1	2876	C
36	1	2887	A
36	1	2897	A
36	1	2898	G
36	1	2899	C
36	1	2916	U
36	1	2923	U
36	1	2925	C
36	1	2935	U
36	1	2936	A
36	1	2940	A
36	1	2942	C
36	1	2943	G
36	1	2947	G
36	1	2960	C
36	1	2971	A
36	1	2977	G
36	1	2979	U
36	1	2983	C
36	1	2990	G
36	1	2996	U
36	1	2997	G
36	1	3011	A
36	1	3012	A
36	1	3025	C
36	1	3030	G
36	1	3040	A
36	1	3050	U
36	1	3056	U
36	1	3059	G
36	1	3065	G
36	1	3074	G
36	1	3078	U
36	1	3079	U

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Mol	Chain	Res	Type
36	1	3080	G
36	1	3086	A
36	1	3092	C
36	1	3097	C
36	1	3098	G
36	1	3104	U
36	1	3122	A
36	1	3129	A
36	1	3130	A
36	1	3131	U
36	1	3141	A
36	1	3142	A
36	1	3143	C
36	1	3151	U
36	1	3153	U
36	1	3154	C
36	1	3155	U
36	1	3156	U
36	1	3157	U
36	1	3164	C
36	1	3165	A
36	1	3167	A
36	1	3168	A
36	1	3170	A
36	1	3171	U
36	1	3173	G
36	1	3174	A
36	1	3176	G
36	1	3179	U
36	1	3181	C
36	1	3187	A
36	1	3196	U
36	1	3207	U
36	1	3210	A
36	1	3217	C
36	1	3218	A
36	1	3219	G
36	1	3229	G
36	1	3239	G
36	1	3243	A
36	1	3244	A
36	1	3245	A

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Mol	Chain	Res	Type
36	1	3246	G
36	1	3247	G
36	1	3253	G
36	1	3257	C
36	1	3259	U
36	1	3269	U
36	1	3270	U
36	1	3276	G
36	1	3281	U
36	1	3286	G
36	1	3289	G
36	1	3294	A
36	1	3303	G
36	1	3304	U
36	1	3307	A
36	1	3313	U
36	1	3316	A
36	1	3318	G
36	1	3319	U
36	1	3320	A
36	1	3341	U
36	1	3342	A
36	1	3345	G
36	1	3347	A
36	1	3350	C
36	1	3351	U
36	1	3352	U
36	1	3353	G
36	1	3354	U
36	1	3355	U
36	1	3356	G
36	1	3368	U
36	1	3369	G
36	1	3375	A
36	1	3376	A
36	1	3378	C
36	1	3382	U
36	1	3383	G
36	1	3388	C
36	1	3389	U
36	1	3396	U
37	3	7	G

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Mol	Chain	Res	Type
37	3	10	C
37	3	11	A
37	3	13	A
37	3	22	A
37	3	29	C
37	3	41	G
37	3	53	U
37	3	55	A
37	3	60	G
37	3	65	G
37	3	68	C
37	3	74	C
37	3	76	A
37	3	90	U
37	3	101	G
37	3	102	A
37	3	104	A
37	3	112	G
37	3	121	U
38	4	16	G
38	4	23	U
38	4	34	U
38	4	35	C
38	4	51	G
38	4	59	A
38	4	62	C
38	4	63	G
38	4	69	U
38	4	70	G
38	4	71	A
38	4	75	G
38	4	80	A
38	4	81	U
38	4	82	U
38	4	83	C
38	4	85	G
38	4	86	U
38	4	87	G
38	4	90	U
38	4	95	G
38	4	96	A
38	4	102	U

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Mol	Chain	Res	Type
38	4	104	A
38	4	106	C
38	4	111	A
38	4	113	U
38	4	125	U
38	4	126	A
38	4	128	U
38	4	138	A
38	4	152	G
38	4	155	A
1	6	2	A
1	6	11	A
1	6	17	C
1	6	25	C
1	6	26	A
1	6	27	U
1	6	34	G
1	6	47	A
1	6	57	G
1	6	60	U
1	6	63	G
1	6	65	A
1	6	67	A
1	6	68	A
1	6	69	G
1	6	72	A
1	6	75	U
1	6	76	A
1	6	77	U
1	6	101	U
1	6	104	A
1	6	114	C
1	6	115	G
1	6	132	U
1	6	137	U
1	6	138	A
1	6	140	A
1	6	141	U
1	6	142	G
1	6	143	G
1	6	144	U
1	6	145	A

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Mol	Chain	Res	Type
1	6	146	U
1	6	153	G
1	6	159	U
1	6	161	U
1	6	162	A
1	6	166	C
1	6	178	U
1	6	179	A
1	6	181	A
1	6	184	C
1	6	185	U
1	6	187	G
1	6	188	A
1	6	190	C
1	6	191	C
1	6	192	U
1	6	193	U
1	6	194	U
1	6	195	G
1	6	196	G
1	6	199	G
1	6	200	A
1	6	215	A
1	6	216	U
1	6	217	A
1	6	218	A
1	6	219	A
1	6	220	A
1	6	226	A
1	6	227	U
1	6	228	G
1	6	230	C
1	6	232	U
1	6	233	C
1	6	234	G
1	6	235	G
1	6	238	U
1	6	240	U
1	6	241	U
1	6	250	C
1	6	261	U
1	6	262	U

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Mol	Chain	Res	Type
1	6	265	A
1	6	266	A
1	6	267	U
1	6	270	C
1	6	271	A
1	6	272	U
1	6	273	G
1	6	277	U
1	6	278	U
1	6	280	U
1	6	287	G
1	6	299	A
1	6	302	U
1	6	314	C
1	6	316	A
1	6	319	U
1	6	320	U
1	6	321	C
1	6	322	G
1	6	337	G
1	6	338	C
1	6	341	A
1	6	344	A
1	6	352	A
1	6	359	A
1	6	360	A
1	6	361	C
1	6	378	A
1	6	385	A
1	6	390	G
1	6	400	A
1	6	401	A
1	6	402	C
1	6	404	G
1	6	416	A
1	6	423	G
1	6	424	C
1	6	425	A
1	6	426	G
1	6	434	G
1	6	438	A
1	6	439	U

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Mol	Chain	Res	Type
1	6	444	C
1	6	448	C
1	6	454	U
1	6	468	A
1	6	475	A
1	6	477	A
1	6	480	G
1	6	484	C
1	6	486	G
1	6	488	G
1	6	489	C
1	6	490	C
1	6	492	A
1	6	493	U
1	6	494	U
1	6	496	G
1	6	500	C
1	6	501	U
1	6	504	U
1	6	505	A
1	6	506	A
1	6	508	U
1	6	510	G
1	6	511	A
1	6	512	A
1	6	513	U
1	6	515	A
1	6	519	C
1	6	536	C
1	6	538	A
1	6	539	G
1	6	540	G
1	6	541	A
1	6	542	A
1	6	543	C
1	6	544	A
1	6	548	G
1	6	555	A
1	6	556	A
1	6	557	G
1	6	558	U
1	6	559	C

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Mol	Chain	Res	Type
1	6	565	C
1	6	568	G
1	6	570	A
1	6	574	G
1	6	577	G
1	6	579	A
1	6	580	A
1	6	594	A
1	6	595	G
1	6	597	G
1	6	606	A
1	6	609	U
1	6	610	G
1	6	611	U
1	6	619	A
1	6	620	A
1	6	623	A
1	6	624	G
1	6	637	C
1	6	639	U
1	6	651	G
1	6	652	G
1	6	653	C
1	6	659	C
1	6	660	G
1	6	661	A
1	6	662	U
1	6	665	U
1	6	667	U
1	6	669	G
1	6	670	U
1	6	676	G
1	6	679	U
1	6	681	U
1	6	682	C
1	6	683	C
1	6	684	A
1	6	685	A
1	6	687	G
1	6	690	G
1	6	695	U
1	6	696	C

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Mol	Chain	Res	Type
1	6	697	C
1	6	698	U
1	6	709	C
1	6	710	U
1	6	711	U
1	6	717	C
1	6	719	U
1	6	720	G
1	6	721	U
1	6	722	G
1	6	730	G
1	6	742	U
1	6	743	U
1	6	751	G
1	6	754	A
1	6	755	A
1	6	756	A
1	6	765	G
1	6	766	U
1	6	767	U
1	6	774	A
1	6	775	G
1	6	780	A
1	6	781	U
1	6	782	U
1	6	783	G
1	6	787	G
1	6	789	A
1	6	792	U
1	6	793	A
1	6	794	U
1	6	811	A
1	6	812	A
1	6	814	A
1	6	815	G
1	6	821	U
1	6	823	G
1	6	825	U
1	6	826	U
1	6	829	A
1	6	830	U
1	6	832	U

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Mol	Chain	Res	Type
1	6	833	U
1	6	834	G
1	6	835	U
1	6	842	C
1	6	844	A
1	6	861	U
1	6	862	A
1	6	863	A
1	6	864	U
1	6	865	A
1	6	871	G
1	6	876	G
1	6	886	U
1	6	898	A
1	6	906	A
1	6	911	U
1	6	913	G
1	6	914	G
1	6	933	A
1	6	935	U
1	6	942	G
1	6	944	A
1	6	946	U
1	6	958	U
1	6	959	U
1	6	960	U
1	6	966	A
1	6	969	C
1	6	992	A
1	6	993	A
1	6	997	G
1	6	1003	A
1	6	1004	U
1	6	1005	A
1	6	1020	A
1	6	1021	C
1	6	1026	A
1	6	1028	C
1	6	1029	U
1	6	1032	G
1	6	1039	A
1	6	1040	G

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Mol	Chain	Res	Type
1	6	1052	U
1	6	1053	G
1	6	1057	U
1	6	1058	U
1	6	1059	U
1	6	1060	U
1	6	1061	A
1	6	1063	U
1	6	1071	U
1	6	1081	A
1	6	1082	C
1	6	1091	A
1	6	1092	A
1	6	1096	C
1	6	1097	U
1	6	1098	U
1	6	1099	U
1	6	1100	G
1	6	1137	A
1	6	1138	A
1	6	1149	G
1	6	1151	A
1	6	1154	G
1	6	1155	G
1	6	1158	C
1	6	1159	C
1	6	1160	A
1	6	1164	G
1	6	1167	G
1	6	1185	U
1	6	1191	U
1	6	1194	A
1	6	1196	A
1	6	1197	C
1	6	1199	G
1	6	1200	G
1	6	1202	A
1	6	1207	C
1	6	1217	A
1	6	1218	G
1	6	1227	A
1	6	1228	G

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Mol	Chain	Res	Type
1	6	1229	G
1	6	1230	A
1	6	1235	C
1	6	1239	U
1	6	1240	U
1	6	1243	G
1	6	1244	A
1	6	1245	G
1	6	1246	C
1	6	1256	A
1	6	1257	U
1	6	1258	U
1	6	1273	G
1	6	1275	A
1	6	1284	C
1	6	1285	U
1	6	1286	U
1	6	1288	G
1	6	1291	G
1	6	1293	U
1	6	1314	U
1	6	1315	U
1	6	1316	G
1	6	1320	U
1	6	1321	A
1	6	1335	U
1	6	1344	A
1	6	1345	A
1	6	1354	G
1	6	1361	U
1	6	1362	U
1	6	1363	U
1	6	1364	G
1	6	1367	G
1	6	1370	U
1	6	1371	A
1	6	1388	A
1	6	1390	U
1	6	1398	U
1	6	1399	C
1	6	1400	A
1	6	1402	G

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Mol	Chain	Res	Type
1	6	1413	U
1	6	1414	U
1	6	1415	U
1	6	1427	A
1	6	1428	G
1	6	1445	G
1	6	1446	A
1	6	1448	G
1	6	1458	G
1	6	1459	C
1	6	1461	C
1	6	1469	A
1	6	1471	A
1	6	1473	U
1	6	1481	C
1	6	1482	C
1	6	1486	G
1	6	1490	C
1	6	1491	U
1	6	1492	A
1	6	1493	A
1	6	1494	C
1	6	1506	G
1	6	1514	U
1	6	1515	A
1	6	1516	A
1	6	1517	U
1	6	1521	G
1	6	1523	G
1	6	1524	A
1	6	1535	U
1	6	1536	G
1	6	1537	C
1	6	1538	U
1	6	1540	G
1	6	1554	U
1	6	1557	U
1	6	1559	A
1	6	1569	A
1	6	1574	G
1	6	1582	U
1	6	1584	G

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Mol	Chain	Res	Type
1	6	1600	A
1	6	1601	G
1	6	1603	U
1	6	1621	U
1	6	1634	C
1	6	1636	C
1	6	1637	C
1	6	1638	G
1	6	1657	U
1	6	1658	G
1	6	1697	G
1	6	1698	G
1	6	1699	G
1	6	1700	C
1	6	1701	A
1	6	1702	A
1	6	1712	A
1	6	1713	G
1	6	1716	C
1	6	1717	G
1	6	1736	G
1	6	1754	A
1	6	1755	A
1	6	1760	G
1	6	1762	A
1	6	1766	A
1	6	1767	G
1	6	1769	U
1	6	1780	G
1	6	1782	A
1	6	1783	C
1	6	1788	G
1	6	1789	G
1	6	1791	A
1	6	1792	G
1	6	1793	G
1	6	1794	A
1	6	1796	C
1	6	1799	U
1	6	1800	A
36	5	14	U
36	5	15	C

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Mol	Chain	Res	Type
36	5	26	A
36	5	30	G
36	5	31	C
36	5	40	A
36	5	49	A
36	5	57	A
36	5	59	G
36	5	60	A
36	5	65	A
36	5	66	A
36	5	72	C
36	5	73	C
36	5	74	G
36	5	76	G
36	5	89	A
36	5	92	G
36	5	93	C
36	5	96	G
36	5	99	A
36	5	109	A
36	5	110	G
36	5	111	C
36	5	116	A
36	5	120	G
36	5	121	A
36	5	122	A
36	5	124	U
36	5	133	U
36	5	134	U
36	5	135	C
36	5	136	G
36	5	150	A
36	5	152	U
36	5	156	G
36	5	157	A
36	5	165	A
36	5	166	C
36	5	170	G
36	5	171	G
36	5	173	G
36	5	174	C
36	5	181	U

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Mol	Chain	Res	Type
36	5	182	U
36	5	184	U
36	5	187	A
36	5	190	U
36	5	191	U
36	5	210	U
36	5	213	A
36	5	218	G
36	5	219	A
36	5	221	A
36	5	231	G
36	5	235	A
36	5	236	G
36	5	239	G
36	5	240	U
36	5	243	G
36	5	245	U
36	5	248	U
36	5	249	U
36	5	250	U
36	5	251	G
36	5	252	U
36	5	253	A
36	5	254	A
36	5	269	G
36	5	284	A
36	5	286	U
36	5	295	A
36	5	323	A
36	5	329	U
36	5	334	A
36	5	338	A
36	5	339	C
36	5	349	A
36	5	350	C
36	5	351	A
36	5	374	A
36	5	375	A
36	5	376	G
36	5	382	U
36	5	398	A
36	5	399	A

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Mol	Chain	Res	Type
36	5	401	U
36	5	402	A
36	5	403	C
36	5	421	G
36	5	422	A
36	5	436	A
36	5	437	G
36	5	438	A
36	5	439	C
36	5	441	U
36	5	442	G
36	5	492	U
36	5	496	C
36	5	507	U
36	5	520	U
36	5	521	A
36	5	523	A
36	5	531	G
36	5	532	A
36	5	533	A
36	5	543	C
36	5	546	C
36	5	547	G
36	5	548	G
36	5	553	U
36	5	555	U
36	5	557	A
36	5	559	A
36	5	565	U
36	5	569	A
36	5	578	A
36	5	579	G
36	5	589	A
36	5	592	A
36	5	594	U
36	5	595	G
36	5	600	G
36	5	604	G
36	5	607	A
36	5	609	G
36	5	611	A
36	5	612	U

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Mol	Chain	Res	Type
36	5	619	A
36	5	620	U
36	5	636	C
36	5	649	A
36	5	660	A
36	5	677	A
36	5	681	U
36	5	691	A
36	5	692	A
36	5	705	A
36	5	708	G
36	5	712	G
36	5	715	A
36	5	716	A
36	5	720	A
36	5	726	G
36	5	727	G
36	5	741	U
36	5	742	G
36	5	758	C
36	5	763	G
36	5	766	U
36	5	767	U
36	5	768	C
36	5	776	U
36	5	777	U
36	5	781	G
36	5	785	G
36	5	786	A
36	5	806	A
36	5	817	A
36	5	830	A
36	5	850	U
36	5	861	C
36	5	869	G
36	5	874	U
36	5	879	U
36	5	891	G
36	5	895	A
36	5	896	A
36	5	897	U
36	5	907	G

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Mol	Chain	Res	Type
36	5	908	G
36	5	910	G
36	5	913	A
36	5	914	A
36	5	916	G
36	5	917	A
36	5	924	G
36	5	936	A
36	5	937	G
36	5	944	C
36	5	959	C
36	5	960	U
36	5	963	G
36	5	968	G
36	5	974	G
36	5	979	U
36	5	981	U
36	5	993	G
36	5	994	G
36	5	1001	G
36	5	1002	A
36	5	1006	A
36	5	1010	G
36	5	1014	U
36	5	1015	U
36	5	1016	C
36	5	1017	C
36	5	1018	G
36	5	1019	G
36	5	1021	G
36	5	1024	G
36	5	1025	A
36	5	1026	A
36	5	1028	U
36	5	1029	G
36	5	1032	C
36	5	1035	G
36	5	1047	A
36	5	1049	C
36	5	1064	A
36	5	1065	A
36	5	1072	G

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Mol	Chain	Res	Type
36	5	1081	U
36	5	1082	U
36	5	1085	A
36	5	1093	A
36	5	1095	U
36	5	1097	G
36	5	1098	A
36	5	1103	A
36	5	1104	G
36	5	1117	G
36	5	1131	G
36	5	1152	G
36	5	1153	A
36	5	1159	A
36	5	1160	C
36	5	1161	G
36	5	1174	G
36	5	1180	A
36	5	1181	U
36	5	1191	U
36	5	1192	C
36	5	1193	A
36	5	1196	C
36	5	1201	C
36	5	1202	A
36	5	1209	G
36	5	1222	G
36	5	1223	A
36	5	1232	C
36	5	1235	U
36	5	1236	G
36	5	1237	G
36	5	1239	C
36	5	1241	U
36	5	1242	G
36	5	1245	A
36	5	1246	G
36	5	1248	C
36	5	1253	U
36	5	1258	U
36	5	1262	G
36	5	1263	A

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Mol	Chain	Res	Type
36	5	1264	G
36	5	1265	U
36	5	1266	G
36	5	1281	G
36	5	1285	G
36	5	1305	U
36	5	1307	G
36	5	1308	A
36	5	1309	U
36	5	1313	G
36	5	1324	U
36	5	1330	A
36	5	1331	U
36	5	1349	G
36	5	1351	U
36	5	1352	A
36	5	1353	U
36	5	1355	A
36	5	1356	U
36	5	1357	G
36	5	1368	U
36	5	1380	G
36	5	1385	C
36	5	1386	A
36	5	1387	G
36	5	1399	A
36	5	1400	G
36	5	1419	A
36	5	1421	G
36	5	1431	G
36	5	1433	A
36	5	1434	G
36	5	1437	C
36	5	1438	U
36	5	1446	A
36	5	1450	G
36	5	1481	A
36	5	1482	A
36	5	1508	C
36	5	1527	C
36	5	1536	G
36	5	1548	C

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Mol	Chain	Res	Type
36	5	1554	U
36	5	1555	U
36	5	1556	C
36	5	1557	A
36	5	1560	G
36	5	1561	G
36	5	1562	C
36	5	1567	U
36	5	1568	U
36	5	1570	U
36	5	1571	A
36	5	1572	U
36	5	1574	C
36	5	1575	A
36	5	1576	G
36	5	1577	G
36	5	1578	C
36	5	1579	C
36	5	1580	A
36	5	1581	C
36	5	1582	C
36	5	1583	A
36	5	1587	A
36	5	1589	A
36	5	1605	A
36	5	1607	U
36	5	1620	U
36	5	1629	U
36	5	1639	C
36	5	1643	A
36	5	1644	C
36	5	1645	U
36	5	1675	G
36	5	1677	G
36	5	1683	A
36	5	1713	G
36	5	1716	U
36	5	1724	U
36	5	1725	C
36	5	1736	G
36	5	1750	A
36	5	1751	G

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Mol	Chain	Res	Type
36	5	1761	C
36	5	1762	C
36	5	1764	U
36	5	1765	U
36	5	1766	G
36	5	1770	G
36	5	1775	G
36	5	1780	G
36	5	1793	C
36	5	1797	A
36	5	1810	A
36	5	1813	A
36	5	1814	A
36	5	1815	U
36	5	1816	A
36	5	1817	G
36	5	1818	U
36	5	1821	U
36	5	1839	A
36	5	1841	A
36	5	1842	A
36	5	1846	C
36	5	1849	C
36	5	1850	A
36	5	1863	G
36	5	1864	A
36	5	1878	G
36	5	1879	A
36	5	1880	U
36	5	1893	A
36	5	1906	G
36	5	1926	C
36	5	2100	A
36	5	2101	C
36	5	2102	U
36	5	2111	G
36	5	2112	U
36	5	2113	A
36	5	2114	C
36	5	2121	G
36	5	2122	G
36	5	2129	U

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Mol	Chain	Res	Type
36	5	2131	A
36	5	2134	G
36	5	2144	A
36	5	2149	A
36	5	2158	A
36	5	2169	G
36	5	2170	U
36	5	2187	G
36	5	2188	A
36	5	2192	C
36	5	2201	G
36	5	2203	U
36	5	2205	U
36	5	2206	G
36	5	2208	A
36	5	2210	G
36	5	2222	A
36	5	2223	A
36	5	2229	A
36	5	2244	A
36	5	2249	G
36	5	2250	G
36	5	2251	G
36	5	2252	A
36	5	2253	G
36	5	2255	A
36	5	2256	A
36	5	2269	U
36	5	2270	A
36	5	2273	G
36	5	2276	G
36	5	2279	A
36	5	2280	A
36	5	2288	G
36	5	2301	U
36	5	2307	G
36	5	2310	U
36	5	2313	A
36	5	2315	G
36	5	2318	U
36	5	2335	G
36	5	2336	U

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Mol	Chain	Res	Type
36	5	2338	C
36	5	2347	U
36	5	2372	A
36	5	2373	A
36	5	2374	C
36	5	2375	G
36	5	2385	G
36	5	2392	C
36	5	2393	G
36	5	2394	G
36	5	2397	A
36	5	2401	A
36	5	2402	A
36	5	2403	G
36	5	2404	A
36	5	2405	C
36	5	2411	U
36	5	2418	G
36	5	2419	A
36	5	2438	A
36	5	2439	A
36	5	2441	A
36	5	2443	A
36	5	2444	C
36	5	2505	U
36	5	2506	U
36	5	2507	C
36	5	2508	U
36	5	2510	U
36	5	2511	A
36	5	2512	C
36	5	2514	U
36	5	2515	A
36	5	2522	G
36	5	2523	A
36	5	2524	A
36	5	2525	G
36	5	2526	C
36	5	2531	C
36	5	2532	U
36	5	2535	A
36	5	2538	U

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Mol	Chain	Res	Type
36	5	2539	C
36	5	2540	A
36	5	2541	U
36	5	2543	U
36	5	2544	U
36	5	2549	G
36	5	2552	C
36	5	2555	G
36	5	2567	C
36	5	2568	C
36	5	2569	A
36	5	2570	U
36	5	2571	U
36	5	2572	C
36	5	2573	G
36	5	2574	G
36	5	2584	G
36	5	2585	G
36	5	2587	U
36	5	2589	G
36	5	2593	A
36	5	2594	C
36	5	2606	G
36	5	2607	G
36	5	2614	G
36	5	2638	C
36	5	2652	U
36	5	2656	A
36	5	2657	A
36	5	2674	A
36	5	2675	C
36	5	2676	A
36	5	2677	G
36	5	2678	A
36	5	2680	A
36	5	2689	A
36	5	2690	G
36	5	2691	A
36	5	2694	A
36	5	2696	A
36	5	2705	A
36	5	2714	G

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Mol	Chain	Res	Type
36	5	2719	U
36	5	2720	G
36	5	2727	A
36	5	2728	G
36	5	2729	U
36	5	2752	U
36	5	2753	G
36	5	2762	A
36	5	2772	C
36	5	2773	C
36	5	2776	C
36	5	2777	G
36	5	2778	G
36	5	2779	A
36	5	2782	U
36	5	2796	G
36	5	2799	A
36	5	2800	G
36	5	2801	A
36	5	2802	A
36	5	2803	A
36	5	2804	A
36	5	2810	C
36	5	2814	G
36	5	2816	G
36	5	2817	A
36	5	2818	U
36	5	2829	U
36	5	2844	C
36	5	2845	A
36	5	2847	A
36	5	2849	C
36	5	2853	A
36	5	2865	U
36	5	2871	G
36	5	2872	A
36	5	2875	U
36	5	2887	A
36	5	2889	C
36	5	2899	C
36	5	2900	A
36	5	2922	G

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Mol	Chain	Res	Type
36	5	2923	U
36	5	2928	C
36	5	2935	U
36	5	2936	A
36	5	2942	C
36	5	2945	G
36	5	2947	G
36	5	2960	C
36	5	2964	G
36	5	2971	A
36	5	2979	U
36	5	2983	C
36	5	2990	G
36	5	2996	U
36	5	2997	G
36	5	3012	A
36	5	3049	A
36	5	3056	U
36	5	3057	U
36	5	3059	G
36	5	3078	U
36	5	3079	U
36	5	3086	A
36	5	3092	C
36	5	3098	G
36	5	3102	G
36	5	3113	A
36	5	3119	U
36	5	3122	A
36	5	3130	A
36	5	3131	U
36	5	3142	A
36	5	3143	C
36	5	3150	A
36	5	3153	U
36	5	3155	U
36	5	3156	U
36	5	3157	U
36	5	3158	G
36	5	3162	C
36	5	3164	C
36	5	3165	A

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Mol	Chain	Res	Type
36	5	3168	A
36	5	3172	A
36	5	3173	G
36	5	3174	A
36	5	3176	G
36	5	3177	G
36	5	3178	A
36	5	3179	U
36	5	3181	C
36	5	3185	U
36	5	3187	A
36	5	3195	U
36	5	3196	U
36	5	3206	C
36	5	3207	U
36	5	3217	C
36	5	3218	A
36	5	3219	G
36	5	3224	G
36	5	3227	A
36	5	3229	G
36	5	3234	A
36	5	3238	G
36	5	3239	G
36	5	3244	A
36	5	3245	A
36	5	3246	G
36	5	3247	G
36	5	3259	U
36	5	3260	G
36	5	3265	C
36	5	3266	G
36	5	3269	U
36	5	3270	U
36	5	3275	U
36	5	3276	G
36	5	3277	U
36	5	3278	C
36	5	3280	U
36	5	3281	U
36	5	3282	U
36	5	3284	G

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Mol	Chain	Res	Type
36	5	3285	C
36	5	3286	G
36	5	3287	U
36	5	3288	G
36	5	3289	G
36	5	3290	G
36	5	3293	U
36	5	3304	U
36	5	3313	U
36	5	3316	A
36	5	3317	U
36	5	3318	G
36	5	3320	A
36	5	3341	U
36	5	3342	A
36	5	3345	G
36	5	3348	G
36	5	3351	U
36	5	3352	U
36	5	3353	G
36	5	3354	U
36	5	3355	U
36	5	3356	G
36	5	3358	U
36	5	3368	U
36	5	3369	G
36	5	3378	C
36	5	3389	U
36	5	3396	U
37	7	22	A
37	7	33	U
37	7	41	G
37	7	50	U
37	7	54	U
37	7	60	G
37	7	64	A
37	7	65	G
37	7	73	C
37	7	74	C
37	7	76	A
37	7	93	C
37	7	102	A

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Mol	Chain	Res	Type
37	7	112	G
37	7	121	U
38	8	13	A
38	8	21	C
38	8	34	U
38	8	35	C
38	8	48	A
38	8	50	C
38	8	51	G
38	8	52	A
38	8	59	A
38	8	62	C
38	8	63	G
38	8	79	A
38	8	80	A
38	8	81	U
38	8	82	U
38	8	83	C
38	8	84	C
38	8	85	G
38	8	86	U
38	8	87	G
38	8	95	G
38	8	104	A
38	8	105	A
38	8	106	C
38	8	111	A
38	8	113	U
38	8	116	G
38	8	125	U
38	8	126	A
38	8	156	U
38	8	157	U
38	8	158	U
84	B	75	C

All (213) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	25	C
1	2	68	A
1	2	73	U

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Mol	Chain	Res	Type
1	2	74	U
1	2	130	C
1	2	131	C
1	2	139	C
1	2	158	U
1	2	192	U
1	2	218	A
1	2	240	U
1	2	242	U
1	2	278	U
1	2	322	G
1	2	417	A
1	2	499	U
1	2	501	U
1	2	503	G
1	2	512	A
1	2	555	A
1	2	704	C
1	2	720	G
1	2	721	U
1	2	811	A
1	2	829	A
1	2	913	G
1	2	1058	U
1	2	1081	A
1	2	1157	A
1	2	1207	C
1	2	1244	A
1	2	1250	U
1	2	1344	A
1	2	1481	C
1	2	1489	U
1	2	1568	C
1	2	1573	A
1	2	1615	C
1	2	1657	U
1	2	1698	G
1	2	1711	C
1	2	1761	U
36	1	13	A
36	1	65	A
36	1	210	U

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Mol	Chain	Res	Type
36	1	239	G
36	1	269	G
36	1	285	A
36	1	397	A
36	1	594	U
36	1	619	A
36	1	637	C
36	1	715	A
36	1	763	G
36	1	873	C
36	1	896	A
36	1	916	G
36	1	979	U
36	1	981	U
36	1	993	G
36	1	1064	A
36	1	1094	U
36	1	1097	G
36	1	1103	A
36	1	1196	C
36	1	1273	A
36	1	1329	U
36	1	1331	U
36	1	1352	A
36	1	1355	A
36	1	1481	A
36	1	1484	U
36	1	1507	G
36	1	1562	C
36	1	1582	C
36	1	1716	U
36	1	1820	U
36	1	1841	A
36	1	2101	C
36	1	2112	U
36	1	2208	A
36	1	2209	U
36	1	2249	G
36	1	2281	A
36	1	2372	A
36	1	2400	G
36	1	2404	A

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Mol	Chain	Res	Type
36	1	2418	G
36	1	2513	U
36	1	2537	U
36	1	2541	U
36	1	2554	A
36	1	2585	G
36	1	2593	A
36	1	2801	A
36	1	2818	U
36	1	3078	U
36	1	3121	U
36	1	3195	U
36	1	3218	A
36	1	3228	C
36	1	3269	U
36	1	3319	U
36	1	3350	C
36	1	3351	U
36	1	3353	G
36	1	3375	A
37	3	52	G
38	4	80	A
38	4	85	G
38	4	125	U
1	6	25	C
1	6	75	U
1	6	76	A
1	6	139	C
1	6	158	U
1	6	187	G
1	6	192	U
1	6	217	A
1	6	272	U
1	6	277	U
1	6	512	A
1	6	542	A
1	6	555	A
1	6	558	U
1	6	678	A
1	6	697	C
1	6	755	A
1	6	829	A

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Mol	Chain	Res	Type
1	6	834	G
1	6	1031	U
1	6	1051	G
1	6	1058	U
1	6	1097	U
1	6	1196	A
1	6	1244	A
1	6	1255	G
1	6	1344	A
1	6	1481	C
1	6	1535	U
1	6	1568	C
1	6	1573	A
1	6	1620	C
1	6	1657	U
1	6	1698	G
1	6	1754	A
36	5	43	A
36	5	151	A
36	5	183	G
36	5	238	A
36	5	438	A
36	5	546	C
36	5	588	G
36	5	715	A
36	5	765	C
36	5	816	A
36	5	873	C
36	5	896	A
36	5	916	G
36	5	993	G
36	5	1017	C
36	5	1027	A
36	5	1064	A
36	5	1081	U
36	5	1152	G
36	5	1222	G
36	5	1238	C
36	5	1241	U
36	5	1284	C
36	5	1307	G
36	5	1329	U

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Mol	Chain	Res	Type
36	5	1352	A
36	5	1355	A
36	5	1367	G
36	5	1481	A
36	5	1554	U
36	5	1560	G
36	5	1571	A
36	5	1774	C
36	5	1815	U
36	5	1816	A
36	5	2101	C
36	5	2112	U
36	5	2209	U
36	5	2249	G
36	5	2255	A
36	5	2281	A
36	5	2440	G
36	5	2507	C
36	5	2513	U
36	5	2531	C
36	5	2539	C
36	5	2586	G
36	5	2728	G
36	5	2772	C
36	5	2801	A
36	5	2818	U
36	5	2874	G
36	5	3056	U
36	5	3078	U
36	5	3154	C
36	5	3195	U
36	5	3228	C
36	5	3269	U
36	5	3275	U
36	5	3276	G
36	5	3289	G
36	5	3317	U
36	5	3340	G
36	5	3341	U
36	5	3357	U
37	7	49	G
38	8	156	U

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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
83	5CT	f	51	83	13,14,15	2.47	3 (23%)	9,15,17	2.36	4 (44%)
84	8AN	C	76	89,85,84	19,24,25	1.07	1 (5%)	13,35,38	1.48	3 (23%)
84	8AN	B	76	89,85,84	19,24,25	1.00	1 (5%)	13,35,38	1.52	2 (15%)

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
83	5CT	f	51	83	1/1/2/4	6/13/14/16	-
84	8AN	C	76	89,85,84	-	3/3/25/26	0/3/3/3
84	8AN	B	76	89,85,84	-	2/3/25/26	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	f	51	5CT	O1-C2	-6.86	1.22	1.43
83	f	51	5CT	CB-CA	3.74	1.58	1.53
83	f	51	5CT	C1-NZ	-3.36	1.41	1.47
84	C	76	8AN	C5-C4	2.44	1.47	1.40
84	B	76	8AN	C5-C4	2.25	1.46	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	f	51	5CT	C3-C2-C1	5.22	124.06	112.16
83	f	51	5CT	O1-C2-C1	3.20	120.25	109.32
84	B	76	8AN	C4-C5-N7	-3.10	106.17	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	C	76	8AN	N3-C2-N1	-3.03	123.94	128.68
84	B	76	8AN	N3-C2-N1	-2.94	124.09	128.68
84	C	76	8AN	C4-C5-N7	-2.40	106.90	109.40
83	f	51	5CT	O1-C2-C3	2.27	115.69	109.21
83	f	51	5CT	C1-NZ-CE	-2.24	108.41	113.42
84	C	76	8AN	C2'-C3'-C4'	2.12	105.64	102.68

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
83	f	51	5CT	C2

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
83	f	51	5CT	CD-CE-NZ-C1
83	f	51	5CT	O1-C2-C3-C4
83	f	51	5CT	C2-C3-C4-N1
83	f	51	5CT	CG-CD-CE-NZ
83	f	51	5CT	NZ-C1-C2-O1
84	C	76	8AN	C4'-C5'-O5'-P
84	B	76	8AN	C4'-C5'-O5'-P
84	C	76	8AN	C3'-C4'-C5'-O5'
84	C	76	8AN	O4'-C4'-C5'-O5'
83	f	51	5CT	C2-C1-NZ-CE
84	B	76	8AN	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2284 ligands modelled in this entry, 1109 are monoatomic - leaving 1175 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
89	PRO	5	4173	89	5,7,8	0.41	0	7,8,10	1.30	1 (14%)
86	OHX	1	3965	-	0,6,6	-	-	-	-	-
86	OHX	2	2095	-	0,6,6	-	-	-	-	-
86	OHX	5	3836	-	0,6,6	-	-	-	-	-
86	OHX	1	3834	-	0,6,6	-	-	-	-	-
86	OHX	1	3992	-	0,6,6	-	-	-	-	-
86	OHX	3	217	-	0,6,6	-	-	-	-	-
86	OHX	1	3995	-	0,6,6	-	-	-	-	-
86	OHX	5	3833	-	0,6,6	-	-	-	-	-
86	OHX	5	3929	-	0,6,6	-	-	-	-	-
86	OHX	5	4031	-	0,6,6	-	-	-	-	-
86	OHX	8	225	-	0,6,6	-	-	-	-	-
86	OHX	1	4060	-	0,6,6	-	-	-	-	-
86	OHX	2	2043	-	0,6,6	-	-	-	-	-
86	OHX	2	2139	-	0,6,6	-	-	-	-	-
86	OHX	5	4127	-	0,6,6	-	-	-	-	-
86	OHX	1	3892	-	0,6,6	-	-	-	-	-
86	OHX	5	4132	-	0,6,6	-	-	-	-	-
86	OHX	5	3912	-	0,6,6	-	-	-	-	-
86	OHX	D9	102	-	0,6,6	-	-	-	-	-
86	OHX	2	2022	-	0,6,6	-	-	-	-	-
86	OHX	1	3947	-	0,6,6	-	-	-	-	-
86	OHX	1	3982	-	0,6,6	-	-	-	-	-
86	OHX	5	4107	-	0,6,6	-	-	-	-	-
86	OHX	2	2131	-	0,6,6	-	-	-	-	-
86	OHX	1	3987	-	0,6,6	-	-	-	-	-
86	OHX	5	4133	-	0,6,6	-	-	-	-	-
86	OHX	2	2057	-	0,6,6	-	-	-	-	-
86	OHX	1	3763	-	0,6,6	-	-	-	-	-
89	PRO	B	101	89,84	5,7,8	0.51	0	7,8,10	1.30	1 (14%)
86	OHX	1	3857	-	0,6,6	-	-	-	-	-
86	OHX	1	4085	-	0,6,6	-	-	-	-	-
86	OHX	6	2045	-	0,6,6	-	-	-	-	-
86	OHX	6	2076	-	0,6,6	-	-	-	-	-
86	OHX	5	3842	-	0,6,6	-	-	-	-	-
86	OHX	5	3996	-	0,6,6	-	-	-	-	-
86	OHX	6	2072	-	0,6,6	-	-	-	-	-
86	OHX	5	3878	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3939	-	0,6,6	-	-	-		
86	OHX	5	3924	-	0,6,6	-	-	-		
86	OHX	5	4035	-	0,6,6	-	-	-		
86	OHX	5	3906	-	0,6,6	-	-	-		
86	OHX	1	4011	-	0,6,6	-	-	-		
86	OHX	M7	205	-	0,6,6	-	-	-		
86	OHX	1	4013	-	0,6,6	-	-	-		
86	OHX	1	3826	-	0,6,6	-	-	-		
86	OHX	5	3993	-	0,6,6	-	-	-		
86	OHX	5	4026	-	0,6,6	-	-	-		
86	OHX	5	4169	-	0,6,6	-	-	-		
86	OHX	1	3919	-	0,6,6	-	-	-		
86	OHX	6	2054	-	0,6,6	-	-	-		
86	OHX	5	4055	-	0,6,6	-	-	-		
86	OHX	8	211	-	0,6,6	-	-	-		
86	OHX	8	215	-	0,6,6	-	-	-		
86	OHX	2	2002	-	0,6,6	-	-	-		
86	OHX	5	3848	-	0,6,6	-	-	-		
86	OHX	5	4070	-	0,6,6	-	-	-		
86	OHX	7	217	-	0,6,6	-	-	-		
86	OHX	1	3762	-	0,6,6	-	-	-		
86	OHX	2	2127	-	0,6,6	-	-	-		
86	OHX	1	3820	-	0,6,6	-	-	-		
86	OHX	2	2016	-	0,6,6	-	-	-		
86	OHX	5	3898	-	0,6,6	-	-	-		
86	OHX	6	2037	-	0,6,6	-	-	-		
86	OHX	5	3956	-	0,6,6	-	-	-		
86	OHX	1	3906	-	0,6,6	-	-	-		
86	OHX	5	4052	-	0,6,6	-	-	-		
86	OHX	5	4056	-	0,6,6	-	-	-		
86	OHX	1	4050	-	0,6,6	-	-	-		
86	OHX	6	2036	-	0,6,6	-	-	-		
86	OHX	5	4170	-	0,6,6	-	-	-		
86	OHX	1	3946	-	0,6,6	-	-	-		
86	OHX	1	3948	-	0,6,6	-	-	-		
86	OHX	4	221	-	0,6,6	-	-	-		
86	OHX	2	2086	-	0,6,6	-	-	-		
86	OHX	1	4006	-	0,6,6	-	-	-		
86	OHX	5	4017	-	0,6,6	-	-	-		
86	OHX	6	2170	-	0,6,6	-	-	-		
86	OHX	7	219	-	0,6,6	-	-	-		
86	OHX	5	4075	-	0,6,6	-	-	-		
86	OHX	5	4111	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	s1	301	-	0,6,6	-	-	-		
86	OHX	5	4002	-	0,6,6	-	-	-		
86	OHX	5	3998	-	0,6,6	-	-	-		
86	OHX	2	2042	-	0,6,6	-	-	-		
86	OHX	2	2136	-	0,6,6	-	-	-		
86	OHX	5	3864	-	0,6,6	-	-	-		
86	OHX	1	3913	-	0,6,6	-	-	-		
86	OHX	5	3959	-	0,6,6	-	-	-		
86	OHX	5	4013	-	0,6,6	-	-	-		
86	OHX	5	4045	-	0,6,6	-	-	-		
86	OHX	1	3788	-	0,6,6	-	-	-		
86	OHX	1	3882	-	0,6,6	-	-	-		
86	OHX	1	4075	-	0,6,6	-	-	-		
86	OHX	2	2040	-	0,6,6	-	-	-		
86	OHX	1	4067	-	0,6,6	-	-	-		
86	OHX	1	3876	-	0,6,6	-	-	-		
86	OHX	5	3936	-	0,6,6	-	-	-		
86	OHX	o7	503	-	0,6,6	-	-	-		
86	OHX	5	4108	-	0,6,6	-	-	-		
86	OHX	5	3962	-	0,6,6	-	-	-		
86	OHX	5	4051	-	0,6,6	-	-	-		
86	OHX	5	4016	-	0,6,6	-	-	-		
86	OHX	2	2038	-	0,6,6	-	-	-		
86	OHX	1	4095	-	0,6,6	-	-	-		
86	OHX	n9	101	-	0,6,6	-	-	-		
86	OHX	5	3855	-	0,6,6	-	-	-		
86	OHX	5	3927	-	0,6,6	-	-	-		
86	OHX	5	3989	-	0,6,6	-	-	-		
86	OHX	2	2072	-	0,6,6	-	-	-		
86	OHX	1	4032	-	0,6,6	-	-	-		
86	OHX	6	2058	-	0,6,6	-	-	-		
86	OHX	6	2031	-	0,6,6	-	-	-		
86	OHX	5	4059	-	0,6,6	-	-	-		
86	OHX	6	2128	-	0,6,6	-	-	-		
86	OHX	5	4147	-	0,6,6	-	-	-		
86	OHX	1	3815	-	0,6,6	-	-	-		
86	OHX	5	4050	-	0,6,6	-	-	-		
86	OHX	2	2011	-	0,6,6	-	-	-		
86	OHX	1	4057	-	0,6,6	-	-	-		
86	OHX	1	3962	-	0,6,6	-	-	-		
86	OHX	6	2100	-	0,6,6	-	-	-		
86	OHX	5	4087	-	0,6,6	-	-	-		
86	OHX	1	3791	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4018	-	0,6,6	-	-	-		
86	OHX	6	2152	-	0,6,6	-	-	-		
86	OHX	2	2082	-	0,6,6	-	-	-		
86	OHX	4	226	-	0,6,6	-	-	-		
86	OHX	5	3821	-	0,6,6	-	-	-		
86	OHX	1	3996	-	0,6,6	-	-	-		
86	OHX	1	3766	-	0,6,6	-	-	-		
86	OHX	2	2110	-	0,6,6	-	-	-		
86	OHX	6	2077	-	0,6,6	-	-	-		
86	OHX	1	3953	-	0,6,6	-	-	-		
86	OHX	1	3885	-	0,6,6	-	-	-		
86	OHX	6	2113	-	0,6,6	-	-	-		
86	OHX	1	3955	-	0,6,6	-	-	-		
86	OHX	1	3933	-	0,6,6	-	-	-		
86	OHX	sR	401	-	0,6,6	-	-	-		
86	OHX	1	3782	-	0,6,6	-	-	-		
86	OHX	2	2059	-	0,6,6	-	-	-		
86	OHX	5	3831	-	0,6,6	-	-	-		
86	OHX	7	221	-	0,6,6	-	-	-		
86	OHX	1	3835	-	0,6,6	-	-	-		
86	OHX	5	3846	-	0,6,6	-	-	-		
86	OHX	5	3903	-	0,6,6	-	-	-		
86	OHX	1	4109	-	0,6,6	-	-	-		
86	OHX	5	4166	-	0,6,6	-	-	-		
86	OHX	1	3798	-	0,6,6	-	-	-		
86	OHX	6	2025	-	0,6,6	-	-	-		
86	OHX	O1	201	-	0,6,6	-	-	-		
86	OHX	m0	303	-	0,6,6	-	-	-		
86	OHX	5	4069	-	0,6,6	-	-	-		
86	OHX	1	3874	-	0,6,6	-	-	-		
86	OHX	5	3837	-	0,6,6	-	-	-		
86	OHX	6	2093	-	0,6,6	-	-	-		
86	OHX	5	4128	-	0,6,6	-	-	-		
86	OHX	5	3883	-	0,6,6	-	-	-		
86	OHX	1	3938	-	0,6,6	-	-	-		
86	OHX	8	223	-	0,6,6	-	-	-		
86	OHX	5	3975	-	0,6,6	-	-	-		
86	OHX	2	2115	-	0,6,6	-	-	-		
86	OHX	5	3981	-	0,6,6	-	-	-		
86	OHX	5	4082	-	0,6,6	-	-	-		
86	OHX	5	4157	-	0,6,6	-	-	-		
86	OHX	1	3849	-	0,6,6	-	-	-		
86	OHX	1	3998	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3905	-	0,6,6	-	-	-	-	-
86	OHX	6	2163	-	0,6,6	-	-	-	-	-
86	OHX	5	4151	-	0,6,6	-	-	-	-	-
86	OHX	6	2035	-	0,6,6	-	-	-	-	-
86	OHX	2	2064	-	0,6,6	-	-	-	-	-
86	OHX	6	2081	-	0,6,6	-	-	-	-	-
86	OHX	1	3864	-	0,6,6	-	-	-	-	-
86	OHX	5	3873	-	0,6,6	-	-	-	-	-
86	OHX	6	2127	-	0,6,6	-	-	-	-	-
86	OHX	1	3880	-	0,6,6	-	-	-	-	-
86	OHX	Q2	503	-	0,6,6	-	-	-	-	-
86	OHX	5	4115	-	0,6,6	-	-	-	-	-
86	OHX	5	3817	-	0,6,6	-	-	-	-	-
86	OHX	5	4071	-	0,6,6	-	-	-	-	-
86	OHX	6	2147	-	0,6,6	-	-	-	-	-
86	OHX	5	4154	-	0,6,6	-	-	-	-	-
86	OHX	2	1992	-	0,6,6	-	-	-	-	-
86	OHX	5	3829	-	0,6,6	-	-	-	-	-
86	OHX	5	4160	-	0,6,6	-	-	-	-	-
86	OHX	1	3931	-	0,6,6	-	-	-	-	-
86	OHX	5	4131	-	0,6,6	-	-	-	-	-
86	OHX	1	3783	-	0,6,6	-	-	-	-	-
86	OHX	6	2179	-	0,6,6	-	-	-	-	-
86	OHX	5	3850	-	0,6,6	-	-	-	-	-
86	OHX	5	3972	-	0,6,6	-	-	-	-	-
86	OHX	5	4077	-	0,6,6	-	-	-	-	-
86	OHX	8	226	-	0,6,6	-	-	-	-	-
86	OHX	5	3967	-	0,6,6	-	-	-	-	-
86	OHX	5	3932	-	0,6,6	-	-	-	-	-
86	OHX	5	3856	-	0,6,6	-	-	-	-	-
86	OHX	1	4033	-	0,6,6	-	-	-	-	-
86	OHX	6	2120	-	0,6,6	-	-	-	-	-
86	OHX	6	2134	-	0,6,6	-	-	-	-	-
86	OHX	6	2136	-	0,6,6	-	-	-	-	-
86	OHX	1	3767	-	0,6,6	-	-	-	-	-
86	OHX	3	216	-	0,6,6	-	-	-	-	-
86	OHX	5	3914	-	0,6,6	-	-	-	-	-
86	OHX	2	2054	-	0,6,6	-	-	-	-	-
86	OHX	7	215	-	0,6,6	-	-	-	-	-
86	OHX	5	3859	-	0,6,6	-	-	-	-	-
86	OHX	1	3829	-	0,6,6	-	-	-	-	-
86	OHX	2	2061	-	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	c8	203	-	0,6,6	-	-	-		
86	OHX	5	4144	-	0,6,6	-	-	-		
86	OHX	8	214	-	0,6,6	-	-	-		
86	OHX	1	4026	-	0,6,6	-	-	-		
86	OHX	6	2115	-	0,6,6	-	-	-		
86	OHX	6	2049	-	0,6,6	-	-	-		
86	OHX	6	2133	-	0,6,6	-	-	-		
86	OHX	1	3802	-	0,6,6	-	-	-		
86	OHX	5	3860	-	0,6,6	-	-	-		
86	OHX	1	3832	-	0,6,6	-	-	-		
86	OHX	1	3856	-	0,6,6	-	-	-		
86	OHX	1	4103	-	0,6,6	-	-	-		
86	OHX	2	2149	-	0,6,6	-	-	-		
86	OHX	2	2123	-	0,6,6	-	-	-		
86	OHX	1	4015	-	0,6,6	-	-	-		
86	OHX	4	231	-	0,6,6	-	-	-		
86	OHX	5	4023	-	0,6,6	-	-	-		
86	OHX	2	2037	-	0,6,6	-	-	-		
86	OHX	6	2052	-	0,6,6	-	-	-		
86	OHX	4	227	-	0,6,6	-	-	-		
86	OHX	1	4065	-	0,6,6	-	-	-		
86	OHX	5	4094	-	0,6,6	-	-	-		
86	OHX	2	2046	-	0,6,6	-	-	-		
86	OHX	1	3859	-	0,6,6	-	-	-		
86	OHX	5	4119	-	0,6,6	-	-	-		
86	OHX	5	4122	-	0,6,6	-	-	-		
86	OHX	5	4105	-	0,6,6	-	-	-		
86	OHX	6	2042	-	0,6,6	-	-	-		
86	OHX	5	4114	-	0,6,6	-	-	-		
86	OHX	2	2077	-	0,6,6	-	-	-		
86	OHX	1	4041	-	0,6,6	-	-	-		
86	OHX	1	3952	-	0,6,6	-	-	-		
86	OHX	1	4052	-	0,6,6	-	-	-		
86	OHX	4	219	-	0,6,6	-	-	-		
88	SPS	5	3403	-	20,23,23	3.38	10 (50%)	18,30,30	3.11	10 (55%)
86	OHX	6	2056	-	0,6,6	-	-	-		
86	OHX	1	4055	-	0,6,6	-	-	-		
86	OHX	6	2154	-	0,6,6	-	-	-		
86	OHX	1	3810	-	0,6,6	-	-	-		
86	OHX	2	2067	-	0,6,6	-	-	-		
86	OHX	2	2117	-	0,6,6	-	-	-		
86	OHX	6	2063	-	0,6,6	-	-	-		
86	OHX	6	2157	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2008	-	0,6,6	-	-	-		
86	OHX	5	4106	-	0,6,6	-	-	-		
86	OHX	1	4039	-	0,6,6	-	-	-		
86	OHX	5	3843	-	0,6,6	-	-	-		
86	OHX	m8	201	-	0,6,6	-	-	-		
86	OHX	1	4088	-	0,6,6	-	-	-		
86	OHX	4	230	-	0,6,6	-	-	-		
86	OHX	4	225	-	0,6,6	-	-	-		
86	OHX	5	4061	-	0,6,6	-	-	-		
86	OHX	S1	301	-	0,6,6	-	-	-		
86	OHX	1	3951	-	0,6,6	-	-	-		
86	OHX	5	3946	-	0,6,6	-	-	-		
86	OHX	1	3902	-	0,6,6	-	-	-		
86	OHX	2	2093	-	0,6,6	-	-	-		
86	OHX	6	2140	-	0,6,6	-	-	-		
86	OHX	1	3875	-	0,6,6	-	-	-		
86	OHX	6	2167	-	0,6,6	-	-	-		
86	OHX	2	2044	-	0,6,6	-	-	-		
86	OHX	6	2014	-	0,6,6	-	-	-		
86	OHX	5	3988	-	0,6,6	-	-	-		
86	OHX	5	4049	-	0,6,6	-	-	-		
86	OHX	5	3943	-	0,6,6	-	-	-		
86	OHX	2	2023	-	0,6,6	-	-	-		
86	OHX	1	3803	-	0,6,6	-	-	-		
86	OHX	5	3866	-	0,6,6	-	-	-		
86	OHX	5	3947	-	0,6,6	-	-	-		
86	OHX	2	2066	-	0,6,6	-	-	-		
86	OHX	2	2114	-	0,6,6	-	-	-		
86	OHX	1	3878	-	0,6,6	-	-	-		
86	OHX	6	2103	-	0,6,6	-	-	-		
86	OHX	5	4141	-	0,6,6	-	-	-		
86	OHX	1	4035	-	0,6,6	-	-	-		
86	OHX	1	4009	-	0,6,6	-	-	-		
86	OHX	O3	201	-	0,6,6	-	-	-		
86	OHX	1	3945	-	0,6,6	-	-	-		
86	OHX	1	3863	-	0,6,6	-	-	-		
86	OHX	m6	201	-	0,6,6	-	-	-		
86	OHX	1	3993	-	0,6,6	-	-	-		
86	OHX	1	3973	-	0,6,6	-	-	-		
86	OHX	5	3953	-	0,6,6	-	-	-		
86	OHX	1	3936	-	0,6,6	-	-	-		
86	OHX	5	3841	-	0,6,6	-	-	-		
86	OHX	2	2071	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3764	-	0,6,6	-	-	-	-	-
86	OHX	5	4024	-	0,6,6	-	-	-	-	-
86	OHX	5	3822	-	0,6,6	-	-	-	-	-
86	OHX	5	3838	-	0,6,6	-	-	-	-	-
86	OHX	1	4051	-	0,6,6	-	-	-	-	-
86	OHX	8	221	-	0,6,6	-	-	-	-	-
86	OHX	1	3768	-	0,6,6	-	-	-	-	-
86	OHX	6	2074	-	0,6,6	-	-	-	-	-
86	OHX	m7	204	-	0,6,6	-	-	-	-	-
86	OHX	2	2150	-	0,6,6	-	-	-	-	-
86	OHX	5	3949	-	0,6,6	-	-	-	-	-
86	OHX	2	2105	-	0,6,6	-	-	-	-	-
86	OHX	5	4063	-	0,6,6	-	-	-	-	-
86	OHX	SR	401	-	0,6,6	-	-	-	-	-
86	OHX	3	215	-	0,6,6	-	-	-	-	-
86	OHX	1	4020	-	0,6,6	-	-	-	-	-
86	OHX	S6	301	-	0,6,6	-	-	-	-	-
86	OHX	2	2012	-	0,6,6	-	-	-	-	-
86	OHX	6	2024	-	0,6,6	-	-	-	-	-
86	OHX	6	2121	-	0,6,6	-	-	-	-	-
86	OHX	5	3839	-	0,6,6	-	-	-	-	-
86	OHX	6	2089	-	0,6,6	-	-	-	-	-
86	OHX	15	303	-	0,6,6	-	-	-	-	-
86	OHX	1	4084	-	0,6,6	-	-	-	-	-
86	OHX	6	2160	-	0,6,6	-	-	-	-	-
86	OHX	2	2108	-	0,6,6	-	-	-	-	-
86	OHX	1	4038	-	0,6,6	-	-	-	-	-
86	OHX	3	212	-	0,6,6	-	-	-	-	-
86	OHX	1	4028	-	0,6,6	-	-	-	-	-
86	OHX	2	2013	-	0,6,6	-	-	-	-	-
86	OHX	7	224	-	0,6,6	-	-	-	-	-
86	OHX	6	2034	-	0,6,6	-	-	-	-	-
86	OHX	5	3830	-	0,6,6	-	-	-	-	-
86	OHX	5	3994	-	0,6,6	-	-	-	-	-
86	OHX	5	3891	-	0,6,6	-	-	-	-	-
86	OHX	5	3966	-	0,6,6	-	-	-	-	-
86	OHX	1	4001	-	0,6,6	-	-	-	-	-
86	OHX	5	3955	36	0,6,6	-	-	-	-	-
86	OHX	6	2126	-	0,6,6	-	-	-	-	-
86	OHX	5	4098	-	0,6,6	-	-	-	-	-
86	OHX	1	3825	-	0,6,6	-	-	-	-	-
86	OHX	6	2086	-	0,6,6	-	-	-	-	-
86	OHX	1	3883	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3899	-	0,6,6	-	-	-		
86	OHX	2	2034	-	0,6,6	-	-	-		
86	OHX	5	3861	-	0,6,6	-	-	-		
86	OHX	5	3918	-	0,6,6	-	-	-		
86	OHX	6	2028	-	0,6,6	-	-	-		
86	OHX	1	3796	-	0,6,6	-	-	-		
86	OHX	2	2014	-	0,6,6	-	-	-		
86	OHX	5	4163	-	0,6,6	-	-	-		
86	OHX	5	4161	-	0,6,6	-	-	-		
86	OHX	5	3980	-	0,6,6	-	-	-		
86	OHX	1	4100	-	0,6,6	-	-	-		
86	OHX	2	2146	-	0,6,6	-	-	-		
86	OHX	5	4005	-	0,6,6	-	-	-		
86	OHX	5	3869	-	0,6,6	-	-	-		
86	OHX	2	2128	-	0,6,6	-	-	-		
86	OHX	1	4002	-	0,6,6	-	-	-		
86	OHX	5	4064	-	0,6,6	-	-	-		
86	OHX	5	4104	-	0,6,6	-	-	-		
86	OHX	5	4136	-	0,6,6	-	-	-		
86	OHX	7	216	-	0,6,6	-	-	-		
86	OHX	4	222	-	0,6,6	-	-	-		
86	OHX	1	3837	-	0,6,6	-	-	-		
86	OHX	6	2027	-	0,6,6	-	-	-		
86	OHX	1	4078	-	0,6,6	-	-	-		
86	OHX	1	4081	-	0,6,6	-	-	-		
86	OHX	6	2181	-	0,6,6	-	-	-		
86	OHX	5	4113	-	0,6,6	-	-	-		
86	OHX	2	2028	-	0,6,6	-	-	-		
86	OHX	4	218	-	0,6,6	-	-	-		
86	OHX	d9	102	-	0,6,6	-	-	-		
86	OHX	1	3943	-	0,6,6	-	-	-		
86	OHX	5	4006	-	0,6,6	-	-	-		
86	OHX	1	4082	-	0,6,6	-	-	-		
86	OHX	6	2182	-	0,6,6	-	-	-		
86	OHX	6	2168	-	0,6,6	-	-	-		
86	OHX	5	4088	-	0,6,6	-	-	-		
86	OHX	6	2038	-	0,6,6	-	-	-		
86	OHX	1	3865	-	0,6,6	-	-	-		
86	OHX	6	2098	-	0,6,6	-	-	-		
86	OHX	8	230	-	0,6,6	-	-	-		
86	OHX	6	2125	-	0,6,6	-	-	-		
86	OHX	1	4099	-	0,6,6	-	-	-		
86	OHX	1	4073	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3875	-	0,6,6	-	-	-		
86	OHX	6	2172	-	0,6,6	-	-	-		
86	OHX	1	3805	-	0,6,6	-	-	-		
86	OHX	2	2104	-	0,6,6	-	-	-		
86	OHX	5	4072	-	0,6,6	-	-	-		
86	OHX	1	3845	-	0,6,6	-	-	-		
86	OHX	6	2135	-	0,6,6	-	-	-		
86	OHX	1	3817	-	0,6,6	-	-	-		
86	OHX	2	2091	-	0,6,6	-	-	-		
86	OHX	6	2169	-	0,6,6	-	-	-		
86	OHX	8	219	-	0,6,6	-	-	-		
86	OHX	6	2075	-	0,6,6	-	-	-		
86	OHX	5	3926	-	0,6,6	-	-	-		
86	OHX	2	2080	-	0,6,6	-	-	-		
86	OHX	5	3923	-	0,6,6	-	-	-		
86	OHX	2	2125	-	0,6,6	-	-	-		
86	OHX	5	4041	-	0,6,6	-	-	-		
89	PRO	C	101	89,84	5,7,8	0.48	0	7,8,10	1.39	1 (14%)
86	OHX	2	2021	-	0,6,6	-	-	-		
86	OHX	1	3967	-	0,6,6	-	-	-		
86	OHX	2	2006	-	0,6,6	-	-	-		
86	OHX	2	2007	-	0,6,6	-	-	-		
86	OHX	1	3840	-	0,6,6	-	-	-		
86	OHX	5	3979	-	0,6,6	-	-	-		
86	OHX	2	2074	-	0,6,6	-	-	-		
86	OHX	3	211	-	0,6,6	-	-	-		
86	OHX	2	1993	-	0,6,6	-	-	-		
86	OHX	2	2050	-	0,6,6	-	-	-		
86	OHX	2	2133	-	0,6,6	-	-	-		
86	OHX	2	2099	-	0,6,6	-	-	-		
86	OHX	1	3813	-	0,6,6	-	-	-		
86	OHX	1	4097	-	0,6,6	-	-	-		
86	OHX	2	2005	-	0,6,6	-	-	-		
86	OHX	6	2095	-	0,6,6	-	-	-		
86	OHX	5	3851	-	0,6,6	-	-	-		
86	OHX	5	4040	-	0,6,6	-	-	-		
86	OHX	5	4102	-	0,6,6	-	-	-		
86	OHX	5	4117	-	0,6,6	-	-	-		
86	OHX	c5	202	17	0,6,6	-	-	-		
86	OHX	6	2138	-	0,6,6	-	-	-		
86	OHX	6	2173	-	0,6,6	-	-	-		
86	OHX	5	3920	-	0,6,6	-	-	-		
86	OHX	1	3950	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2096	-	0,6,6	-	-	-		
86	OHX	1	3814	-	0,6,6	-	-	-		
86	OHX	6	2059	-	0,6,6	-	-	-		
86	OHX	5	4025	-	0,6,6	-	-	-		
86	OHX	1	3836	-	0,6,6	-	-	-		
86	OHX	1	4048	-	0,6,6	-	-	-		
86	OHX	1	3809	-	0,6,6	-	-	-		
86	OHX	5	3832	-	0,6,6	-	-	-		
86	OHX	2	2068	-	0,6,6	-	-	-		
86	OHX	5	3913	-	0,6,6	-	-	-		
86	OHX	5	4101	-	0,6,6	-	-	-		
86	OHX	m5	305	-	0,6,6	-	-	-		
86	OHX	5	3961	-	0,6,6	-	-	-		
86	OHX	5	3922	-	0,6,6	-	-	-		
86	OHX	5	3858	-	0,6,6	-	-	-		
86	OHX	1	3811	-	0,6,6	-	-	-		
86	OHX	1	3769	-	0,6,6	-	-	-		
86	OHX	5	3887	-	0,6,6	-	-	-		
86	OHX	1	4110	-	0,6,6	-	-	-		
86	OHX	2	2047	-	0,6,6	-	-	-		
86	OHX	4	216	-	0,6,6	-	-	-		
86	OHX	6	2109	-	0,6,6	-	-	-		
86	OHX	6	2069	-	0,6,6	-	-	-		
86	OHX	1	3957	-	0,6,6	-	-	-		
86	OHX	5	3888	-	0,6,6	-	-	-		
86	OHX	6	2048	-	0,6,6	-	-	-		
86	OHX	5	3890	-	0,6,6	-	-	-		
86	OHX	6	2171	-	0,6,6	-	-	-		
86	OHX	5	4004	-	0,6,6	-	-	-		
86	OHX	5	4091	-	0,6,6	-	-	-		
86	OHX	8	217	-	0,6,6	-	-	-		
86	OHX	2	2116	-	0,6,6	-	-	-		
86	OHX	2	2051	-	0,6,6	-	-	-		
86	OHX	5	3825	-	0,6,6	-	-	-		
86	OHX	1	3958	-	0,6,6	-	-	-		
86	OHX	1	3860	-	0,6,6	-	-	-		
86	OHX	5	4029	-	0,6,6	-	-	-		
86	OHX	5	4168	-	0,6,6	-	-	-		
86	OHX	1	3772	-	0,6,6	-	-	-		
86	OHX	5	4139	-	0,6,6	-	-	-		
86	OHX	6	2021	-	0,6,6	-	-	-		
86	OHX	5	4044	-	0,6,6	-	-	-		
86	OHX	1	3846	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3887	-	0,6,6	-	-	-		
86	OHX	1	4105	-	0,6,6	-	-	-		
86	OHX	8	212	-	0,6,6	-	-	-		
86	OHX	5	3934	-	0,6,6	-	-	-		
86	OHX	5	4028	-	0,6,6	-	-	-		
86	OHX	5	4081	-	0,6,6	-	-	-		
86	OHX	1	3804	-	0,6,6	-	-	-		
86	OHX	1	3940	-	0,6,6	-	-	-		
86	OHX	2	2102	-	0,6,6	-	-	-		
86	OHX	6	2174	-	0,6,6	-	-	-		
86	OHX	2	2130	-	0,6,6	-	-	-		
86	OHX	S9	201	-	0,6,6	-	-	-		
86	OHX	1	3792	-	0,6,6	-	-	-		
86	OHX	1	4003	-	0,6,6	-	-	-		
86	OHX	1	3828	-	0,6,6	-	-	-		
86	OHX	5	4100	-	0,6,6	-	-	-		
86	OHX	6	2166	-	0,6,6	-	-	-		
86	OHX	2	2112	-	0,6,6	-	-	-		
86	OHX	1	4031	-	0,6,6	-	-	-		
86	OHX	5	3990	-	0,6,6	-	-	-		
86	OHX	5	4172	-	0,6,6	-	-	-		
86	OHX	5	3944	-	0,6,6	-	-	-		
86	OHX	6	2030	-	0,6,6	-	-	-		
86	OHX	1	3935	-	0,6,6	-	-	-		
86	OHX	6	2079	-	0,6,6	-	-	-		
86	OHX	2	2075	-	0,6,6	-	-	-		
86	OHX	5	4110	-	0,6,6	-	-	-		
86	OHX	1	3841	-	0,6,6	-	-	-		
86	OHX	1	3934	-	0,6,6	-	-	-		
86	OHX	1	3790	-	0,6,6	-	-	-		
86	OHX	1	4108	-	0,6,6	-	-	-		
86	OHX	5	4080	-	0,6,6	-	-	-		
86	OHX	19	201	-	0,6,6	-	-	-		
86	OHX	1	4044	-	0,6,6	-	-	-		
86	OHX	5	4086	-	0,6,6	-	-	-		
86	OHX	1	4061	-	0,6,6	-	-	-		
86	OHX	1	4093	-	0,6,6	-	-	-		
86	OHX	6	2012	-	0,6,6	-	-	-		
86	OHX	1	3816	-	0,6,6	-	-	-		
86	OHX	1	3960	-	0,6,6	-	-	-		
86	OHX	5	3937	-	0,6,6	-	-	-		
86	OHX	1	3984	-	0,6,6	-	-	-		
86	OHX	5	4015	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	n3	202	-	0,6,6	-	-	-		
86	OHX	1	3850	-	0,6,6	-	-	-		
86	OHX	2	2009	-	0,6,6	-	-	-		
86	OHX	5	3974	-	0,6,6	-	-	-		
86	OHX	2	2118	-	0,6,6	-	-	-		
86	OHX	2	2029	-	0,6,6	-	-	-		
86	OHX	5	3992	-	0,6,6	-	-	-		
86	OHX	6	2124	-	0,6,6	-	-	-		
86	OHX	2	2045	-	0,6,6	-	-	-		
86	OHX	2	2076	-	0,6,6	-	-	-		
86	OHX	5	3995	-	0,6,6	-	-	-		
86	OHX	5	4019	-	0,6,6	-	-	-		
86	OHX	1	3861	-	0,6,6	-	-	-		
86	OHX	2	2070	-	0,6,6	-	-	-		
86	OHX	6	2106	-	0,6,6	-	-	-		
86	OHX	6	2102	-	0,6,6	-	-	-		
86	OHX	1	3852	-	0,6,6	-	-	-		
86	OHX	1	3830	-	0,6,6	-	-	-		
86	OHX	5	4146	-	0,6,6	-	-	-		
86	OHX	5	4000	-	0,6,6	-	-	-		
86	OHX	M0	304	-	0,6,6	-	-	-		
86	OHX	2	1991	-	0,6,6	-	-	-		
86	OHX	1	3855	-	0,6,6	-	-	-		
86	OHX	1	3980	-	0,6,6	-	-	-		
86	OHX	5	4099	-	0,6,6	-	-	-		
86	OHX	6	2132	-	0,6,6	-	-	-		
86	OHX	d4	201	-	0,6,6	-	-	-		
86	OHX	6	2047	-	0,6,6	-	-	-		
86	OHX	8	231	-	0,6,6	-	-	-		
86	OHX	M0	303	-	0,6,6	-	-	-		
86	OHX	2	2049	-	0,6,6	-	-	-		
86	OHX	1	3891	-	0,6,6	-	-	-		
86	OHX	1	3966	-	0,6,6	-	-	-		
86	OHX	5	3845	-	0,6,6	-	-	-		
86	OHX	5	3905	-	0,6,6	-	-	-		
86	OHX	8	224	-	0,6,6	-	-	-		
86	OHX	5	4046	-	0,6,6	-	-	-		
86	OHX	1	3886	-	0,6,6	-	-	-		
86	OHX	6	2057	-	0,6,6	-	-	-		
86	OHX	6	2146	-	0,6,6	-	-	-		
86	OHX	1	3976	-	0,6,6	-	-	-		
86	OHX	2	2052	-	0,6,6	-	-	-		
86	OHX	1	4019	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	4074	-	0,6,6	-	-	-		
86	OHX	6	2040	-	0,6,6	-	-	-		
86	OHX	1	4058	-	0,6,6	-	-	-		
86	OHX	1	3895	-	0,6,6	-	-	-		
86	OHX	L3	403	-	0,6,6	-	-	-		
86	OHX	2	2135	-	0,6,6	-	-	-		
86	OHX	1	3956	-	0,6,6	-	-	-		
86	OHX	C5	201	17	0,6,6	-	-	-		
86	OHX	6	2026	-	0,6,6	-	-	-		
86	OHX	6	2131	-	0,6,6	-	-	-		
86	OHX	2	2094	-	0,6,6	-	-	-		
86	OHX	5	4068	-	0,6,6	-	-	-		
86	OHX	5	3824	-	0,6,6	-	-	-		
86	OHX	6	2020	-	0,6,6	-	-	-		
86	OHX	1	3866	-	0,6,6	-	-	-		
86	OHX	1	4064	-	0,6,6	-	-	-		
86	OHX	5	3919	-	0,6,6	-	-	-		
86	OHX	5	3877	-	0,6,6	-	-	-		
86	OHX	5	4043	-	0,6,6	-	-	-		
86	OHX	6	2176	-	0,6,6	-	-	-		
86	OHX	1	3978	-	0,6,6	-	-	-		
86	OHX	5	4156	-	0,6,6	-	-	-		
86	OHX	1	3898	-	0,6,6	-	-	-		
86	OHX	5	4134	-	0,6,6	-	-	-		
86	OHX	6	2180	-	0,6,6	-	-	-		
86	OHX	1	3926	-	0,6,6	-	-	-		
86	OHX	2	2097	-	0,6,6	-	-	-		
86	OHX	6	2032	-	0,6,6	-	-	-		
86	OHX	6	2053	-	0,6,6	-	-	-		
86	OHX	5	3986	-	0,6,6	-	-	-		
86	OHX	2	2119	-	0,6,6	-	-	-		
86	OHX	1	4083	-	0,6,6	-	-	-		
86	OHX	5	4027	-	0,6,6	-	-	-		
86	OHX	1	3979	-	0,6,6	-	-	-		
86	OHX	5	4158	-	0,6,6	-	-	-		
86	OHX	1	4024	-	0,6,6	-	-	-		
86	OHX	6	2091	-	0,6,6	-	-	-		
86	OHX	1	3884	-	0,6,6	-	-	-		
86	OHX	1	3787	-	0,6,6	-	-	-		
86	OHX	2	1995	-	0,6,6	-	-	-		
86	OHX	5	4092	-	0,6,6	-	-	-		
86	OHX	2	2141	-	0,6,6	-	-	-		
86	OHX	2	2056	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3797	-	0,6,6	-	-	-		
86	OHX	1	3928	-	0,6,6	-	-	-		
86	OHX	1	3990	-	0,6,6	-	-	-		
86	OHX	5	3886	-	0,6,6	-	-	-		
86	OHX	15	302	-	0,6,6	-	-	-		
86	OHX	5	3940	-	0,6,6	-	-	-		
86	OHX	1	3923	-	0,6,6	-	-	-		
86	OHX	5	4103	-	0,6,6	-	-	-		
86	OHX	5	3965	-	0,6,6	-	-	-		
86	OHX	5	3827	-	0,6,6	-	-	-		
86	OHX	1	3939	-	0,6,6	-	-	-		
86	OHX	1	3779	-	0,6,6	-	-	-		
86	OHX	1	3823	-	0,6,6	-	-	-		
86	OHX	1	3924	-	0,6,6	-	-	-		
86	OHX	5	3818	-	0,6,6	-	-	-		
86	OHX	5	3952	-	0,6,6	-	-	-		
86	OHX	2	2031	-	0,6,6	-	-	-		
86	OHX	4	228	-	0,6,6	-	-	-		
86	OHX	6	2105	-	0,6,6	-	-	-		
86	OHX	5	3823	-	0,6,6	-	-	-		
86	OHX	2	2085	-	0,6,6	-	-	-		
86	OHX	1	4080	-	0,6,6	-	-	-		
86	OHX	6	2142	-	0,6,6	-	-	-		
86	OHX	1	4018	-	0,6,6	-	-	-		
86	OHX	2	2109	-	0,6,6	-	-	-		
86	OHX	6	2143	-	0,6,6	-	-	-		
86	OHX	1	3869	-	0,6,6	-	-	-		
86	OHX	2	2069	-	0,6,6	-	-	-		
86	OHX	5	4067	-	0,6,6	-	-	-		
86	OHX	1	4040	-	0,6,6	-	-	-		
86	OHX	2	2030	-	0,6,6	-	-	-		
86	OHX	5	4090	-	0,6,6	-	-	-		
86	OHX	1	4059	-	0,6,6	-	-	-		
86	OHX	6	2156	-	0,6,6	-	-	-		
86	OHX	1	3858	-	0,6,6	-	-	-		
86	OHX	1	3971	-	0,6,6	-	-	-		
86	OHX	5	3960	-	0,6,6	-	-	-		
86	OHX	2	2001	-	0,6,6	-	-	-		
86	OHX	1	4098	-	0,6,6	-	-	-		
86	OHX	6	2064	-	0,6,6	-	-	-		
86	OHX	2	2137	-	0,6,6	-	-	-		
86	OHX	M9	202	-	0,6,6	-	-	-		
86	OHX	5	3872	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3897	-	0,6,6	-	-	-		
86	OHX	6	2073	-	0,6,6	-	-	-		
86	OHX	5	4014	-	0,6,6	-	-	-		
86	OHX	M5	303	-	0,6,6	-	-	-		
86	OHX	1	4086	-	0,6,6	-	-	-		
86	OHX	5	4076	-	0,6,6	-	-	-		
86	OHX	m1	201	-	0,6,6	-	-	-		
86	OHX	5	4126	-	0,6,6	-	-	-		
86	OHX	5	3969	-	0,6,6	-	-	-		
86	OHX	2	2000	-	0,6,6	-	-	-		
86	OHX	1	4037	-	0,6,6	-	-	-		
86	OHX	5	3942	-	0,6,6	-	-	-		
86	OHX	5	3963	-	0,6,6	-	-	-		
86	OHX	5	3985	-	0,6,6	-	-	-		
86	OHX	2	2004	-	0,6,6	-	-	-		
86	OHX	1	3999	-	0,6,6	-	-	-		
86	OHX	7	223	-	0,6,6	-	-	-		
86	OHX	1	4111	-	0,6,6	-	-	-		
86	OHX	5	3844	-	0,6,6	-	-	-		
86	OHX	6	2178	-	0,6,6	-	-	-		
86	OHX	1	4023	-	0,6,6	-	-	-		
86	OHX	1	3991	-	0,6,6	-	-	-		
86	OHX	6	2111	-	0,6,6	-	-	-		
86	OHX	5	3867	-	0,6,6	-	-	-		
86	OHX	6	2129	-	0,6,6	-	-	-		
86	OHX	2	2101	-	0,6,6	-	-	-		
86	OHX	6	2110	-	0,6,6	-	-	-		
86	OHX	5	3983	-	0,6,6	-	-	-		
86	OHX	1	3773	-	0,6,6	-	-	-		
86	OHX	1	3774	-	0,6,6	-	-	-		
86	OHX	1	3827	-	0,6,6	-	-	-		
86	OHX	1	3929	-	0,6,6	-	-	-		
86	OHX	1	3942	-	0,6,6	-	-	-		
86	OHX	2	2079	-	0,6,6	-	-	-		
86	OHX	6	2107	-	0,6,6	-	-	-		
86	OHX	5	4036	-	0,6,6	-	-	-		
86	OHX	1	3975	-	0,6,6	-	-	-		
86	OHX	1	4029	-	0,6,6	-	-	-		
86	OHX	5	3865	-	0,6,6	-	-	-		
86	OHX	5	4135	-	0,6,6	-	-	-		
86	OHX	5	3893	-	0,6,6	-	-	-		
86	OHX	1	3870	-	0,6,6	-	-	-		
86	OHX	6	2065	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2129	-	0,6,6	-	-	-		
86	OHX	5	4079	-	0,6,6	-	-	-		
86	OHX	1	3915	-	0,6,6	-	-	-		
86	OHX	1	4054	-	0,6,6	-	-	-		
86	OHX	5	3819	-	0,6,6	-	-	-		
86	OHX	1	3808	-	0,6,6	-	-	-		
86	OHX	1	4089	-	0,6,6	-	-	-		
86	OHX	6	2055	-	0,6,6	-	-	-		
86	OHX	5	3828	-	0,6,6	-	-	-		
86	OHX	2	2089	-	0,6,6	-	-	-		
86	OHX	1	3912	-	0,6,6	-	-	-		
86	OHX	2	2124	-	0,6,6	-	-	-		
86	OHX	8	213	-	0,6,6	-	-	-		
86	OHX	1	4077	-	0,6,6	-	-	-		
86	OHX	5	3910	-	0,6,6	-	-	-		
86	OHX	1	4107	-	0,6,6	-	-	-		
86	OHX	6	2083	-	0,6,6	-	-	-		
86	OHX	1	4092	-	0,6,6	-	-	-		
86	OHX	5	3941	-	0,6,6	-	-	-		
86	OHX	5	3826	-	0,6,6	-	-	-		
86	OHX	1	4021	-	0,6,6	-	-	-		
86	OHX	6	2067	1	0,6,6	-	-	-		
86	OHX	5	4129	-	0,6,6	-	-	-		
86	OHX	6	2159	-	0,6,6	-	-	-		
86	OHX	2	2132	-	0,6,6	-	-	-		
86	OHX	5	3954	-	0,6,6	-	-	-		
86	OHX	1	3888	-	0,6,6	-	-	-		
86	OHX	1	4007	-	0,6,6	-	-	-		
86	OHX	1	3881	-	0,6,6	-	-	-		
86	OHX	6	2175	-	0,6,6	-	-	-		
86	OHX	5	3871	-	0,6,6	-	-	-		
86	OHX	5	4042	-	0,6,6	-	-	-		
86	OHX	14	403	-	0,6,6	-	-	-		
86	OHX	1	3807	-	0,6,6	-	-	-		
86	OHX	1	3937	-	0,6,6	-	-	-		
86	OHX	2	1998	-	0,6,6	-	-	-		
86	OHX	5	4153	-	0,6,6	-	-	-		
86	OHX	6	2033	-	0,6,6	-	-	-		
86	OHX	4	220	-	0,6,6	-	-	-		
86	OHX	1	3775	-	0,6,6	-	-	-		
86	OHX	2	2145	-	0,6,6	-	-	-		
86	OHX	5	3840	-	0,6,6	-	-	-		
86	OHX	6	2114	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4008	-	0,6,6	-	-	-		
86	OHX	2	2024	-	0,6,6	-	-	-		
86	OHX	5	3916	-	0,6,6	-	-	-		
86	OHX	2	2017	-	0,6,6	-	-	-		
86	OHX	1	3910	-	0,6,6	-	-	-		
86	OHX	5	4022	-	0,6,6	-	-	-		
86	OHX	1	3833	-	0,6,6	-	-	-		
86	OHX	6	2039	-	0,6,6	-	-	-		
86	OHX	1	3785	-	0,6,6	-	-	-		
86	OHX	3	209	-	0,6,6	-	-	-		
86	OHX	6	2165	-	0,6,6	-	-	-		
86	OHX	5	4123	-	0,6,6	-	-	-		
86	OHX	1	3822	-	0,6,6	-	-	-		
86	OHX	5	4033	-	0,6,6	-	-	-		
86	OHX	2	1999	-	0,6,6	-	-	-		
86	OHX	6	2019	-	0,6,6	-	-	-		
86	OHX	2	2020	-	0,6,6	-	-	-		
86	OHX	6	2090	-	0,6,6	-	-	-		
86	OHX	4	217	-	0,6,6	-	-	-		
86	OHX	C8	201	-	0,6,6	-	-	-		
86	OHX	5	4062	-	0,6,6	-	-	-		
86	OHX	1	3819	-	0,6,6	-	-	-		
86	OHX	5	4130	-	0,6,6	-	-	-		
86	OHX	5	4162	-	0,6,6	-	-	-		
86	OHX	2	2151	-	0,6,6	-	-	-		
86	OHX	1	4000	-	0,6,6	-	-	-		
86	OHX	5	4020	-	0,6,6	-	-	-		
86	OHX	7	220	-	0,6,6	-	-	-		
86	OHX	o6	201	-	0,6,6	-	-	-		
86	OHX	5	4155	-	0,6,6	-	-	-		
86	OHX	6	2104	-	0,6,6	-	-	-		
86	OHX	2	2032	-	0,6,6	-	-	-		
86	OHX	7	222	-	0,6,6	-	-	-		
86	OHX	1	3977	-	0,6,6	-	-	-		
86	OHX	2	2053	-	0,6,6	-	-	-		
86	OHX	1	3959	-	0,6,6	-	-	-		
86	OHX	1	4043	-	0,6,6	-	-	-		
86	OHX	1	3921	-	0,6,6	-	-	-		
86	OHX	1	3981	-	0,6,6	-	-	-		
86	OHX	1	3985	-	0,6,6	-	-	-		
86	OHX	1	4025	-	0,6,6	-	-	-		
86	OHX	7	218	-	0,6,6	-	-	-		
86	OHX	1	3784	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3964	-	0,6,6	-	-	-		
86	OHX	5	4149	-	0,6,6	-	-	-		
86	OHX	2	2147	-	0,6,6	-	-	-		
86	OHX	6	2046	-	0,6,6	-	-	-		
86	OHX	6	2150	-	0,6,6	-	-	-		
86	OHX	2	2111	-	0,6,6	-	-	-		
86	OHX	1	4056	-	0,6,6	-	-	-		
86	OHX	2	2078	-	0,6,6	-	-	-		
86	OHX	5	3948	-	0,6,6	-	-	-		
86	OHX	1	4068	-	0,6,6	-	-	-		
86	OHX	1	3994	-	0,6,6	-	-	-		
86	OHX	8	228	-	0,6,6	-	-	-		
86	OHX	2	2107	-	0,6,6	-	-	-		
86	OHX	2	2003	-	0,6,6	-	-	-		
86	OHX	1	3777	-	0,6,6	-	-	-		
86	OHX	1	3989	-	0,6,6	-	-	-		
86	OHX	6	2078	-	0,6,6	-	-	-		
86	OHX	5	3991	-	0,6,6	-	-	-		
86	OHX	5	4066	-	0,6,6	-	-	-		
86	OHX	5	3899	-	0,6,6	-	-	-		
86	OHX	5	4120	-	0,6,6	-	-	-		
86	OHX	5	3997	-	0,6,6	-	-	-		
86	OHX	1	3907	-	0,6,6	-	-	-		
86	OHX	5	3868	-	0,6,6	-	-	-		
86	OHX	5	3987	-	0,6,6	-	-	-		
86	OHX	2	1997	-	0,6,6	-	-	-		
86	OHX	5	4152	-	0,6,6	-	-	-		
86	OHX	1	3944	-	0,6,6	-	-	-		
86	OHX	1	4087	-	0,6,6	-	-	-		
86	OHX	c3	201	-	0,6,6	-	-	-		
86	OHX	2	2120	-	0,6,6	-	-	-		
86	OHX	2	2152	-	0,6,6	-	-	-		
86	OHX	1	4053	-	0,6,6	-	-	-		
86	OHX	6	2066	-	0,6,6	-	-	-		
86	OHX	1	3778	-	0,6,6	-	-	-		
86	OHX	6	2141	-	0,6,6	-	-	-		
86	OHX	1	3909	-	0,6,6	-	-	-		
86	OHX	C3	201	-	0,6,6	-	-	-		
86	OHX	5	4074	-	0,6,6	-	-	-		
86	OHX	5	4165	-	0,6,6	-	-	-		
86	OHX	1	3771	-	0,6,6	-	-	-		
86	OHX	6	2118	-	0,6,6	-	-	-		
86	OHX	5	3880	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3907	-	0,6,6	-	-	-		
86	OHX	m0	302	-	0,6,6	-	-	-		
86	OHX	1	3941	-	0,6,6	-	-	-		
86	OHX	5	3863	-	0,6,6	-	-	-		
86	OHX	5	4083	-	0,6,6	-	-	-		
86	OHX	1	4094	-	0,6,6	-	-	-		
86	OHX	4	224	-	0,6,6	-	-	-		
86	OHX	6	2070	-	0,6,6	-	-	-		
86	OHX	1	4034	-	0,6,6	-	-	-		
86	OHX	1	4036	-	0,6,6	-	-	-		
86	OHX	1	3854	-	0,6,6	-	-	-		
86	OHX	6	2116	-	0,6,6	-	-	-		
86	OHX	1	3831	-	0,6,6	-	-	-		
86	OHX	6	2177	-	0,6,6	-	-	-		
86	OHX	5	3945	-	0,6,6	-	-	-		
86	OHX	1	3903	-	0,6,6	-	-	-		
86	OHX	5	4009	-	0,6,6	-	-	-		
86	OHX	5	4138	-	0,6,6	-	-	-		
86	OHX	5	4171	-	0,6,6	-	-	-		
86	OHX	1	3824	-	0,6,6	-	-	-		
86	OHX	3	218	-	0,6,6	-	-	-		
86	OHX	1	3877	-	0,6,6	-	-	-		
86	OHX	1	4063	-	0,6,6	-	-	-		
86	OHX	1	3821	-	0,6,6	-	-	-		
86	OHX	6	2108	-	0,6,6	-	-	-		
86	OHX	5	3930	-	0,6,6	-	-	-		
86	OHX	6	2148	-	0,6,6	-	-	-		
86	OHX	1	3897	-	0,6,6	-	-	-		
86	OHX	1	3844	-	0,6,6	-	-	-		
86	OHX	1	3900	-	0,6,6	-	-	-		
86	OHX	1	4014	-	0,6,6	-	-	-		
86	OHX	2	2019	-	0,6,6	-	-	-		
86	OHX	1	4062	-	0,6,6	-	-	-		
86	OHX	6	2123	-	0,6,6	-	-	-		
86	OHX	5	4053	-	0,6,6	-	-	-		
86	OHX	1	4076	-	0,6,6	-	-	-		
86	OHX	5	4150	-	0,6,6	-	-	-		
86	OHX	5	3938	-	0,6,6	-	-	-		
86	OHX	2	2065	-	0,6,6	-	-	-		
86	OHX	1	3851	-	0,6,6	-	-	-		
86	OHX	2	2126	-	0,6,6	-	-	-		
86	OHX	1	3969	-	0,6,6	-	-	-		
86	OHX	1	4102	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2060	-	0,6,6	-	-	-		
86	OHX	5	3896	-	0,6,6	-	-	-		
86	OHX	2	2140	-	0,6,6	-	-	-		
86	OHX	1	3963	-	0,6,6	-	-	-		
86	OHX	6	2183	-	0,6,6	-	-	-		
86	OHX	6	2017	-	0,6,6	-	-	-		
86	OHX	2	2039	-	0,6,6	-	-	-		
86	OHX	2	2055	-	0,6,6	-	-	-		
86	OHX	2	2106	-	0,6,6	-	-	-		
86	OHX	1	3799	-	0,6,6	-	-	-		
86	OHX	5	4096	-	0,6,6	-	-	-		
86	OHX	3	210	-	0,6,6	-	-	-		
88	SPS	1	4113	85	20,23,23	3.43	11 (55%)	18,30,30	3.22	7 (38%)
86	OHX	1	3983	-	0,6,6	-	-	-		
86	OHX	1	3972	-	0,6,6	-	-	-		
86	OHX	5	3854	-	0,6,6	-	-	-		
86	OHX	o7	502	-	0,6,6	-	-	-		
86	OHX	2	2035	-	0,6,6	-	-	-		
86	OHX	4	232	-	0,6,6	-	-	-		
86	OHX	5	3881	-	0,6,6	-	-	-		
86	OHX	6	2151	-	0,6,6	-	-	-		
86	OHX	5	3982	-	0,6,6	-	-	-		
86	OHX	1	3986	-	0,6,6	-	-	-		
86	OHX	q2	203	-	0,6,6	-	-	-		
86	OHX	1	3893	-	0,6,6	-	-	-		
86	OHX	6	2041	-	0,6,6	-	-	-		
86	OHX	5	4030	-	0,6,6	-	-	-		
86	OHX	6	2044	-	0,6,6	-	-	-		
86	OHX	6	2015	-	0,6,6	-	-	-		
86	OHX	6	2092	-	0,6,6	-	-	-		
86	OHX	6	2097	-	0,6,6	-	-	-		
86	OHX	5	3911	-	0,6,6	-	-	-		
86	OHX	5	4038	-	0,6,6	-	-	-		
86	OHX	6	2062	-	0,6,6	-	-	-		
86	OHX	8	229	-	0,6,6	-	-	-		
86	OHX	3	214	-	0,6,6	-	-	-		
86	OHX	o3	202	-	0,6,6	-	-	-		
86	OHX	L5	301	-	0,6,6	-	-	-		
86	OHX	5	4142	-	0,6,6	-	-	-		
86	OHX	5	4078	-	0,6,6	-	-	-		
86	OHX	8	216	-	0,6,6	-	-	-		
86	OHX	1	3818	-	0,6,6	-	-	-		
86	OHX	1	3795	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	2	2063	-	0,6,6	-	-	-		
86	OHX	5	3908	-	0,6,6	-	-	-		
86	OHX	8	218	-	0,6,6	-	-	-		
86	OHX	5	3973	-	0,6,6	-	-	-		
86	OHX	1	4030	-	0,6,6	-	-	-		
86	OHX	6	2080	-	0,6,6	-	-	-		
86	OHX	1	3793	-	0,6,6	-	-	-		
86	OHX	1	3914	-	0,6,6	-	-	-		
86	OHX	6	2155	-	0,6,6	-	-	-		
86	OHX	6	2122	-	0,6,6	-	-	-		
86	OHX	5	3909	-	0,6,6	-	-	-		
86	OHX	1	3917	-	0,6,6	-	-	-		
86	OHX	6	2130	-	0,6,6	-	-	-		
86	OHX	5	4148	-	0,6,6	-	-	-		
86	OHX	8	222	-	0,6,6	-	-	-		
86	OHX	6	2051	-	0,6,6	-	-	-		
86	OHX	5	4143	-	0,6,6	-	-	-		
86	OHX	1	4090	-	0,6,6	-	-	-		
86	OHX	1	3801	-	0,6,6	-	-	-		
86	OHX	1	3776	-	0,6,6	-	-	-		
86	OHX	1	3904	-	0,6,6	-	-	-		
86	OHX	6	2149	-	0,6,6	-	-	-		
86	OHX	1	3871	-	0,6,6	-	-	-		
86	OHX	1	3968	-	0,6,6	-	-	-		
86	OHX	5	4089	-	0,6,6	-	-	-		
86	OHX	5	3957	-	0,6,6	-	-	-		
86	OHX	1	3872	-	0,6,6	-	-	-		
86	OHX	6	2013	-	0,6,6	-	-	-		
86	OHX	2	2073	-	0,6,6	-	-	-		
86	OHX	1	3901	-	0,6,6	-	-	-		
86	OHX	1	3949	-	0,6,6	-	-	-		
86	OHX	5	3862	-	0,6,6	-	-	-		
86	OHX	m5	306	-	0,6,6	-	-	-		
86	OHX	1	3853	-	0,6,6	-	-	-		
86	OHX	1	3842	-	0,6,6	-	-	-		
86	OHX	5	3857	-	0,6,6	-	-	-		
86	OHX	1	3786	-	0,6,6	-	-	-		
86	OHX	1	3918	-	0,6,6	-	-	-		
86	OHX	5	4021	-	0,6,6	-	-	-		
86	OHX	M6	203	-	0,6,6	-	-	-		
86	OHX	5	4034	-	0,6,6	-	-	-		
86	OHX	O4	202	-	0,6,6	-	-	-		
86	OHX	5	3870	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3839	-	0,6,6	-	-	-		
86	OHX	8	220	-	0,6,6	-	-	-		
86	OHX	1	3988	-	0,6,6	-	-	-		
86	OHX	5	4011	-	0,6,6	-	-	-		
86	OHX	5	4012	-	0,6,6	-	-	-		
86	OHX	1	3961	-	0,6,6	-	-	-		
86	OHX	1	3843	-	0,6,6	-	-	-		
86	OHX	1	4005	-	0,6,6	-	-	-		
86	OHX	6	2117	-	0,6,6	-	-	-		
86	OHX	m4	201	-	0,6,6	-	-	-		
86	OHX	6	2084	-	0,6,6	-	-	-		
86	OHX	6	2029	-	0,6,6	-	-	-		
86	OHX	O9	101	-	0,6,6	-	-	-		
86	OHX	6	2112	-	0,6,6	-	-	-		
86	OHX	1	3848	-	0,6,6	-	-	-		
86	OHX	1	3890	-	0,6,6	-	-	-		
86	OHX	5	3999	-	0,6,6	-	-	-		
86	OHX	5	3900	-	0,6,6	-	-	-		
86	OHX	5	3950	-	0,6,6	-	-	-		
86	OHX	5	4007	-	0,6,6	-	-	-		
86	OHX	5	4085	-	0,6,6	-	-	-		
86	OHX	1	3997	-	0,6,6	-	-	-		
86	OHX	2	2092	-	0,6,6	-	-	-		
86	OHX	1	3964	-	0,6,6	-	-	-		
86	OHX	5	4047	-	0,6,6	-	-	-		
86	OHX	13	404	-	0,6,6	-	-	-		
86	OHX	2	2088	-	0,6,6	-	-	-		
86	OHX	m9	201	-	0,6,6	-	-	-		
86	OHX	1	3838	-	0,6,6	-	-	-		
86	OHX	5	3904	-	0,6,6	-	-	-		
86	OHX	6	2023	-	0,6,6	-	-	-		
86	OHX	1	4072	-	0,6,6	-	-	-		
89	PRO	1	4114	89	5,7,8	0.57	0	7,8,10	1.06	0
86	OHX	3	213	-	0,6,6	-	-	-		
86	OHX	1	4049	-	0,6,6	-	-	-		
86	OHX	1	3879	-	0,6,6	-	-	-		
86	OHX	2	2041	-	0,6,6	-	-	-		
86	OHX	5	4010	-	0,6,6	-	-	-		
86	OHX	5	3931	-	0,6,6	-	-	-		
86	OHX	5	4054	-	0,6,6	-	-	-		
86	OHX	2	2018	-	0,6,6	-	-	-		
86	OHX	5	4140	-	0,6,6	-	-	-		
86	OHX	1	3889	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3935	-	0,6,6	-	-	-	-	-
86	OHX	3	219	-	0,6,6	-	-	-	-	-
86	OHX	2	2084	-	0,6,6	-	-	-	-	-
86	OHX	2	2048	-	0,6,6	-	-	-	-	-
86	OHX	s1	302	-	0,6,6	-	-	-	-	-
86	OHX	6	2119	-	0,6,6	-	-	-	-	-
86	OHX	5	4060	-	0,6,6	-	-	-	-	-
86	OHX	2	1996	-	0,6,6	-	-	-	-	-
86	OHX	1	3873	-	0,6,6	-	-	-	-	-
86	OHX	5	3892	-	0,6,6	-	-	-	-	-
86	OHX	6	2153	-	0,6,6	-	-	-	-	-
86	OHX	S8	301	-	0,6,6	-	-	-	-	-
86	OHX	1	3789	-	0,6,6	-	-	-	-	-
86	OHX	1	4104	-	0,6,6	-	-	-	-	-
86	OHX	5	4145	-	0,6,6	-	-	-	-	-
86	OHX	2	2148	-	0,6,6	-	-	-	-	-
86	OHX	6	2161	-	0,6,6	-	-	-	-	-
86	OHX	1	3920	-	0,6,6	-	-	-	-	-
86	OHX	1	4079	-	0,6,6	-	-	-	-	-
86	OHX	6	2085	-	0,6,6	-	-	-	-	-
86	OHX	5	4037	-	0,6,6	-	-	-	-	-
86	OHX	L3	402	-	0,6,6	-	-	-	-	-
86	OHX	2	2087	-	0,6,6	-	-	-	-	-
86	OHX	5	4095	-	0,6,6	-	-	-	-	-
86	OHX	5	3834	-	0,6,6	-	-	-	-	-
86	OHX	1	4022	-	0,6,6	-	-	-	-	-
86	OHX	2	2060	-	0,6,6	-	-	-	-	-
86	OHX	5	4116	-	0,6,6	-	-	-	-	-
86	OHX	2	2081	-	0,6,6	-	-	-	-	-
86	OHX	1	4101	-	0,6,6	-	-	-	-	-
86	OHX	5	3958	-	0,6,6	-	-	-	-	-
86	OHX	O7	104	73	0,6,6	-	-	-	-	-
86	OHX	2	2103	-	0,6,6	-	-	-	-	-
86	OHX	1	3922	-	0,6,6	-	-	-	-	-
86	OHX	N9	101	-	0,6,6	-	-	-	-	-
86	OHX	5	3917	-	0,6,6	-	-	-	-	-
86	OHX	6	2094	-	0,6,6	-	-	-	-	-
86	OHX	5	3984	-	0,6,6	-	-	-	-	-
86	OHX	6	2099	-	0,6,6	-	-	-	-	-
86	OHX	6	2139	-	0,6,6	-	-	-	-	-
86	OHX	5	3951	-	0,6,6	-	-	-	-	-
86	OHX	s8	303	-	0,6,6	-	-	-	-	-
86	OHX	2	2122	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	1	3780	-	0,6,6	-	-	-	-	-
86	OHX	1	4042	-	0,6,6	-	-	-	-	-
86	OHX	1	3868	-	0,6,6	-	-	-	-	-
86	OHX	1	3806	-	0,6,6	-	-	-	-	-
86	OHX	5	4093	-	0,6,6	-	-	-	-	-
86	OHX	1	3765	-	0,6,6	-	-	-	-	-
86	OHX	s9	201	-	0,6,6	-	-	-	-	-
86	OHX	5	3977	-	0,6,6	-	-	-	-	-
86	OHX	2	1994	-	0,6,6	-	-	-	-	-
86	OHX	5	4137	-	0,6,6	-	-	-	-	-
86	OHX	1	3761	-	0,6,6	-	-	-	-	-
86	OHX	2	2015	-	0,6,6	-	-	-	-	-
86	OHX	1	4070	-	0,6,6	-	-	-	-	-
86	OHX	6	2068	-	0,6,6	-	-	-	-	-
86	OHX	5	3820	-	0,6,6	-	-	-	-	-
86	OHX	6	2101	-	0,6,6	-	-	-	-	-
86	OHX	2	2033	-	0,6,6	-	-	-	-	-
86	OHX	2	2083	-	0,6,6	-	-	-	-	-
86	OHX	1	3781	-	0,6,6	-	-	-	-	-
86	OHX	6	2087	-	0,6,6	-	-	-	-	-
86	OHX	1	3770	-	0,6,6	-	-	-	-	-
86	OHX	1	3896	-	0,6,6	-	-	-	-	-
86	OHX	1	3916	-	0,6,6	-	-	-	-	-
86	OHX	N8	204	-	0,6,6	-	-	-	-	-
86	OHX	5	4167	-	0,6,6	-	-	-	-	-
86	OHX	2	2113	-	0,6,6	-	-	-	-	-
86	OHX	5	3925	-	0,6,6	-	-	-	-	-
86	OHX	5	3852	-	0,6,6	-	-	-	-	-
86	OHX	5	4073	-	0,6,6	-	-	-	-	-
86	OHX	2	2090	-	0,6,6	-	-	-	-	-
86	OHX	1	4096	-	0,6,6	-	-	-	-	-
86	OHX	m5	304	-	0,6,6	-	-	-	-	-
86	OHX	5	3921	-	0,6,6	-	-	-	-	-
86	OHX	1	4071	36	0,6,6	-	-	-	-	-
86	OHX	5	4112	-	0,6,6	-	-	-	-	-
86	OHX	14	402	-	0,6,6	-	-	-	-	-
86	OHX	1	4106	-	0,6,6	-	-	-	-	-
86	OHX	2	2025	-	0,6,6	-	-	-	-	-
86	OHX	1	3812	-	0,6,6	-	-	-	-	-
86	OHX	5	3894	-	0,6,6	-	-	-	-	-
86	OHX	5	3901	-	0,6,6	-	-	-	-	-
86	OHX	5	3849	-	0,6,6	-	-	-	-	-
86	OHX	1	3932	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	3853	-	0,6,6	-	-	-		
86	OHX	1	3908	-	0,6,6	-	-	-		
86	OHX	5	3976	-	0,6,6	-	-	-		
86	OHX	M8	201	-	0,6,6	-	-	-		
86	OHX	5	3876	-	0,6,6	-	-	-		
86	OHX	2	2138	-	0,6,6	-	-	-		
86	OHX	2	2144	-	0,6,6	-	-	-		
86	OHX	4	223	-	0,6,6	-	-	-		
86	OHX	1	3911	-	0,6,6	-	-	-		
86	OHX	L4	401	-	0,6,6	-	-	-		
86	OHX	5	4058	-	0,6,6	-	-	-		
86	OHX	5	3970	-	0,6,6	-	-	-		
86	OHX	2	2121	-	0,6,6	-	-	-		
86	OHX	6	2043	-	0,6,6	-	-	-		
86	OHX	s4	602	-	0,6,6	-	-	-		
86	OHX	1	3894	-	0,6,6	-	-	-		
86	OHX	2	2134	-	0,6,6	-	-	-		
86	OHX	1	3974	-	0,6,6	-	-	-		
86	OHX	2	2143	-	0,6,6	-	-	-		
86	OHX	5	3933	-	0,6,6	-	-	-		
86	OHX	6	2162	-	0,6,6	-	-	-		
86	OHX	5	3884	-	0,6,6	-	-	-		
86	OHX	1	4046	-	0,6,6	-	-	-		
86	OHX	6	2022	-	0,6,6	-	-	-		
86	OHX	5	4121	-	0,6,6	-	-	-		
86	OHX	1	3970	-	0,6,6	-	-	-		
86	OHX	2	2027	-	0,6,6	-	-	-		
86	OHX	2	2010	-	0,6,6	-	-	-		
86	OHX	5	4084	36	0,6,6	-	-	-		
86	OHX	5	3847	-	0,6,6	-	-	-		
86	OHX	5	3968	-	0,6,6	-	-	-		
86	OHX	4	233	-	0,6,6	-	-	-		
86	OHX	1	4066	-	0,6,6	-	-	-		
86	OHX	5	4097	-	0,6,6	-	-	-		
86	OHX	2	2142	-	0,6,6	-	-	-		
86	OHX	1	4004	-	0,6,6	-	-	-		
86	OHX	2	2098	-	0,6,6	-	-	-		
86	OHX	1	4091	-	0,6,6	-	-	-		
86	OHX	5	4032	-	0,6,6	-	-	-		
86	OHX	6	2158	-	0,6,6	-	-	-		
86	OHX	5	3928	-	0,6,6	-	-	-		
86	OHX	1	3862	-	0,6,6	-	-	-		
86	OHX	6	2050	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	5	4057	-	0,6,6	-	-	-		
86	OHX	2	2062	-	0,6,6	-	-	-		
86	OHX	2	2036	-	0,6,6	-	-	-		
86	OHX	1	3847	-	0,6,6	-	-	-		
86	OHX	6	2144	-	0,6,6	-	-	-		
86	OHX	5	4001	-	0,6,6	-	-	-		
86	OHX	5	3882	-	0,6,6	-	-	-		
86	OHX	1	3800	-	0,6,6	-	-	-		
86	OHX	6	2137	-	0,6,6	-	-	-		
86	OHX	5	4048	-	0,6,6	-	-	-		
86	OHX	1	3794	-	0,6,6	-	-	-		
86	OHX	1	3954	-	0,6,6	-	-	-		
86	OHX	1	4012	-	0,6,6	-	-	-		
86	OHX	6	2018	-	0,6,6	-	-	-		
86	OHX	L3	404	-	0,6,6	-	-	-		
86	OHX	5	4164	-	0,6,6	-	-	-		
86	OHX	5	3889	-	0,6,6	-	-	-		
86	OHX	1	3927	-	0,6,6	-	-	-		
86	OHX	6	2016	-	0,6,6	-	-	-		
86	OHX	2	2026	-	0,6,6	-	-	-		
86	OHX	1	4017	-	0,6,6	-	-	-		
86	OHX	4	229	-	0,6,6	-	-	-		
86	OHX	6	2082	-	0,6,6	-	-	-		
86	OHX	1	3930	-	0,6,6	-	-	-		
86	OHX	5	3915	-	0,6,6	-	-	-		
86	OHX	5	4125	-	0,6,6	-	-	-		
86	OHX	5	3874	-	0,6,6	-	-	-		
86	OHX	1	3867	-	0,6,6	-	-	-		
86	OHX	5	3885	-	0,6,6	-	-	-		
86	OHX	5	3971	-	0,6,6	-	-	-		
86	OHX	2	2096	-	0,6,6	-	-	-		
86	OHX	1	4069	-	0,6,6	-	-	-		
86	OHX	c5	201	-	0,6,6	-	-	-		
86	OHX	5	4159	-	0,6,6	-	-	-		
86	OHX	1	4010	-	0,6,6	-	-	-		
86	OHX	8	227	-	0,6,6	-	-	-		
86	OHX	7	214	-	0,6,6	-	-	-		
86	OHX	6	2061	-	0,6,6	-	-	-		
86	OHX	1	4045	-	0,6,6	-	-	-		
86	OHX	6	2071	-	0,6,6	-	-	-		
86	OHX	1	4008	-	0,6,6	-	-	-		
86	OHX	1	4027	-	0,6,6	-	-	-		
86	OHX	5	4039	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OHX	6	2145	-	0,6,6	-	-	-	-	-
86	OHX	1	4047	-	0,6,6	-	-	-	-	-
86	OHX	5	3835	-	0,6,6	-	-	-	-	-
86	OHX	5	4003	-	0,6,6	-	-	-	-	-
86	OHX	5	4065	-	0,6,6	-	-	-	-	-
86	OHX	5	4124	-	0,6,6	-	-	-	-	-
86	OHX	5	4109	-	0,6,6	-	-	-	-	-
86	OHX	13	403	-	0,6,6	-	-	-	-	-
86	OHX	6	2164	-	0,6,6	-	-	-	-	-
86	OHX	5	3895	-	0,6,6	-	-	-	-	-
86	OHX	5	3879	-	0,6,6	-	-	-	-	-
86	OHX	5	3902	-	0,6,6	-	-	-	-	-
86	OHX	5	4118	-	0,6,6	-	-	-	-	-
86	OHX	6	2088	-	0,6,6	-	-	-	-	-
86	OHX	1	4016	-	0,6,6	-	-	-	-	-
86	OHX	1	3925	-	0,6,6	-	-	-	-	-
86	OHX	M5	304	-	0,6,6	-	-	-	-	-
86	OHX	2	2100	-	0,6,6	-	-	-	-	-
86	OHX	5	3978	-	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
89	PRO	C	101	89,84	-	0/0/9/11	0/1/1/1
89	PRO	5	4173	89	-	0/0/9/11	0/1/1/1
88	SPS	5	3403	-	-	2/15/18/18	0/1/1/1
89	PRO	B	101	89,84	-	0/0/9/11	0/1/1/1
89	PRO	1	4114	89	-	0/0/9/11	0/1/1/1
88	SPS	1	4113	85	-	3/15/18/18	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	1	4113	SPS	C9-C10	-8.24	1.31	1.48
88	5	3403	SPS	C9-C10	-8.07	1.31	1.48
88	5	3403	SPS	C9-C8	7.40	1.52	1.33
88	1	4113	SPS	C9-C8	7.23	1.51	1.33
88	5	3403	SPS	O13-C13	-5.41	1.19	1.42
88	1	4113	SPS	O13-C13	-5.33	1.19	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	1	4113	SPS	O15-S15	4.33	1.65	1.50
88	1	4113	SPS	C10-N11	4.29	1.44	1.34
88	5	3403	SPS	C10-N11	4.08	1.44	1.34
88	5	3403	SPS	O15-S15	4.00	1.64	1.50
88	1	4113	SPS	C3-N4	-2.97	1.32	1.38
88	5	3403	SPS	O10-C10	-2.85	1.19	1.24
88	1	4113	SPS	O10-C10	-2.73	1.19	1.24
88	5	3403	SPS	C6-C8	2.69	1.53	1.47
88	1	4113	SPS	C6-C8	2.67	1.53	1.47
88	5	3403	SPS	C3-N4	-2.46	1.33	1.38
88	1	4113	SPS	C6-C1	-2.36	1.37	1.43
88	5	3403	SPS	O1-C1	-2.24	1.18	1.24
88	1	4113	SPS	O1-C1	-2.23	1.18	1.24
88	5	3403	SPS	C3-N2	-2.10	1.34	1.38
88	1	4113	SPS	C6-C5	-2.01	1.37	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	1	4113	SPS	C3-N2-C1	8.00	121.90	115.14
88	1	4113	SPS	C6-C1-N2	-7.95	118.86	124.40
88	5	3403	SPS	C3-N2-C1	7.08	121.12	115.14
88	5	3403	SPS	C6-C1-N2	-6.34	119.98	124.40
88	5	3403	SPS	C12-N11-C10	-4.66	116.01	122.57
88	1	4113	SPS	C18-S17-C16	3.76	110.52	100.10
88	1	4113	SPS	O13-C13-C12	3.40	120.73	111.95
88	5	3403	SPS	C9-C10-N11	3.25	120.80	114.56
88	5	3403	SPS	C18-S17-C16	3.20	108.95	100.10
88	5	3403	SPS	O13-C13-C12	3.00	119.70	111.95
89	5	4173	PRO	O-C-CA	-2.66	117.80	124.78
89	C	101	PRO	O-C-CA	-2.62	117.92	124.78
88	5	3403	SPS	O10-C10-N11	-2.57	118.95	122.35
88	1	4113	SPS	O15-S15-C16	2.52	109.47	106.47
88	5	3403	SPS	O15-S15-C16	2.46	109.39	106.47
89	B	101	PRO	O-C-CA	-2.34	118.65	124.78
88	1	4113	SPS	C12-N11-C10	-2.33	119.29	122.57
88	5	3403	SPS	C8-C9-C10	-2.20	117.25	121.56
88	5	3403	SPS	C7-C5-N4	2.13	119.78	116.49
88	1	4113	SPS	C8-C9-C10	-2.00	117.64	121.56

There are no chirality outliers.

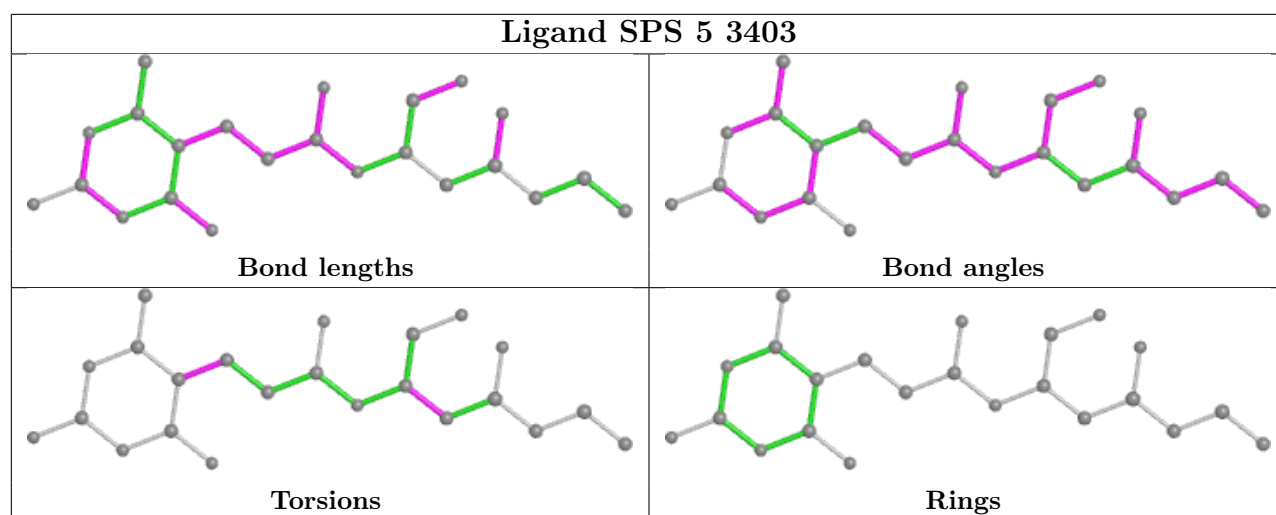
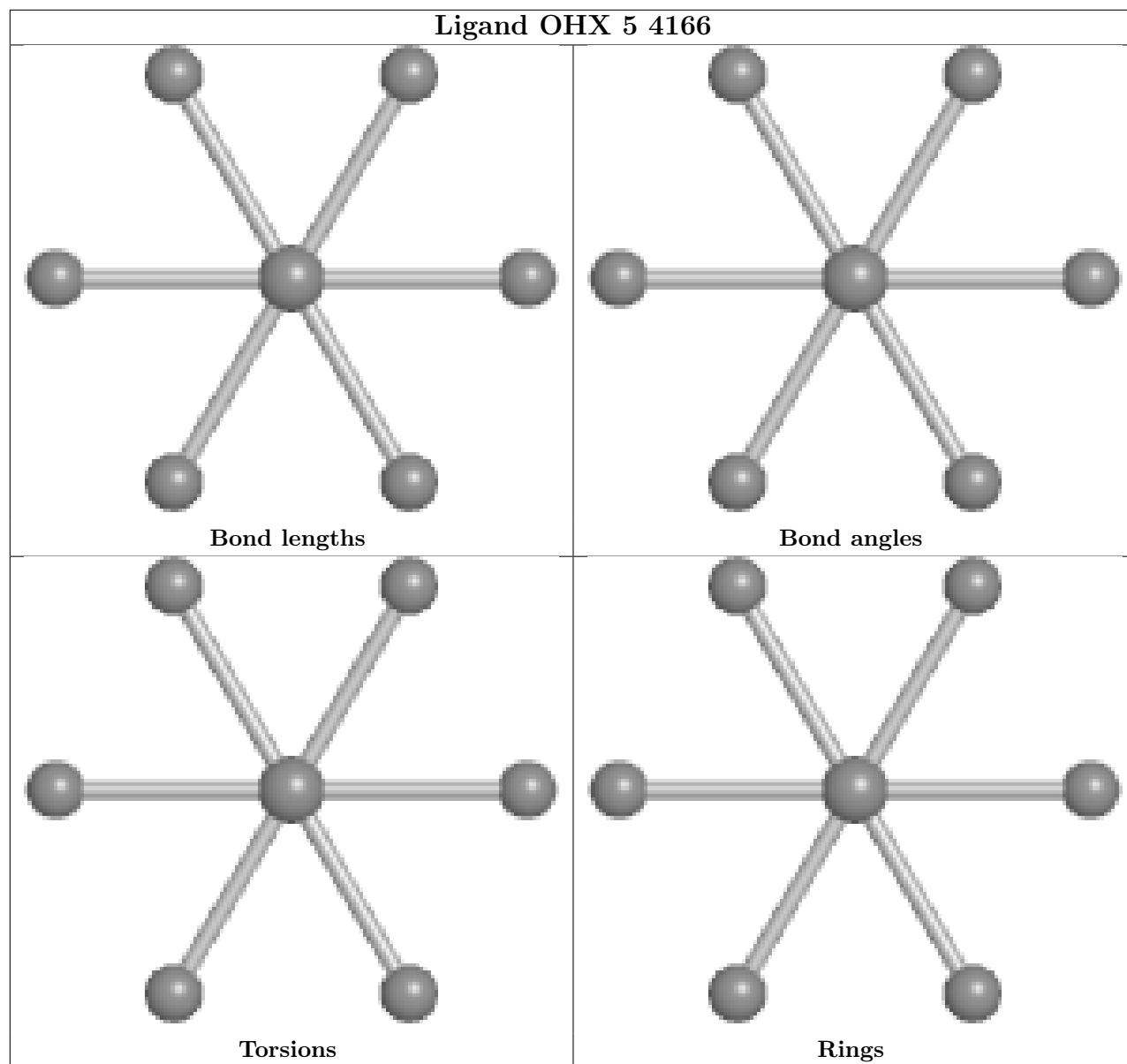
All (5) torsion outliers are listed below:

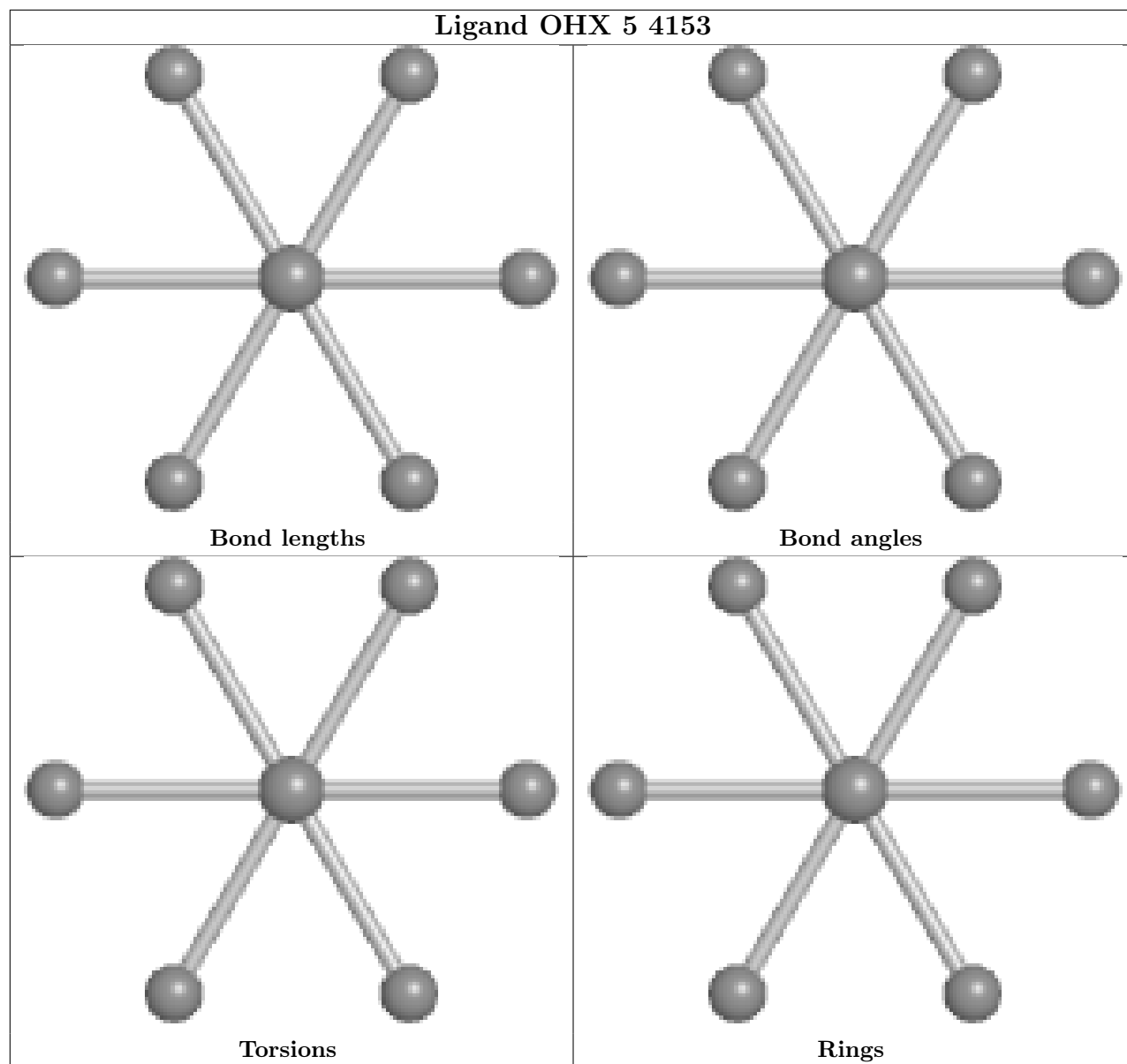
Mol	Chain	Res	Type	Atoms
88	1	4113	SPS	N11-C12-C13-O13
88	1	4113	SPS	C14-C12-C13-O13
88	1	4113	SPS	N11-C12-C14-S15
88	5	3403	SPS	N11-C12-C14-S15
88	5	3403	SPS	C5-C6-C8-C9

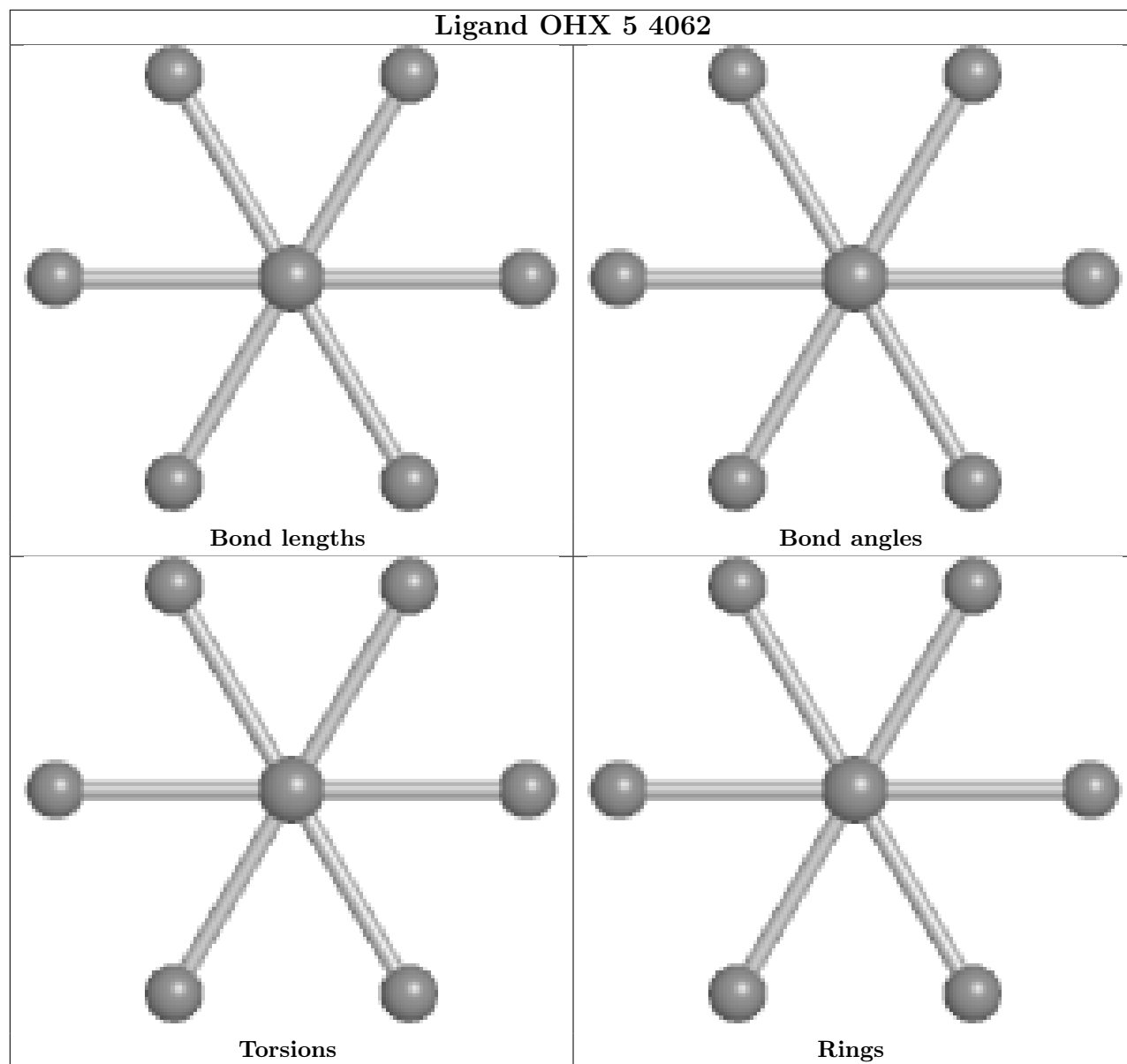
There are no ring outliers.

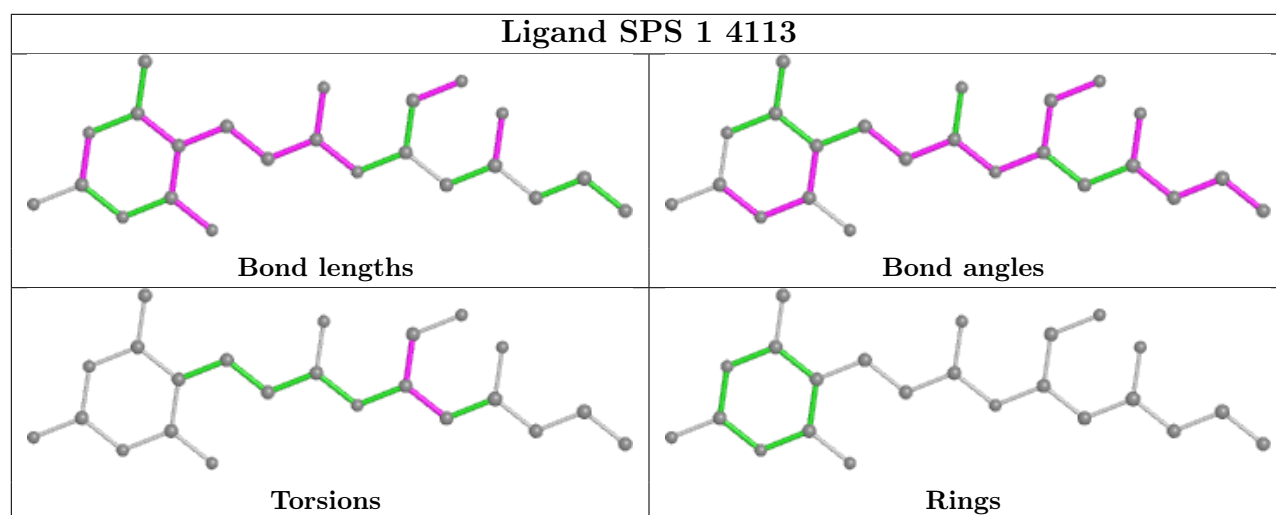
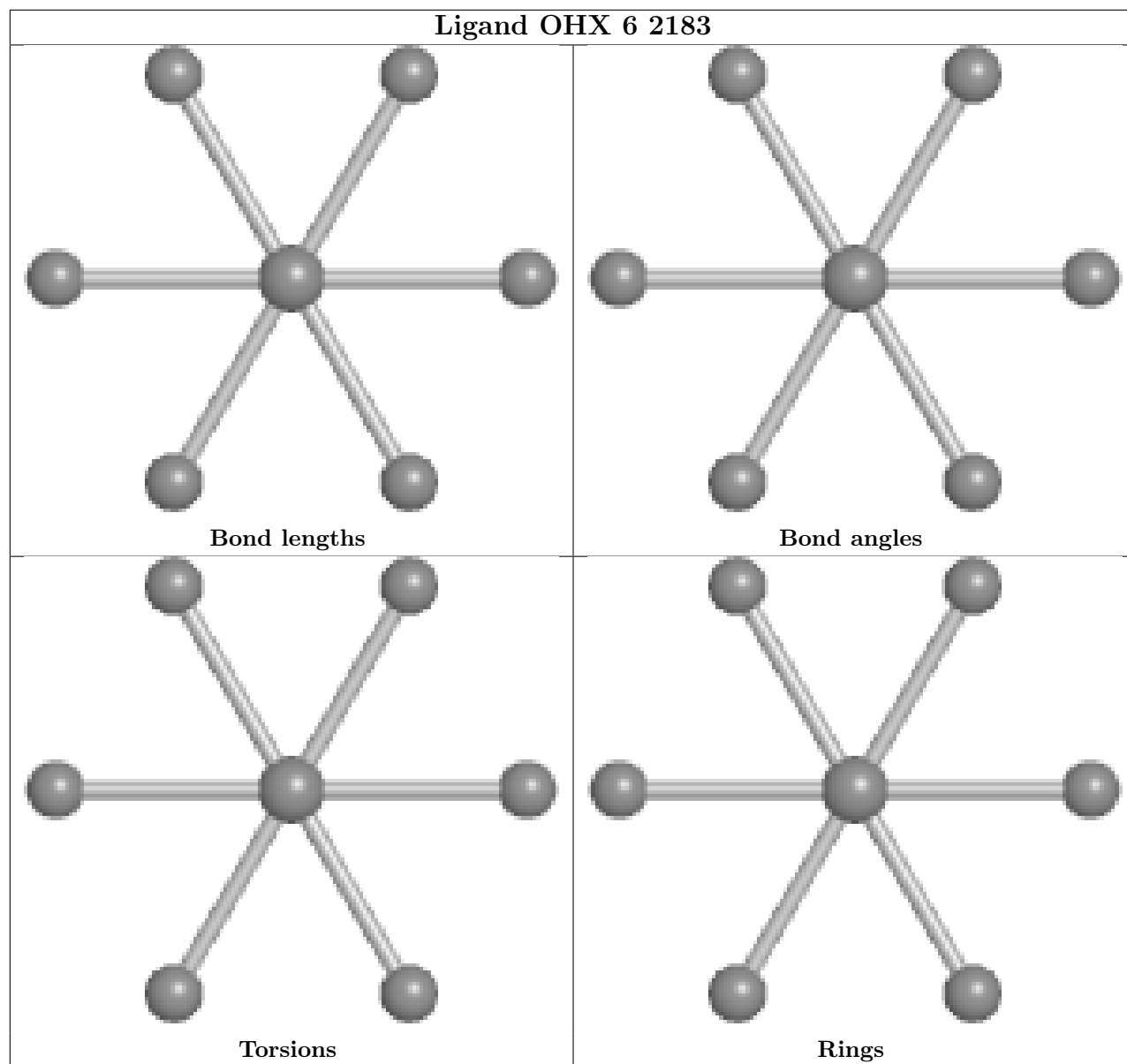
No monomer is involved in short contacts.

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2	2
80	m2	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1716:C	O3'	1717:G	P	5.10
1	m2	23:LEU	C	28:ARG	N	3.71
1	m2	52:LYS	C	54:LYS	N	3.25
1	2	1685:G	O3'	1686:C	P	2.98

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	2	1781/1800 (98%)	0.35	83 (4%) 31 31	58, 100, 190, 245	0
1	6	1795/1800 (99%)	0.15	46 (2%) 56 53	41, 84, 172, 231	0
2	S0	206/251 (82%)	1.29	52 (25%) 0 0	99, 112, 122, 125	0
2	s0	206/251 (82%)	0.46	14 (6%) 17 19	78, 93, 107, 115	0
3	S1	214/254 (84%)	1.32	59 (27%) 0 0	114, 152, 175, 179	0
3	s1	216/254 (85%)	0.61	25 (11%) 4 6	80, 93, 110, 126	0
4	S2	217/253 (85%)	0.31	8 (3%) 41 40	79, 95, 109, 118	0
4	s2	217/253 (85%)	0.49	20 (9%) 9 11	63, 79, 90, 99	0
5	S3	223/239 (93%)	0.95	38 (17%) 1 2	90, 103, 122, 135	0
5	s3	223/239 (93%)	1.10	50 (22%) 0 0	83, 108, 131, 139	0
6	S4	260/260 (100%)	1.86	109 (41%) 0 0	78, 101, 111, 133	0
6	s4	260/260 (100%)	1.19	60 (23%) 0 0	56, 79, 94, 113	0
7	S5	206/224 (91%)	2.38	108 (52%) 0 0	107, 122, 134, 144	0
7	s5	206/224 (91%)	1.69	82 (39%) 0 0	88, 106, 123, 134	0
8	S6	226/236 (95%)	0.75	27 (11%) 4 6	77, 113, 131, 142	0
8	s6	218/236 (92%)	0.50	23 (10%) 6 8	56, 85, 110, 123	0
9	S7	184/189 (97%)	0.92	33 (17%) 1 2	96, 127, 147, 152	0
9	s7	186/189 (98%)	0.37	7 (3%) 40 39	70, 103, 132, 139	0
10	S8	188/200 (94%)	1.21	45 (23%) 0 0	68, 88, 122, 139	0
10	s8	188/200 (94%)	0.71	15 (7%) 12 14	52, 69, 110, 129	0
11	S9	185/196 (94%)	1.72	73 (39%) 0 0	91, 107, 137, 157	0
11	s9	185/196 (94%)	0.87	21 (11%) 5 7	68, 87, 125, 146	0
12	C0	96/105 (91%)	1.54	29 (30%) 0 0	96, 121, 141, 151	0
12	c0	96/105 (91%)	1.86	37 (38%) 0 0	105, 136, 149, 150	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	C1	155/155 (100%)	1.30	36 (23%) 0 0	71, 84, 118, 130	0
13	c1	146/155 (94%)	0.74	16 (10%) 5 7	54, 66, 94, 115	0
14	C2	124/142 (87%)	1.15	25 (20%) 1 1	149, 161, 174, 180	0
14	c2	124/142 (87%)	2.34	68 (54%) 0 0	180, 196, 211, 215	0
15	C3	150/150 (100%)	0.99	29 (19%) 1 1	79, 94, 109, 115	0
15	c3	150/150 (100%)	0.25	6 (4%) 38 36	62, 76, 93, 96	0
16	C4	127/136 (93%)	1.41	44 (34%) 0 0	83, 146, 158, 162	0
16	c4	128/136 (94%)	0.81	16 (12%) 3 6	64, 96, 104, 109	0
17	C5	124/141 (87%)	0.85	13 (10%) 6 8	87, 103, 120, 130	0
17	c5	135/141 (95%)	1.18	33 (24%) 0 0	72, 107, 122, 123	0
18	C6	141/142 (99%)	2.33	75 (53%) 0 0	92, 110, 116, 118	0
18	c6	142/142 (100%)	1.74	49 (34%) 0 0	82, 104, 118, 136	0
19	C7	120/136 (88%)	1.04	22 (18%) 1 2	95, 110, 129, 131	0
19	c7	117/136 (86%)	0.41	12 (10%) 6 9	85, 102, 114, 122	0
20	C8	145/145 (100%)	0.93	25 (17%) 1 2	85, 109, 135, 142	0
20	c8	145/145 (100%)	1.03	26 (17%) 1 2	83, 101, 117, 124	0
21	C9	143/143 (100%)	2.00	71 (49%) 0 0	95, 110, 125, 133	0
21	c9	143/143 (100%)	0.93	22 (15%) 2 3	82, 98, 115, 123	0
22	D0	107/120 (89%)	0.93	19 (17%) 1 2	86, 114, 136, 138	0
22	d0	110/120 (91%)	1.13	27 (24%) 0 0	85, 115, 144, 149	0
23	D1	87/87 (100%)	0.75	12 (13%) 2 4	96, 103, 117, 122	0
23	d1	87/87 (100%)	-0.06	0 100 100	71, 82, 104, 111	0
24	D2	129/129 (100%)	0.84	14 (10%) 5 8	80, 92, 101, 111	0
24	d2	129/129 (100%)	0.28	3 (2%) 60 58	59, 68, 75, 84	0
25	D3	144/144 (100%)	1.44	51 (35%) 0 0	70, 78, 90, 102	0
25	d3	144/144 (100%)	0.79	12 (8%) 11 14	52, 57, 70, 81	0
26	D4	134/134 (100%)	1.55	44 (32%) 0 0	89, 111, 123, 127	0
26	d4	134/134 (100%)	0.51	15 (11%) 5 7	65, 88, 100, 105	0
27	D5	70/107 (65%)	2.26	37 (52%) 0 0	118, 134, 141, 146	0
27	d5	69/107 (64%)	1.88	27 (39%) 0 0	98, 112, 124, 126	0
28	D6	97/97 (100%)	1.49	33 (34%) 0 0	86, 108, 160, 162	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)		Q<0.9	
28	d6	97/97 (100%)	0.82	12 (12%)	4	6	67, 84, 111, 116	0
29	D7	81/81 (100%)	1.54	29 (35%)	0	0	95, 113, 139, 143	0
29	d7	81/81 (100%)	0.93	15 (18%)	1	2	72, 89, 127, 128	0
30	D8	63/66 (95%)	1.98	28 (44%)	0	0	114, 131, 139, 144	0
30	d8	63/66 (95%)	2.08	27 (42%)	0	0	105, 118, 125, 128	0
31	D9	53/55 (96%)	1.08	10 (18%)	1	2	85, 90, 108, 114	0
31	d9	53/55 (96%)	1.81	23 (43%)	0	0	82, 92, 128, 145	0
32	E0	60/63 (95%)	2.11	31 (51%)	0	0	80, 110, 134, 137	0
32	e0	62/63 (98%)	1.51	17 (27%)	0	0	60, 88, 117, 120	0
33	E1	71/76 (93%)	1.45	21 (29%)	0	0	115, 142, 155, 157	0
33	e1	76/76 (100%)	2.39	37 (48%)	0	0	117, 168, 186, 187	0
34	SR	318/318 (100%)	1.38	83 (26%)	0	0	109, 122, 138, 156	0
34	sR	318/318 (100%)	2.10	152 (47%)	0	0	112, 127, 141, 153	0
35	SM	159/273 (58%)	1.18	43 (27%)	0	0	58, 100, 159, 163	0
35	sM	104/273 (38%)	1.25	25 (24%)	0	0	51, 115, 188, 197	0
36	1	3149/3396 (92%)	0.11	57 (1%)	68	65	33, 58, 136, 238	0
36	5	3150/3396 (92%)	0.09	35 (1%)	80	77	28, 52, 127, 213	0
37	3	121/121 (100%)	-0.05	0	100	100	42, 77, 90, 98	0
37	7	121/121 (100%)	-0.14	0	100	100	33, 55, 66, 75	0
38	4	158/158 (100%)	-0.01	1 (0%)	89	87	42, 63, 102, 146	0
38	8	158/158 (100%)	-0.03	0	100	100	42, 63, 101, 131	0
39	L2	252/253 (99%)	0.47	13 (5%)	27	27	40, 60, 78, 84	0
39	l2	252/253 (99%)	0.26	2 (0%)	86	82	36, 55, 73, 80	0
40	L3	386/386 (100%)	0.20	9 (2%)	60	58	37, 62, 77, 88	0
40	l3	386/386 (100%)	0.14	6 (1%)	72	69	28, 45, 60, 81	0
41	L4	361/361 (100%)	0.11	4 (1%)	80	77	38, 54, 69, 74	0
41	l4	361/361 (100%)	0.05	2 (0%)	89	87	37, 56, 74, 82	0
42	L5	296/296 (100%)	1.31	87 (29%)	0	0	58, 80, 98, 119	0
42	l5	294/296 (99%)	0.45	12 (4%)	37	36	42, 56, 82, 97	0
43	L6	156/175 (89%)	0.52	7 (4%)	33	32	46, 56, 72, 87	0
43	l6	157/175 (89%)	0.48	9 (5%)	23	23	48, 57, 78, 93	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	L7	222/243 (91%)	0.17	1 (0%) 91 89	38, 47, 77, 104	0
44	l7	223/243 (91%)	-0.08	0 100 100	33, 45, 82, 112	0
45	L8	233/255 (91%)	0.86	32 (13%) 3 4	68, 84, 110, 120	0
45	l8	231/255 (90%)	1.06	41 (17%) 1 2	69, 82, 107, 117	0
46	L9	191/191 (100%)	0.46	15 (7%) 12 15	59, 71, 82, 94	0
46	l9	191/191 (100%)	0.12	3 (1%) 72 69	41, 51, 68, 78	0
47	M0	211/220 (95%)	0.51	15 (7%) 16 18	44, 63, 94, 105	0
47	m0	213/220 (96%)	0.27	4 (1%) 66 64	39, 54, 78, 94	0
48	M1	169/173 (97%)	1.19	30 (17%) 1 2	68, 85, 97, 103	0
48	m1	169/173 (97%)	0.33	3 (1%) 68 65	47, 66, 77, 81	0
49	M3	193/198 (97%)	0.45	4 (2%) 63 61	36, 63, 101, 122	0
49	m3	194/198 (97%)	0.52	11 (5%) 23 23	38, 67, 104, 119	0
50	M4	136/137 (99%)	-0.14	0 100 100	50, 59, 72, 83	0
50	m4	137/137 (100%)	-0.19	0 100 100	43, 50, 66, 84	0
51	M5	203/203 (100%)	0.58	16 (7%) 12 15	39, 56, 67, 71	0
51	m5	203/203 (100%)	1.04	39 (19%) 1 1	40, 58, 68, 73	0
52	M6	197/198 (99%)	-0.13	1 (0%) 91 89	25, 32, 46, 49	0
52	m6	197/198 (99%)	-0.14	1 (0%) 91 89	18, 24, 45, 52	0
53	M7	183/183 (100%)	0.72	24 (13%) 3 5	44, 52, 105, 133	0
53	m7	155/183 (84%)	0.05	1 (0%) 89 87	36, 45, 55, 77	0
54	M8	185/185 (100%)	0.23	3 (1%) 72 69	42, 51, 68, 88	0
54	m8	185/185 (100%)	0.37	4 (2%) 62 59	39, 53, 64, 72	0
55	M9	188/188 (100%)	0.83	31 (16%) 1 2	64, 78, 147, 156	0
55	m9	188/188 (100%)	0.26	10 (5%) 26 26	50, 62, 123, 138	0
56	N0	172/172 (100%)	0.41	5 (2%) 51 49	37, 56, 70, 75	0
56	n0	172/172 (100%)	0.02	1 (0%) 89 87	32, 45, 57, 67	0
57	N1	159/159 (100%)	0.13	1 (0%) 89 87	41, 56, 99, 105	0
57	n1	159/159 (100%)	0.09	1 (0%) 89 87	37, 45, 82, 88	0
58	N2	100/120 (83%)	1.33	27 (27%) 0 0	94, 106, 112, 117	0
58	n2	98/120 (81%)	1.09	20 (20%) 1 1	74, 85, 93, 95	0
59	N3	136/136 (100%)	0.17	3 (2%) 62 59	49, 59, 73, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
59	n3	136/136 (100%)	0.11	2 (1%) 73 71	31, 41, 52, 57	0
60	N4	98/155 (63%)	2.01	28 (28%) 0 0	59, 74, 147, 155	0
60	n4	135/155 (87%)	0.75	20 (14%) 2 3	41, 93, 124, 142	0
61	N5	121/141 (85%)	0.83	12 (9%) 7 9	59, 71, 86, 103	0
61	n5	120/141 (85%)	0.60	8 (6%) 17 19	55, 68, 82, 97	0
62	N6	126/126 (100%)	0.57	9 (7%) 16 18	48, 64, 77, 85	0
62	n6	126/126 (100%)	0.09	0 100 100	50, 66, 82, 85	0
63	N7	135/135 (100%)	2.01	66 (48%) 0 0	83, 96, 107, 111	0
63	n7	135/135 (100%)	0.96	23 (17%) 1 2	78, 89, 101, 109	0
64	N8	148/148 (100%)	0.58	11 (7%) 14 17	32, 54, 76, 82	0
64	n8	148/148 (100%)	0.64	13 (8%) 10 12	34, 55, 72, 75	0
65	N9	58/58 (100%)	-0.03	0 100 100	36, 59, 97, 113	0
65	n9	58/58 (100%)	0.00	0 100 100	36, 55, 76, 82	0
66	O0	97/104 (93%)	0.82	14 (14%) 2 3	83, 90, 106, 111	0
66	o0	100/104 (96%)	0.50	8 (8%) 12 14	69, 79, 98, 105	0
67	O1	109/112 (97%)	1.43	32 (29%) 0 0	60, 73, 94, 101	0
67	o1	109/112 (97%)	1.21	18 (16%) 1 2	44, 56, 89, 97	0
68	O2	127/129 (98%)	0.28	3 (2%) 59 56	34, 48, 63, 79	0
68	o2	127/129 (98%)	0.49	3 (2%) 59 56	32, 52, 67, 78	0
69	O3	106/106 (100%)	0.19	0 100 100	39, 46, 70, 82	0
69	o3	106/106 (100%)	0.59	3 (2%) 53 51	36, 44, 71, 82	0
70	O4	112/121 (92%)	1.55	40 (35%) 0 0	57, 74, 110, 117	0
70	o4	112/121 (92%)	0.96	24 (21%) 0 1	50, 66, 101, 108	0
71	O5	119/119 (100%)	0.17	1 (0%) 86 82	56, 73, 80, 83	0
71	o5	119/119 (100%)	0.10	2 (1%) 70 67	58, 71, 86, 96	0
72	O6	99/99 (100%)	0.80	13 (13%) 3 5	59, 70, 100, 111	0
72	o6	99/99 (100%)	0.83	13 (13%) 3 5	62, 72, 91, 110	0
73	O7	87/87 (100%)	0.10	0 100 100	41, 49, 70, 80	0
73	o7	87/87 (100%)	0.07	0 100 100	37, 48, 79, 85	0
74	O8	77/77 (100%)	0.52	3 (3%) 39 38	85, 97, 107, 108	0
74	o8	77/77 (100%)	1.84	32 (41%) 0 0	75, 85, 94, 97	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
75	O9	50/50 (100%)	0.39	0 100 100	51, 57, 61, 62	0
75	o9	50/50 (100%)	0.10	1 (2%) 65 63	49, 54, 63, 64	0
76	Q0	52/52 (100%)	0.84	7 (13%) 3 4	53, 59, 74, 82	0
76	q0	52/52 (100%)	0.08	1 (1%) 66 64	38, 42, 52, 57	0
77	Q1	25/25 (100%)	0.23	0 100 100	62, 66, 72, 74	0
77	q1	25/25 (100%)	-0.20	0 100 100	49, 53, 54, 55	0
78	Q2	105/105 (100%)	0.42	8 (7%) 13 16	41, 55, 76, 97	0
78	q2	105/105 (100%)	0.14	1 (0%) 82 79	40, 53, 69, 96	0
79	Q3	91/91 (100%)	0.29	2 (2%) 62 59	49, 65, 79, 85	0
79	q3	91/91 (100%)	0.10	0 100 100	40, 55, 71, 81	0
80	m2	150/165 (90%)	1.15	38 (25%) 0 0	102, 138, 156, 161	0
81	p0	143/311 (45%)	1.98	67 (46%) 0 0	100, 125, 220, 229	0
82	p1	47/106 (44%)	4.08	35 (74%) 0 0	179, 224, 242, 245	0
82	p2	46/106 (43%)	4.88	35 (76%) 0 0	275, 283, 288, 289	0
83	f	147/157 (93%)	2.14	69 (46%) 0 0	47, 99, 167, 169	74 (50%)
84	B	2/3 (66%)	0.68	0 100 100	45, 45, 45, 48	0
84	C	2/3 (66%)	0.33	0 100 100	43, 43, 43, 49	0
All	All	33488/35639 (93%)	0.61	3755 (11%) 5 7	18, 74, 141, 289	74 (0%)

All (3755) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
82	p2	31	ASN	22.6
82	p2	30	THR	19.2
82	p1	17	SER	14.0
82	p2	32	ALA	13.3
82	p2	12	LEU	12.9
82	p1	16	ASP	12.9
60	N4	86	SER	12.5
82	p1	12	LEU	12.1
60	N4	88	ASP	12.0
82	p2	8	SER	12.0
60	N4	76	VAL	11.9
53	M7	161	ALA	11.9
1	2	1698	G	10.8
60	N4	75	THR	10.8

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Mol	Chain	Res	Type	RSRZ
1	2	1694	A	10.8
18	C6	20	ALA	10.7
36	5	2505	U	10.6
36	5	2503	G	10.3
1	2	1702	A	10.3
13	C1	147	ALA	9.9
1	2	1695	G	9.9
83	f	157	ASP	9.9
1	2	1696	G	9.8
1	2	1709	C	9.8
82	p1	1	MET	9.6
33	e1	77	GLY	9.5
7	S5	71	ALA	9.5
1	2	1693	A	9.3
1	2	1699	G	9.1
60	N4	85	ALA	9.1
3	S1	20	VAL	9.0
53	M7	162	GLU	8.9
1	2	1692	G	8.9
82	p2	29	LEU	8.9
82	p2	9	TYR	8.8
60	N4	90	ILE	8.7
13	c1	3	THR	8.7
1	2	1708	U	8.7
82	p1	15	ALA	8.7
60	N4	83	THR	8.6
60	N4	89	LEU	8.5
81	p0	211	SER	8.5
1	2	1710	U	8.4
1	2	1697	G	8.4
1	2	715	U	8.3
14	c2	126	TRP	8.2
36	5	2504	U	8.2
60	N4	84	GLY	8.0
35	sM	83	LYS	8.0
35	SM	85	SER	7.9
7	S5	152	GLY	7.8
53	M7	160	ALA	7.8
81	p0	212	HIS	7.8
12	c0	25	LYS	7.8
7	S5	70	VAL	7.8
20	C8	2	SER	7.7

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Mol	Chain	Res	Type	RSRZ
10	S8	152	ILE	7.7
16	C4	15	GLY	7.7
35	sM	85	SER	7.6
34	sR	313	TRP	7.5
60	N4	87	LEU	7.5
18	c6	142	TYR	7.5
34	sR	25	THR	7.5
30	d8	9	LEU	7.5
12	c0	64	TYR	7.5
3	S1	91	VAL	7.4
3	S1	47	LEU	7.4
60	N4	78	ALA	7.4
82	p1	14	LEU	7.3
34	sR	24	ALA	7.2
34	sR	214	ALA	7.2
83	f	149	SER	7.2
7	S5	155	ALA	7.2
35	SM	89	ARG	7.2
17	c5	134	THR	7.1
80	m2	91	SER	7.1
34	sR	252	LEU	7.1
13	C1	145	ALA	7.1
34	sR	303	ALA	7.0
7	S5	37	GLN	7.0
16	C4	75	GLY	7.0
35	SM	84	LYS	7.0
14	c2	112	ALA	6.9
13	C1	146	ALA	6.9
82	p2	33	ALA	6.9
78	Q2	106	PHE	6.9
4	s2	88	LYS	6.9
13	c1	4	GLU	6.9
34	sR	314	GLN	6.8
82	p2	19	ILE	6.8
33	e1	85	TYR	6.8
35	SM	88	ARG	6.8
36	5	2506	U	6.7
82	p2	11	ALA	6.7
1	2	913	G	6.7
82	p1	5	SER	6.6
34	sR	32	LEU	6.6
34	SR	33	LEU	6.6

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Mol	Chain	Res	Type	RSRZ
35	SM	87	THR	6.6
31	d9	4	GLU	6.6
12	c0	22	VAL	6.6
22	d0	67	THR	6.5
22	D0	121	ASN	6.5
33	e1	80	ARG	6.5
34	sR	202	LEU	6.5
35	sM	84	LYS	6.4
4	s2	90	THR	6.4
82	p2	5	SER	6.4
7	s5	37	GLN	6.4
14	c2	105	LYS	6.4
34	SR	45	TRP	6.3
4	s2	87	GLN	6.3
12	c0	23	ALA	6.3
14	C2	41	LEU	6.2
1	2	719	U	6.2
60	n4	69	LYS	6.2
82	p2	4	GLU	6.2
14	c2	123	VAL	6.2
18	C6	21	HIS	6.2
34	sR	302	PHE	6.1
36	5	1567	U	6.1
5	S3	217	ILE	6.1
33	e1	83	LYS	6.1
1	2	1703	C	6.1
33	E1	85	TYR	6.1
12	c0	65	TYR	6.0
36	1	1570	U	6.0
30	d8	33	LEU	6.0
33	e1	81	LYS	6.0
34	sR	212	ALA	6.0
34	SR	79	TYR	6.0
30	D8	16	LEU	6.0
60	n4	68	ALA	6.0
82	p1	2	SER	6.0
1	2	1701	A	6.0
27	d5	50	ILE	6.0
81	p0	88	PHE	5.9
36	5	1569	U	5.9
13	C1	2	SER	5.9
16	C4	76	ILE	5.9

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Mol	Chain	Res	Type	RSRZ
28	D6	49	ALA	5.9
34	SR	44	SER	5.9
60	N4	77	LYS	5.9
8	S6	78	THR	5.8
34	SR	25	THR	5.8
18	C6	66	ARG	5.8
20	c8	146	ALA	5.8
60	N4	74	LYS	5.8
56	N0	1	MET	5.8
18	c6	49	TYR	5.8
81	p0	218	SER	5.8
82	p2	28	THR	5.7
20	c8	22	VAL	5.7
82	p1	43	ASP	5.7
7	S5	41	LYS	5.7
34	sR	168	THR	5.7
34	sR	244	ALA	5.7
18	c6	139	GLN	5.7
82	p2	3	THR	5.7
5	s3	148	LYS	5.7
25	D3	48	HIS	5.7
60	N4	68	ALA	5.7
1	6	663	U	5.7
11	s9	148	VAL	5.7
14	c2	122	VAL	5.7
60	N4	72	SER	5.7
32	e0	62	VAL	5.6
62	N6	127	GLU	5.6
21	C9	105	LEU	5.6
18	c6	141	SER	5.6
82	p1	37	VAL	5.6
17	C5	8	LYS	5.6
81	p0	209	LEU	5.6
34	sR	167	VAL	5.6
82	p1	23	SER	5.6
34	SR	32	LEU	5.6
81	p0	216	ALA	5.6
83	f	155	ARG	5.6
7	S5	69	PHE	5.6
63	N7	92	PHE	5.6
81	p0	86	PHE	5.6
53	M7	157	VAL	5.5

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Mol	Chain	Res	Type	RSRZ
81	p0	205	THR	5.5
81	p0	219	THR	5.5
3	S1	103	MET	5.5
22	D0	82	TYR	5.5
48	M1	127	PHE	5.5
6	S4	54	TYR	5.5
8	S6	77	LEU	5.5
33	e1	96	LYS	5.5
30	D8	7	VAL	5.5
63	N7	46	ILE	5.5
1	2	506	A	5.4
30	d8	43	ASN	5.4
42	L5	146	LEU	5.4
7	S5	154	ALA	5.4
7	S5	151	GLY	5.4
35	SM	16	ASP	5.4
33	e1	145	HIS	5.4
1	2	1705	C	5.4
30	D8	66	LEU	5.4
82	p2	2	SER	5.4
5	s3	180	GLY	5.4
14	c2	117	GLY	5.4
11	S9	181	ALA	5.4
34	sR	292	LEU	5.4
60	N4	70	LYS	5.3
21	C9	5	SER	5.3
13	c1	5	LEU	5.3
34	sR	33	LEU	5.3
18	C6	18	ALA	5.3
21	C9	28	LEU	5.3
1	2	717	C	5.3
18	C6	96	TYR	5.3
6	S4	44	LEU	5.3
36	5	2507	C	5.3
70	O4	23	VAL	5.3
27	D5	58	ARG	5.3
26	D4	31	ASN	5.2
26	D4	70	VAL	5.2
30	d8	7	VAL	5.2
26	D4	34	ASN	5.2
32	E0	61	SER	5.2
34	sR	82	SER	5.2

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Mol	Chain	Res	Type	RSRZ
82	p2	20	GLU	5.2
83	f	87	ARG	5.2
1	6	1694	A	5.2
5	s3	150	MET	5.2
12	C0	64	TYR	5.2
12	C0	66	TYR	5.2
83	f	115	ALA	5.2
21	C9	4	VAL	5.2
36	1	1568	U	5.2
1	2	716	C	5.1
36	1	1563	C	5.1
34	SR	83	ALA	5.1
3	S1	59	ASP	5.1
18	C6	52	LEU	5.1
7	s5	137	ILE	5.1
36	5	1568	U	5.1
82	p1	11	ALA	5.1
1	2	1707	A	5.1
35	sM	82	THR	5.1
3	S1	50	LYS	5.1
33	E1	87	THR	5.1
34	sR	121	MET	5.1
18	c6	44	LEU	5.1
74	o8	26	LYS	5.1
55	M9	181	ARG	5.1
34	sR	301	LEU	5.1
8	s6	169	TYR	5.1
34	SR	43	ILE	5.1
58	N2	33	TYR	5.1
1	2	1690	G	5.1
80	m2	74	GLN	5.1
5	S3	218	LEU	5.1
6	s4	183	VAL	5.1
11	S9	141	VAL	5.1
13	C1	156	PHE	5.0
5	s3	176	LEU	5.0
14	C2	82	PRO	5.0
34	sR	170	ILE	5.0
63	n7	96	VAL	5.0
81	p0	70	LEU	5.0
36	1	1569	U	5.0
21	C9	71	VAL	5.0

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Mol	Chain	Res	Type	RSRZ
55	M9	186	LYS	5.0
11	S9	138	LYS	5.0
36	5	2539	C	5.0
27	d5	51	LEU	5.0
14	c2	106	ILE	5.0
82	p2	1	MET	5.0
5	S3	143	ARG	5.0
34	sR	213	SER	5.0
27	D5	60	VAL	5.0
3	S1	92	GLN	5.0
12	c0	57	THR	5.0
83	f	18	THR	5.0
80	m2	19	LYS	5.0
32	e0	51	ASN	4.9
13	C1	152	GLN	4.9
18	C6	68	ARG	4.9
15	C3	23	PRO	4.9
1	6	1695	G	4.9
18	C6	39	VAL	4.9
34	sR	71	CYS	4.9
34	SR	42	LEU	4.9
1	2	1059	U	4.9
14	C2	32	LEU	4.9
18	C6	116	LEU	4.9
34	SR	81	LEU	4.9
7	s5	68	ILE	4.9
12	C0	1	MET	4.9
82	p2	26	LEU	4.9
33	E1	86	THR	4.9
3	S1	90	GLU	4.9
7	S5	68	ILE	4.9
83	f	90	TYR	4.9
36	1	2507	C	4.9
55	M9	182	ASP	4.9
18	C6	7	VAL	4.9
1	2	1686	C	4.9
7	s5	145	ASP	4.9
34	sR	166	SER	4.9
11	S9	36	LEU	4.8
34	sR	72	THR	4.8
7	S5	199	ILE	4.8
31	d9	27	HIS	4.8

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Mol	Chain	Res	Type	RSRZ
33	e1	146	SER	4.8
18	c6	143	ARG	4.8
34	sR	253	ALA	4.8
2	S0	201	LEU	4.8
6	S4	111	VAL	4.8
14	c2	28	LEU	4.8
14	c2	61	VAL	4.8
29	d7	33	LEU	4.8
27	D5	88	ILE	4.8
14	c2	104	ALA	4.8
21	C9	50	ALA	4.8
15	C3	25	TRP	4.8
2	S0	98	ILE	4.8
48	M1	96	PHE	4.8
60	N4	81	PRO	4.8
81	p0	191	TYR	4.8
27	d5	89	ILE	4.8
63	N7	26	VAL	4.8
7	S5	137	ILE	4.8
26	D4	6	THR	4.8
33	e1	87	THR	4.8
20	C8	146	ALA	4.8
83	f	105	MET	4.8
34	sR	61	PHE	4.7
7	s5	130	ILE	4.7
7	S5	86	GLN	4.7
21	C9	104	VAL	4.7
1	2	1700	C	4.7
63	n7	68	ILE	4.7
17	c5	52	LYS	4.7
26	D4	4	ALA	4.7
33	e1	98	VAL	4.7
5	s3	152	PHE	4.7
32	E0	6	GLY	4.7
7	S5	100	ASN	4.7
34	SR	46	LYS	4.7
63	N7	42	LEU	4.7
33	e1	110	ALA	4.7
42	L5	145	PHE	4.7
82	p1	6	ALA	4.7
60	n4	70	LYS	4.7
4	s2	89	GLN	4.7

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Mol	Chain	Res	Type	RSRZ
1	2	1704	U	4.7
27	D5	97	LYS	4.7
1	2	1711	C	4.7
25	D3	107	PHE	4.7
71	o5	120	ALA	4.7
27	D5	67	ASP	4.7
30	d8	66	LEU	4.7
34	sR	157	VAL	4.7
21	C9	92	LYS	4.7
34	SR	115	ILE	4.7
3	S1	93	GLY	4.7
60	N4	73	ARG	4.7
1	6	678	A	4.7
3	S1	86	LEU	4.7
3	S1	55	LYS	4.7
6	S4	64	ILE	4.7
82	p2	7	LEU	4.7
29	D7	51	GLN	4.6
21	c9	18	TYR	4.6
1	2	714	G	4.6
83	f	136	VAL	4.6
12	C0	24	LYS	4.6
47	M0	36	LEU	4.6
42	L5	95	TRP	4.6
22	D0	84	MET	4.6
80	m2	11	PRO	4.6
34	SR	34	LEU	4.6
1	2	718	U	4.6
5	S3	25	PHE	4.6
70	O4	93	PHE	4.6
22	d0	78	THR	4.6
33	e1	84	VAL	4.6
83	f	152	GLU	4.6
18	C6	54	LEU	4.6
34	sR	310	ILE	4.6
83	f	148	ILE	4.6
12	C0	62	GLN	4.6
15	C3	62	GLN	4.6
6	s4	39	ARG	4.6
30	D8	44	VAL	4.6
33	e1	86	THR	4.6
34	sR	227	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
78	q2	106	PHE	4.6
6	S4	65	LEU	4.6
30	D8	67	ARG	4.6
14	c2	121	VAL	4.6
20	C8	22	VAL	4.6
70	O4	21	LYS	4.6
19	C7	60	ARG	4.6
26	D4	35	VAL	4.6
82	p1	36	PRO	4.6
5	s3	153	ALA	4.6
16	C4	98	GLY	4.6
60	n4	132	GLY	4.6
5	s3	138	VAL	4.6
14	c2	63	VAL	4.6
83	f	156	THR	4.6
18	C6	12	LYS	4.6
15	C3	54	LEU	4.6
19	C7	2	GLY	4.6
14	C2	59	LEU	4.6
82	p1	19	ILE	4.5
60	N4	66	GLU	4.5
12	c0	93	GLN	4.5
28	D6	44	ILE	4.5
14	c2	20	ALA	4.5
45	l8	121	SER	4.5
34	sR	79	TYR	4.5
33	E1	145	HIS	4.5
42	L5	51	LEU	4.5
51	m5	6	TYR	4.5
6	S4	8	HIS	4.5
6	S4	66	MET	4.5
11	S9	140	ILE	4.5
1	6	1228	G	4.5
55	M9	51	VAL	4.5
8	S6	175	ILE	4.5
22	d0	76	SER	4.5
26	D4	67	GLY	4.5
80	m2	18	VAL	4.5
70	o4	57	LEU	4.5
82	p1	31	ASN	4.5
6	S4	90	ILE	4.5
42	L5	64	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
6	S4	56	LEU	4.5
20	c8	18	LEU	4.5
35	SM	19	VAL	4.4
81	p0	188	VAL	4.4
18	C6	13	LYS	4.4
3	S1	46	THR	4.4
29	D7	41	LEU	4.4
6	s4	15	PRO	4.4
14	C2	122	VAL	4.4
60	n4	67	VAL	4.4
4	s2	96	THR	4.4
7	s5	36	ALA	4.4
32	e0	63	GLN	4.4
83	f	153	ALA	4.4
28	D6	62	TYR	4.4
16	C4	97	GLY	4.4
10	S8	151	LYS	4.4
35	SM	18	VAL	4.4
81	p0	87	VAL	4.4
61	N5	24	LEU	4.4
13	C1	154	ALA	4.4
5	s3	184	ILE	4.4
7	S5	153	GLY	4.4
31	d9	29	GLY	4.4
3	S1	54	LEU	4.4
74	o8	43	PHE	4.4
7	S5	54	LYS	4.4
43	l6	129	GLU	4.4
1	2	656	G	4.4
14	c2	41	LEU	4.4
60	N4	69	LYS	4.4
82	p1	34	ASN	4.4
9	S7	98	ILE	4.4
34	sR	254	ALA	4.4
5	s3	142	LEU	4.4
6	S4	123	LEU	4.4
18	c6	36	ILE	4.4
16	C4	39	ILE	4.4
28	d6	69	ASN	4.4
30	D8	28	VAL	4.4
83	f	151	LYS	4.4
3	S1	101	HIS	4.4

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Mol	Chain	Res	Type	RSRZ
22	d0	77	LYS	4.4
34	SR	181	TRP	4.3
35	SM	97	THR	4.3
11	S9	110	GLN	4.3
80	m2	10	PRO	4.3
45	L8	116	VAL	4.3
55	M9	50	ILE	4.3
63	N7	136	PHE	4.3
35	SM	90	ALA	4.3
48	M1	66	ALA	4.3
63	N7	70	PRO	4.3
30	d8	44	VAL	4.3
18	C6	49	TYR	4.3
5	s3	151	LYS	4.3
33	e1	99	LYS	4.3
7	s5	90	ILE	4.3
26	D4	26	ASP	4.3
35	sM	52	PRO	4.3
12	C0	2	LEU	4.3
34	sR	211	ILE	4.3
80	m2	157	ASP	4.3
7	s5	198	LEU	4.3
21	C9	3	GLY	4.3
3	S1	98	THR	4.3
6	S4	101	LEU	4.3
33	E1	130	VAL	4.3
67	O1	14	ILE	4.3
33	e1	90	LYS	4.3
21	C9	8	ASP	4.3
1	2	1691	A	4.3
3	S1	53	GLY	4.3
38	4	158	U	4.3
11	S9	180	LYS	4.3
12	C0	23	ALA	4.3
74	o8	45	VAL	4.3
18	C6	65	ILE	4.2
18	c6	114	ARG	4.2
22	d0	98	GLN	4.2
18	C6	40	GLU	4.2
7	S5	165	LEU	4.2
12	c0	67	THR	4.2
45	l8	192	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
7	s5	152	GLY	4.2
74	o8	2	ALA	4.2
32	e0	53	LYS	4.2
7	S5	53	VAL	4.2
18	C6	36	ILE	4.2
21	C9	2	PRO	4.2
32	E0	54	ARG	4.2
36	1	2506	U	4.2
16	C4	47	LYS	4.2
6	S4	226	PHE	4.2
17	c5	101	ALA	4.2
7	s5	43	PHE	4.2
18	c6	90	VAL	4.2
18	c6	29	ILE	4.2
76	Q0	77	ILE	4.2
83	f	11	ALA	4.2
2	S0	189	VAL	4.2
12	C0	25	LYS	4.2
26	D4	97	ALA	4.2
18	C6	105	LEU	4.2
20	c8	15	LEU	4.2
34	SR	102	ARG	4.2
7	S5	43	PHE	4.2
25	D3	130	VAL	4.2
30	d8	32	PHE	4.2
18	C6	123	ARG	4.2
11	S9	134	ILE	4.2
17	c5	133	ALA	4.2
34	sR	294	TRP	4.2
67	O1	20	LEU	4.2
58	N2	108	TYR	4.2
32	E0	55	ARG	4.1
32	E0	56	MET	4.1
21	C9	108	LEU	4.1
82	p1	33	ALA	4.1
33	e1	88	PRO	4.1
1	6	662	U	4.1
5	s3	149	ALA	4.1
18	C6	15	SER	4.1
60	n4	97	LYS	4.1
81	p0	26	PHE	4.1
5	S3	216	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
21	C9	9	VAL	4.1
82	p1	13	ILE	4.1
17	c5	10	ARG	4.1
34	sR	92	TRP	4.1
3	S1	28	GLU	4.1
29	D7	33	LEU	4.1
7	S5	96	SER	4.1
10	S8	109	PHE	4.1
17	c5	136	SER	4.1
6	S4	55	ALA	4.1
81	p0	221	ALA	4.1
7	s5	48	PHE	4.1
12	C0	44	LYS	4.1
15	C3	59	GLY	4.1
33	E1	88	PRO	4.1
27	D5	69	LEU	4.1
1	2	1706	C	4.1
36	1	1762	C	4.1
58	N2	27	VAL	4.1
3	S1	140	ILE	4.1
34	SR	213	SER	4.1
34	sR	134	TRP	4.1
34	sR	243	LEU	4.1
68	O2	128	LEU	4.1
2	s0	166	GLY	4.1
14	c2	21	GLU	4.1
83	f	42	VAL	4.1
40	L3	387	LEU	4.1
42	L5	131	LEU	4.1
32	E0	60	PRO	4.1
63	N7	118	PHE	4.1
28	d6	45	VAL	4.1
3	S1	217	LEU	4.1
6	S4	38	LEU	4.1
7	S5	122	ASN	4.1
27	D5	98	GLN	4.1
28	D6	20	PRO	4.1
56	N0	2	ALA	4.1
3	s1	89	ASP	4.1
7	s5	156	ARG	4.1
42	L5	144	VAL	4.1
60	n4	131	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
11	S9	128	LEU	4.1
27	D5	89	ILE	4.1
33	e1	100	LEU	4.1
26	D4	12	VAL	4.0
12	c0	66	TYR	4.0
1	2	261	U	4.0
6	S4	199	GLU	4.0
18	c6	11	GLY	4.0
34	SR	262	VAL	4.0
34	SR	313	TRP	4.0
14	c2	113	ARG	4.0
14	c2	52	LEU	4.0
16	C4	105	LEU	4.0
19	C7	101	ASN	4.0
6	S4	102	VAL	4.0
15	C3	61	THR	4.0
29	D7	58	SER	4.0
63	N7	91	ALA	4.0
5	s3	178	ARG	4.0
11	S9	3	ARG	4.0
18	C6	47	LYS	4.0
55	M9	52	LYS	4.0
21	c9	55	TYR	4.0
21	C9	6	VAL	4.0
13	C1	155	LYS	4.0
7	S5	190	ILE	4.0
1	2	134	U	4.0
4	s2	84	LYS	4.0
7	S5	116	HIS	4.0
45	L8	58	VAL	4.0
83	f	24	SER	4.0
53	M7	163	LYS	4.0
30	d8	10	ALA	4.0
36	5	1566	A	4.0
45	l8	162	LEU	4.0
47	m0	221	ALA	4.0
3	S1	95	ASN	4.0
5	S3	87	TYR	4.0
5	s3	179	GLN	4.0
6	S4	99	PHE	4.0
17	c5	5	VAL	4.0
45	l8	196	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
43	L6	130	ILE	4.0
60	N4	82	ILE	4.0
7	s5	69	PHE	4.0
11	S9	158	PHE	4.0
15	c3	40	TYR	4.0
45	l8	120	LYS	4.0
14	c2	59	LEU	4.0
27	D5	100	ILE	4.0
83	f	86	LYS	4.0
14	c2	40	GLY	4.0
2	S0	122	ILE	4.0
27	D5	81	ARG	4.0
27	d5	94	LYS	4.0
7	S5	97	LEU	4.0
26	D4	18	LEU	4.0
7	S5	212	LYS	4.0
15	C3	26	PHE	4.0
29	D7	32	PHE	4.0
58	n2	14	THR	4.0
34	SR	35	SER	4.0
30	D8	43	ASN	3.9
55	M9	185	LEU	3.9
36	1	1239	C	3.9
58	N2	93	ILE	3.9
14	c2	64	SER	3.9
3	S1	96	LEU	3.9
5	s3	143	ARG	3.9
9	S7	58	LEU	3.9
18	C6	38	LEU	3.9
30	D8	6	PRO	3.9
6	S4	143	ASP	3.9
11	S9	156	ILE	3.9
21	C9	94	ILE	3.9
34	sR	123	ILE	3.9
83	f	43	ASP	3.9
33	e1	95	HIS	3.9
4	s2	94	GLN	3.9
5	S3	183	GLY	3.9
7	s5	93	LEU	3.9
18	C6	132	LYS	3.9
32	e0	55	ARG	3.9
35	SM	98	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
51	m5	2	GLY	3.9
27	D5	101	TYR	3.9
7	s5	138	THR	3.9
17	c5	135	THR	3.9
28	D6	45	VAL	3.9
29	D7	70	LYS	3.9
34	SR	74	THR	3.9
30	D8	9	LEU	3.9
34	sR	28	GLY	3.9
34	sR	81	LEU	3.9
82	p2	45	PHE	3.9
7	S5	87	CYS	3.9
35	SM	86	ASN	3.9
80	m2	121	GLU	3.9
81	p0	20	GLU	3.9
34	sR	163	ASP	3.9
34	sR	311	ARG	3.9
42	L5	101	THR	3.9
27	D5	61	SER	3.9
7	S5	36	ALA	3.9
11	S9	144	PRO	3.9
18	C6	5	PRO	3.9
80	m2	90	ALA	3.9
20	c8	144	ARG	3.9
63	N7	23	VAL	3.9
3	S1	100	PHE	3.9
13	C1	3	THR	3.9
33	e1	82	LYS	3.9
53	M7	158	ALA	3.9
53	M7	184	ALA	3.9
60	n4	85	ALA	3.9
63	N7	65	ARG	3.9
13	C1	68	GLY	3.9
19	C7	63	LYS	3.9
83	f	23	CYS	3.9
20	c8	20	THR	3.9
42	L5	89	THR	3.9
34	sR	204	ALA	3.9
82	p2	41	TRP	3.9
36	1	1579	C	3.9
7	S5	72	HIS	3.9
13	C1	148	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
45	l8	155	ASN	3.9
30	D8	27	GLN	3.9
70	o4	33	GLN	3.9
10	S8	179	CYS	3.9
83	f	142	MET	3.9
22	d0	79	TRP	3.9
26	D4	69	SER	3.9
82	p2	22	SER	3.9
35	SM	106	VAL	3.9
1	6	659	C	3.9
25	D3	89	ASN	3.9
6	S4	110	ALA	3.9
9	s7	58	LEU	3.9
9	s7	93	LEU	3.9
14	C2	37	VAL	3.9
42	L5	122	VAL	3.9
16	C4	14	PHE	3.9
9	S7	33	GLU	3.9
21	C9	84	LYS	3.9
81	p0	220	ILE	3.9
1	6	1199	G	3.9
1	2	1687	U	3.8
45	l8	197	VAL	3.8
18	C6	29	ILE	3.8
26	D4	32	ARG	3.8
7	S5	111	VAL	3.8
82	p1	38	GLU	3.8
11	S9	147	MET	3.8
7	s5	62	VAL	3.8
83	f	134	LEU	3.8
36	1	2502	A	3.8
1	6	658	C	3.8
49	m3	191	ALA	3.8
18	c6	46	PHE	3.8
22	D0	69	LYS	3.8
48	M1	104	PHE	3.8
29	D7	38	PRO	3.8
36	5	1350	A	3.8
18	C6	57	LEU	3.8
70	O4	79	SER	3.8
81	p0	25	LEU	3.8
42	L5	90	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
7	S5	91	GLU	3.8
7	S5	132	VAL	3.8
19	C7	62	GLN	3.8
30	D8	5	THR	3.8
36	1	1955	U	3.8
66	o0	7	GLN	3.8
6	S4	167	GLY	3.8
5	s3	134	CYS	3.8
2	S0	99	ALA	3.8
8	S6	79	LYS	3.8
18	C6	14	LYS	3.8
83	f	106	ASP	3.8
6	S4	208	VAL	3.8
45	L8	182	GLY	3.8
70	O4	73	SER	3.8
36	1	2205	U	3.8
70	O4	72	VAL	3.8
34	sR	263	PHE	3.8
34	SR	71	CYS	3.8
83	f	81	GLU	3.8
12	c0	43	ILE	3.8
26	d4	18	LEU	3.8
36	5	1571	A	3.8
33	e1	78	LYS	3.8
1	6	1709	C	3.8
18	C6	6	SER	3.8
32	e0	49	LEU	3.8
34	sR	112	SER	3.8
22	d0	64	LYS	3.8
80	m2	58	ASP	3.8
58	n2	11	ILE	3.8
35	SM	99	LYS	3.7
28	D6	63	ALA	3.7
63	N7	45	GLY	3.7
80	m2	57	GLU	3.7
12	C0	61	TRP	3.7
31	d9	5	ASN	3.7
27	D5	51	LEU	3.7
18	c6	140	LYS	3.7
5	s3	177	MET	3.7
34	sR	26	SER	3.7
7	s5	153	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
34	sR	70	ASP	3.7
34	sR	90	ARG	3.7
51	m5	55	ALA	3.7
58	N2	92	TRP	3.7
14	c2	116	VAL	3.7
18	c6	19	VAL	3.7
15	C3	24	ALA	3.7
28	D6	46	GLU	3.7
3	s1	84	ILE	3.7
15	C3	50	ILE	3.7
27	D5	65	LEU	3.7
36	5	1764	U	3.7
21	C9	72	GLY	3.7
5	S3	144	ALA	3.7
6	S4	180	LEU	3.7
23	D1	34	ILE	3.7
34	sR	34	LEU	3.7
76	Q0	128	LYS	3.7
5	s3	182	LEU	3.7
16	C4	102	LEU	3.7
18	C6	117	LEU	3.7
34	sR	7	LEU	3.7
74	o8	54	LEU	3.7
2	s0	170	ILE	3.7
16	C4	13	VAL	3.7
63	N7	113	VAL	3.7
72	o6	2	THR	3.7
13	C1	4	GLU	3.7
33	e1	94	LYS	3.7
81	p0	19	LEU	3.7
5	S3	184	ILE	3.7
3	S1	225	VAL	3.7
11	S9	130	THR	3.7
27	d5	101	TYR	3.7
2	S0	97	PRO	3.7
9	S7	43	PHE	3.7
33	e1	79	LYS	3.7
58	n2	27	VAL	3.7
72	O6	99	ARG	3.7
7	s5	165	LEU	3.7
14	c2	103	LEU	3.7
18	C6	16	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
25	D3	132	LEU	3.7
35	SM	15	ALA	3.7
7	S5	121	ILE	3.7
18	c6	132	LYS	3.7
35	SM	105	LYS	3.7
11	S9	148	VAL	3.7
17	C5	76	VAL	3.7
21	c9	23	GLN	3.7
42	L5	63	GLN	3.7
1	6	1217	A	3.7
58	N2	80	THR	3.7
81	p0	16	ARG	3.7
14	C2	42	ALA	3.7
7	S5	61	TYR	3.7
34	sR	241	PHE	3.7
45	L8	67	ILE	3.7
23	D1	39	VAL	3.7
14	c2	96	GLN	3.7
30	d8	65	ARG	3.7
16	C4	77	THR	3.7
26	D4	30	PRO	3.7
34	sR	116	ASP	3.7
35	sM	123	ALA	3.7
27	D5	71	ILE	3.7
81	p0	51	VAL	3.7
47	M0	112	GLN	3.7
83	f	53	GLY	3.6
1	6	679	U	3.6
36	1	1764	U	3.6
3	S1	29	TRP	3.6
7	S5	67	PRO	3.6
2	S0	203	PHE	3.6
24	D2	25	VAL	3.6
34	sR	113	VAL	3.6
83	f	41	ILE	3.6
11	S9	112	GLN	3.6
30	D8	17	GLY	3.6
8	S6	80	ASN	3.6
6	S4	52	LEU	3.6
10	S8	141	ARG	3.6
11	S9	164	PHE	3.6
14	c2	118	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
27	D5	102	THR	3.6
60	N4	98	PRO	3.6
60	n4	83	THR	3.6
80	m2	13	PHE	3.6
81	p0	215	SER	3.6
80	m2	104	ASP	3.6
21	c9	25	GLN	3.6
70	O4	24	LYS	3.6
14	C2	28	LEU	3.6
12	c0	3	MET	3.6
31	D9	55	PHE	3.6
32	E0	2	ALA	3.6
34	SR	61	PHE	3.6
45	L8	131	ALA	3.6
47	M0	84	ALA	3.6
81	p0	60	ARG	3.6
5	s3	185	LYS	3.6
81	p0	69	ASP	3.6
45	l8	200	LEU	3.6
34	sR	224	ASN	3.6
3	S1	60	ALA	3.6
10	s8	200	LYS	3.6
81	p0	59	VAL	3.6
36	1	3275	U	3.6
63	N7	49	TYR	3.6
5	S3	185	LYS	3.6
13	C1	153	PHE	3.6
6	S4	181	VAL	3.6
15	C3	33	VAL	3.6
27	d5	92	ILE	3.6
7	S5	207	THR	3.6
14	c2	43	ARG	3.6
23	D1	55	LEU	3.6
30	D8	56	LEU	3.6
60	n4	133	THR	3.6
63	N7	132	SER	3.6
53	M7	165	VAL	3.6
7	s5	44	ASN	3.6
28	D6	69	ASN	3.6
7	S5	158	GLN	3.6
70	o4	21	LYS	3.6
10	S8	72	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
27	D5	36	ALA	3.6
35	SM	96	ARG	3.6
5	S3	142	LEU	3.6
7	S5	150	GLY	3.6
7	s5	129	PRO	3.6
78	Q2	104	LEU	3.6
81	p0	85	GLY	3.6
83	f	70	LEU	3.6
18	C6	109	PHE	3.6
83	f	12	ASP	3.6
20	C8	145	ARG	3.6
74	o8	73	LEU	3.6
2	S0	15	GLN	3.6
3	S1	138	PHE	3.6
17	c5	11	VAL	3.6
30	d8	13	ILE	3.6
34	sR	203	THR	3.6
66	o0	6	SER	3.6
81	p0	100	ILE	3.6
1	6	1700	C	3.6
7	s5	159	ALA	3.6
34	sR	23	LEU	3.6
45	L8	130	TYR	3.6
58	N2	28	PHE	3.6
7	S5	140	THR	3.6
21	C9	40	SER	3.6
63	n7	12	VAL	3.6
42	L5	77	ALA	3.6
63	n7	11	ALA	3.6
28	d6	68	TYR	3.6
31	d9	36	LEU	3.6
58	N2	89	LEU	3.6
18	c6	138	PHE	3.6
26	D4	58	PHE	3.6
26	D4	61	ARG	3.6
8	S6	91	GLU	3.6
16	C4	16	VAL	3.6
7	s5	141	GLY	3.6
30	d8	8	THR	3.6
81	p0	197	PHE	3.5
10	S8	67	TRP	3.5
12	c0	24	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
14	c2	42	ALA	3.5
34	sR	183	LEU	3.5
7	S5	92	ARG	3.5
42	l5	235	SER	3.5
17	C5	9	LYS	3.5
35	SM	83	LYS	3.5
11	S9	186	GLU	3.5
83	f	22	GLN	3.5
14	c2	110	ALA	3.5
20	C8	15	LEU	3.5
67	O1	71	LEU	3.5
55	M9	49	THR	3.5
60	N4	67	VAL	3.5
26	D4	22	GLN	3.5
16	C4	27	PHE	3.5
36	5	1016	C	3.5
18	C6	141	SER	3.5
34	sR	300	THR	3.5
82	p1	8	SER	3.5
34	SR	136	ILE	3.5
18	c6	89	LEU	3.5
24	D2	60	LYS	3.5
1	6	1708	U	3.5
83	f	131	GLY	3.5
12	C0	41	TYR	3.5
26	D4	3	ASP	3.5
29	d7	57	GLU	3.5
72	O6	100	HIS	3.5
23	D1	65	SER	3.5
32	E0	7	SER	3.5
34	sR	115	ILE	3.5
63	N7	25	ILE	3.5
72	o6	27	SER	3.5
2	S0	146	LEU	3.5
6	S4	67	GLN	3.5
53	M7	180	LYS	3.5
11	S9	135	ALA	3.5
32	e0	2	ALA	3.5
7	s5	31	GLU	3.5
31	d9	31	ILE	3.5
59	N3	2	SER	3.5
1	2	1712	A	3.5

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Mol	Chain	Res	Type	RSRZ
32	E0	44	PHE	3.5
5	s3	141	LYS	3.5
2	S0	170	ILE	3.5
4	s2	93	GLY	3.5
13	c1	2	SER	3.5
18	C6	51	PRO	3.5
27	D5	99	ALA	3.5
32	e0	52	GLY	3.5
63	N7	117	ALA	3.5
22	D0	83	GLU	3.5
51	m5	30	TYR	3.5
6	s4	208	VAL	3.5
16	c4	79	VAL	3.5
6	S4	23	LEU	3.5
14	c2	23	THR	3.5
17	c5	132	GLY	3.5
34	sR	293	ALA	3.5
27	d5	88	ILE	3.5
1	6	232	U	3.5
21	C9	62	ALA	3.5
23	D1	53	TYR	3.5
34	sR	35	SER	3.5
6	S4	9	LEU	3.5
17	c5	4	ALA	3.5
34	SR	80	ALA	3.5
2	S0	106	SER	3.5
6	S4	220	THR	3.5
18	C6	92	TYR	3.5
34	sR	171	SER	3.5
35	SM	17	VAL	3.5
6	S4	45	ILE	3.5
16	C4	41	ARG	3.5
21	C9	65	ILE	3.5
74	o8	51	LEU	3.5
12	C0	27	PHE	3.5
20	c8	73	MET	3.5
25	d3	60	GLU	3.4
83	f	133	ASP	3.4
21	C9	80	TYR	3.4
19	C7	120	SER	3.4
18	c6	26	LYS	3.4
20	c8	17	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
26	D4	7	ILE	3.4
26	D4	72	PHE	3.4
42	L5	203	HIS	3.4
21	c9	37	VAL	3.4
28	D6	65	PRO	3.4
1	2	711	U	3.4
3	S1	84	ILE	3.4
36	5	1565	G	3.4
18	C6	74	HIS	3.4
18	c6	18	ALA	3.4
27	D5	82	HIS	3.4
60	N4	71	ARG	3.4
2	S0	161	PRO	3.4
2	s0	164	ASN	3.4
22	d0	72	ASN	3.4
34	sR	240	VAL	3.4
80	m2	75	LEU	3.4
36	1	1567	U	3.4
66	o0	105	ALA	3.4
67	o1	82	GLU	3.4
61	N5	124	VAL	3.4
72	O6	57	LEU	3.4
83	f	120	LEU	3.4
6	s4	18	TRP	3.4
10	s8	176	SER	3.4
15	C3	51	GLY	3.4
31	d9	16	LYS	3.4
34	SR	27	ALA	3.4
63	N7	2	ALA	3.4
25	D3	133	LEU	3.4
63	N7	5	LEU	3.4
6	S4	79	ASP	3.4
34	sR	53	LYS	3.4
6	s4	184	THR	3.4
6	s4	102	VAL	3.4
15	C3	53	LEU	3.4
36	1	1564	U	3.4
36	1	2505	U	3.4
36	1	1581	C	3.4
81	p0	210	VAL	3.4
7	S5	90	ILE	3.4
14	c2	89	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
4	s2	95	ARG	3.4
42	L5	158	ARG	3.4
34	SR	308	ASN	3.4
34	SR	72	THR	3.4
23	D1	33	GLN	3.4
81	p0	63	ILE	3.4
20	c8	25	ASN	3.4
55	M9	23	TRP	3.4
7	s5	70	VAL	3.4
14	C2	52	LEU	3.4
55	M9	24	LEU	3.4
22	D0	81	THR	3.4
31	d9	20	GLN	3.4
48	M1	65	ILE	3.4
9	S7	134	GLU	3.4
36	1	1243	G	3.4
36	1	2503	G	3.4
5	s3	175	VAL	3.4
7	S5	134	VAL	3.4
31	d9	40	ARG	3.4
34	SR	252	LEU	3.4
35	sM	119	ALA	3.4
63	N7	95	VAL	3.4
7	s5	89	ILE	3.4
18	c6	85	ILE	3.4
26	D4	2	SER	3.4
40	L3	49	TYR	3.4
7	S5	75	GLY	3.4
5	S3	186	VAL	3.4
7	S5	107	LYS	3.4
14	c2	128	ALA	3.4
27	d5	90	LYS	3.4
51	m5	48	ALA	3.4
63	N7	133	LYS	3.4
81	p0	192	ASP	3.4
6	S4	82	TYR	3.4
28	d6	59	TYR	3.4
58	n2	33	TYR	3.4
11	s9	184	SER	3.4
14	c2	127	GLY	3.4
36	5	2540	A	3.4
6	S4	48	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
6	S4	225	VAL	3.4
7	S5	62	VAL	3.4
25	D3	104	LEU	3.4
30	d8	54	LEU	3.4
42	L5	83	LEU	3.4
6	S4	228	ILE	3.4
48	M1	95	ASN	3.4
4	s2	181	SER	3.4
22	d0	80	GLU	3.4
7	S5	94	THR	3.4
36	1	1349	G	3.4
10	S8	168	CYS	3.4
22	D0	85	ARG	3.4
22	d0	68	ARG	3.4
83	f	137	THR	3.4
8	s6	162	VAL	3.3
18	C6	19	VAL	3.3
34	sR	104	VAL	3.3
82	p2	46	ALA	3.3
2	S0	197	ILE	3.3
42	L5	129	TYR	3.3
70	O4	64	THR	3.3
6	S4	88	ASP	3.3
21	c9	24	ARG	3.3
6	S4	80	THR	3.3
8	s6	163	THR	3.3
14	c2	30	VAL	3.3
18	c6	39	VAL	3.3
34	sR	111	MET	3.3
45	l8	238	LEU	3.3
51	M5	22	LEU	3.3
82	p1	3	THR	3.3
1	2	658	C	3.3
15	C3	37	ILE	3.3
7	S5	181	GLU	3.3
82	p2	18	GLU	3.3
7	s5	158	GLN	3.3
39	L2	253	GLN	3.3
81	p0	217	VAL	3.3
25	D3	47	SER	3.3
1	6	794	U	3.3
7	S5	25	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
11	S9	116	LEU	3.3
18	c6	54	LEU	3.3
7	S5	95	ASN	3.3
83	f	135	MET	3.3
26	D4	33	ALA	3.3
6	s4	54	TYR	3.3
7	S5	55	ASP	3.3
18	C6	44	LEU	3.3
6	S4	89	VAL	3.3
7	S5	162	VAL	3.3
30	d8	45	LYS	3.3
51	m5	147	ARG	3.3
3	s1	141	ALA	3.3
7	S5	129	PRO	3.3
18	C6	17	THR	3.3
3	S1	89	ASP	3.3
21	C9	64	HIS	3.3
7	S5	106	LYS	3.3
30	D8	59	SER	3.3
74	o8	36	LYS	3.3
13	c1	116	ARG	3.3
14	c2	62	LEU	3.3
3	S1	38	PHE	3.3
34	SR	263	PHE	3.3
21	C9	29	GLU	3.3
34	sR	36	ALA	3.3
53	M7	156	ALA	3.3
11	s9	6	ARG	3.3
29	D7	42	ASN	3.3
60	n4	104	ASN	3.3
7	s5	57	SER	3.3
5	s3	136	VAL	3.3
13	c1	117	VAL	3.3
34	sR	74	THR	3.3
81	p0	187	VAL	3.3
2	s0	173	ILE	3.3
3	S1	102	GLY	3.3
30	D8	45	LYS	3.3
11	S9	126	ARG	3.3
5	s3	25	PHE	3.3
11	S9	5	PRO	3.3
31	d9	28	THR	3.3

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Mol	Chain	Res	Type	RSRZ
42	L5	55	PHE	3.3
34	SR	214	ALA	3.3
2	S0	182	LEU	3.3
61	N5	123	TYR	3.3
7	s5	133	VAL	3.3
18	c6	55	VAL	3.3
32	E0	45	VAL	3.3
74	O8	43	PHE	3.3
36	1	1572	U	3.3
82	p2	25	LYS	3.3
82	p1	20	GLU	3.3
82	p2	6	ALA	3.3
34	SR	225	LEU	3.3
15	C3	27	LYS	3.3
34	sR	46	LYS	3.3
36	1	1270	A	3.2
1	2	238	U	3.2
1	2	1370	U	3.2
17	c5	80	MET	3.2
10	S8	43	ILE	3.2
81	p0	24	SER	3.2
45	l8	194	THR	3.2
6	s4	103	TYR	3.2
9	S7	41	LEU	3.2
48	M1	167	TYR	3.2
10	s8	46	VAL	3.2
6	S4	57	ASN	3.2
6	s4	101	LEU	3.2
11	s9	146	PHE	3.2
12	c0	27	PHE	3.2
14	c2	115	VAL	3.2
18	c6	48	VAL	3.2
42	L5	147	ASP	3.2
63	n7	13	VAL	3.2
2	S0	23	HIS	3.2
2	S0	198	MET	3.2
21	C9	100	ILE	3.2
67	O1	60	TRP	3.2
67	o1	60	TRP	3.2
74	o8	69	LEU	3.2
11	S9	12	TYR	3.2
16	C4	81	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
36	1	1240	A	3.2
63	N7	131	PHE	3.2
1	6	1697	G	3.2
2	S0	84	ARG	3.2
6	S4	11	ARG	3.2
13	C1	38	ALA	3.2
27	d5	69	LEU	3.2
34	sR	42	LEU	3.2
46	l9	191	LEU	3.2
58	n2	89	LEU	3.2
30	d8	49	ARG	3.2
19	C7	110	VAL	3.2
30	d8	55	VAL	3.2
48	M1	11	ASP	3.2
6	S4	162	ILE	3.2
48	M1	125	MET	3.2
6	s4	92	LEU	3.2
13	C1	116	ARG	3.2
39	L2	71	LEU	3.2
42	L5	150	LEU	3.2
5	S3	152	PHE	3.2
17	c5	126	VAL	3.2
21	C9	14	PHE	3.2
28	D6	8	ASN	3.2
10	S8	66	SER	3.2
30	d8	48	VAL	3.2
34	sR	6	VAL	3.2
1	2	657	U	3.2
6	S4	22	LYS	3.2
27	d5	105	THR	3.2
36	1	1351	U	3.2
67	O1	61	LYS	3.2
28	D6	82	ARG	3.2
33	E1	129	GLY	3.2
2	S0	199	PRO	3.2
6	s4	35	PRO	3.2
10	S8	145	ALA	3.2
29	D7	37	CYS	3.2
51	m5	45	PRO	3.2
5	s3	186	VAL	3.2
7	S5	133	VAL	3.2
14	c2	25	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
74	o8	42	LYS	3.2
14	c2	36	LEU	3.2
28	d6	44	ILE	3.2
34	sR	73	LEU	3.2
72	o6	9	ILE	3.2
70	O4	33	GLN	3.2
21	C9	83	ALA	3.2
48	M1	102	PHE	3.2
7	s5	41	LYS	3.2
48	M1	153	LYS	3.2
51	M5	30	TYR	3.2
7	S5	144	GLU	3.2
33	E1	146	SER	3.2
34	sR	124	SER	3.2
6	S4	25	GLY	3.2
11	S9	143	ILE	3.2
30	d8	24	GLY	3.2
61	N5	82	LEU	3.2
18	c6	13	LYS	3.2
34	SR	36	ALA	3.2
83	f	65	PHE	3.2
6	S4	15	PRO	3.2
81	p0	80	VAL	3.2
81	p0	214	VAL	3.2
4	S2	144	TRP	3.2
5	s3	103	GLU	3.2
30	d8	67	ARG	3.2
3	S1	207	LEU	3.2
22	d0	121	ASN	3.2
28	D6	83	ILE	3.2
39	L2	104	LEU	3.2
42	L5	247	ILE	3.2
45	L8	152	LEU	3.2
34	sR	201	THR	3.2
74	o8	44	LYS	3.2
34	SR	78	ALA	3.2
45	L8	198	ALA	3.2
26	D4	90	ARG	3.2
32	E0	35	TYR	3.2
51	m5	26	ARG	3.2
8	s6	216	LEU	3.2
10	S8	21	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
6	S4	252	ARG	3.2
7	S5	131	GLN	3.2
46	L9	31	ARG	3.2
18	c6	124	PRO	3.2
6	S4	261	LEU	3.2
15	C3	66	ILE	3.2
21	c9	15	ILE	3.2
47	M0	87	LEU	3.2
48	M1	83	GLY	3.2
16	C4	34	SER	3.2
20	C8	21	ASN	3.2
34	SR	196	ASN	3.2
6	S4	60	GLU	3.2
1	6	1701	A	3.2
7	S5	209	TYR	3.2
12	c0	74	GLU	3.2
75	o9	2	ALA	3.2
51	m5	129	TYR	3.2
81	p0	18	TYR	3.2
6	s4	207	LEU	3.1
7	S5	211	ILE	3.1
9	S7	77	LEU	3.1
21	C9	103	LYS	3.1
42	L5	181	PRO	3.1
10	S8	181	GLY	3.1
82	p1	21	ILE	3.1
63	N7	135	ARG	3.1
28	d6	40	ALA	3.1
81	p0	68	SER	3.1
19	c7	25	THR	3.1
20	c8	140	THR	3.1
29	D7	44	THR	3.1
6	s4	164	LEU	3.1
7	s5	58	LEU	3.1
34	SR	47	LEU	3.1
34	sR	210	LEU	3.1
5	S3	173	ARG	3.1
61	n5	142	ILE	3.1
83	f	139	ILE	3.1
3	S1	30	PHE	3.1
11	S9	29	LYS	3.1
12	C0	75	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
21	C9	66	TYR	3.1
33	e1	92	LYS	3.1
70	O4	71	THR	3.1
3	s1	140	ILE	3.1
11	s9	5	PRO	3.1
6	S4	18	TRP	3.1
58	N2	107	PHE	3.1
33	E1	90	LYS	3.1
6	S4	259	GLN	3.1
28	D6	64	LEU	3.1
34	sR	291	SER	3.1
45	L8	93	LEU	3.1
2	S0	192	THR	3.1
7	s5	126	ASP	3.1
49	m3	182	ILE	3.1
82	p2	43	ASP	3.1
29	d7	32	PHE	3.1
20	C8	73	MET	3.1
67	o1	12	TYR	3.1
26	D4	40	LEU	3.1
42	l5	236	LEU	3.1
13	C1	42	PHE	3.1
60	n4	84	GLY	3.1
67	o1	75	ILE	3.1
13	c1	59	PRO	3.1
7	S5	108	LEU	3.1
11	s9	48	GLN	3.1
13	c1	138	ASN	3.1
16	c4	27	PHE	3.1
63	N7	72	ILE	3.1
11	S9	122	VAL	3.1
14	c2	67	THR	3.1
17	c5	125	PRO	3.1
21	C9	131	ASP	3.1
25	D3	72	VAL	3.1
25	D3	124	VAL	3.1
27	d5	54	VAL	3.1
29	D7	45	THR	3.1
74	o8	55	VAL	3.1
42	L5	162	ALA	3.1
17	c5	104	GLN	3.1
26	d4	68	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
34	SR	62	LYS	3.1
17	c5	129	GLY	3.1
6	S4	76	VAL	3.1
7	S5	139	ASN	3.1
7	s5	83	ARG	3.1
7	S5	161	ASP	3.1
14	c2	65	SER	3.1
16	C4	79	VAL	3.1
42	L5	124	GLU	3.1
83	f	72	ASP	3.1
27	d5	59	TYR	3.1
34	SR	73	LEU	3.1
35	sM	67	GLY	3.1
60	n4	134	GLN	3.1
12	c0	59	PHE	3.1
7	S5	128	ASN	3.1
18	C6	55	VAL	3.1
33	e1	134	ASN	3.1
34	sR	156	VAL	3.1
13	C1	151	LYS	3.1
19	C7	86	PRO	3.1
83	f	16	SER	3.1
83	f	38	PRO	3.1
14	C2	128	ALA	3.1
80	m2	82	ALA	3.1
82	p1	30	THR	3.1
82	p1	32	ALA	3.1
16	C4	115	ILE	3.1
28	D6	85	ARG	3.1
4	s2	121	VAL	3.1
28	D6	50	VAL	3.1
83	f	85	VAL	3.1
21	C9	27	LYS	3.1
33	e1	97	LYS	3.1
14	C2	26	ASP	3.1
36	1	2504	U	3.1
59	n3	2	SER	3.1
63	N7	82	PRO	3.1
6	S4	182	TYR	3.1
82	p1	41	TRP	3.1
2	S0	107	PHE	3.1
16	c4	112	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
34	sR	169	ILE	3.1
7	S5	225	ARG	3.1
10	S8	73	SER	3.1
34	sR	251	TRP	3.1
35	SM	175	ASP	3.1
36	5	1570	U	3.1
42	L5	62	CYS	3.1
70	O4	62	TYR	3.1
46	L9	144	ILE	3.1
81	p0	73	PHE	3.1
19	C7	74	GLN	3.1
60	N4	79	GLN	3.1
60	N4	65	GLU	3.1
12	c0	68	LEU	3.1
18	C6	89	LEU	3.1
29	d7	24	LEU	3.1
36	1	1571	A	3.1
63	N7	122	HIS	3.1
29	d7	38	PRO	3.0
41	l4	26	PHE	3.0
16	C4	112	ILE	3.0
74	o8	32	ASN	3.0
83	f	88	ASN	3.0
21	C9	39	THR	3.0
30	D8	55	VAL	3.0
1	6	1699	G	3.0
21	C9	132	LEU	3.0
29	D7	50	ALA	3.0
51	m5	37	HIS	3.0
63	N7	124	ALA	3.0
74	o8	35	GLY	3.0
7	s5	161	ASP	3.0
7	s5	168	VAL	3.0
17	C5	104	GLN	3.0
60	n4	95	SER	3.0
27	d5	102	THR	3.0
34	sR	309	VAL	3.0
9	S7	126	LEU	3.0
25	D3	57	LEU	3.0
18	C6	79	TYR	3.0
18	c6	129	PHE	3.0
48	M1	64	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
21	C9	41	SER	3.0
22	d0	120	SER	3.0
63	N7	123	GLN	3.0
70	o4	58	ARG	3.0
42	L5	254	LYS	3.0
42	L5	180	PHE	3.0
45	L8	91	PHE	3.0
20	c8	129	TRP	3.0
43	L6	135	VAL	3.0
22	d0	63	LEU	3.0
48	M1	17	LEU	3.0
7	S5	125	THR	3.0
32	E0	48	THR	3.0
11	s9	19	TYR	3.0
42	L5	119	TYR	3.0
83	f	147	ALA	3.0
14	C2	108	ARG	3.0
25	D3	59	ILE	3.0
34	sR	16	HIS	3.0
55	M9	173	ARG	3.0
7	s5	33	VAL	3.0
30	D8	15	VAL	3.0
81	p0	28	VAL	3.0
7	S5	175	LEU	3.0
10	S8	143	TRP	3.0
11	S9	97	LEU	3.0
35	SM	95	SER	3.0
63	N7	101	PHE	3.0
34	sR	284	ALA	3.0
1	6	1227	A	3.0
66	O0	59	TYR	3.0
74	o8	52	TYR	3.0
83	f	71	GLU	3.0
25	D3	140	LYS	3.0
80	m2	156	VAL	3.0
8	s6	147	LEU	3.0
21	c9	22	LEU	3.0
7	S5	46	TRP	3.0
6	S4	86	PHE	3.0
6	S4	87	MET	3.0
27	D5	93	SER	3.0
34	sR	246	SER	3.0

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Mol	Chain	Res	Type	RSRZ
51	m5	130	PHE	3.0
2	S0	144	ILE	3.0
6	S4	91	THR	3.0
6	s4	121	TYR	3.0
10	s8	117	TYR	3.0
14	c2	68	GLU	3.0
18	c6	79	TYR	3.0
22	D0	65	ILE	3.0
22	D0	67	THR	3.0
22	D0	80	GLU	3.0
29	D7	43	ILE	3.0
29	d7	52	THR	3.0
58	n2	106	ALA	3.0
81	p0	49	ALA	3.0
64	N8	126	LYS	3.0
82	p1	9	TYR	3.0
82	p2	13	ILE	3.0
83	f	89	GLU	3.0
33	e1	147	VAL	3.0
36	5	1763	U	3.0
58	n2	54	VAL	3.0
34	sR	158	PRO	3.0
58	N2	37	LEU	3.0
7	s5	167	ARG	3.0
40	L3	386	ASP	3.0
6	s4	84	ALA	3.0
7	S5	172	ILE	3.0
16	C4	101	ALA	3.0
21	C9	44	GLU	3.0
63	n7	41	ALA	3.0
3	S1	215	VAL	3.0
9	S7	129	LEU	3.0
11	S9	105	LEU	3.0
21	C9	70	GLN	3.0
2	S0	174	TRP	3.0
25	D3	106	GLY	3.0
27	D5	94	LYS	3.0
33	e1	112	GLY	3.0
12	C0	63	TYR	3.0
15	c3	16	ILE	3.0
35	SM	176	ALA	3.0
82	p2	15	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
21	c9	9	VAL	3.0
83	f	57	VAL	3.0
27	D5	105	THR	3.0
42	L5	92	LEU	3.0
58	N2	105	LEU	3.0
2	S0	11	PRO	3.0
18	C6	140	LYS	3.0
29	d7	47	PHE	3.0
34	SR	121	MET	3.0
7	S5	89	ILE	3.0
12	c0	26	ASP	3.0
34	sR	80	ALA	3.0
19	C7	99	VAL	3.0
3	S1	42	ASN	3.0
7	s5	79	ASN	3.0
11	S9	111	THR	3.0
18	C6	10	PHE	3.0
42	L5	3	PHE	3.0
42	L5	153	THR	3.0
53	M7	164	LYS	3.0
21	C9	31	PRO	3.0
34	sR	105	GLY	3.0
1	2	194	U	3.0
11	S9	6	ARG	3.0
21	C9	15	ILE	3.0
12	C0	22	VAL	3.0
25	D3	49	ALA	3.0
31	D9	44	ARG	3.0
32	E0	49	LEU	3.0
34	sR	68	VAL	3.0
51	m5	53	TYR	3.0
71	O5	120	ALA	3.0
72	O6	68	ARG	3.0
20	C8	101	LEU	3.0
81	p0	76	LEU	3.0
14	c2	111	ASN	3.0
7	s5	140	THR	3.0
34	SR	63	GLY	2.9
39	l2	164	GLY	2.9
42	L5	126	GLU	3.0
42	L5	226	TYR	2.9
45	l8	134	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
53	M7	183	ALA	2.9
3	S1	58	SER	2.9
4	s2	208	GLU	2.9
6	S4	173	ILE	2.9
43	l6	11	PRO	2.9
3	s1	217	LEU	2.9
5	S3	137	VAL	2.9
6	S4	127	LYS	2.9
14	C2	36	LEU	2.9
30	D8	48	VAL	2.9
33	e1	108	VAL	2.9
40	l3	387	LEU	2.9
36	1	1028	U	2.9
6	S4	41	SER	2.9
53	M7	181	ARG	2.9
2	S0	168	HIS	2.9
3	S1	137	ILE	2.9
35	SM	91	THR	2.9
13	C1	144	ALA	2.9
34	sR	47	LEU	2.9
34	sR	236	ALA	2.9
17	c5	127	ARG	2.9
9	s7	2	SER	2.9
11	S9	37	LYS	2.9
34	sR	52	GLN	2.9
53	M7	159	LYS	2.9
62	N6	125	LYS	2.9
18	c6	20	ALA	2.9
81	p0	93	LEU	2.9
36	5	1352	A	2.9
14	c2	124	LYS	2.9
4	s2	92	ALA	2.9
18	C6	48	VAL	2.9
7	s5	61	TYR	2.9
42	L5	100	ALA	2.9
3	s1	100	PHE	2.9
32	E0	18	THR	2.9
10	S8	160	PHE	2.9
14	c2	125	ASN	2.9
26	D4	85	PHE	2.9
42	l5	200	PHE	2.9
83	f	54	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
7	s5	144	GLU	2.9
34	SR	92	TRP	2.9
18	C6	122	ARG	2.9
32	E0	38	LEU	2.9
83	f	138	ILE	2.9
2	S0	187	ALA	2.9
1	2	1362	U	2.9
1	6	493	U	2.9
5	s3	108	LYS	2.9
4	s2	85	PRO	2.9
27	D5	59	TYR	2.9
31	D9	52	PHE	2.9
61	N5	30	ALA	2.9
14	c2	56	GLU	2.9
5	S3	90	ARG	2.9
7	s5	162	VAL	2.9
35	sM	25	ILE	2.9
45	L8	197	VAL	2.9
83	f	92	LEU	2.9
1	2	239	C	2.9
14	c2	95	LYS	2.9
70	O4	52	GLN	2.9
78	Q2	105	GLN	2.9
70	o4	62	TYR	2.9
11	S9	133	HIS	2.9
30	D8	21	SER	2.9
70	o4	42	PRO	2.9
30	d8	26	THR	2.9
39	L2	252	THR	2.9
18	c6	28	LEU	2.9
53	M7	176	ILE	2.9
7	S5	191	ALA	2.9
8	s6	145	PHE	2.9
45	l8	154	ALA	2.9
46	l9	190	ASP	2.9
82	p2	10	ALA	2.9
11	S9	182	GLU	2.9
70	o4	31	ARG	2.9
7	S5	93	LEU	2.9
26	D4	68	LYS	2.9
7	S5	130	ILE	2.9
28	D6	21	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
29	D7	46	VAL	2.9
83	f	93	LEU	2.9
26	d4	72	PHE	2.9
42	L5	79	TYR	2.9
61	n5	90	ALA	2.9
18	C6	120	ASP	2.9
34	sR	155	ARG	2.9
67	O1	82	GLU	2.9
11	S9	2	PRO	2.9
21	c9	92	LYS	2.9
70	O4	55	SER	2.9
70	O4	70	LYS	2.9
4	S2	86	VAL	2.9
9	S7	93	LEU	2.9
32	E0	46	ASN	2.9
36	1	1238	C	2.9
83	f	76	SER	2.9
42	L5	52	VAL	2.9
18	C6	46	PHE	2.9
7	s5	71	ALA	2.9
13	C1	149	ALA	2.9
35	SM	60	ALA	2.9
69	o3	60	ARG	2.9
9	S7	32	PRO	2.9
5	s3	164	VAL	2.8
6	s4	173	ILE	2.8
12	c0	60	SER	2.8
7	S5	184	PHE	2.8
11	S9	146	PHE	2.8
6	s4	37	LYS	2.8
11	S9	20	GLU	2.8
12	C0	45	ALA	2.8
16	C4	40	ALA	2.8
74	o8	53	THR	2.8
67	O1	34	LYS	2.8
14	c2	26	ASP	2.8
35	sM	75	ASP	2.8
83	f	129	ASP	2.8
47	m0	206	LEU	2.8
5	s3	137	VAL	2.8
33	e1	102	VAL	2.8
70	O4	20	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
39	L2	63	PHE	2.8
11	S9	95	TYR	2.8
36	5	620	U	2.8
34	SR	55	GLY	2.8
6	S4	71	LYS	2.8
7	S5	48	PHE	2.8
36	1	1580	A	2.8
36	1	1605	A	2.8
42	L5	200	PHE	2.8
67	O1	10	ARG	2.8
6	s4	149	TYR	2.8
12	c0	63	TYR	2.8
28	D6	59	TYR	2.8
55	M9	174	ALA	2.8
70	O4	6	THR	2.8
70	o4	25	THR	2.8
14	C2	78	LEU	2.8
63	N7	80	LEU	2.8
7	s5	64	VAL	2.8
18	C6	114	ARG	2.8
25	D3	102	VAL	2.8
27	D5	68	ARG	2.8
27	D5	92	ILE	2.8
29	d7	46	VAL	2.8
45	l8	140	VAL	2.8
35	SM	21	PRO	2.8
66	o0	42	ILE	2.8
69	o3	64	ILE	2.8
12	C0	3	MET	2.8
7	S5	182	ALA	2.8
30	D8	10	ALA	2.8
34	sR	181	TRP	2.8
70	O4	63	ALA	2.8
21	c9	101	ASN	2.8
11	S9	86	LEU	2.8
29	D7	69	GLY	2.8
80	m2	32	GLY	2.8
6	S4	70	VAL	2.8
6	S4	129	VAL	2.8
12	c0	21	VAL	2.8
19	C7	69	ILE	2.8
63	N7	61	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
63	n7	136	PHE	2.8
76	Q0	78	ILE	2.8
83	f	82	VAL	2.8
7	S5	66	GLN	2.8
10	S8	166	TYR	2.8
14	C2	57	ALA	2.8
12	c0	62	GLN	2.8
21	C9	25	GLN	2.8
22	d0	82	TYR	2.8
34	sR	83	ALA	2.8
58	N2	106	ALA	2.8
10	S8	200	LYS	2.8
26	D4	17	LEU	2.8
34	SR	194	GLY	2.8
53	M7	168	LEU	2.8
58	N2	84	LEU	2.8
3	S1	66	VAL	2.8
3	S1	121	ILE	2.8
16	C4	31	THR	2.8
18	C6	22	VAL	2.8
82	p1	44	ILE	2.8
5	s3	105	MET	2.8
2	S0	92	HIS	2.8
14	c2	82	PRO	2.8
55	M9	187	GLU	2.8
5	S3	145	ALA	2.8
6	S4	27	TYR	2.8
68	O2	127	ALA	2.8
4	S2	145	GLY	2.8
10	S8	159	GLN	2.8
22	D0	54	GLY	2.8
33	E1	116	LYS	2.8
67	O1	102	LYS	2.8
18	C6	85	ILE	2.8
27	D5	40	VAL	2.8
31	d9	38	ILE	2.8
18	C6	9	THR	2.8
36	1	1352	A	2.8
2	S0	157	ASP	2.8
43	L6	8	LYS	2.8
63	n7	21	LYS	2.8
2	S0	188	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
16	c4	15	GLY	2.8
34	sR	304	GLY	2.8
55	m9	24	LEU	2.8
70	O4	51	LEU	2.8
22	D0	86	ILE	2.8
33	E1	91	ILE	2.8
18	c6	37	THR	2.8
63	N7	52	LYS	2.8
28	D6	52	ASP	2.8
45	L8	99	PRO	2.8
1	6	194	U	2.8
34	SR	23	LEU	2.8
45	L8	61	GLN	2.8
18	C6	81	ILE	2.8
2	S0	113	ARG	2.8
11	s9	20	GLU	2.8
21	C9	79	LEU	2.8
31	d9	30	LEU	2.8
45	l8	113	ALA	2.8
51	m5	3	ALA	2.8
61	n5	23	ALA	2.8
63	N7	11	ALA	2.8
1	2	713	A	2.8
2	S0	158	VAL	2.8
45	l8	94	PHE	2.8
63	N7	71	PHE	2.8
22	D0	68	ARG	2.8
34	SR	137	LYS	2.8
3	s1	47	LEU	2.8
9	S7	154	LEU	2.8
10	S8	167	ALA	2.8
28	D6	67	THR	2.8
48	M1	91	LEU	2.8
7	s5	72	HIS	2.8
9	S7	155	ASP	2.8
14	c2	87	PRO	2.8
26	d4	67	GLY	2.8
83	f	25	ALA	2.8
13	C1	16	GLN	2.8
14	c2	107	ASP	2.8
20	c8	4	VAL	2.8
35	SM	101	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
36	1	1565	G	2.8
20	c8	123	ARG	2.8
34	sR	188	ILE	2.8
45	l8	153	ILE	2.8
42	L5	123	GLU	2.8
82	p1	18	GLU	2.8
7	S5	194	LEU	2.8
19	c7	26	LEU	2.8
79	Q3	58	SER	2.8
5	s3	114	ALA	2.8
3	S1	219	LYS	2.8
5	S3	54	ARG	2.8
33	E1	99	LYS	2.8
61	n5	110	VAL	2.8
70	O4	7	PHE	2.8
6	S4	192	ILE	2.7
7	s5	34	GLN	2.7
72	O6	9	ILE	2.7
81	p0	58	MET	2.7
9	s7	154	LEU	2.7
2	S0	166	GLY	2.7
3	S1	45	LYS	2.7
5	s3	106	LYS	2.7
34	sR	27	ALA	2.7
68	o2	93	ALA	2.7
83	f	74	SER	2.7
42	L5	240	TYR	2.7
67	O1	33	VAL	2.7
5	S3	50	ILE	2.7
19	C7	83	GLN	2.7
34	SR	131	ILE	2.7
42	L5	168	ASP	2.7
1	2	132	U	2.7
3	s1	94	LYS	2.7
25	D3	103	LEU	2.7
35	sM	69	ARG	2.7
72	o6	99	ARG	2.7
63	n7	20	GLY	2.7
7	s5	29	ILE	2.7
10	S8	185	GLU	2.7
17	c5	84	ILE	2.7
22	D0	71	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
24	D2	27	ILE	2.7
31	D9	20	GLN	2.7
34	sR	189	GLU	2.7
35	sM	122	GLU	2.7
67	o1	95	PRO	2.7
25	D3	71	CYS	2.7
5	s3	113	LEU	2.7
7	S5	112	ARG	2.7
18	c6	52	LEU	2.7
32	E0	20	LYS	2.7
58	N2	94	ARG	2.7
58	n2	105	LEU	2.7
74	o8	31	LEU	2.7
6	S4	260	GLY	2.7
18	C6	67	VAL	2.7
21	C9	21	PHE	2.7
42	L5	127	GLY	2.7
11	S9	87	SER	2.7
15	c3	37	ILE	2.7
1	6	660	G	2.7
1	6	1466	G	2.7
33	E1	93	HIS	2.7
33	e1	93	HIS	2.7
1	6	1702	A	2.7
3	S1	41	ARG	2.7
3	s1	52	THR	2.7
66	o0	22	LYS	2.7
11	s9	109	LEU	2.7
18	c6	38	LEU	2.7
20	c8	32	LEU	2.7
12	c0	54	TYR	2.7
17	c5	93	VAL	2.7
21	C9	91	TYR	2.7
34	SR	24	ALA	2.7
10	s8	61	GLU	2.7
66	O0	100	ILE	2.7
70	o4	16	ARG	2.7
80	m2	85	SER	2.7
3	s1	61	LEU	2.7
5	s3	174	HIS	2.7
6	S4	197	HIS	2.7
16	C4	80	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
34	sR	50	ASP	2.7
35	SM	100	THR	2.7
40	L3	48	GLY	2.7
5	s3	181	VAL	2.7
55	M9	170	ARG	2.7
66	o0	100	ILE	2.7
81	p0	81	LYS	2.7
1	6	1473	U	2.7
5	s3	139	SER	2.7
25	D3	135	LEU	2.7
36	5	1351	U	2.7
45	L8	26	LEU	2.7
76	Q0	121	LEU	2.7
19	c7	104	ASN	2.7
10	S8	30	GLY	2.7
10	S8	95	THR	2.7
29	d7	55	THR	2.7
34	sR	165	ASP	2.7
11	s9	4	ALA	2.7
12	C0	65	TYR	2.7
15	C3	60	VAL	2.7
16	C4	42	VAL	2.7
6	S4	191	ARG	2.7
26	D4	19	ALA	2.7
30	D8	41	VAL	2.7
34	SR	20	VAL	2.7
42	L5	27	LYS	2.7
42	L5	98	ALA	2.7
51	M5	60	VAL	2.7
51	m5	5	LYS	2.7
55	M9	183	ALA	2.7
63	n7	7	ALA	2.7
70	O4	5	VAL	2.7
74	o8	74	LYS	2.7
83	f	32	VAL	2.7
74	O8	5	ILE	2.7
36	1	1025	A	2.7
9	S7	74	GLN	2.7
23	D1	69	LEU	2.7
51	m5	15	GLN	2.7
82	p2	23	SER	2.7
6	s4	122	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
8	S6	149	LYS	2.7
32	E0	14	VAL	2.7
35	SM	170	LYS	2.7
35	sM	50	ASN	2.7
45	l8	137	ASN	2.7
10	S8	56	ARG	2.7
11	S9	4	ALA	2.7
14	C2	123	VAL	2.7
9	S7	91	ILE	2.7
11	S9	106	GLU	2.7
14	c2	92	ALA	2.7
16	C4	18	ARG	2.7
18	C6	143	ARG	2.7
23	D1	23	ILE	2.7
42	L5	61	ILE	2.7
46	L9	187	ILE	2.7
49	M3	95	ILE	2.7
3	s1	54	LEU	2.7
27	d5	37	GLN	2.7
34	sR	234	LEU	2.7
16	C4	29	HIS	2.7
25	D3	86	PHE	2.7
26	d4	99	LYS	2.7
33	e1	89	LYS	2.7
45	l8	159	PRO	2.7
49	m3	179	PHE	2.7
67	O1	66	GLY	2.7
70	O4	67	LYS	2.7
70	o4	26	PRO	2.7
80	m2	140	SER	2.7
27	d5	40	VAL	2.7
42	L5	125	VAL	2.7
81	p0	48	ARG	2.7
3	S1	67	GLU	2.7
21	C9	107	ALA	2.7
81	p0	94	THR	2.7
2	S0	104	PRO	2.7
4	s2	98	PHE	2.7
12	c0	1	MET	2.7
16	C4	12	GLN	2.7
9	S7	69	GLY	2.7
14	c2	102	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
18	c6	60	PHE	2.7
34	SR	103	PHE	2.7
35	sM	79	SER	2.7
46	L9	178	GLY	2.7
74	o8	70	PRO	2.7
6	S4	26	CYS	2.7
10	S8	149	SER	2.7
16	c4	42	VAL	2.7
63	N7	96	VAL	2.7
70	o4	23	VAL	2.7
20	C8	44	ASN	2.7
21	C9	96	ALA	2.7
24	D2	53	ILE	2.7
24	d2	86	ILE	2.7
34	SR	93	ASP	2.7
45	l8	179	ILE	2.7
55	M9	171	ASP	2.7
58	N2	38	ILE	2.7
6	S4	128	LYS	2.7
9	S7	81	LEU	2.7
18	c6	115	THR	2.7
72	O6	59	ASP	2.7
34	sR	13	LEU	2.7
36	5	1349	G	2.7
45	l8	65	LEU	2.7
58	n2	13	LYS	2.7
83	f	114	LYS	2.7
7	s5	35	GLN	2.7
10	S8	2	GLY	2.7
14	c2	22	VAL	2.7
26	d4	57	VAL	2.7
40	L3	294	GLY	2.7
28	D6	17	HIS	2.7
42	L5	130	GLU	2.7
7	S5	74	ALA	2.7
25	D3	117	ILE	2.7
34	sR	67	ILE	2.7
70	o4	2	ALA	2.7
6	S4	77	ARG	2.7
7	s5	94	THR	2.7
11	S9	28	LEU	2.7
33	E1	82	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
30	d8	5	THR	2.7
36	5	1580	A	2.7
45	l8	152	LEU	2.7
51	m5	43	THR	2.7
58	n2	15	PHE	2.7
11	S9	32	GLY	2.7
2	s0	97	PRO	2.7
5	S3	138	VAL	2.7
21	C9	42	GLY	2.7
25	D3	51	GLY	2.7
10	S8	140	GLU	2.7
18	C6	50	GLU	2.7
30	d8	28	VAL	2.7
48	m1	108	GLU	2.7
61	N5	107	VAL	2.7
5	s3	3	ALA	2.7
17	c5	128	HIS	2.7
11	S9	184	SER	2.6
25	D3	114	LYS	2.6
72	o6	100	HIS	2.7
11	s9	80	LEU	2.6
15	C3	14	SER	2.6
16	c4	102	LEU	2.6
34	sR	45	TRP	2.6
80	m2	89	SER	2.6
7	S5	147	THR	2.6
9	S7	70	PHE	2.6
34	sR	54	PHE	2.6
61	N5	31	THR	2.6
63	N7	130	PHE	2.6
26	D4	25	VAL	2.6
48	M1	131	MET	2.6
5	S3	208	ILE	2.6
6	s4	162	ILE	2.6
14	c2	114	LYS	2.6
15	C3	16	ILE	2.6
35	SM	22	PRO	2.6
42	L5	148	ILE	2.6
61	N5	81	ILE	2.6
80	m2	12	LYS	2.6
11	S9	118	LEU	2.6
12	c0	49	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
70	O4	76	TYR	2.6
82	p1	22	SER	2.6
5	S3	24	PHE	2.6
7	s5	82	PHE	2.6
2	s0	162	CYS	2.6
20	C8	142	GLY	2.6
21	C9	67	MET	2.6
25	d3	71	CYS	2.6
45	L8	90	THR	2.6
70	o4	28	GLY	2.6
60	n4	66	GLU	2.6
2	s0	20	ALA	2.6
5	s3	50	ILE	2.6
20	C8	40	ARG	2.6
21	C9	47	PRO	2.6
29	D7	73	LEU	2.6
63	N7	79	HIS	2.6
83	f	58	HIS	2.6
2	S0	54	TRP	2.6
16	c4	23	PHE	2.6
7	s5	24	VAL	2.6
31	d9	37	ASN	2.6
33	e1	125	THR	2.6
36	1	1573	G	2.6
58	N2	91	ASP	2.6
25	D3	84	THR	2.6
51	M5	15	GLN	2.6
2	S0	126	PRO	2.6
8	s6	172	ALA	2.6
10	S8	144	ALA	2.6
28	D6	71	LEU	2.6
33	E1	148	TYR	2.6
34	sR	9	LEU	2.6
51	m5	22	LEU	2.6
66	O0	23	TYR	2.6
66	O0	42	ILE	2.6
67	O1	104	LEU	2.6
15	C3	58	HIS	2.6
47	M0	136	PHE	2.6
63	N7	4	PHE	2.6
67	o1	90	PHE	2.6
1	2	724	C	2.6

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Mol	Chain	Res	Type	RSRZ
35	SM	53	ARG	2.6
36	1	1016	C	2.6
48	M1	75	LYS	2.6
6	s4	143	ASP	2.6
18	C6	31	VAL	2.6
21	C9	114	VAL	2.6
26	d4	27	VAL	2.6
27	D5	64	VAL	2.6
39	L2	72	ARG	2.6
7	s5	169	ASN	2.6
58	N2	88	GLN	2.6
5	s3	109	LEU	2.6
19	C7	100	LEU	2.6
24	D2	26	LEU	2.6
63	n7	72	ILE	2.6
6	S4	53	LYS	2.6
25	D3	139	LYS	2.6
3	S1	21	VAL	2.6
6	s4	111	VAL	2.6
7	s5	53	VAL	2.6
25	D3	96	VAL	2.6
25	D3	141	GLU	2.6
66	O0	88	GLY	2.6
81	p0	50	VAL	2.6
8	S6	182	GLN	2.6
18	c6	94	GLN	2.6
21	C9	95	ASP	2.6
22	D0	63	LEU	2.6
24	D2	61	ILE	2.6
6	s4	182	TYR	2.6
8	S6	100	ALA	2.6
10	S8	62	THR	2.6
47	M0	152	LEU	2.6
6	S4	47	PHE	2.6
13	C1	69	LYS	2.6
51	m5	148	TYR	2.6
26	D4	16	PRO	2.6
45	L8	68	ARG	2.6
58	N2	30	PRO	2.6
61	N5	32	PHE	2.6
6	S4	69	HIS	2.6
1	6	234	G	2.6

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Mol	Chain	Res	Type	RSRZ
42	L5	133	GLU	2.6
55	M9	22	VAL	2.6
70	O4	65	VAL	2.6
3	s1	110	LEU	2.6
12	c0	35	ILE	2.6
5	s3	171	ALA	2.6
3	s1	98	THR	2.6
13	C1	13	PHE	2.6
18	C6	112	TYR	2.6
18	C6	142	TYR	2.6
34	sR	180	ALA	2.6
39	L2	69	TYR	2.6
80	m2	20	TYR	2.6
18	C6	45	ARG	2.6
30	d8	42	ARG	2.6
5	s3	37	VAL	2.6
8	s6	165	GLY	2.6
31	d9	17	GLY	2.6
49	m3	192	GLU	2.6
34	sR	223	TRP	2.6
19	c7	38	ILE	2.6
25	D3	123	LYS	2.6
27	d5	80	LEU	2.6
33	e1	91	ILE	2.6
42	L5	297	GLN	2.6
83	f	15	SER	2.6
3	s1	142	PHE	2.6
7	s5	157	ARG	2.6
11	S9	125	ALA	2.6
61	N5	23	ALA	2.6
11	S9	136	VAL	2.6
16	C4	113	GLY	2.6
34	sR	30	PRO	2.6
45	l8	144	GLU	2.6
51	m5	58	GLY	2.6
12	c0	44	LYS	2.6
18	c6	12	LYS	2.6
31	D9	56	ARG	2.6
70	O4	61	GLN	2.6
22	d0	28	SER	2.6
31	d9	14	TYR	2.6
66	o0	59	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
5	s3	112	GLY	2.6
6	S4	78	THR	2.6
16	C4	119	THR	2.6
34	sR	20	VAL	2.6
1	2	1689	A	2.6
7	s5	42	LEU	2.6
10	S8	96	LEU	2.6
42	L5	65	ILE	2.6
67	O1	73	LEU	2.6
1	2	959	U	2.6
7	S5	170	GLN	2.6
29	D7	47	PHE	2.6
63	N7	44	ALA	2.6
67	o1	39	PHE	2.6
34	SR	82	SER	2.6
10	S8	63	GLY	2.6
34	SR	309	VAL	2.6
40	l3	85	VAL	2.6
20	C8	3	LEU	2.6
30	d8	56	LEU	2.6
6	s4	226	PHE	2.6
36	1	1566	A	2.6
1	6	1710	U	2.6
70	O4	32	ALA	2.6
3	S1	51	SER	2.6
23	D1	40	ASP	2.6
53	M7	167	ARG	2.6
7	S5	79	ASN	2.6
42	L5	163	LEU	2.6
64	N8	73	LEU	2.6
27	d5	71	ILE	2.6
29	D7	55	THR	2.6
34	SR	195	HIS	2.6
46	L9	134	ILE	2.6
58	n2	98	THR	2.6
11	s9	104	PHE	2.5
13	C1	60	PHE	2.5
55	M9	169	ALA	2.5
1	6	754	A	2.5
42	L5	159	VAL	2.5
58	N2	65	VAL	2.5
67	O1	72	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
72	O6	97	SER	2.5
18	C6	28	LEU	2.5
70	o4	51	LEU	2.5
48	M1	21	ILE	2.5
48	M1	79	ILE	2.5
2	s0	46	HIS	2.5
34	SR	261	LYS	2.5
54	M8	88	THR	2.5
11	S9	174	ARG	2.5
21	c9	17	ALA	2.5
40	l3	179	ALA	2.5
42	L5	86	TYR	2.5
70	O4	60	ARG	2.5
6	S4	61	VAL	2.5
1	6	1059	U	2.5
6	s4	41	SER	2.5
18	c6	116	LEU	2.5
40	l3	178	LEU	2.5
48	M1	12	LEU	2.5
10	s8	60	ILE	2.5
26	d4	102	LYS	2.5
31	d9	52	PHE	2.5
34	SR	302	PHE	2.5
82	p2	44	ILE	2.5
6	S4	59	ARG	2.5
6	s4	36	HIS	2.5
26	D4	15	ASN	2.5
2	S0	195	TRP	2.5
7	S5	196	GLU	2.5
22	D0	15	GLN	2.5
22	d0	83	GLU	2.5
28	d6	67	THR	2.5
29	D7	31	TYR	2.5
34	sR	41	THR	2.5
63	N7	18	TYR	2.5
2	S0	50	VAL	2.5
10	s8	156	VAL	2.5
51	m5	52	GLY	2.5
14	c2	45	LEU	2.5
45	l8	150	LEU	2.5
34	sR	122	ILE	2.5
35	sM	61	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
36	5	3275	U	2.5
76	Q0	81	SER	2.5
1	2	135	A	2.5
31	d9	44	ARG	2.5
34	SR	90	ARG	2.5
51	m5	63	ARG	2.5
6	S4	103	TYR	2.5
17	C5	101	ALA	2.5
21	c9	91	TYR	2.5
31	D9	4	GLU	2.5
32	e0	11	ALA	2.5
80	m2	65	GLU	2.5
82	p1	10	ALA	2.5
17	c5	86	VAL	2.5
36	1	2522	G	2.5
15	C3	39	LYS	2.5
25	D3	50	LYS	2.5
49	m3	190	LYS	2.5
67	O1	62	ARG	2.5
70	o4	29	ILE	2.5
32	e0	30	PRO	2.5
36	1	1765	U	2.5
3	s1	68	VAL	2.5
6	S4	112	HIS	2.5
6	S4	6	LYS	2.5
7	s5	128	ASN	2.5
8	S6	36	VAL	2.5
22	d0	18	GLN	2.5
5	s3	21	LEU	2.5
6	s4	123	LEU	2.5
63	N7	66	THR	2.5
7	s5	190	ILE	2.5
17	c5	83	MET	2.5
34	sR	186	PHE	2.5
36	1	1242	G	2.5
47	M0	31	ILE	2.5
67	O1	59	ILE	2.5
11	s9	152	SER	2.5
6	s4	14	ALA	2.5
7	S5	64	VAL	2.5
13	c1	145	ALA	2.5
18	C6	127	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
19	C7	116	LYS	2.5
70	O4	37	LYS	2.5
83	f	83	PRO	2.5
42	L5	53	VAL	2.5
27	d5	42	LEU	2.5
29	D7	49	HIS	2.5
34	SR	58	VAL	2.5
80	m2	126	ALA	2.5
8	s6	193	LEU	2.5
25	d3	103	LEU	2.5
61	n5	82	LEU	2.5
64	n8	120	ASN	2.5
6	s4	159	THR	2.5
45	l8	74	THR	2.5
67	O1	79	ARG	2.5
80	m2	72	THR	2.5
7	s5	20	PHE	2.5
12	C0	11	ILE	2.5
22	d0	65	ILE	2.5
47	M0	46	PHE	2.5
14	C2	56	GLU	2.5
25	D3	137	LYS	2.5
46	L9	189	GLU	2.5
51	m5	54	LYS	2.5
7	S5	88	PRO	2.5
1	6	1601	G	2.5
3	s1	225	VAL	2.5
6	S4	34	GLY	2.5
11	s9	2	PRO	2.5
21	C9	33	TYR	2.5
25	D3	85	ALA	2.5
51	m5	121	VAL	2.5
81	p0	22	TYR	2.5
6	S4	42	LEU	2.5
6	S4	130	GLN	2.5
20	C8	41	ARG	2.5
20	c8	116	LEU	2.5
21	c9	105	LEU	2.5
34	sR	29	GLN	2.5
42	L5	50	ARG	2.5
55	M9	44	LEU	2.5
34	sR	12	THR	2.5

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Mol	Chain	Res	Type	RSRZ
34	sR	245	PHE	2.5
83	f	150	PHE	2.5
33	e1	107	LYS	2.5
34	sR	14	GLU	2.5
2	s0	165	ARG	2.5
6	s4	107	GLY	2.5
27	d5	91	PRO	2.5
29	d7	59	CYS	2.5
32	E0	4	VAL	2.5
51	M5	58	GLY	2.5
58	n2	17	VAL	2.5
81	p0	27	VAL	2.5
21	C9	54	PHE	2.5
1	2	1685	G	2.5
2	S0	22	THR	2.5
6	s4	90	ILE	2.5
7	S5	200	ASN	2.5
34	sR	136	ILE	2.5
42	L5	190	ILE	2.5
49	m3	147	ILE	2.5
3	S1	26	ARG	2.5
3	S1	88	VAL	2.5
48	M1	133	ARG	2.5
1	2	31	C	2.5
1	2	1426	C	2.5
8	S6	75	LEU	2.5
8	S6	198	ALA	2.5
1	6	1707	A	2.5
12	c0	58	GLN	2.5
18	C6	41	PRO	2.5
32	E0	39	LEU	2.5
62	N6	126	LEU	2.5
63	N7	77	TYR	2.5
2	S0	102	PHE	2.5
3	S1	130	SER	2.5
42	L5	185	PHE	2.5
19	C7	38	ILE	2.5
43	l6	9	TRP	2.5
45	L8	64	ILE	2.5
1	6	718	U	2.5
25	D3	28	ASN	2.5
36	1	1241	U	2.5

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Mol	Chain	Res	Type	RSRZ
64	n8	104	THR	2.5
74	o8	22	THR	2.5
14	C2	60	VAL	2.5
45	L8	226	TYR	2.5
51	M5	135	VAL	2.5
14	C2	81	ASP	2.5
26	D4	56	SER	2.5
34	sR	44	SER	2.5
67	o1	76	SER	2.5
11	S9	132	ARG	2.5
30	D8	60	GLU	2.5
1	2	494	U	2.5
1	2	558	U	2.5
6	s4	225	VAL	2.5
7	S5	44	ASN	2.5
7	S5	176	THR	2.5
10	S8	64	ASN	2.5
15	C3	65	VAL	2.5
33	E1	98	VAL	2.5
34	sR	135	THR	2.5
36	5	1353	U	2.5
45	L8	86	THR	2.5
6	S4	138	TYR	2.5
34	sR	305	TYR	2.5
35	SM	103	LYS	2.5
66	O0	14	LEU	2.5
43	l6	176	PHE	2.5
70	O4	42	PRO	2.5
80	m2	118	GLN	2.5
6	S4	256	ARG	2.5
17	C5	84	ILE	2.5
21	C9	124	ILE	2.5
29	D7	62	ILE	2.5
63	N7	68	ILE	2.5
1	2	1527	C	2.4
11	s9	147	MET	2.4
60	n4	135	SER	2.5
12	C0	42	VAL	2.4
36	1	1575	A	2.4
51	m5	7	LEU	2.4
55	m9	22	VAL	2.4
62	N6	124	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
14	c2	57	ALA	2.4
21	C9	55	TYR	2.4
29	d7	61	THR	2.4
34	sR	255	ALA	2.4
46	L9	188	THR	2.4
58	N2	12	ALA	2.4
74	o8	15	THR	2.4
7	S5	114	ILE	2.4
9	S7	135	ILE	2.4
26	D4	106	GLN	2.4
58	N2	9	GLN	2.4
70	O4	4	ARG	2.4
74	o8	37	PRO	2.4
55	M9	72	GLU	2.4
20	c8	137	HIS	2.4
3	S1	216	LYS	2.4
9	S7	84	LYS	2.4
34	SR	221	MET	2.4
1	6	1229	G	2.4
3	s1	97	LEU	2.4
12	C0	40	LEU	2.4
16	C4	67	VAL	2.4
26	d4	35	VAL	2.4
45	l8	230	LYS	2.4
51	m5	10	LEU	2.4
63	N7	126	LYS	2.4
6	S4	149	TYR	2.4
13	c1	146	ALA	2.4
15	C3	40	TYR	2.4
18	C6	108	ALA	2.4
34	SR	198	ASN	2.4
36	5	1579	C	2.4
5	s3	116	ARG	2.4
7	S5	76	ARG	2.4
7	s5	180	ARG	2.4
8	S6	154	ARG	2.4
19	c7	3	ARG	2.4
22	d0	70	THR	2.4
45	l8	78	PHE	2.4
81	p0	104	ARG	2.4
18	C6	124	PRO	2.4
21	c9	111	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
28	D6	31	PRO	2.4
34	sR	239	GLU	2.4
34	SR	66	HIS	2.4
42	l5	125	VAL	2.4
47	M0	148	VAL	2.4
54	m8	2	GLY	2.4
59	n3	3	GLY	2.4
64	n8	121	VAL	2.4
66	O0	90	VAL	2.4
6	S4	84	ALA	2.4
10	s8	166	TYR	2.4
25	D3	105	ALA	2.4
67	O1	12	TYR	2.4
12	c0	28	ASN	2.4
45	L8	240	ASN	2.4
1	2	195	G	2.4
4	s2	120	GLU	2.4
16	C4	83	ILE	2.4
17	c5	85	ILE	2.4
32	E0	25	GLU	2.4
42	L5	151	GLN	2.4
45	l8	122	LYS	2.4
2	s0	23	HIS	2.4
3	S1	212	VAL	2.4
19	C7	24	LEU	2.4
46	L9	90	MET	2.4
21	C9	7	ARG	2.4
21	C9	57	ARG	2.4
21	c9	64	HIS	2.4
32	e0	54	ARG	2.4
51	m5	31	ARG	2.4
4	S2	66	PHE	2.4
4	s2	118	ALA	2.4
20	c8	42	TYR	2.4
21	c9	66	TYR	2.4
31	d9	34	TYR	2.4
34	SR	186	PHE	2.4
63	N7	94	SER	2.4
66	O0	9	SER	2.4
42	L5	78	ALA	2.4
53	M7	178	ALA	2.4
83	f	31	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
6	S4	169	ILE	2.4
6	s4	71	LYS	2.4
14	c2	24	ILE	2.4
16	C4	82	LYS	2.4
20	c8	141	THR	2.4
35	SM	54	PRO	2.4
7	S5	198	LEU	2.4
20	c8	54	LEU	2.4
36	1	1574	C	2.4
51	m5	186	GLY	2.4
63	n7	10	VAL	2.4
66	O0	101	LEU	2.4
66	o0	90	VAL	2.4
6	s4	17	HIS	2.4
18	c6	74	HIS	2.4
34	SR	114	ASP	2.4
11	S9	104	PHE	2.4
81	p0	66	PHE	2.4
6	S4	7	LYS	2.4
55	m9	21	LYS	2.4
10	S8	70	GLU	2.4
11	S9	129	ILE	2.4
34	SR	310	ILE	2.4
42	L5	60	ILE	2.4
13	C1	22	ASN	2.4
57	N1	127	GLN	2.4
2	S0	18	LEU	2.4
16	c4	28	VAL	2.4
18	c6	130	GLY	2.4
30	D8	30	VAL	2.4
45	L8	132	VAL	2.4
80	m2	71	VAL	2.4
1	2	493	U	2.4
9	s7	43	PHE	2.4
12	c0	36	ASP	2.4
42	L5	223	PHE	2.4
51	M5	37	HIS	2.4
2	S0	85	ALA	2.4
7	s5	39	GLU	2.4
25	D3	145	SER	2.4
30	d8	59	SER	2.4
18	C6	8	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
4	S2	63	VAL	2.4
5	S3	37	VAL	2.4
25	D3	125	VAL	2.4
43	L6	55	LEU	2.4
58	n2	76	LEU	2.4
76	Q0	85	LEU	2.4
32	E0	32	GLY	2.4
34	sR	125	GLY	2.4
81	p0	190	VAL	2.4
13	c1	115	PHE	2.4
67	O1	39	PHE	2.4
70	o4	93	PHE	2.4
12	c0	94	GLU	2.4
26	d4	26	ASP	2.4
36	1	1555	U	2.4
48	M1	111	ASP	2.4
1	6	495	C	2.4
16	c4	83	ILE	2.4
21	C9	63	ARG	2.4
10	S8	111	GLN	2.4
10	S8	165	LEU	2.4
10	s8	58	LEU	2.4
17	C5	105	VAL	2.4
30	D8	25	VAL	2.4
63	N7	51	LEU	2.4
63	N7	87	LEU	2.4
18	c6	14	LYS	2.4
25	D3	58	GLY	2.4
45	l8	70	LYS	2.4
5	s3	24	PHE	2.4
19	C7	118	PRO	2.4
20	C8	25	ASN	2.4
20	c8	21	ASN	2.4
64	n8	116	GLY	2.4
39	l2	59	ALA	2.4
44	L7	27	ALA	2.4
70	O4	34	HIS	2.4
1	2	280	U	2.4
25	D3	136	TRP	2.4
35	SM	110	TRP	2.4
36	5	2538	U	2.4
64	N8	79	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
5	S3	110	LEU	2.4
9	S7	38	LEU	2.4
10	S8	121	LEU	2.4
22	d0	14	GLN	2.4
27	D5	52	LYS	2.4
29	d7	58	SER	2.4
34	sR	94	VAL	2.4
39	L2	68	LYS	2.4
49	M3	190	LYS	2.4
63	N7	116	LYS	2.4
80	m2	92	SER	2.4
81	p0	29	GLY	2.4
12	C0	28	ASN	2.4
42	L5	94	ASN	2.4
66	O0	35	ARG	2.4
82	p2	34	ASN	2.4
7	S5	77	TYR	2.4
8	s6	208	TYR	2.4
14	c2	99	GLU	2.4
28	d6	63	ALA	2.4
42	l5	126	GLU	2.4
70	o4	39	ALA	2.4
9	S7	181	ILE	2.4
5	s3	69	LEU	2.4
8	s6	76	LEU	2.4
14	c2	29	LYS	2.4
19	c7	59	LYS	2.4
40	l3	106	TRP	2.4
74	o8	27	ILE	2.4
27	D5	83	LEU	2.4
40	L3	47	LEU	2.4
6	S4	24	SER	2.4
19	C7	85	VAL	2.4
19	c7	105	GLN	2.4
34	sR	69	GLN	2.4
42	L5	201	GLY	2.4
45	L8	40	VAL	2.4
70	O4	3	GLN	2.4
70	O4	22	VAL	2.4
80	m2	73	VAL	2.4
7	S5	219	ARG	2.4
25	d3	42	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
28	D6	92	ARG	2.4
25	D3	67	ALA	2.4
64	N8	146	GLU	2.4
29	D7	36	LYS	2.4
42	L5	262	LYS	2.4
63	N7	22	LYS	2.4
67	o1	61	LYS	2.4
5	S3	182	LEU	2.4
6	S4	92	LEU	2.4
21	c9	108	LEU	2.4
49	M3	98	ASP	2.4
60	n4	96	LEU	2.4
83	f	26	LEU	2.4
6	s4	185	GLY	2.4
9	S7	90	VAL	2.4
16	C4	74	VAL	2.4
24	D2	129	VAL	2.4
55	m9	51	VAL	2.4
7	s5	127	GLN	2.4
9	S7	42	GLN	2.4
9	S7	187	SER	2.4
13	C1	115	PHE	2.4
30	D8	65	ARG	2.4
36	5	1572	U	2.4
39	L2	70	ARG	2.4
25	D3	88	PRO	2.4
32	e0	3	LYS	2.4
46	L9	143	GLU	2.4
32	e0	40	TYR	2.4
34	SR	283	LYS	2.4
63	n7	115	LYS	2.4
67	o1	92	TYR	2.4
68	o2	2	ALA	2.4
70	o4	19	LYS	2.4
82	p1	4	GLU	2.4
36	5	1762	C	2.4
11	S9	24	LEU	2.4
26	D4	9	THR	2.4
43	l6	130	ILE	2.4
34	sR	222	LEU	2.4
42	L5	75	LEU	2.4
72	o6	11	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
82	p1	28	THR	2.4
18	c6	64	ASP	2.3
26	D4	66	GLY	2.3
36	1	1271	A	2.3
36	1	2445	A	2.3
67	O1	23	VAL	2.3
42	L5	160	PHE	2.3
74	o8	39	ARG	2.3
3	S1	85	LYS	2.3
12	c0	48	SER	2.3
42	L5	82	GLU	2.3
43	l6	8	LYS	2.3
81	p0	44	GLU	2.3
83	f	45	SER	2.3
1	2	1584	G	2.3
6	S4	210	ILE	2.3
15	c3	15	ALA	2.3
20	c8	121	ALA	2.3
34	SR	296	ALA	2.3
45	L8	46	LEU	2.3
70	O4	95	ILE	2.3
2	S0	181	VAL	2.3
11	S9	11	THR	2.3
17	c5	103	ASN	2.3
6	s4	163	ASP	2.3
1	6	506	A	2.3
23	D1	10	GLU	2.3
28	d6	46	GLU	2.3
63	N7	128	GLN	2.3
5	S3	188	ILE	2.3
6	s4	2	ALA	2.3
7	S5	113	ILE	2.3
11	s9	183	ALA	2.3
24	D2	52	TYR	2.3
32	e0	61	SER	2.3
25	D3	68	ILE	2.3
28	D6	98	PRO	2.3
42	L5	99	TYR	2.3
51	M5	10	LEU	2.3
51	M5	61	ILE	2.3
7	s5	143	ARG	2.3
10	S8	195	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
70	O4	30	LEU	2.3
2	S0	156	VAL	2.3
8	S6	97	VAL	2.3
7	S5	213	LYS	2.3
8	s6	156	PHE	2.3
13	C1	64	VAL	2.3
17	c5	6	ASN	2.3
18	C6	60	PHE	2.3
21	C9	61	VAL	2.3
41	L4	263	GLY	2.3
66	O0	89	VAL	2.3
53	M7	169	THR	2.3
3	s1	64	ARG	2.3
7	S5	143	ARG	2.3
7	S5	185	ARG	2.3
13	c1	147	ALA	2.3
14	c2	119	SER	2.3
18	c6	2	SER	2.3
28	d6	73	TYR	2.3
36	1	1350	A	2.3
43	l6	66	SER	2.3
49	m3	183	ARG	2.3
3	s1	53	GLY	2.3
4	s2	64	LYS	2.3
9	s7	92	PHE	2.3
20	c8	5	VAL	2.3
33	E1	96	LYS	2.3
47	M0	50	VAL	2.3
48	M1	54	VAL	2.3
63	N7	114	VAL	2.3
67	o1	93	VAL	2.3
74	o8	25	VAL	2.3
13	C1	21	ASN	2.3
21	C9	53	TRP	2.3
10	s8	159	GLN	2.3
22	d0	35	GLU	2.3
63	N7	83	THR	2.3
80	m2	155	ARG	2.3
8	S6	73	ILE	2.3
8	S6	101	ILE	2.3
17	C5	66	ALA	2.3
20	c8	14	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
27	d5	47	TYR	2.3
28	D6	73	TYR	2.3
29	d7	53	ALA	2.3
42	l5	294	ALA	2.3
54	m8	67	ILE	2.3
15	C3	52	VAL	2.3
25	D3	42	PRO	2.3
12	C0	19	GLY	2.3
36	5	1025	A	2.3
42	L5	175	HIS	2.3
45	L8	202	GLU	2.3
7	s5	176	THR	2.3
8	S6	199	GLN	2.3
8	s6	88	ARG	2.3
42	L5	28	THR	2.3
51	m5	49	ARG	2.3
58	N2	64	THR	2.3
81	p0	89	THR	2.3
81	p0	195	GLN	2.3
5	S3	21	LEU	2.3
14	c2	94	ALA	2.3
24	D2	104	LEU	2.3
45	L8	65	LEU	2.3
48	M1	112	LEU	2.3
48	M1	142	LYS	2.3
67	o1	20	LEU	2.3
34	SR	156	VAL	2.3
58	n2	56	VAL	2.3
1	6	1696	G	2.3
42	L5	182	GLY	2.3
17	c5	89	MET	2.3
63	N7	99	GLU	2.3
3	s1	86	LEU	2.3
6	S4	159	THR	2.3
6	s4	23	LEU	2.3
7	s5	80	LYS	2.3
19	c7	24	LEU	2.3
21	C9	110	LYS	2.3
51	m5	122	ASN	2.3
34	sR	226	ALA	2.3
72	o6	93	ILE	2.3
9	S7	62	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
17	C5	41	VAL	2.3
42	l5	159	VAL	2.3
63	n7	23	VAL	2.3
7	s5	163	SER	2.3
23	D1	68	SER	2.3
31	d9	18	SER	2.3
34	sR	205	SER	2.3
35	SM	93	ARG	2.3
60	N4	92	GLU	2.3
21	C9	38	LYS	2.3
21	c9	84	LYS	2.3
32	E0	31	LYS	2.3
61	n5	36	LYS	2.3
10	S8	112	TRP	2.3
36	1	252	U	2.3
6	S4	13	ALA	2.3
10	s8	78	ILE	2.3
16	c4	85	ALA	2.3
18	C6	24	ALA	2.3
20	C8	69	ILE	2.3
36	1	1577	G	2.3
36	5	2440	G	2.3
51	M5	28	TRP	2.3
67	o1	55	LEU	2.3
25	D3	95	PHE	2.3
25	D3	113	ALA	2.3
35	SM	102	THR	2.3
35	sM	60	ALA	2.3
67	O1	32	ALA	2.3
72	o6	53	TYR	2.3
45	L8	94	PHE	2.3
5	s3	117	ARG	2.3
6	S4	39	ARG	2.3
24	d2	123	GLY	2.3
9	S7	115	SER	2.3
10	s8	199	LYS	2.3
26	D4	81	GLU	2.3
28	D6	66	LYS	2.3
32	E0	3	LYS	2.3
34	sR	5	GLU	2.3
61	N5	29	SER	2.3
1	6	239	C	2.3

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Mol	Chain	Res	Type	RSRZ
6	s4	9	LEU	2.3
17	C5	128	HIS	2.3
24	D2	126	LEU	2.3
63	n7	42	LEU	2.3
72	o6	50	LEU	2.3
79	Q3	86	LEU	2.3
5	s3	188	ILE	2.3
18	C6	43	ILE	2.3
7	s5	122	ASN	2.3
8	S6	67	VAL	2.3
21	c9	33	TYR	2.3
27	d5	78	ILE	2.3
63	n7	18	TYR	2.3
64	n8	124	ILE	2.3
1	2	1713	G	2.3
25	D3	91	GLY	2.3
27	D5	87	GLY	2.3
31	D9	28	THR	2.3
53	M7	174	GLY	2.3
67	O1	50	ARG	2.3
70	O4	78	GLY	2.3
7	s5	45	LYS	2.3
29	D7	57	GLU	2.3
35	SM	58	GLU	2.3
32	e0	56	MET	2.3
45	l8	246	MET	2.3
45	l8	142	LEU	2.3
3	S1	32	ILE	2.3
11	S9	171	ARG	2.3
26	D4	13	ILE	2.3
27	d5	82	HIS	2.3
55	M9	118	HIS	2.3
58	N2	41	ILE	2.3
66	O0	43	ILE	2.3
4	s2	86	VAL	2.3
7	s5	154	ALA	2.3
29	d7	50	ALA	2.3
34	SR	56	VAL	2.3
34	sR	154	VAL	2.3
34	sR	315	VAL	2.3
54	m8	81	VAL	2.3
67	o1	109	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	2	1340	U	2.3
2	s0	22	THR	2.3
22	d0	73	GLY	2.3
83	f	80	MET	2.3
18	c6	68	ARG	2.3
32	E0	42	ARG	2.3
36	5	1573	G	2.3
17	c5	119	PHE	2.3
18	c6	83	GLN	2.3
25	D3	52	ILE	2.3
3	s1	38	PHE	2.3
25	D3	131	SER	2.3
6	S4	33	ALA	2.3
7	s5	123	VAL	2.3
10	s8	67	TRP	2.3
11	S9	96	VAL	2.3
34	SR	253	ALA	2.3
55	M9	177	VAL	2.3
58	N2	13	LYS	2.3
63	n7	74	VAL	2.3
64	N8	111	LYS	2.3
72	O6	53	TYR	2.3
51	M5	137	PRO	2.3
6	s4	22	LYS	2.3
6	s4	228	ILE	2.3
20	c8	125	ILE	2.3
5	S3	174	HIS	2.3
7	S5	136	ALA	2.3
8	S6	84	TYR	2.3
11	S9	43	TYR	2.3
16	C4	78	ALA	2.3
19	C7	70	SER	2.3
25	d3	86	PHE	2.3
27	d5	52	LYS	2.3
67	O1	37	LYS	2.3
34	SR	65	SER	2.3
45	L8	223	ALA	2.3
47	M0	138	VAL	2.3
48	M1	136	ALA	2.3
52	m6	183	ALA	2.3
67	o1	91	SER	2.3
29	D7	40	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
3	s1	46	THR	2.2
6	s4	42	LEU	2.2
6	s4	65	LEU	2.2
8	S6	92	ARG	2.2
19	C7	123	ASN	2.2
25	d3	90	ASP	2.2
29	D7	67	THR	2.2
34	SR	76	ASP	2.2
35	SM	92	ASP	2.2
45	l8	166	LEU	2.2
80	m2	127	ARG	2.2
81	p0	98	ASN	2.2
6	S4	83	PRO	2.2
6	S4	198	LYS	2.2
13	c1	69	LYS	2.2
22	D0	64	LYS	2.2
27	D5	78	ILE	2.2
63	n7	130	PHE	2.2
67	O1	75	ILE	2.2
42	L5	96	ALA	2.2
51	M5	40	ALA	2.2
51	M5	148	TYR	2.2
7	s5	46	TRP	2.2
18	C6	61	SER	2.2
51	m5	39	ALA	2.2
55	m9	23	TRP	2.2
72	O6	98	ARG	2.2
74	o8	46	ARG	2.2
6	s4	26	CYS	2.2
12	C0	5	LYS	2.2
34	SR	7	LEU	2.2
34	SR	117	LYS	2.2
34	sR	221	MET	2.2
45	L8	69	LEU	2.2
51	m5	56	LYS	2.2
78	Q2	100	LYS	2.2
8	s6	144	PHE	2.2
11	s9	141	VAL	2.2
14	c2	66	VAL	2.2
14	c2	120	VAL	2.2
32	E0	27	PRO	2.2
34	sR	178	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
36	1	1763	U	2.2
58	n2	66	VAL	2.2
58	n2	71	PHE	2.2
63	N7	10	VAL	2.2
6	s4	124	GLY	2.2
14	c2	35	ALA	2.2
24	D2	59	GLY	2.2
47	m0	195	ALA	2.2
63	N7	106	GLN	2.2
63	n7	2	ALA	2.2
64	N8	109	TYR	2.2
82	p2	42	ALA	2.2
7	S5	81	ARG	2.2
7	s5	219	ARG	2.2
17	c5	137	ARG	2.2
45	L8	28	HIS	2.2
53	M7	170	SER	2.2
6	s4	238	LEU	2.2
60	N4	91	LYS	2.2
62	N6	35	LEU	2.2
1	2	1337	A	2.2
1	6	1226	A	2.2
34	sR	184	ASN	2.2
34	sR	220	ILE	2.2
9	S7	73	VAL	2.2
16	C4	28	VAL	2.2
7	s5	151	GLY	2.2
13	C1	127	GLN	2.2
18	c6	27	GLY	2.2
56	n0	2	ALA	2.2
7	S5	222	LYS	2.2
1	2	575	C	2.2
5	s3	110	LEU	2.2
7	s5	118	LEU	2.2
14	c2	74	LEU	2.2
26	D4	125	LEU	2.2
35	sM	28	SER	2.2
42	L5	242	SER	2.2
9	S7	24	PHE	2.2
2	S0	143	VAL	2.2
4	S2	178	ILE	2.2
10	S8	102	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
16	C4	48	VAL	2.2
17	c5	96	ILE	2.2
28	D6	84	VAL	2.2
40	L3	328	ILE	2.2
31	D9	40	ARG	2.2
45	L8	45	ASN	2.2
63	N7	75	VAL	2.2
35	sM	64	LYS	2.2
36	1	2207	A	2.2
70	O4	31	ARG	2.2
70	O4	80	ARG	2.2
7	s5	85	ALA	2.2
7	s5	179	ALA	2.2
14	c2	85	LYS	2.2
16	C4	63	ALA	2.2
16	C4	104	ALA	2.2
39	L2	47	GLN	2.2
55	M9	53	LYS	2.2
74	o8	30	LYS	2.2
81	p0	11	TYR	2.2
83	f	17	ALA	2.2
1	2	133	U	2.2
1	2	193	U	2.2
60	n4	87	LEU	2.2
1	2	1610	G	2.2
24	d2	122	SER	2.2
27	d5	93	SER	2.2
3	s1	30	PHE	2.2
3	S1	48	VAL	2.2
7	s5	160	VAL	2.2
8	s6	175	ILE	2.2
13	c1	137	PHE	2.2
36	1	1576	G	2.2
14	c2	33	ARG	2.2
67	O1	64	VAL	2.2
74	O8	56	ILE	2.2
2	S0	51	GLY	2.2
16	c4	59	ALA	2.2
26	D4	71	GLY	2.2
28	d6	62	TYR	2.2
63	N7	47	GLU	2.2
67	O1	27	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
81	p0	208	GLU	2.2
34	SR	244	ALA	2.2
42	L5	246	ALA	2.2
60	n4	103	ALA	2.2
61	n5	111	ASN	2.2
72	O6	96	ALA	2.2
1	2	474	A	2.2
8	s6	133	LEU	2.2
48	m1	91	LEU	2.2
55	m9	184	LEU	2.2
58	n2	37	LEU	2.2
6	s4	127	LYS	2.2
11	S9	113	VAL	2.2
12	c0	56	LYS	2.2
14	c2	72	ILE	2.2
27	d5	60	VAL	2.2
53	M7	16	SER	2.2
63	N7	48	ARG	2.2
70	o4	22	VAL	2.2
7	s5	181	GLU	2.2
42	L5	268	GLU	2.2
20	C8	30	TYR	2.2
28	D6	35	ALA	2.2
34	sR	287	PRO	2.2
61	n5	40	LEU	2.2
1	2	599	A	2.2
7	s5	199	ILE	2.2
11	S9	120	LYS	2.2
13	C1	137	PHE	2.2
83	f	78	HIS	2.2
13	C1	66	ILE	2.2
30	d8	25	VAL	2.2
41	L4	249	ILE	2.2
43	l6	2	SER	2.2
58	n2	97	SER	2.2
67	O1	67	VAL	2.2
34	sR	11	GLY	2.2
11	S9	8	TYR	2.2
51	m5	62	TYR	2.2
1	2	584	C	2.2
14	c2	133	LEU	2.2
17	C5	75	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
8	S6	197	ASN	2.2
2	S0	81	PHE	2.2
4	S2	88	LYS	2.2
16	C4	103	ARG	2.2
30	D8	29	ARG	2.2
33	e1	151	ASN	2.2
36	5	2442	G	2.2
63	N7	67	LYS	2.2
69	o3	65	ARG	2.2
12	c0	16	PHE	2.2
26	d4	23	PHE	2.2
8	s6	161	GLU	2.2
14	C2	83	GLU	2.2
15	c3	25	TRP	2.2
28	d6	17	HIS	2.2
40	L3	78	VAL	2.2
54	m8	101	VAL	2.2
62	N6	45	ILE	2.2
81	p0	53	MET	2.2
2	S0	196	SER	2.2
18	C6	121	SER	2.2
36	1	1269	U	2.2
55	M9	59	SER	2.2
64	N8	116	GLY	2.2
11	S9	183	ALA	2.2
27	D5	79	ALA	2.2
34	sR	172	ALA	2.2
42	L5	172	TYR	2.2
45	l8	198	ALA	2.2
55	m9	35	ALA	2.2
8	S6	86	PRO	2.2
10	S8	103	GLN	2.2
26	d4	135	ASP	2.2
33	E1	149	LYS	2.2
63	N7	17	ARG	2.2
64	n8	119	PRO	2.2
74	o8	40	GLN	2.2
25	D3	65	ASN	2.2
58	N2	49	ASN	2.2
58	N2	87	ASN	2.2
78	Q2	3	ASN	2.2
21	C9	113	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
28	D6	41	ILE	2.2
42	L5	231	ILE	2.2
80	m2	96	THR	2.2
46	L9	85	GLY	2.2
1	6	1232	U	2.2
6	S4	51	ARG	2.2
16	c4	49	LYS	2.2
20	C8	54	LEU	2.2
47	M0	139	ARG	2.2
48	M1	85	LYS	2.2
58	n2	108	TYR	2.2
70	O4	2	ALA	2.2
81	p0	199	SER	2.2
1	2	1410	A	2.2
1	6	1469	A	2.2
16	c4	99	GLN	2.2
25	d3	118	PRO	2.2
35	sM	40	PRO	2.2
70	o4	7	PHE	2.2
74	o8	11	PHE	2.2
6	S4	236	ILE	2.2
11	s9	7	THR	2.2
23	D1	32	VAL	2.2
64	N8	82	ILE	2.2
64	N8	104	THR	2.2
3	s1	153	HIS	2.2
20	C8	129	TRP	2.2
42	L5	161	GLY	2.2
5	S3	69	LEU	2.2
8	S6	208	TYR	2.2
11	S9	39	LYS	2.2
12	c0	79	TYR	2.2
28	D6	68	TYR	2.2
51	m5	41	ARG	2.2
15	C3	75	LEU	2.2
16	c4	33	LEU	2.2
22	d0	93	LEU	2.2
25	D3	93	LEU	2.2
25	d3	104	LEU	2.2
34	sR	274	LEU	2.2
6	S4	175	PHE	2.2
6	s4	175	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
7	S5	82	PHE	2.2
64	n8	89	GLN	2.2
8	s6	135	PRO	2.2
6	S4	147	ILE	2.2
6	s4	73	ASP	2.2
31	d9	11	PRO	2.2
11	S9	77	ILE	2.2
12	c0	55	VAL	2.2
27	D5	41	ILE	2.2
34	sR	51	ASP	2.2
34	sR	312	VAL	2.2
42	L5	221	GLU	2.2
46	L9	99	ILE	2.2
64	n8	112	ILE	2.2
3	S1	49	ASN	2.2
7	S5	138	THR	2.2
15	C3	69	ASN	2.2
30	D8	26	THR	2.2
33	E1	115	THR	2.2
39	L2	85	GLY	2.2
53	M7	29	THR	2.2
70	o4	41	ARG	2.2
33	e1	148	TYR	2.1
34	SR	301	LEU	2.1
64	n8	79	TRP	2.1
70	o4	38	LEU	2.1
2	S0	83	GLN	2.1
54	M8	96	PHE	2.1
36	1	1265	U	2.1
55	M9	175	GLN	2.1
3	S1	65	VAL	2.1
7	S5	119	ASP	2.1
15	C3	71	ILE	2.1
31	D9	23	VAL	2.1
35	sM	168	GLU	2.1
42	L5	204	VAL	2.1
43	L6	65	ILE	2.1
51	m5	42	PRO	2.1
27	D5	103	ARG	2.1
78	Q2	92	GLU	2.1
80	m2	125	ILE	2.1
6	S4	207	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
35	sM	57	ASN	2.1
34	SR	212	ALA	2.1
45	l8	80	TYR	2.1
45	l8	110	THR	2.1
72	o6	92	ASN	2.1
17	c5	97	TYR	2.1
58	N2	36	TYR	2.1
2	S0	116	LYS	2.1
7	s5	23	VAL	2.1
11	s9	33	GLU	2.1
13	C1	46	LYS	2.1
18	C6	69	VAL	2.1
22	D0	62	VAL	2.1
22	d0	69	LYS	2.1
28	D6	51	ARG	2.1
32	E0	50	VAL	2.1
34	SR	6	VAL	2.1
46	L9	10	ILE	2.1
62	N6	113	LYS	2.1
66	O0	40	LYS	2.1
67	O1	28	ARG	2.1
82	p1	40	ILE	2.1
20	c8	124	GLY	2.1
21	c9	67	MET	2.1
29	D7	68	GLY	2.1
51	m5	46	ASP	2.1
22	D0	26	LEU	2.1
27	D5	75	LEU	2.1
72	O6	50	LEU	2.1
10	S8	138	ASN	2.1
34	SR	99	THR	2.1
72	O6	48	ALA	2.1
80	m2	79	ASN	2.1
21	c9	21	PHE	2.1
81	p0	213	PHE	2.1
1	2	1583	A	2.1
6	s4	187	ARG	2.1
17	c5	130	ARG	2.1
22	d0	74	GLU	2.1
32	e0	17	GLN	2.1
36	1	1026	A	2.1
81	p0	23	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
55	M9	41	ILE	2.1
63	N7	12	VAL	2.1
63	N7	43	VAL	2.1
6	s4	34	GLY	2.1
8	s6	134	GLY	2.1
11	S9	117	GLY	2.1
47	m0	124	GLY	2.1
55	m9	26	PRO	2.1
18	c6	98	ASP	2.1
20	C8	45	LEU	2.1
81	p0	15	LEU	2.1
32	E0	5	HIS	2.1
34	sR	31	ASN	2.1
34	sR	85	TRP	2.1
52	M6	184	THR	2.1
53	M7	177	ALA	2.1
63	n7	49	TYR	2.1
6	s4	145	ARG	2.1
76	q0	128	LYS	2.1
25	D3	63	GLN	2.1
34	sR	43	ILE	2.1
63	n7	26	VAL	2.1
72	O6	58	ILE	2.1
1	2	175	G	2.1
1	2	576	G	2.1
18	C6	33	GLY	2.1
19	c7	2	GLY	2.1
20	C8	124	GLY	2.1
24	D2	111	MET	2.1
32	E0	58	PRO	2.1
1	2	174	U	2.1
1	2	742	U	2.1
5	S3	141	LYS	2.1
11	S9	31	ALA	2.1
19	c7	28	PHE	2.1
35	sM	78	ASP	2.1
42	L5	134	ALA	2.1
42	L5	142	PHE	2.1
45	l8	91	PHE	2.1
55	M9	54	ALA	2.1
81	p0	79	PHE	2.1
7	S5	52	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
11	S9	85	VAL	2.1
17	C5	78	THR	2.1
21	C9	37	VAL	2.1
64	n8	146	GLU	2.1
22	d0	17	GLN	2.1
30	D8	57	MET	2.1
64	N8	110	GLY	2.1
83	f	39	CYS	2.1
2	s0	146	LEU	2.1
10	s8	184	LEU	2.1
14	C2	62	LEU	2.1
3	S1	64	ARG	2.1
6	S4	62	LYS	2.1
8	S6	95	LYS	2.1
11	S9	121	SER	2.1
3	S1	142	PHE	2.1
21	C9	130	ARG	2.1
67	O1	76	SER	2.1
34	sR	75	ALA	2.1
71	o5	2	ALA	2.1
6	S4	17	HIS	2.1
10	s8	102	VAL	2.1
26	D4	29	HIS	2.1
5	S3	26	THR	2.1
15	C3	74	ILE	2.1
40	l3	162	VAL	2.1
45	l8	157	VAL	2.1
59	N3	137	VAL	2.1
22	d0	81	THR	2.1
29	D7	52	THR	2.1
81	p0	96	ILE	2.1
3	S1	97	LEU	2.1
10	S8	184	LEU	2.1
11	S9	80	LEU	2.1
13	C1	141	LYS	2.1
21	C9	134	ARG	2.1
34	SR	176	LYS	2.1
46	L9	161	LEU	2.1
8	s6	27	PHE	2.1
15	c3	14	SER	2.1
7	S5	85	ALA	2.1
21	C9	18	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
35	sM	66	ALA	2.1
68	o2	92	TYR	2.1
14	C2	75	VAL	2.1
25	D3	120	VAL	2.1
42	L5	189	GLU	2.1
41	L4	250	TRP	2.1
48	M1	138	VAL	2.1
70	o4	90	ILE	2.1
72	o6	58	ILE	2.1
1	6	668	C	2.1
3	S1	99	ASN	2.1
3	s1	111	ARG	2.1
6	S4	58	GLY	2.1
8	S6	178	LEU	2.1
12	C0	37	THR	2.1
15	C3	43	LYS	2.1
18	C6	77	GLN	2.1
18	c6	8	GLN	2.1
20	C8	8	GLN	2.1
25	d3	4	GLY	2.1
31	D9	36	LEU	2.1
32	E0	43	ARG	2.1
32	e0	24	THR	2.1
35	sM	70	ASN	2.1
40	L3	50	LYS	2.1
42	L5	118	THR	2.1
42	L5	222	LEU	2.1
64	n8	117	ARG	2.1
66	O0	38	LYS	2.1
70	O4	68	THR	2.1
74	o8	72	THR	2.1
13	C1	23	PRO	2.1
28	D6	2	PRO	2.1
43	L6	101	PHE	2.1
21	C9	58	ALA	2.1
55	m9	59	SER	2.1
8	s6	79	LYS	2.1
33	E1	95	HIS	2.1
42	l5	247	ILE	2.1
45	l8	203	VAL	2.1
5	S3	109	LEU	2.1
11	S9	150	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
18	C6	82	ARG	2.1
35	SM	67	GLY	2.1
70	O4	9	ARG	2.1
9	S7	92	PHE	2.1
14	C2	140	PHE	2.1
26	d4	9	THR	2.1
34	SR	17	ASN	2.1
57	n1	66	ASN	2.1
80	m2	16	ASN	2.1
1	2	1199	G	2.1
35	sM	39	PRO	2.1
13	C1	48	ALA	2.1
45	L8	55	TYR	2.1
25	d3	125	VAL	2.1
29	D7	54	VAL	2.1
30	d8	12	VAL	2.1
54	M8	63	SER	2.1
63	N7	62	VAL	2.1
83	f	84	VAL	2.1
6	S4	131	LEU	2.1
12	C0	26	ASP	2.1
12	c0	46	LEU	2.1
14	c2	93	ASP	2.1
16	C4	95	GLY	2.1
16	c4	62	LEU	2.1
42	L5	113	LEU	2.1
56	N0	76	GLY	2.1
39	L2	115	ASN	2.1
56	N0	4	PHE	2.1
1	6	1196	A	2.1
13	C1	59	PRO	2.1
34	sR	247	PRO	2.1
42	l5	129	TYR	2.1
43	L6	131	LYS	2.1
33	E1	84	VAL	2.1
45	l8	114	ALA	2.1
1	2	1481	C	2.1
63	n7	75	VAL	2.1
74	o8	75	VAL	2.1
27	D5	50	ILE	2.1
2	s0	17	LEU	2.1
7	S5	118	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
7	s5	55	ASP	2.1
26	d4	96	LEU	2.1
36	5	2437	G	2.1
49	m3	170	LEU	2.1
6	s4	87	MET	2.1
48	M1	152	HIS	2.1
9	s7	24	PHE	2.1
53	m7	55	GLN	2.1
1	2	232	U	2.1
6	s4	153	ASN	2.1
7	S5	148	ARG	2.1
7	s5	102	ARG	2.1
17	c5	98	ASN	2.1
35	SM	27	LYS	2.1
42	l5	198	TYR	2.1
51	M5	131	GLU	2.1
83	f	104	ASN	2.1
6	S4	46	VAL	2.1
9	S7	4	PRO	2.1
11	S9	169	PRO	2.1
63	N7	28	PRO	2.1
68	O2	2	ALA	2.1
74	o8	34	ALA	2.1
6	s4	44	LEU	2.1
19	C7	26	LEU	2.1
34	SR	89	LEU	2.1
51	m5	61	ILE	2.1
51	m5	142	ILE	2.1
9	S7	158	ASP	2.1
2	S0	56	LYS	2.0
4	S2	64	LYS	2.0
5	S3	75	LYS	2.0
34	SR	85	TRP	2.0
27	d5	68	ARG	2.0
35	SM	46	LYS	2.0
35	SM	94	HIS	2.1
48	m1	90	GLN	2.0
63	N7	29	HIS	2.1
64	n8	126	LYS	2.0
20	c8	98	TYR	2.0
26	D4	86	GLU	2.0
2	S0	103	THR	2.0

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Mol	Chain	Res	Type	RSRZ
8	s6	153	VAL	2.0
34	sR	130	THR	2.0
55	M9	35	ALA	2.0
55	m9	36	ASN	2.0
64	N8	107	ALA	2.0
4	s2	178	ILE	2.0
45	l8	136	LEU	2.0
46	l9	74	LEU	2.0
76	Q0	80	PRO	2.0
6	S4	243	GLY	2.0
5	S3	150	MET	2.0
5	s3	107	PHE	2.0
6	S4	109	PHE	2.0
49	m3	177	LYS	2.0
60	n4	102	LYS	2.0
63	N7	27	LYS	2.0
7	S5	102	ARG	2.0
11	S9	123	HIS	2.0
13	c1	127	GLN	2.0
20	C8	16	ARG	2.0
61	N5	33	ARG	2.0
72	o6	62	ARG	2.0
80	m2	133	SER	2.0
12	C0	34	GLU	2.0
12	C0	78	GLU	2.0
5	S3	181	VAL	2.0
7	s5	134	VAL	2.0
26	D4	82	ALA	2.0
28	D6	48	ALA	2.0
48	M1	128	TYR	2.0
51	M5	62	TYR	2.0
78	Q2	2	VAL	2.0
2	s0	49	ASN	2.0
39	L2	79	ASN	2.0
47	M0	33	ILE	2.0
51	M5	36	ILE	2.0
49	M3	74	GLY	2.0
64	n8	91	LEU	2.0
80	m2	122	ILE	2.0
1	6	1435	G	2.0
8	S6	66	GLY	2.0
17	c5	9	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
27	d5	97	LYS	2.0
36	1	1237	G	2.0
42	l5	169	GLY	2.0
78	Q2	15	LYS	2.0
21	C9	45	MET	2.0
49	m3	180	ARG	2.0
56	N0	90	MET	2.0
63	n7	107	ARG	2.0
67	O1	25	PHE	2.0
6	S4	253	ASP	2.0
18	c6	121	SER	2.0
21	C9	60	SER	2.0
29	D7	74	SER	2.0
34	sR	114	ASP	2.0
55	M9	116	ASP	2.0
70	o4	34	HIS	2.0
25	d3	72	VAL	2.0
5	s3	208	ILE	2.0
7	S5	177	ILE	2.0
13	C1	43	LYS	2.0
16	C4	33	LEU	2.0
20	C8	18	LEU	2.0
25	d3	85	ALA	2.0
31	d9	6	VAL	2.0
35	SM	141	ALA	2.0
8	s6	164	LYS	2.0
16	c4	98	GLY	2.0
20	C8	56	LYS	2.0
21	C9	78	LYS	2.0
30	d8	11	LYS	2.0
45	l8	181	LYS	2.0
67	o1	73	LEU	2.0
6	s4	220	THR	2.0
19	C7	78	ARG	2.0
34	sR	48	THR	2.0
34	sR	233	THR	2.0
58	n2	101	ASN	2.0
67	O1	103	GLY	2.0
1	2	551	G	2.0
33	e1	111	GLU	2.0
42	l5	151	GLN	2.0
10	S8	44	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
11	S9	124	HIS	2.0
7	S5	33	VAL	2.0
11	s9	51	LYS	2.0
12	C0	43	ILE	2.0
13	c1	40	LEU	2.0
15	C3	15	ALA	2.0
20	C8	113	LEU	2.0
25	D3	126	LYS	2.0
26	d4	12	VAL	2.0
55	M9	188	ASP	2.0
62	N6	82	VAL	2.0
2	S0	160	ILE	2.0
3	S1	110	LEU	2.0
1	6	1189	A	2.0
5	S3	27	ARG	2.0
5	s3	115	ILE	2.0
17	C5	99	GLY	2.0
24	D2	68	ARG	2.0
26	D4	44	LEU	2.0
27	D5	76	ALA	2.0
34	SR	13	LEU	2.0
35	SM	20	LEU	2.0
42	L5	103	LEU	2.0
45	l8	237	ILE	2.0
46	L9	146	LEU	2.0
51	m5	51	LEU	2.0
63	N7	64	LYS	2.0
6	S4	254	ARG	2.0
67	O1	36	ILE	2.0
82	p2	27	LEU	2.0
36	5	1696	A	2.0
7	s5	67	PRO	2.0
9	S7	183	PHE	2.0
26	D4	64	PHE	2.0
5	S3	177	MET	2.0
11	s9	74	ASN	2.0
14	C2	53	THR	2.0
16	C4	89	THR	2.0
34	sR	159	ASN	2.0
80	m2	63	THR	2.0
6	s4	60	GLU	2.0
19	c7	87	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
21	C9	109	GLU	2.0
1	2	231	U	2.0
8	S6	102	VAL	2.0
6	s4	38	LEU	2.0
10	S8	192	TYR	2.0
16	C4	108	SER	2.0
29	d7	54	VAL	2.0
31	d9	23	VAL	2.0
32	E0	53	LYS	2.0
41	L4	42	VAL	2.0
43	l6	128	LYS	2.0
31	d9	12	ARG	2.0
34	SR	165	ASP	2.0
41	l4	244	LEU	2.0
46	L9	177	ASP	2.0
47	M0	68	ALA	2.0
47	M0	142	ASP	2.0
51	m5	66	VAL	2.0
67	o1	108	VAL	2.0
11	S9	98	ALA	2.0
14	C2	89	ILE	2.0
19	c7	60	ARG	2.0
49	m3	193	ALA	2.0
55	M9	168	ALA	2.0
67	o1	112	ASP	2.0
1	2	1364	G	2.0
59	N3	3	GLY	2.0
6	s4	83	PRO	2.0
45	L8	161	GLU	2.0
1	6	1711	C	2.0
5	S3	187	LYS	2.0
10	S8	142	LYS	2.0
18	C6	30	LYS	2.0
34	sR	228	LYS	2.0
36	1	3154	C	2.0
72	o6	25	LYS	2.0
2	S0	184	LEU	2.0
6	S4	12	LEU	2.0
12	c0	20	VAL	2.0
21	C9	24	ARG	2.0
21	C9	123	ARG	2.0
24	D2	69	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
34	SR	91	LEU	2.0
34	sR	89	LEU	2.0
62	N6	99	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
83	5CT	f	51	15/16	0.71	0.36	44,44,44,44	15
84	8AN	C	76	22/23	0.95	0.24	40,42,43,43	0
84	8AN	B	76	22/23	0.97	0.20	44,44,45,45	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
85	MG	2	1943	1/1	0.35	0.41	115,115,115,115	0
85	MG	2	1987	1/1	0.35	0.31	104,104,104,104	0
85	MG	2	1986	1/1	0.40	0.39	118,118,118,118	0
85	MG	6	1980	1/1	0.40	0.27	76,76,76,76	0
85	MG	5	3462	1/1	0.40	0.22	109,109,109,109	0
85	MG	6	1984	1/1	0.44	0.26	109,109,109,109	0
85	MG	6	1974	1/1	0.46	0.34	94,94,94,94	0
85	MG	5	3680	1/1	0.46	0.44	70,70,70,70	0
85	MG	1	3600	1/1	0.47	0.36	60,60,60,60	0
85	MG	6	1990	1/1	0.48	0.53	79,79,79,79	0
85	MG	1	3742	1/1	0.53	0.70	44,44,44,44	0
85	MG	6	1972	1/1	0.53	0.34	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	6	2004	1/1	0.54	0.80	74,74,74,74	0
85	MG	2	1965	1/1	0.55	0.87	76,76,76,76	0
85	MG	5	3638	1/1	0.55	0.42	50,50,50,50	0
85	MG	4	203	1/1	0.55	0.67	57,57,57,57	0
85	MG	2	1969	1/1	0.56	0.28	108,108,108,108	0
85	MG	2	1939	1/1	0.56	0.55	130,130,130,130	0
85	MG	6	1937	1/1	0.56	0.88	98,98,98,98	0
85	MG	5	3757	1/1	0.56	0.18	73,73,73,73	0
85	MG	5	3816	1/1	0.56	0.45	39,39,39,39	0
85	MG	5	3674	1/1	0.57	0.23	65,65,65,65	0
85	MG	2	1985	1/1	0.57	0.53	86,86,86,86	0
85	MG	17	2200	1/1	0.58	0.32	50,50,50,50	0
85	MG	2	1978	1/1	0.59	0.33	74,74,74,74	0
85	MG	6	1996	1/1	0.59	0.68	70,70,70,70	0
85	MG	2	1927	1/1	0.60	0.24	85,85,85,85	0
85	MG	1	3407	1/1	0.61	0.54	33,33,33,33	0
85	MG	2	1953	1/1	0.62	0.21	89,89,89,89	0
85	MG	1	3523	1/1	0.64	0.41	54,54,54,54	0
85	MG	2	1958	1/1	0.64	0.53	104,104,104,104	0
85	MG	6	1915	1/1	0.64	0.41	75,75,75,75	0
85	MG	1	3695	1/1	0.65	0.39	58,58,58,58	0
85	MG	5	3446	1/1	0.66	0.48	64,64,64,64	0
85	MG	6	1986	1/1	0.67	0.95	93,93,93,93	0
85	MG	5	3637	1/1	0.67	0.57	36,36,36,36	0
86	OHX	2	2135	7/7	0.67	0.15	188,188,188,188	6
85	MG	2	1989	1/1	0.68	0.47	65,65,65,65	0
85	MG	2	1973	1/1	0.68	0.45	80,80,80,80	0
85	MG	5	3741	1/1	0.68	0.52	66,66,66,66	0
85	MG	2	1974	1/1	0.68	0.41	83,83,83,83	0
85	MG	2	1904	1/1	0.68	0.44	90,90,90,90	0
85	MG	6	1932	1/1	0.68	0.40	72,72,72,72	0
85	MG	1	3662	1/1	0.68	0.79	101,101,101,101	0
86	OHX	6	2178	7/7	0.68	0.28	145,145,145,145	6
85	MG	M7	201	1/1	0.69	0.59	71,71,71,71	0
85	MG	5	3448	1/1	0.69	0.47	36,36,36,36	0
85	MG	D3	201	1/1	0.69	0.43	54,54,54,54	0
85	MG	o3	201	1/1	0.69	0.31	51,51,51,51	0
85	MG	5	3481	1/1	0.69	0.24	76,76,76,76	0
85	MG	5	3613	1/1	0.69	0.54	42,42,42,42	0
85	MG	5	3423	1/1	0.70	0.22	43,43,43,43	0
85	MG	1	3743	1/1	0.70	0.37	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
85	MG	1	3754	1/1	0.70	0.43	71,71,71,71	0
85	MG	5	3460	1/1	0.70	0.48	36,36,36,36	0
85	MG	1	3714	1/1	0.70	0.68	46,46,46,46	0
85	MG	4	205	1/1	0.70	0.61	58,58,58,58	0
87	ZN	D7	101	1/1	0.70	0.37	161,161,161,161	0
85	MG	5	3746	1/1	0.71	0.48	76,76,76,76	0
85	MG	1	3679	1/1	0.71	0.26	59,59,59,59	0
86	OHX	2	2149	7/7	0.71	0.28	137,137,137,137	6
85	MG	5	3685	1/1	0.71	0.69	48,48,48,48	0
85	MG	6	1985	1/1	0.71	0.49	55,55,55,55	0
85	MG	5	3464	1/1	0.72	0.15	125,125,125,125	0
85	MG	c8	202	1/1	0.72	0.31	84,84,84,84	0
85	MG	5	3483	1/1	0.72	0.87	52,52,52,52	0
85	MG	1	3708	1/1	0.72	0.45	42,42,42,42	0
85	MG	5	3444	1/1	0.72	0.46	34,34,34,34	0
85	MG	2	1959	1/1	0.72	0.29	87,87,87,87	0
85	MG	5	3672	1/1	0.72	0.54	62,62,62,62	0
85	MG	2	1938	1/1	0.72	0.26	72,72,72,72	0
85	MG	1	3692	1/1	0.72	0.54	61,61,61,61	0
85	MG	1	3608	1/1	0.72	0.43	46,46,46,46	0
85	MG	2	1936	1/1	0.73	0.14	83,83,83,83	0
86	OHX	2	2133	7/7	0.73	0.20	214,214,214,214	6
85	MG	2	1950	1/1	0.73	0.31	108,108,108,108	0
85	MG	5	3784	1/1	0.73	0.34	35,35,35,35	0
85	MG	5	3715	1/1	0.73	0.32	62,62,62,62	0
86	OHX	6	2183	7/7	0.73	0.59	76,76,76,76	5
85	MG	6	1960	1/1	0.73	0.14	65,65,65,65	0
85	MG	2	1912	1/1	0.74	0.49	88,88,88,88	0
85	MG	2	1930	1/1	0.74	0.40	72,72,72,72	0
85	MG	5	3503	1/1	0.74	0.47	57,57,57,57	0
85	MG	5	3599	1/1	0.74	0.56	39,39,39,39	0
85	MG	1	3642	1/1	0.74	0.57	32,32,32,32	0
85	MG	1	3423	1/1	0.74	0.48	46,46,46,46	0
85	MG	2	1960	1/1	0.74	0.28	76,76,76,76	0
85	MG	5	3426	1/1	0.74	0.47	45,45,45,45	0
85	MG	5	3807	1/1	0.74	0.24	54,54,54,54	0
85	MG	6	1993	1/1	0.75	0.26	66,66,66,66	0
85	MG	1	3747	1/1	0.75	0.34	48,48,48,48	0
85	MG	6	1961	1/1	0.75	0.15	95,95,95,95	0
85	MG	5	3698	1/1	0.75	0.61	42,42,42,42	0
86	OHX	2	2150	7/7	0.75	0.14	151,151,151,151	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	5	3649	1/1	0.75	0.68	47,47,47,47	0
85	MG	8	207	1/1	0.75	0.43	43,43,43,43	0
85	MG	1	3700	1/1	0.75	0.34	51,51,51,51	0
85	MG	7	207	1/1	0.76	0.41	55,55,55,55	0
85	MG	5	3552	1/1	0.76	0.50	52,52,52,52	0
85	MG	5	3690	1/1	0.76	0.61	75,75,75,75	0
85	MG	5	3401	1/1	0.76	0.21	53,53,53,53	0
85	MG	1	3591	1/1	0.76	0.32	53,53,53,53	0
85	MG	1	3723	1/1	0.76	0.52	67,67,67,67	0
85	MG	5	3468	1/1	0.76	0.43	47,47,47,47	0
85	MG	1	3737	1/1	0.76	0.42	63,63,63,63	0
85	MG	6	2008	1/1	0.76	0.95	61,61,61,61	0
85	MG	6	1982	1/1	0.76	1.00	53,53,53,53	0
85	MG	5	3543	1/1	0.76	0.55	41,41,41,41	0
85	MG	5	3469	1/1	0.77	0.54	38,38,38,38	1
85	MG	5	3573	1/1	0.77	0.27	48,48,48,48	0
85	MG	1	3634	1/1	0.77	0.69	41,41,41,41	0
85	MG	1	3639	1/1	0.77	0.71	56,56,56,56	0
86	OHX	3	219	7/7	0.77	0.24	82,82,82,82	5
85	MG	14	401	1/1	0.77	0.45	42,42,42,42	0
85	MG	5	3418	1/1	0.77	0.50	36,36,36,36	0
86	OHX	5	4159	7/7	0.77	0.39	48,48,48,48	4
86	OHX	5	4162	7/7	0.77	0.36	100,100,100,100	7
85	MG	2	1957	1/1	0.77	0.34	99,99,99,99	0
85	MG	5	3714	1/1	0.78	0.42	36,36,36,36	0
85	MG	1	3729	1/1	0.78	0.46	69,69,69,69	0
85	MG	5	3651	1/1	0.78	0.36	42,42,42,42	0
85	MG	1	3617	1/1	0.78	0.49	41,41,41,41	0
85	MG	1	3661	1/1	0.78	0.29	51,51,51,51	0
85	MG	5	3773	1/1	0.78	0.77	52,52,52,52	0
85	MG	5	3778	1/1	0.78	0.33	115,115,115,115	0
85	MG	1	3449	1/1	0.78	0.41	57,57,57,57	0
85	MG	5	3790	1/1	0.78	0.32	69,69,69,69	0
85	MG	1	3663	1/1	0.78	0.97	44,44,44,44	0
86	OHX	5	4153	7/7	0.78	0.43	35,35,35,35	4
85	MG	5	3686	1/1	0.78	0.32	92,92,92,92	0
85	MG	1	3665	1/1	0.78	0.69	48,48,48,48	0
86	OHX	5	4166	7/7	0.78	0.52	49,49,49,49	4
85	MG	1	3612	1/1	0.78	0.30	55,55,55,55	0
85	MG	M6	202	1/1	0.79	0.29	40,40,40,40	0
85	MG	2	1967	1/1	0.79	0.29	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	5	3598	1/1	0.79	0.40	48,48,48,48	0
85	MG	5	3723	1/1	0.79	0.40	52,52,52,52	0
85	MG	3	203	1/1	0.79	0.76	42,42,42,42	0
85	MG	1	3491	1/1	0.79	0.64	51,51,51,51	0
85	MG	5	3750	1/1	0.79	0.42	37,37,37,37	0
85	MG	5	3625	1/1	0.79	0.40	51,51,51,51	0
85	MG	2	1949	1/1	0.79	1.00	86,86,86,86	0
86	OHX	2	2104	7/7	0.79	0.20	119,119,119,119	5
85	MG	4	214	1/1	0.79	0.53	41,41,41,41	0
85	MG	2	1963	1/1	0.80	0.19	83,83,83,83	0
85	MG	8	209	1/1	0.80	0.69	55,55,55,55	0
85	MG	M9	201	1/1	0.80	0.31	75,75,75,75	0
85	MG	N6	201	1/1	0.80	0.47	70,70,70,70	0
85	MG	2	1932	1/1	0.80	0.61	64,64,64,64	0
85	MG	5	3600	1/1	0.80	0.43	37,37,37,37	0
85	MG	4	201	1/1	0.80	0.34	36,36,36,36	0
85	MG	2	1945	1/1	0.80	0.22	107,107,107,107	0
85	MG	6	1992	1/1	0.80	0.33	61,61,61,61	0
85	MG	6	1944	1/1	0.80	0.27	63,63,63,63	0
86	OHX	1	4089	7/7	0.80	0.34	55,55,55,55	6
85	MG	6	1954	1/1	0.80	0.65	64,64,64,64	0
85	MG	1	3459	1/1	0.80	0.66	60,60,60,60	0
85	MG	1	3745	1/1	0.80	0.46	53,53,53,53	0
86	OHX	5	4062	7/7	0.80	0.47	56,56,56,56	3
85	MG	6	1965	1/1	0.80	0.39	48,48,48,48	0
85	MG	4	215	1/1	0.80	0.85	55,55,55,55	0
85	MG	2	1909	1/1	0.80	0.48	83,83,83,83	0
85	MG	5	3545	1/1	0.80	0.53	57,57,57,57	0
86	OHX	m1	201	7/7	0.80	0.32	78,78,78,78	3
85	MG	8	203	1/1	0.80	0.36	57,57,57,57	0
85	MG	3	202	1/1	0.81	0.43	56,56,56,56	0
85	MG	5	3681	1/1	0.81	0.35	43,43,43,43	0
85	MG	5	3500	1/1	0.81	0.40	40,40,40,40	0
85	MG	d6	102	1/1	0.81	0.61	68,68,68,68	0
85	MG	6	1978	1/1	0.81	0.56	77,77,77,77	0
85	MG	5	3694	1/1	0.81	0.28	55,55,55,55	0
85	MG	5	3696	1/1	0.81	0.57	45,45,45,45	0
85	MG	5	3697	1/1	0.81	0.16	61,61,61,61	0
85	MG	5	3405	1/1	0.81	0.72	49,49,49,49	0
85	MG	5	3412	1/1	0.81	0.25	47,47,47,47	0
85	MG	O7	101	1/1	0.81	0.45	62,62,62,62	0
85	MG	1	3483	1/1	0.81	0.83	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	1	3971	7/7	0.81	0.37	47,47,47,47	4
85	MG	2	1916	1/1	0.81	0.68	63,63,63,63	0
85	MG	1	3739	1/1	0.81	0.39	72,72,72,72	0
86	OHX	L3	404	7/7	0.81	0.27	84,84,84,84	6
86	OHX	O9	101	7/7	0.81	0.35	51,51,51,51	6
86	OHX	6	2161	7/7	0.81	0.35	84,84,84,84	6
85	MG	2	1921	1/1	0.81	0.63	63,63,63,63	0
85	MG	1	3573	1/1	0.81	0.71	40,40,40,40	0
85	MG	2	1908	1/1	0.81	0.30	90,90,90,90	0
86	OHX	5	4086	7/7	0.81	0.47	70,70,70,70	4
86	OHX	5	4095	7/7	0.81	0.41	41,41,41,41	2
85	MG	5	3777	1/1	0.81	0.40	41,41,41,41	0
85	MG	1	3638	1/1	0.81	0.91	48,48,48,48	0
85	MG	1	3675	1/1	0.81	0.37	49,49,49,49	0
85	MG	6	1970	1/1	0.81	1.00	64,64,64,64	0
85	MG	1	3760	1/1	0.81	0.13	62,62,62,62	0
85	MG	6	2011	1/1	0.81	0.72	48,48,48,48	0
85	MG	5	3641	1/1	0.82	1.16	55,55,55,55	0
85	MG	5	3726	1/1	0.82	0.55	46,46,46,46	0
85	MG	6	1914	1/1	0.82	0.77	62,62,62,62	0
86	OHX	2	2142	7/7	0.82	0.16	132,132,132,132	7
85	MG	4	212	1/1	0.82	0.39	60,60,60,60	0
85	MG	5	3670	1/1	0.82	0.41	35,35,35,35	0
85	MG	6	1919	1/1	0.82	1.05	64,64,64,64	0
85	MG	5	3673	1/1	0.82	0.30	78,78,78,78	0
86	OHX	1	4098	7/7	0.82	0.34	61,61,61,61	5
85	MG	5	3774	1/1	0.82	0.65	55,55,55,55	0
85	MG	1	3410	1/1	0.82	0.56	39,39,39,39	0
86	OHX	M0	304	7/7	0.82	0.29	101,101,101,101	6
85	MG	1	3711	1/1	0.82	0.36	54,54,54,54	0
85	MG	L6	201	1/1	0.82	0.19	57,57,57,57	0
85	MG	5	3577	1/1	0.82	0.44	31,31,31,31	0
85	MG	5	3795	1/1	0.82	0.27	41,41,41,41	0
85	MG	1	3629	1/1	0.82	0.92	33,33,33,33	0
85	MG	1	3420	1/1	0.82	0.44	45,45,45,45	0
85	MG	1	3543	1/1	0.82	0.14	58,58,58,58	0
85	MG	2	1901	1/1	0.82	0.30	87,87,87,87	0
85	MG	5	3623	1/1	0.82	0.37	42,42,42,42	0
85	MG	4	206	1/1	0.82	0.74	44,44,44,44	0
85	MG	5	3712	1/1	0.82	0.35	67,67,67,67	0
86	OHX	8	230	7/7	0.82	0.37	68,68,68,68	3
85	MG	5	3487	1/1	0.82	0.69	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	5	3491	1/1	0.82	0.65	41,41,41,41	0
85	MG	2	1902	1/1	0.83	0.94	49,49,49,49	0
85	MG	1	3505	1/1	0.83	0.78	38,38,38,38	0
86	OHX	2	2122	7/7	0.83	0.30	91,91,91,91	7
85	MG	2	1964	1/1	0.83	0.38	92,92,92,92	0
85	MG	5	3640	1/1	0.83	0.16	50,50,50,50	0
85	MG	5	3730	1/1	0.83	0.52	41,41,41,41	0
85	MG	s8	302	1/1	0.83	0.45	49,49,49,49	0
85	MG	1	3535	1/1	0.83	0.51	39,39,39,39	0
85	MG	1	3428	1/1	0.83	0.37	52,52,52,52	0
86	OHX	1	4062	7/7	0.83	0.40	51,51,51,51	3
86	OHX	1	4073	7/7	0.83	0.44	71,71,71,71	5
85	MG	5	3663	1/1	0.83	0.27	48,48,48,48	0
85	MG	5	3763	1/1	0.83	0.68	38,38,38,38	0
85	MG	5	3769	1/1	0.83	0.96	50,50,50,50	0
85	MG	1	3567	1/1	0.83	0.40	48,48,48,48	0
85	MG	2	1929	1/1	0.83	0.38	83,83,83,83	0
85	MG	5	3409	1/1	0.83	0.51	45,45,45,45	0
85	MG	5	3410	1/1	0.83	0.28	29,29,29,29	0
86	OHX	6	2163	7/7	0.83	0.39	61,61,61,61	4
85	MG	2	1906	1/1	0.83	0.35	68,68,68,68	0
85	MG	6	1925	1/1	0.83	0.31	49,49,49,49	0
86	OHX	5	3948	7/7	0.83	0.40	49,49,49,49	2
85	MG	6	1931	1/1	0.83	0.18	92,92,92,92	0
85	MG	1	3461	1/1	0.83	0.41	57,57,57,57	0
85	MG	5	3436	1/1	0.83	0.41	44,44,44,44	0
86	OHX	5	4143	7/7	0.83	0.33	50,50,50,50	4
85	MG	1	3467	1/1	0.83	0.51	42,42,42,42	0
85	MG	2	1910	1/1	0.83	0.62	69,69,69,69	0
85	MG	1	3489	1/1	0.83	0.73	67,67,67,67	0
85	MG	8	208	1/1	0.83	0.50	51,51,51,51	0
85	MG	5	3456	1/1	0.83	0.53	31,31,31,31	0
85	MG	5	3702	1/1	0.83	0.35	54,54,54,54	0
85	MG	1	3746	1/1	0.83	0.48	43,43,43,43	0
85	MG	5	3767	1/1	0.84	0.34	43,43,43,43	0
85	MG	3	208	1/1	0.84	0.82	42,42,42,42	0
85	MG	1	3707	1/1	0.84	0.53	48,48,48,48	0
86	OHX	2	2151	7/7	0.84	0.29	112,112,112,112	7
85	MG	2	1923	1/1	0.84	0.89	45,45,45,45	0
86	OHX	1	3975	7/7	0.84	0.24	88,88,88,88	3
85	MG	6	1917	1/1	0.84	0.47	64,64,64,64	0
85	MG	1	3710	1/1	0.84	0.24	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	5	3402	1/1	0.84	0.07	54,54,54,54	0
85	MG	5	3630	1/1	0.84	0.41	56,56,56,56	0
85	MG	1	3677	1/1	0.84	0.36	46,46,46,46	0
85	MG	5	3802	1/1	0.84	0.74	44,44,44,44	0
85	MG	1	3533	1/1	0.84	0.78	49,49,49,49	0
85	MG	5	3813	1/1	0.84	0.62	31,31,31,31	0
85	MG	5	3706	1/1	0.84	0.43	32,32,32,32	0
85	MG	1	3750	1/1	0.84	0.79	48,48,48,48	0
85	MG	7	210	1/1	0.84	0.29	43,43,43,43	0
85	MG	6	1933	1/1	0.84	0.63	56,56,56,56	0
85	MG	5	3646	1/1	0.84	0.52	56,56,56,56	0
85	MG	1	3752	1/1	0.84	0.19	64,64,64,64	0
85	MG	5	3502	1/1	0.84	0.86	31,31,31,31	0
85	MG	1	3653	1/1	0.84	1.20	55,55,55,55	0
85	MG	5	3734	1/1	0.84	0.27	45,45,45,45	0
85	MG	1	3755	1/1	0.84	0.33	45,45,45,45	0
85	MG	1	3656	1/1	0.84	0.57	46,46,46,46	0
86	OHX	2	2109	7/7	0.84	0.30	105,105,105,105	6
85	MG	1	3673	1/1	0.84	0.52	39,39,39,39	0
86	OHX	2	2124	7/7	0.84	0.18	128,128,128,128	6
85	MG	1	3702	1/1	0.84	0.52	45,45,45,45	0
85	MG	6	2009	1/1	0.84	0.68	64,64,64,64	0
85	MG	6	1935	1/1	0.85	0.85	44,44,44,44	0
85	MG	5	3661	1/1	0.85	0.35	64,64,64,64	0
85	MG	1	3719	1/1	0.85	0.46	65,65,65,65	0
85	MG	5	3669	1/1	0.85	0.19	36,36,36,36	1
85	MG	1	3607	1/1	0.85	0.56	85,85,85,85	0
85	MG	5	3549	1/1	0.85	0.32	43,43,43,43	0
85	MG	6	1953	1/1	0.85	0.46	63,63,63,63	0
86	OHX	1	3867	7/7	0.85	0.32	51,51,51,51	4
86	OHX	1	3915	7/7	0.85	0.38	66,66,66,66	4
85	MG	1	3471	1/1	0.85	0.50	45,45,45,45	0
85	MG	1	3685	1/1	0.85	0.30	43,43,43,43	0
85	MG	6	2007	1/1	0.85	0.98	51,51,51,51	0
85	MG	O4	201	1/1	0.85	0.15	77,77,77,77	0
85	MG	1	3544	1/1	0.85	0.53	55,55,55,55	0
85	MG	5	3610	1/1	0.85	0.19	49,49,49,49	0
86	OHX	1	4104	7/7	0.85	0.24	73,73,73,73	6
86	OHX	1	4106	7/7	0.85	0.20	72,72,72,72	4
85	MG	1	3657	1/1	0.85	0.63	49,49,49,49	0
86	OHX	4	232	7/7	0.85	0.32	73,73,73,73	5
85	MG	5	3621	1/1	0.85	0.40	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	6	1971	1/1	0.85	0.47	90,90,90,90	0
85	MG	5	3815	1/1	0.85	0.70	44,44,44,44	0
85	MG	1	3615	1/1	0.85	0.29	68,68,68,68	0
85	MG	1	3443	1/1	0.85	0.55	46,46,46,46	0
85	MG	5	3632	1/1	0.85	0.68	36,36,36,36	0
85	MG	5	3635	1/1	0.85	0.17	50,50,50,50	0
85	MG	2	1951	1/1	0.85	0.40	71,71,71,71	0
86	OHX	5	4054	7/7	0.85	0.62	50,50,50,50	2
85	MG	6	1979	1/1	0.85	0.32	101,101,101,101	0
85	MG	1	3534	1/1	0.85	0.27	69,69,69,69	0
85	MG	1	3592	1/1	0.85	0.19	61,61,61,61	0
86	OHX	5	4133	7/7	0.85	0.48	34,34,34,34	3
85	MG	1	3674	1/1	0.85	0.40	68,68,68,68	0
86	OHX	5	4147	7/7	0.85	0.27	89,89,89,89	7
86	OHX	5	4149	7/7	0.85	0.16	145,145,145,145	7
85	MG	n0	201	1/1	0.85	0.34	41,41,41,41	0
85	MG	5	3647	1/1	0.85	0.27	55,55,55,55	0
85	MG	5	3738	1/1	0.85	0.31	42,42,42,42	0
85	MG	1	3457	1/1	0.85	0.64	32,32,32,32	0
86	OHX	2	2117	7/7	0.85	0.31	93,93,93,93	4
85	MG	5	3744	1/1	0.85	0.45	57,57,57,57	0
86	OHX	2	2123	7/7	0.85	0.33	121,121,121,121	5
85	MG	1	3701	1/1	0.86	0.29	52,52,52,52	0
85	MG	1	3551	1/1	0.86	0.55	38,38,38,38	0
85	MG	5	3771	1/1	0.86	0.42	36,36,36,36	0
85	MG	2	1948	1/1	0.86	0.58	72,72,72,72	0
86	OHX	S6	301	7/7	0.86	0.14	117,117,117,117	7
85	MG	1	3572	1/1	0.86	0.74	57,57,57,57	0
85	MG	5	3682	1/1	0.86	0.44	45,45,45,45	0
85	MG	5	3615	1/1	0.86	0.53	35,35,35,35	0
85	MG	5	3782	1/1	0.86	0.22	48,48,48,48	0
86	OHX	1	4009	7/7	0.86	0.22	131,131,131,131	7
86	OHX	1	4029	7/7	0.86	0.28	82,82,82,82	3
85	MG	4	204	1/1	0.86	0.63	64,64,64,64	0
86	OHX	1	4069	7/7	0.86	0.38	58,58,58,58	5
85	MG	6	1988	1/1	0.86	0.26	80,80,80,80	0
86	OHX	1	4079	7/7	0.86	0.25	108,108,108,108	6
85	MG	5	3408	1/1	0.86	0.43	40,40,40,40	0
85	MG	1	3474	1/1	0.86	0.29	48,48,48,48	0
85	MG	5	3804	1/1	0.86	0.28	49,49,49,49	0
85	MG	1	3658	1/1	0.86	0.47	42,42,42,42	0
85	MG	5	3809	1/1	0.86	0.41	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	5	3488	1/1	0.86	0.35	44,44,44,44	0
85	MG	5	3411	1/1	0.86	0.54	44,44,44,44	0
85	MG	6	1967	1/1	0.86	0.41	76,76,76,76	0
86	OHX	M9	202	7/7	0.86	0.20	77,77,77,77	3
85	MG	5	3709	1/1	0.86	0.60	51,51,51,51	0
86	OHX	6	2141	7/7	0.86	0.18	151,151,151,151	7
85	MG	5	3414	1/1	0.86	0.32	33,33,33,33	0
85	MG	1	3682	1/1	0.86	0.28	36,36,36,36	0
86	OHX	6	2164	7/7	0.86	0.37	44,44,44,44	5
86	OHX	6	2168	7/7	0.86	0.27	76,76,76,76	3
85	MG	5	3645	1/1	0.86	0.54	31,31,31,31	0
85	MG	5	3518	1/1	0.86	0.43	38,38,38,38	0
85	MG	2	1955	1/1	0.86	0.89	62,62,62,62	0
86	OHX	5	4048	7/7	0.86	0.23	69,69,69,69	3
85	MG	5	3727	1/1	0.86	0.56	44,44,44,44	0
85	MG	2	1979	1/1	0.86	0.46	70,70,70,70	0
85	MG	m3	201	1/1	0.86	0.49	40,40,40,40	0
85	MG	5	3650	1/1	0.86	0.57	29,29,29,29	0
86	OHX	5	4122	7/7	0.86	0.29	52,52,52,52	3
86	OHX	5	4130	7/7	0.86	0.17	171,171,171,171	7
85	MG	n6	201	1/1	0.86	0.43	56,56,56,56	0
86	OHX	5	4136	7/7	0.86	0.13	180,180,180,180	7
86	OHX	5	4139	7/7	0.86	0.16	108,108,108,108	5
85	MG	1	3726	1/1	0.86	0.27	64,64,64,64	0
86	OHX	2	2072	7/7	0.86	0.19	187,187,187,187	7
85	MG	5	3659	1/1	0.86	0.38	39,39,39,39	0
85	MG	1	3463	1/1	0.86	0.37	39,39,39,39	0
85	MG	5	3555	1/1	0.86	0.25	54,54,54,54	0
85	MG	1	3452	1/1	0.86	0.74	55,55,55,55	0
85	MG	5	3755	1/1	0.86	0.95	55,55,55,55	0
86	OHX	5	4169	7/7	0.86	0.25	81,81,81,81	7
85	MG	s4	601	1/1	0.86	0.14	66,66,66,66	0
85	MG	5	3760	1/1	0.86	0.23	53,53,53,53	0
85	MG	5	3451	1/1	0.86	0.51	40,40,40,40	0
86	OHX	1	4039	7/7	0.87	0.09	278,278,278,278	6
86	OHX	1	4044	7/7	0.87	0.26	108,108,108,108	4
85	MG	1	3577	1/1	0.87	0.66	39,39,39,39	0
86	OHX	1	4067	7/7	0.87	0.27	107,107,107,107	7
85	MG	7	212	1/1	0.87	0.81	51,51,51,51	0
85	MG	1	3713	1/1	0.87	0.99	40,40,40,40	0
85	MG	5	3676	1/1	0.87	0.24	51,51,51,51	0
85	MG	5	3485	1/1	0.87	0.47	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	1	4090	7/7	0.87	0.32	47,47,47,47	4
85	MG	M7	203	1/1	0.87	0.34	46,46,46,46	0
86	OHX	1	4099	7/7	0.87	0.38	53,53,53,53	3
85	MG	1	3641	1/1	0.87	0.46	49,49,49,49	0
85	MG	1	3508	1/1	0.87	0.61	38,38,38,38	0
86	OHX	1	4108	7/7	0.87	0.23	59,59,59,59	5
85	MG	2	1940	1/1	0.87	0.67	80,80,80,80	0
85	MG	m5	302	1/1	0.87	0.35	46,46,46,46	0
85	MG	5	3687	1/1	0.87	0.69	37,37,37,37	0
85	MG	1	3444	1/1	0.87	0.52	35,35,35,35	0
85	MG	5	3691	1/1	0.87	0.68	38,38,38,38	0
86	OHX	2	2049	7/7	0.87	0.29	100,100,100,100	4
86	OHX	6	2135	7/7	0.87	0.25	94,94,94,94	7
85	MG	6	1907	1/1	0.87	0.42	51,51,51,51	0
86	OHX	6	2158	7/7	0.87	0.31	131,131,131,131	7
85	MG	5	3432	1/1	0.87	0.30	32,32,32,32	0
86	OHX	2	2105	7/7	0.87	0.24	87,87,87,87	3
85	MG	5	3775	1/1	0.87	0.61	40,40,40,40	0
85	MG	1	3690	1/1	0.87	0.48	63,63,63,63	0
86	OHX	6	2173	7/7	0.87	0.28	64,64,64,64	5
85	MG	2	1925	1/1	0.87	0.30	67,67,67,67	0
85	MG	2	1919	1/1	0.87	0.35	62,62,62,62	0
85	MG	1	3475	1/1	0.87	0.51	44,44,44,44	0
86	OHX	2	2130	7/7	0.87	0.30	84,84,84,84	4
85	MG	5	3449	1/1	0.87	0.43	32,32,32,32	0
86	OHX	2	2134	7/7	0.87	0.30	74,74,74,74	4
85	MG	5	3792	1/1	0.87	0.35	55,55,55,55	0
85	MG	2	1946	1/1	0.87	0.07	108,108,108,108	0
86	OHX	5	4116	7/7	0.87	0.34	52,52,52,52	4
86	OHX	2	2143	7/7	0.87	0.29	84,84,84,84	5
86	OHX	5	4123	7/7	0.87	0.41	76,76,76,76	5
86	OHX	2	2145	7/7	0.87	0.25	103,103,103,103	4
85	MG	5	3801	1/1	0.87	0.35	44,44,44,44	0
85	MG	c9	201	1/1	0.87	0.12	83,83,83,83	0
85	MG	5	3803	1/1	0.87	0.36	35,35,35,35	0
86	OHX	2	2152	7/7	0.87	0.31	122,122,122,122	6
85	MG	1	3487	1/1	0.87	0.39	49,49,49,49	0
85	MG	1	3458	1/1	0.87	0.64	51,51,51,51	0
86	OHX	1	3871	7/7	0.87	0.49	61,61,61,61	2
86	OHX	5	4157	7/7	0.87	0.29	44,44,44,44	5
86	OHX	5	4158	7/7	0.87	0.39	35,35,35,35	3
85	MG	1	3406	1/1	0.87	0.29	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	1	3928	7/7	0.87	0.28	49,49,49,49	3
85	MG	5	3668	1/1	0.87	0.45	33,33,33,33	0
85	MG	5	3603	1/1	0.87	0.27	50,50,50,50	0
86	OHX	5	4172	7/7	0.87	0.66	45,45,45,45	3
86	OHX	8	228	7/7	0.87	0.48	73,73,73,73	5
85	MG	1	3434	1/1	0.87	0.51	62,62,62,62	0
86	OHX	1	4019	7/7	0.87	0.30	47,47,47,47	2
85	MG	1	3751	1/1	0.87	0.90	67,67,67,67	0
85	MG	6	1983	1/1	0.88	0.83	57,57,57,57	0
85	MG	5	3515	1/1	0.88	0.34	42,42,42,42	0
86	OHX	1	4102	7/7	0.88	0.25	65,65,65,65	3
85	MG	1	3618	1/1	0.88	0.36	39,39,39,39	0
85	MG	1	3626	1/1	0.88	0.51	46,46,46,46	0
85	MG	3	206	1/1	0.88	0.17	65,65,65,65	0
85	MG	5	3548	1/1	0.88	0.57	25,25,25,25	0
86	OHX	4	228	7/7	0.88	0.52	51,51,51,51	4
85	MG	1	3586	1/1	0.88	0.30	45,45,45,45	0
85	MG	6	1989	1/1	0.88	0.27	57,57,57,57	0
85	MG	5	3664	1/1	0.88	0.28	62,62,62,62	0
86	OHX	2	2112	7/7	0.88	0.18	121,121,121,121	6
85	MG	5	3554	1/1	0.88	0.61	32,32,32,32	0
86	OHX	6	2130	7/7	0.88	0.15	153,153,153,153	7
85	MG	1	3666	1/1	0.88	0.50	65,65,65,65	0
85	MG	5	3563	1/1	0.88	0.52	44,44,44,44	0
86	OHX	6	2149	7/7	0.88	0.29	95,95,95,95	6
86	OHX	6	2152	7/7	0.88	0.14	107,107,107,107	5
85	MG	1	3672	1/1	0.88	0.44	76,76,76,76	0
85	MG	1	3633	1/1	0.88	0.16	59,59,59,59	0
85	MG	S2	301	1/1	0.88	0.79	62,62,62,62	0
85	MG	1	3636	1/1	0.88	0.76	53,53,53,53	0
85	MG	1	3557	1/1	0.88	0.66	55,55,55,55	0
86	OHX	2	2141	7/7	0.88	0.56	90,90,90,90	6
85	MG	1	3566	1/1	0.88	0.32	47,47,47,47	0
85	MG	5	3604	1/1	0.88	0.35	33,33,33,33	0
86	OHX	5	3926	7/7	0.88	0.28	60,60,60,60	4
85	MG	6	1955	1/1	0.88	0.47	60,60,60,60	0
86	OHX	5	4043	7/7	0.88	0.32	38,38,38,38	4
85	MG	1	3603	1/1	0.88	0.26	63,63,63,63	0
85	MG	1	3604	1/1	0.88	0.69	39,39,39,39	0
85	MG	1	3643	1/1	0.88	0.82	38,38,38,38	0
85	MG	1	3648	1/1	0.88	0.44	42,42,42,42	0
86	OHX	5	4087	7/7	0.88	0.28	39,39,39,39	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
85	MG	1	3693	1/1	0.88	0.20	49,49,49,49	0
85	MG	5	3626	1/1	0.88	0.33	42,42,42,42	0
85	MG	5	3627	1/1	0.88	0.25	47,47,47,47	0
85	MG	5	3628	1/1	0.88	0.52	92,92,92,92	0
85	MG	1	3652	1/1	0.88	0.30	48,48,48,48	0
85	MG	5	3814	1/1	0.88	0.97	42,42,42,42	0
85	MG	5	3631	1/1	0.88	0.20	52,52,52,52	0
85	MG	2	1942	1/1	0.88	0.27	69,69,69,69	0
85	MG	5	3634	1/1	0.88	0.43	36,36,36,36	0
85	MG	7	208	1/1	0.88	0.27	45,45,45,45	0
85	MG	5	3713	1/1	0.88	0.36	38,38,38,38	0
85	MG	1	3568	1/1	0.88	0.44	36,36,36,36	0
86	OHX	1	4048	7/7	0.88	0.23	116,116,116,116	5
86	OHX	1	4050	7/7	0.88	0.29	58,58,58,58	5
85	MG	2	1970	1/1	0.88	0.54	65,65,65,65	0
86	OHX	5	4161	7/7	0.88	0.29	123,123,123,123	7
85	MG	5	3406	1/1	0.88	0.28	47,47,47,47	0
86	OHX	5	4164	7/7	0.88	0.28	61,61,61,61	7
86	OHX	5	4165	7/7	0.88	0.36	51,51,51,51	3
85	MG	2	1975	1/1	0.88	0.40	60,60,60,60	0
86	OHX	1	4070	7/7	0.88	0.17	111,111,111,111	6
85	MG	1	3756	1/1	0.88	0.75	53,53,53,53	0
86	OHX	1	4078	7/7	0.88	0.12	167,167,167,167	7
85	MG	5	3728	1/1	0.88	0.41	44,44,44,44	0
85	MG	5	3643	1/1	0.88	0.70	64,64,64,64	0
85	MG	1	3409	1/1	0.88	0.30	52,52,52,52	0
87	ZN	d7	101	1/1	0.88	0.39	147,147,147,147	0
85	MG	5	3424	1/1	0.89	0.24	56,56,56,56	0
86	OHX	1	4101	7/7	0.89	0.25	66,66,66,66	4
85	MG	n8	202	1/1	0.89	0.31	50,50,50,50	0
85	MG	2	1976	1/1	0.89	0.10	77,77,77,77	0
86	OHX	2	2035	7/7	0.89	0.21	116,116,116,116	5
86	OHX	2	2036	7/7	0.89	0.17	145,145,145,145	5
85	MG	5	3662	1/1	0.89	0.65	42,42,42,42	0
85	MG	1	3473	1/1	0.89	0.31	56,56,56,56	0
85	MG	5	3759	1/1	0.89	0.13	46,46,46,46	0
85	MG	1	3637	1/1	0.89	0.69	46,46,46,46	0
86	OHX	2	2107	7/7	0.89	0.49	66,66,66,66	4
85	MG	5	3762	1/1	0.89	0.59	38,38,38,38	0
85	MG	5	3574	1/1	0.89	0.29	37,37,37,37	0
85	MG	6	1995	1/1	0.89	0.51	47,47,47,47	0
85	MG	1	3419	1/1	0.89	0.24	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	6	2137	7/7	0.89	0.23	95,95,95,95	4
85	MG	6	2001	1/1	0.89	0.39	48,48,48,48	0
85	MG	6	1946	1/1	0.89	0.68	53,53,53,53	0
86	OHX	6	2150	7/7	0.89	0.32	78,78,78,78	6
85	MG	5	3450	1/1	0.89	0.81	45,45,45,45	0
85	MG	2	1933	1/1	0.89	0.45	70,70,70,70	0
85	MG	5	3453	1/1	0.89	0.96	33,33,33,33	0
85	MG	1	3478	1/1	0.89	0.18	60,60,60,60	0
86	OHX	2	2137	7/7	0.89	0.17	219,219,219,219	7
85	MG	5	3781	1/1	0.89	0.49	43,43,43,43	0
85	MG	2	1972	1/1	0.89	0.50	57,57,57,57	0
86	OHX	6	2177	7/7	0.89	0.16	141,141,141,141	7
85	MG	5	3616	1/1	0.89	0.22	42,42,42,42	0
86	OHX	6	2179	7/7	0.89	0.25	61,61,61,61	7
85	MG	5	3788	1/1	0.89	0.30	68,68,68,68	0
86	OHX	s1	302	7/7	0.89	0.23	99,99,99,99	6
85	MG	5	3620	1/1	0.89	0.64	39,39,39,39	0
85	MG	5	3791	1/1	0.89	0.20	46,46,46,46	0
86	OHX	5	4017	7/7	0.89	0.41	36,36,36,36	2
86	OHX	5	4034	7/7	0.89	0.28	66,66,66,66	4
85	MG	5	3461	1/1	0.89	0.28	57,57,57,57	0
85	MG	5	3622	1/1	0.89	0.35	62,62,62,62	0
85	MG	1	3605	1/1	0.89	0.26	44,44,44,44	0
85	MG	1	3691	1/1	0.89	0.23	64,64,64,64	0
86	OHX	5	4078	7/7	0.89	0.35	68,68,68,68	3
85	MG	5	3695	1/1	0.89	0.59	54,54,54,54	0
85	MG	s8	301	1/1	0.89	0.39	52,52,52,52	0
86	OHX	5	4091	7/7	0.89	0.38	45,45,45,45	2
86	OHX	1	3924	7/7	0.89	0.25	71,71,71,71	4
85	MG	2	1903	1/1	0.89	0.58	43,43,43,43	0
85	MG	1	3748	1/1	0.89	0.43	67,67,67,67	0
85	MG	5	3700	1/1	0.89	0.32	43,43,43,43	0
86	OHX	5	4127	7/7	0.89	0.42	44,44,44,44	3
86	OHX	1	3983	7/7	0.89	0.46	77,77,77,77	2
86	OHX	5	4132	7/7	0.89	0.47	45,45,45,45	4
85	MG	1	3650	1/1	0.89	0.24	47,47,47,47	0
85	MG	1	3558	1/1	0.89	0.52	35,35,35,35	0
85	MG	1	3565	1/1	0.89	0.49	40,40,40,40	0
86	OHX	5	4141	7/7	0.89	0.43	49,49,49,49	4
85	MG	1	3613	1/1	0.89	0.78	58,58,58,58	0
85	MG	1	3433	1/1	0.89	0.46	34,34,34,34	0
85	MG	1	3460	1/1	0.89	0.35	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	7	211	1/1	0.89	0.50	57,57,57,57	0
85	MG	2	1911	1/1	0.89	0.84	77,77,77,77	0
86	OHX	1	4063	7/7	0.89	0.12	159,159,159,159	7
86	OHX	1	4066	7/7	0.89	0.28	63,63,63,63	6
85	MG	1	3622	1/1	0.89	0.67	44,44,44,44	0
85	MG	1	3437	1/1	0.89	0.66	44,44,44,44	0
85	MG	6	1920	1/1	0.89	0.44	46,46,46,46	0
85	MG	5	3522	1/1	0.89	0.35	36,36,36,36	0
86	OHX	1	4076	7/7	0.89	0.26	45,45,45,45	5
85	MG	6	1923	1/1	0.89	0.64	46,46,46,46	0
86	OHX	5	4171	7/7	0.89	0.19	90,90,90,90	5
85	MG	2	1907	1/1	0.89	0.58	62,62,62,62	0
85	MG	1	3630	1/1	0.89	0.42	76,76,76,76	0
86	OHX	8	229	7/7	0.89	0.19	101,101,101,101	6
85	MG	5	3420	1/1	0.89	0.68	26,26,26,26	0
86	OHX	1	4093	7/7	0.89	0.54	64,64,64,64	4
86	OHX	1	4094	7/7	0.89	0.20	77,77,77,77	4
85	MG	1	3529	1/1	0.89	0.54	34,34,34,34	0
86	OHX	2	2064	7/7	0.90	0.20	135,135,135,135	5
86	OHX	1	4107	7/7	0.90	0.14	91,91,91,91	6
85	MG	O7	103	1/1	0.90	0.37	49,49,49,49	0
85	MG	Q2	502	1/1	0.90	0.11	63,63,63,63	0
85	MG	5	3756	1/1	0.90	0.57	42,42,42,42	0
85	MG	1	3680	1/1	0.90	0.68	45,45,45,45	0
85	MG	6	1909	1/1	0.90	0.31	53,53,53,53	0
86	OHX	2	2111	7/7	0.90	0.23	112,112,112,112	5
85	MG	6	1910	1/1	0.90	0.28	91,91,91,91	0
86	OHX	N8	204	7/7	0.90	0.32	90,90,90,90	7
86	OHX	2	2114	7/7	0.90	0.17	103,103,103,103	4
85	MG	5	3521	1/1	0.90	0.51	44,44,44,44	0
85	MG	6	1913	1/1	0.90	0.28	79,79,79,79	0
85	MG	5	3523	1/1	0.90	0.51	29,29,29,29	0
85	MG	2	1917	1/1	0.90	0.50	54,54,54,54	0
86	OHX	2	2125	7/7	0.90	0.24	147,147,147,147	6
85	MG	2	1966	1/1	0.90	0.25	74,74,74,74	0
85	MG	5	3546	1/1	0.90	0.62	46,46,46,46	0
85	MG	3	205	1/1	0.90	0.50	68,68,68,68	0
85	MG	6	1918	1/1	0.90	0.41	41,41,41,41	0
85	MG	5	3422	1/1	0.90	0.43	44,44,44,44	0
86	OHX	2	2138	7/7	0.90	0.26	67,67,67,67	5
85	MG	1	3727	1/1	0.90	0.34	48,48,48,48	0
86	OHX	6	2169	7/7	0.90	0.17	89,89,89,89	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	6	2172	7/7	0.90	0.39	69,69,69,69	3
85	MG	1	3415	1/1	0.90	0.40	43,43,43,43	0
86	OHX	6	2175	7/7	0.90	0.17	100,100,100,100	6
85	MG	6	1987	1/1	0.90	0.53	77,77,77,77	0
86	OHX	2	2144	7/7	0.90	0.37	103,103,103,103	6
85	MG	5	3783	1/1	0.90	0.28	38,38,38,38	0
86	OHX	6	2181	7/7	0.90	0.17	117,117,117,117	7
85	MG	1	3660	1/1	0.90	0.17	82,82,82,82	0
85	MG	1	3442	1/1	0.90	0.18	52,52,52,52	0
86	OHX	c5	201	7/7	0.90	0.14	129,129,129,129	6
86	OHX	c5	202	7/7	0.90	0.42	109,109,109,109	6
85	MG	5	3789	1/1	0.90	0.26	49,49,49,49	0
85	MG	5	3438	1/1	0.90	0.55	39,39,39,39	0
86	OHX	5	4011	7/7	0.90	0.27	120,120,120,120	3
86	OHX	5	4013	7/7	0.90	0.18	119,119,119,119	4
85	MG	5	3580	1/1	0.90	0.64	38,38,38,38	0
86	OHX	1	3856	7/7	0.90	0.34	76,76,76,76	3
85	MG	5	3439	1/1	0.90	0.45	30,30,30,30	0
85	MG	6	1928	1/1	0.90	0.41	57,57,57,57	0
85	MG	1	3539	1/1	0.90	0.46	44,44,44,44	0
85	MG	5	3602	1/1	0.90	0.44	30,30,30,30	0
85	MG	1	3501	1/1	0.90	0.56	26,26,26,26	0
86	OHX	5	4082	7/7	0.90	0.14	92,92,92,92	3
86	OHX	1	3955	7/7	0.90	0.25	71,71,71,71	3
86	OHX	1	3963	7/7	0.90	0.46	51,51,51,51	3
85	MG	1	3614	1/1	0.90	0.56	54,54,54,54	0
85	MG	5	3693	1/1	0.90	0.37	38,38,38,38	0
86	OHX	5	4098	7/7	0.90	0.20	106,106,106,106	5
86	OHX	5	4105	7/7	0.90	0.27	84,84,84,84	4
85	MG	5	3608	1/1	0.90	0.46	50,50,50,50	0
86	OHX	5	4119	7/7	0.90	0.34	52,52,52,52	3
85	MG	1	3476	1/1	0.90	0.30	43,43,43,43	0
85	MG	1	3667	1/1	0.90	0.46	58,58,58,58	0
86	OHX	5	4125	7/7	0.90	0.34	48,48,48,48	5
86	OHX	1	4026	7/7	0.90	0.36	52,52,52,52	5
85	MG	6	2002	1/1	0.90	0.36	66,66,66,66	0
85	MG	5	3454	1/1	0.90	0.51	59,59,59,59	0
85	MG	1	3417	1/1	0.90	0.39	78,78,78,78	0
85	MG	1	3520	1/1	0.90	0.49	35,35,35,35	0
86	OHX	5	4137	7/7	0.90	0.42	50,50,50,50	4
85	MG	6	1947	1/1	0.90	0.43	50,50,50,50	0
86	OHX	1	4061	7/7	0.90	0.21	72,72,72,72	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	5	4142	7/7	0.90	0.29	58,58,58,58	4
85	MG	5	3708	1/1	0.90	0.13	50,50,50,50	0
86	OHX	5	4144	7/7	0.90	0.23	65,65,65,65	5
85	MG	6	1950	1/1	0.90	0.33	66,66,66,66	0
86	OHX	5	4148	7/7	0.90	0.20	100,100,100,100	6
85	MG	8	201	1/1	0.90	0.42	43,43,43,43	0
85	MG	5	3463	1/1	0.90	0.28	39,39,39,39	0
86	OHX	5	4154	7/7	0.90	0.21	111,111,111,111	6
85	MG	6	1951	1/1	0.90	0.57	43,43,43,43	0
85	MG	5	3467	1/1	0.90	0.45	47,47,47,47	0
85	MG	1	3480	1/1	0.90	0.38	46,46,46,46	0
86	OHX	5	4160	7/7	0.90	0.34	37,37,37,37	5
85	MG	5	3721	1/1	0.90	0.30	36,36,36,36	0
86	OHX	1	4077	7/7	0.90	0.24	62,62,62,62	4
85	MG	5	3629	1/1	0.90	0.29	35,35,35,35	0
85	MG	1	3623	1/1	0.90	0.20	57,57,57,57	0
85	MG	1	3753	1/1	0.90	0.79	107,107,107,107	0
85	MG	1	3601	1/1	0.90	0.21	72,72,72,72	0
85	MG	1	3524	1/1	0.90	0.52	44,44,44,44	0
85	MG	5	3486	1/1	0.90	0.33	51,51,51,51	0
86	OHX	7	224	7/7	0.90	0.24	54,54,54,54	5
86	OHX	1	4096	7/7	0.90	0.21	80,80,80,80	4
85	MG	6	1963	1/1	0.90	0.47	80,80,80,80	0
86	OHX	2	2011	7/7	0.90	0.33	83,83,83,83	3
85	MG	1	3717	1/1	0.90	0.56	59,59,59,59	0
85	MG	1	3758	1/1	0.90	0.29	48,48,48,48	0
85	MG	5	3499	1/1	0.90	0.43	42,42,42,42	0
86	OHX	6	2146	7/7	0.91	0.47	48,48,48,48	4
85	MG	5	3575	1/1	0.91	0.56	36,36,36,36	0
85	MG	6	1902	1/1	0.91	0.88	40,40,40,40	0
85	MG	5	3658	1/1	0.91	0.34	27,27,27,27	0
86	OHX	6	2157	7/7	0.91	0.23	90,90,90,90	7
85	MG	6	1904	1/1	0.91	0.53	59,59,59,59	0
86	OHX	1	3891	7/7	0.91	0.16	103,103,103,103	5
86	OHX	1	3899	7/7	0.91	0.33	52,52,52,52	4
85	MG	5	3597	1/1	0.91	0.26	44,44,44,44	0
86	OHX	6	2167	7/7	0.91	0.22	73,73,73,73	7
85	MG	5	3470	1/1	0.91	0.17	56,56,56,56	0
85	MG	5	3480	1/1	0.91	0.10	47,47,47,47	0
86	OHX	6	2171	7/7	0.91	0.35	53,53,53,53	7
85	MG	6	1905	1/1	0.91	0.36	51,51,51,51	0
85	MG	5	3667	1/1	0.91	0.49	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
85	MG	1	3492	1/1	0.91	0.64	32,32,32,32	0
86	OHX	6	2176	7/7	0.91	0.30	62,62,62,62	7
85	MG	5	3754	1/1	0.91	0.45	51,51,51,51	0
85	MG	17	2201	1/1	0.91	0.28	46,46,46,46	0
85	MG	1	3403	1/1	0.91	0.27	42,42,42,42	0
85	MG	5	3421	1/1	0.91	0.38	38,38,38,38	0
86	OHX	6	2182	7/7	0.91	0.33	113,113,113,113	7
86	OHX	1	4021	7/7	0.91	0.42	58,58,58,58	3
86	OHX	1	4024	7/7	0.91	0.29	42,42,42,42	3
85	MG	1	3697	1/1	0.91	0.31	42,42,42,42	0
85	MG	6	1998	1/1	0.91	0.67	42,42,42,42	0
86	OHX	d4	201	7/7	0.91	0.26	90,90,90,90	6
86	OHX	1	4030	7/7	0.91	0.23	130,130,130,130	6
86	OHX	5	3941	7/7	0.91	0.42	34,34,34,34	4
86	OHX	1	4032	7/7	0.91	0.27	52,52,52,52	3
85	MG	5	3612	1/1	0.91	0.32	40,40,40,40	0
85	MG	5	3489	1/1	0.91	0.59	39,39,39,39	0
85	MG	4	211	1/1	0.91	0.37	54,54,54,54	0
85	MG	1	3422	1/1	0.91	0.44	32,32,32,32	0
86	OHX	1	4058	7/7	0.91	0.29	100,100,100,100	4
86	OHX	5	4047	7/7	0.91	0.31	28,28,28,28	1
85	MG	1	3619	1/1	0.91	0.39	53,53,53,53	0
85	MG	5	3683	1/1	0.91	0.38	38,38,38,38	0
86	OHX	5	4061	7/7	0.91	0.22	55,55,55,55	4
85	MG	5	3684	1/1	0.91	0.26	62,62,62,62	0
86	OHX	1	4065	7/7	0.91	0.34	59,59,59,59	5
85	MG	1	3588	1/1	0.91	0.39	39,39,39,39	0
86	OHX	2	2077	7/7	0.91	0.24	108,108,108,108	7
86	OHX	2	2092	7/7	0.91	0.40	73,73,73,73	5
86	OHX	2	2099	7/7	0.91	0.12	185,185,185,185	7
86	OHX	2	2101	7/7	0.91	0.18	110,110,110,110	5
86	OHX	1	4075	7/7	0.91	0.21	75,75,75,75	5
85	MG	1	3416	1/1	0.91	1.00	43,43,43,43	0
86	OHX	5	4107	7/7	0.91	0.23	81,81,81,81	5
85	MG	L7	302	1/1	0.91	0.65	50,50,50,50	0
85	MG	5	3689	1/1	0.91	0.43	40,40,40,40	0
86	OHX	5	4121	7/7	0.91	0.25	68,68,68,68	7
85	MG	6	2010	1/1	0.91	0.24	53,53,53,53	0
86	OHX	1	4080	7/7	0.91	0.25	57,57,57,57	4
86	OHX	1	4085	7/7	0.91	0.17	61,61,61,61	6
85	MG	L7	303	1/1	0.91	0.21	50,50,50,50	0
85	MG	1	3741	1/1	0.91	0.44	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	6	1973	1/1	0.91	0.31	51,51,51,51	0
85	MG	5	3785	1/1	0.91	0.34	57,57,57,57	0
86	OHX	1	4095	7/7	0.91	0.25	55,55,55,55	5
86	OHX	2	2120	7/7	0.91	0.46	87,87,87,87	3
85	MG	5	3535	1/1	0.91	0.49	36,36,36,36	0
85	MG	1	3512	1/1	0.91	0.68	31,31,31,31	0
85	MG	6	1927	1/1	0.91	0.30	63,63,63,63	0
85	MG	1	3709	1/1	0.91	0.20	48,48,48,48	0
85	MG	1	3595	1/1	0.91	0.30	78,78,78,78	0
85	MG	5	3794	1/1	0.91	0.20	45,45,45,45	0
85	MG	1	3644	1/1	0.91	0.28	52,52,52,52	0
85	MG	N8	203	1/1	0.91	0.31	30,30,30,30	0
86	OHX	1	4111	7/7	0.91	0.17	104,104,104,104	7
86	OHX	3	217	7/7	0.91	0.36	78,78,78,78	4
85	MG	5	3707	1/1	0.91	0.40	64,64,64,64	0
85	MG	5	3553	1/1	0.91	0.54	26,26,26,26	0
85	MG	3	207	1/1	0.91	0.33	66,66,66,66	0
85	MG	1	3645	1/1	0.91	0.27	51,51,51,51	0
85	MG	5	3558	1/1	0.91	0.53	31,31,31,31	0
85	MG	6	1943	1/1	0.91	0.55	70,70,70,70	0
85	MG	5	3572	1/1	0.91	0.44	21,21,21,21	0
86	OHX	2	2147	7/7	0.91	0.23	116,116,116,116	6
86	OHX	6	2103	7/7	0.91	0.27	67,67,67,67	4
86	OHX	6	2114	7/7	0.91	0.24	66,66,66,66	3
86	OHX	6	2118	7/7	0.91	0.36	89,89,89,89	5
86	OHX	6	2121	7/7	0.91	0.23	86,86,86,86	5
85	MG	5	3719	1/1	0.91	0.33	63,63,63,63	1
86	OHX	8	218	7/7	0.91	0.36	63,63,63,63	4
86	OHX	6	2133	7/7	0.91	0.32	125,125,125,125	6
85	MG	1	3596	1/1	0.91	0.34	46,46,46,46	0
86	OHX	6	2136	7/7	0.91	0.30	62,62,62,62	4
85	MG	7	201	1/1	0.91	0.54	41,41,41,41	0
85	MG	1	3516	1/1	0.91	0.62	33,33,33,33	0
86	OHX	6	2143	7/7	0.91	0.35	51,51,51,51	3
86	OHX	1	3949	7/7	0.92	0.43	111,111,111,111	7
86	OHX	6	2145	7/7	0.92	0.21	92,92,92,92	4
86	OHX	1	3952	7/7	0.92	0.16	140,140,140,140	5
85	MG	5	3748	1/1	0.92	0.06	124,124,124,124	0
85	MG	5	3569	1/1	0.92	0.59	38,38,38,38	0
85	MG	2	1922	1/1	0.92	0.56	85,85,85,85	0
85	MG	m5	301	1/1	0.92	0.97	56,56,56,56	0
85	MG	1	3532	1/1	0.92	0.33	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	6	2159	7/7	0.92	0.22	93,93,93,93	5
86	OHX	1	4000	7/7	0.92	0.43	55,55,55,55	3
85	MG	m5	303	1/1	0.92	0.25	67,67,67,67	0
86	OHX	1	4014	7/7	0.92	0.28	60,60,60,60	3
86	OHX	6	2166	7/7	0.92	0.26	66,66,66,66	4
85	MG	6	1941	1/1	0.92	0.53	57,57,57,57	0
85	MG	2	1956	1/1	0.92	0.85	70,70,70,70	0
85	MG	1	3704	1/1	0.92	0.41	59,59,59,59	0
85	MG	o2	201	1/1	0.92	0.64	35,35,35,35	1
85	MG	1	3418	1/1	0.92	0.56	47,47,47,47	0
85	MG	o4	201	1/1	0.92	0.28	53,53,53,53	0
86	OHX	6	2174	7/7	0.92	0.32	92,92,92,92	6
85	MG	f	1001	1/1	0.92	0.33	53,53,53,53	0
86	OHX	1	4038	7/7	0.92	0.34	56,56,56,56	4
85	MG	5	3589	1/1	0.92	0.57	28,28,28,28	0
85	MG	M7	204	1/1	0.92	0.45	46,46,46,46	0
86	OHX	1	4047	7/7	0.92	0.16	101,101,101,101	5
85	MG	6	1948	1/1	0.92	0.30	85,85,85,85	0
86	OHX	2	2043	7/7	0.92	0.25	100,100,100,100	4
85	MG	1	3574	1/1	0.92	0.97	30,30,30,30	0
85	MG	5	3465	1/1	0.92	0.81	44,44,44,44	0
86	OHX	2	2065	7/7	0.92	0.20	106,106,106,106	5
85	MG	2	1905	1/1	0.92	0.93	63,63,63,63	0
86	OHX	2	2076	7/7	0.92	0.26	87,87,87,87	5
85	MG	1	3669	1/1	0.92	0.15	59,59,59,59	0
85	MG	1	3757	1/1	0.92	0.44	55,55,55,55	0
86	OHX	5	3942	7/7	0.92	0.29	50,50,50,50	5
86	OHX	1	4068	7/7	0.92	0.28	39,39,39,39	3
86	OHX	5	3971	7/7	0.92	0.31	41,41,41,41	7
86	OHX	5	3988	7/7	0.92	0.20	64,64,64,64	5
85	MG	1	3670	1/1	0.92	0.38	38,38,38,38	0
85	MG	1	3759	1/1	0.92	0.31	48,48,48,48	0
86	OHX	2	2103	7/7	0.92	0.34	118,118,118,118	4
86	OHX	1	4074	7/7	0.92	0.43	38,38,38,38	3
85	MG	1	3537	1/1	0.92	0.42	57,57,57,57	0
86	OHX	5	4046	7/7	0.92	0.19	53,53,53,53	5
85	MG	1	4112	1/1	0.92	0.23	44,44,44,44	0
85	MG	6	1964	1/1	0.92	0.21	82,82,82,82	0
86	OHX	5	4050	7/7	0.92	0.30	45,45,45,45	3
85	MG	1	3408	1/1	0.92	0.46	25,25,25,25	0
85	MG	5	3618	1/1	0.92	0.50	34,34,34,34	0
85	MG	5	3787	1/1	0.92	0.30	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	5	4075	7/7	0.92	0.23	47,47,47,47	3
86	OHX	1	4082	7/7	0.92	0.23	63,63,63,63	5
86	OHX	1	4083	7/7	0.92	0.20	45,45,45,45	4
85	MG	1	3462	1/1	0.92	0.74	44,44,44,44	0
85	MG	2	1977	1/1	0.92	0.97	72,72,72,72	0
85	MG	6	1908	1/1	0.92	0.15	109,109,109,109	0
86	OHX	1	4092	7/7	0.92	0.26	47,47,47,47	3
85	MG	1	3646	1/1	0.92	0.25	39,39,39,39	0
85	MG	5	3494	1/1	0.92	0.42	45,45,45,45	0
85	MG	1	3725	1/1	0.92	0.31	38,38,38,38	0
86	OHX	5	4115	7/7	0.92	0.21	63,63,63,63	6
85	MG	6	1911	1/1	0.92	0.51	49,49,49,49	0
86	OHX	2	2129	7/7	0.92	0.24	87,87,87,87	5
85	MG	1	3678	1/1	0.92	0.44	53,53,53,53	0
85	MG	5	3417	1/1	0.92	0.63	64,64,64,64	0
85	MG	5	3506	1/1	0.92	0.73	27,27,27,27	0
86	OHX	1	4103	7/7	0.92	0.24	53,53,53,53	5
86	OHX	5	4126	7/7	0.92	0.21	98,98,98,98	3
85	MG	1	3485	1/1	0.92	0.27	58,58,58,58	0
86	OHX	5	4128	7/7	0.92	0.23	47,47,47,47	4
85	MG	1	3649	1/1	0.92	0.42	37,37,37,37	0
86	OHX	5	4131	7/7	0.92	0.20	64,64,64,64	5
85	MG	6	1981	1/1	0.92	0.60	54,54,54,54	0
86	OHX	2	2139	7/7	0.92	0.19	114,114,114,114	6
86	OHX	1	4110	7/7	0.92	0.24	55,55,55,55	5
85	MG	1	3620	1/1	0.92	0.34	32,32,32,32	0
85	MG	2	1952	1/1	0.92	0.42	64,64,64,64	0
85	MG	1	3598	1/1	0.92	0.34	39,39,39,39	0
85	MG	5	3540	1/1	0.92	0.33	62,62,62,62	0
85	MG	4	207	1/1	0.92	0.25	41,41,41,41	0
85	MG	6	1921	1/1	0.92	0.45	66,66,66,66	0
86	OHX	2	2148	7/7	0.92	0.24	69,69,69,69	6
85	MG	1	3599	1/1	0.92	0.49	32,32,32,32	0
85	MG	6	1924	1/1	0.92	0.53	48,48,48,48	0
86	OHX	5	4150	7/7	0.92	0.20	62,62,62,62	5
86	OHX	O4	202	7/7	0.92	0.21	82,82,82,82	5
85	MG	2	1941	1/1	0.92	0.13	100,100,100,100	0
86	OHX	6	2071	7/7	0.92	0.38	58,58,58,58	4
86	OHX	6	2080	7/7	0.92	0.41	82,82,82,82	1
86	OHX	6	2086	7/7	0.92	0.27	70,70,70,70	5
86	OHX	6	2087	7/7	0.92	0.26	109,109,109,109	6
86	OHX	6	2088	7/7	0.92	0.28	99,99,99,99	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
85	MG	5	3729	1/1	0.92	0.19	47,47,47,47	0
86	OHX	6	2110	7/7	0.92	0.30	112,112,112,112	6
85	MG	1	3526	1/1	0.92	0.48	45,45,45,45	0
85	MG	5	3445	1/1	0.92	0.43	38,38,38,38	0
86	OHX	6	2120	7/7	0.92	0.20	70,70,70,70	3
85	MG	1	3659	1/1	0.92	0.78	78,78,78,78	0
86	OHX	6	2125	7/7	0.92	0.29	52,52,52,52	5
85	MG	L2	301	1/1	0.92	0.24	37,37,37,37	0
86	OHX	6	2131	7/7	0.92	0.31	89,89,89,89	6
86	OHX	8	223	7/7	0.92	0.28	75,75,75,75	5
85	MG	1	3528	1/1	0.92	0.53	47,47,47,47	0
85	MG	8	210	1/1	0.92	0.19	48,48,48,48	0
85	MG	12	302	1/1	0.92	0.48	45,45,45,45	0
86	OHX	15	302	7/7	0.92	0.12	105,105,105,105	4
86	OHX	19	201	7/7	0.92	0.29	61,61,61,61	2
85	MG	13	401	1/1	0.92	0.50	27,27,27,27	0
86	OHX	m7	204	7/7	0.92	0.32	47,47,47,47	5
86	OHX	m9	201	7/7	0.92	0.22	61,61,61,61	6
86	OHX	o6	201	7/7	0.92	0.22	68,68,68,68	4
86	OHX	6	2140	7/7	0.92	0.29	74,74,74,74	6
85	MG	L7	301	1/1	0.92	0.28	38,38,38,38	0
85	MG	4	202	1/1	0.93	0.17	64,64,64,64	0
86	OHX	1	4037	7/7	0.93	0.34	84,84,84,84	7
86	OHX	6	2165	7/7	0.93	0.34	74,74,74,74	6
85	MG	1	3563	1/1	0.93	0.27	41,41,41,41	0
86	OHX	2	2068	7/7	0.93	0.21	103,103,103,103	7
86	OHX	1	4041	7/7	0.93	0.23	46,46,46,46	4
85	MG	1	3686	1/1	0.93	0.69	35,35,35,35	0
86	OHX	1	4046	7/7	0.93	0.41	50,50,50,50	2
86	OHX	2	2074	7/7	0.93	0.25	85,85,85,85	3
85	MG	1	3687	1/1	0.93	0.38	46,46,46,46	0
85	MG	5	3407	1/1	0.93	0.54	35,35,35,35	0
86	OHX	2	2086	7/7	0.93	0.22	112,112,112,112	5
85	MG	1	3688	1/1	0.93	0.77	39,39,39,39	0
86	OHX	2	2093	7/7	0.93	0.24	110,110,110,110	5
85	MG	1	3421	1/1	0.93	0.20	58,58,58,58	0
85	MG	1	3450	1/1	0.93	0.43	31,31,31,31	0
85	MG	1	3632	1/1	0.93	0.70	47,47,47,47	0
85	MG	4	213	1/1	0.93	0.40	64,64,64,64	0
85	MG	1	3602	1/1	0.93	0.35	58,58,58,58	0
85	MG	5	3692	1/1	0.93	0.32	38,38,38,38	0
86	OHX	s8	303	7/7	0.93	0.23	105,105,105,105	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	c3	201	7/7	0.93	0.25	84,84,84,84	4
85	MG	1	3405	1/1	0.93	0.57	132,132,132,132	0
85	MG	1	3696	1/1	0.93	0.63	30,30,30,30	0
85	MG	5	3495	1/1	0.93	0.39	33,33,33,33	0
86	OHX	2	2113	7/7	0.93	0.11	152,152,152,152	7
85	MG	1	3635	1/1	0.93	0.30	88,88,88,88	0
86	OHX	2	2116	7/7	0.93	0.15	127,127,127,127	7
85	MG	5	3798	1/1	0.93	0.39	42,42,42,42	0
85	MG	1	3498	1/1	0.93	0.66	45,45,45,45	0
85	MG	6	1926	1/1	0.93	0.22	65,65,65,65	0
86	OHX	5	3993	7/7	0.93	0.30	38,38,38,38	4
86	OHX	5	4006	7/7	0.93	0.45	109,109,109,109	5
86	OHX	1	4081	7/7	0.93	0.23	43,43,43,43	5
85	MG	1	3664	1/1	0.93	0.30	39,39,39,39	0
85	MG	1	3570	1/1	0.93	0.52	46,46,46,46	0
86	OHX	5	4026	7/7	0.93	0.29	54,54,54,54	4
85	MG	5	3510	1/1	0.93	0.61	39,39,39,39	0
86	OHX	5	4040	7/7	0.93	0.34	149,149,149,149	6
86	OHX	1	4088	7/7	0.93	0.20	92,92,92,92	7
86	OHX	2	2127	7/7	0.93	0.13	128,128,128,128	7
85	MG	M0	302	1/1	0.93	0.23	50,50,50,50	0
85	MG	5	3517	1/1	0.93	0.41	28,28,28,28	0
85	MG	5	3431	1/1	0.93	0.39	41,41,41,41	0
86	OHX	5	4051	7/7	0.93	0.21	64,64,64,64	6
85	MG	1	3703	1/1	0.93	0.44	40,40,40,40	0
86	OHX	5	4055	7/7	0.93	0.28	56,56,56,56	4
85	MG	5	3435	1/1	0.93	0.32	33,33,33,33	0
85	MG	M6	204	1/1	0.93	0.50	37,37,37,37	0
86	OHX	5	4069	7/7	0.93	0.23	58,58,58,58	5
86	OHX	1	4097	7/7	0.93	0.19	42,42,42,42	6
85	MG	5	3529	1/1	0.93	0.57	45,45,45,45	0
85	MG	5	3532	1/1	0.93	0.62	35,35,35,35	0
86	OHX	5	4083	7/7	0.93	0.28	53,53,53,53	3
86	OHX	1	4100	7/7	0.93	0.25	38,38,38,38	3
86	OHX	2	2140	7/7	0.93	0.28	85,85,85,85	5
85	MG	1	3436	1/1	0.93	0.84	39,39,39,39	0
85	MG	1	3503	1/1	0.93	0.54	37,37,37,37	0
85	MG	5	3440	1/1	0.93	0.38	36,36,36,36	0
86	OHX	5	4099	7/7	0.93	0.24	73,73,73,73	5
86	OHX	5	4100	7/7	0.93	0.33	46,46,46,46	5
86	OHX	5	4104	7/7	0.93	0.36	68,68,68,68	6
85	MG	5	3442	1/1	0.93	0.27	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	5	4106	7/7	0.93	0.31	32,32,32,32	4
85	MG	5	3642	1/1	0.93	0.47	39,39,39,39	0
86	OHX	5	4110	7/7	0.93	0.13	133,133,133,133	5
86	OHX	2	2146	7/7	0.93	0.19	87,87,87,87	7
85	MG	8	205	1/1	0.93	0.32	43,43,43,43	0
85	MG	6	1938	1/1	0.93	0.28	60,60,60,60	0
85	MG	1	3611	1/1	0.93	0.27	41,41,41,41	0
85	MG	5	3731	1/1	0.93	0.44	55,55,55,55	0
85	MG	6	1942	1/1	0.93	0.41	43,43,43,43	0
85	MG	2	1914	1/1	0.93	0.27	83,83,83,83	0
85	MG	1	3576	1/1	0.93	0.48	46,46,46,46	0
86	OHX	S8	301	7/7	0.93	0.12	115,115,115,115	7
86	OHX	M7	205	7/7	0.93	0.19	57,57,57,57	5
86	OHX	C3	201	7/7	0.93	0.26	100,100,100,100	5
85	MG	5	3742	1/1	0.93	0.33	31,31,31,31	1
85	MG	l5	301	1/1	0.93	0.15	63,63,63,63	0
85	MG	1	3440	1/1	0.93	0.48	49,49,49,49	0
86	OHX	5	4134	7/7	0.93	0.10	157,157,157,157	7
86	OHX	5	4135	7/7	0.93	0.23	54,54,54,54	4
86	OHX	6	2051	7/7	0.93	0.36	131,131,131,131	5
85	MG	1	3413	1/1	0.93	0.56	41,41,41,41	0
85	MG	5	3655	1/1	0.93	0.30	42,42,42,42	0
86	OHX	5	4140	7/7	0.93	0.14	88,88,88,88	7
85	MG	1	3429	1/1	0.93	0.28	36,36,36,36	0
85	MG	5	3561	1/1	0.93	0.65	26,26,26,26	0
85	MG	1	3430	1/1	0.93	0.17	57,57,57,57	0
86	OHX	6	2102	7/7	0.93	0.36	97,97,97,97	4
85	MG	1	3718	1/1	0.93	0.60	52,52,52,52	0
86	OHX	6	2107	7/7	0.93	0.27	81,81,81,81	5
85	MG	n3	201	1/1	0.93	0.43	25,25,25,25	0
85	MG	1	3545	1/1	0.93	0.37	31,31,31,31	0
86	OHX	5	4151	7/7	0.93	0.25	53,53,53,53	4
85	MG	n8	201	1/1	0.93	0.31	37,37,37,37	0
86	OHX	1	3966	7/7	0.93	0.28	35,35,35,35	3
86	OHX	5	4155	7/7	0.93	0.14	97,97,97,97	7
86	OHX	5	4156	7/7	0.93	0.20	49,49,49,49	6
85	MG	6	1903	1/1	0.93	0.17	88,88,88,88	0
86	OHX	6	2123	7/7	0.93	0.22	70,70,70,70	4
86	OHX	1	3974	7/7	0.93	0.22	63,63,63,63	5
85	MG	1	3721	1/1	0.93	0.42	43,43,43,43	0
86	OHX	1	3979	7/7	0.93	0.09	197,197,197,197	5
85	MG	1	3448	1/1	0.93	0.88	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	6	2134	7/7	0.93	0.12	163,163,163,163	7
86	OHX	1	3995	7/7	0.93	0.58	50,50,50,50	2
86	OHX	1	3999	7/7	0.93	0.06	215,215,215,215	2
86	OHX	5	4168	7/7	0.93	0.29	64,64,64,64	5
85	MG	6	1906	1/1	0.93	0.34	76,76,76,76	0
86	OHX	6	2138	7/7	0.93	0.22	120,120,120,120	7
85	MG	1	3465	1/1	0.93	0.68	28,28,28,28	0
86	OHX	7	223	7/7	0.93	0.34	54,54,54,54	4
86	OHX	1	4013	7/7	0.93	0.36	54,54,54,54	3
85	MG	1	3525	1/1	0.93	0.68	35,35,35,35	0
86	OHX	1	4016	7/7	0.93	0.32	56,56,56,56	3
85	MG	5	3592	1/1	0.93	0.47	35,35,35,35	0
85	MG	5	3772	1/1	0.93	0.16	37,37,37,37	0
86	OHX	1	4022	7/7	0.93	0.22	71,71,71,71	6
86	OHX	8	231	7/7	0.93	0.29	62,62,62,62	5
86	OHX	13	404	7/7	0.93	0.15	72,72,72,72	4
85	MG	5	3594	1/1	0.93	0.66	35,35,35,35	0
86	OHX	6	2153	7/7	0.93	0.30	67,67,67,67	3
86	OHX	6	2156	7/7	0.93	0.09	150,150,150,150	5
85	MG	5	3595	1/1	0.93	0.51	28,28,28,28	0
86	OHX	2	2050	7/7	0.93	0.22	129,129,129,129	6
86	OHX	2	2054	7/7	0.93	0.26	103,103,103,103	5
86	OHX	07	502	7/7	0.93	0.27	83,83,83,83	4
86	OHX	1	4031	7/7	0.93	0.20	65,65,65,65	6
86	OHX	6	2162	7/7	0.93	0.38	114,114,114,114	5
86	OHX	1	3912	7/7	0.94	0.18	126,126,126,126	4
86	OHX	1	3914	7/7	0.94	0.23	79,79,79,79	3
85	MG	1	3728	1/1	0.94	0.53	47,47,47,47	0
85	MG	6	1994	1/1	0.94	0.71	49,49,49,49	0
86	OHX	1	3927	7/7	0.94	0.37	51,51,51,51	3
85	MG	1	3493	1/1	0.94	0.72	42,42,42,42	0
86	OHX	1	3945	7/7	0.94	0.27	57,57,57,57	5
85	MG	1	3730	1/1	0.94	0.15	36,36,36,36	0
86	OHX	6	2147	7/7	0.94	0.24	64,64,64,64	4
85	MG	5	3579	1/1	0.94	0.40	17,17,17,17	0
85	MG	1	3731	1/1	0.94	0.47	57,57,57,57	0
85	MG	8	204	1/1	0.94	0.83	44,44,44,44	0
86	OHX	1	3964	7/7	0.94	0.18	71,71,71,71	4
86	OHX	6	2154	7/7	0.94	0.27	49,49,49,49	3
86	OHX	6	2155	7/7	0.94	0.38	71,71,71,71	3
86	OHX	1	3965	7/7	0.94	0.35	56,56,56,56	3
85	MG	5	3585	1/1	0.94	0.58	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	1	3967	7/7	0.94	0.16	82,82,82,82	3
85	MG	5	3586	1/1	0.94	0.46	29,29,29,29	0
85	MG	6	1999	1/1	0.94	0.72	36,36,36,36	0
85	MG	5	3590	1/1	0.94	0.51	35,35,35,35	0
85	MG	6	2000	1/1	0.94	0.86	48,48,48,48	0
86	OHX	1	3980	7/7	0.94	0.33	51,51,51,51	1
85	MG	5	3457	1/1	0.94	0.27	38,38,38,38	0
86	OHX	1	3986	7/7	0.94	0.21	76,76,76,76	3
86	OHX	1	3990	7/7	0.94	0.15	92,92,92,92	6
85	MG	5	3705	1/1	0.94	0.17	66,66,66,66	0
85	MG	1	3732	1/1	0.94	0.38	35,35,35,35	0
85	MG	5	3596	1/1	0.94	0.24	47,47,47,47	0
86	OHX	1	4004	7/7	0.94	0.35	75,75,75,75	5
85	MG	1	3683	1/1	0.94	0.14	39,39,39,39	1
85	MG	1	3647	1/1	0.94	0.52	64,64,64,64	0
85	MG	5	3710	1/1	0.94	0.37	55,55,55,55	0
85	MG	5	3711	1/1	0.94	0.48	32,32,32,32	0
86	OHX	1	4017	7/7	0.94	0.28	46,46,46,46	2
86	OHX	1	4018	7/7	0.94	0.23	69,69,69,69	3
85	MG	6	2006	1/1	0.94	0.66	67,67,67,67	0
85	MG	1	3495	1/1	0.94	0.83	34,34,34,34	0
85	MG	1	3497	1/1	0.94	0.83	25,25,25,25	0
85	MG	6	1939	1/1	0.94	0.34	34,34,34,34	0
85	MG	SM	301	1/1	0.94	0.21	58,58,58,58	0
86	OHX	1	4027	7/7	0.94	0.27	75,75,75,75	3
86	OHX	s9	201	7/7	0.94	0.20	71,71,71,71	5
86	OHX	1	4028	7/7	0.94	0.20	58,58,58,58	3
85	MG	M5	302	1/1	0.94	0.74	47,47,47,47	0
85	MG	M6	201	1/1	0.94	0.16	34,34,34,34	0
85	MG	5	3471	1/1	0.94	0.24	51,51,51,51	0
86	OHX	d9	102	7/7	0.94	0.27	106,106,106,106	6
86	OHX	5	3917	7/7	0.94	0.35	49,49,49,49	3
85	MG	5	3472	1/1	0.94	0.38	39,39,39,39	0
86	OHX	5	3932	7/7	0.94	0.26	139,139,139,139	5
86	OHX	5	3936	7/7	0.94	0.22	49,49,49,49	3
86	OHX	1	4033	7/7	0.94	0.18	66,66,66,66	5
86	OHX	1	4036	7/7	0.94	0.13	83,83,83,83	6
85	MG	1	3578	1/1	0.94	0.30	60,60,60,60	0
85	MG	q2	201	1/1	0.94	0.51	43,43,43,43	1
86	OHX	5	3975	7/7	0.94	0.44	85,85,85,85	3
85	MG	2	1913	1/1	0.94	0.35	79,79,79,79	0
86	OHX	5	3989	7/7	0.94	0.22	158,158,158,158	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	5	3991	7/7	0.94	0.40	37,37,37,37	3
85	MG	C	102	1/1	0.94	0.59	39,39,39,39	0
86	OHX	1	4042	7/7	0.94	0.14	70,70,70,70	5
86	OHX	5	4008	7/7	0.94	0.29	66,66,66,66	3
85	MG	1	3654	1/1	0.94	0.45	39,39,39,39	0
85	MG	1	3404	1/1	0.94	0.55	57,57,57,57	0
85	MG	d3	201	1/1	0.94	0.34	50,50,50,50	0
86	OHX	5	4024	7/7	0.94	0.22	66,66,66,66	5
85	MG	5	3736	1/1	0.94	0.73	35,35,35,35	1
86	OHX	5	4031	7/7	0.94	0.24	85,85,85,85	4
86	OHX	5	4033	7/7	0.94	0.15	98,98,98,98	7
86	OHX	2	2044	7/7	0.94	0.18	98,98,98,98	6
86	OHX	5	4037	7/7	0.94	0.18	93,93,93,93	5
86	OHX	1	4052	7/7	0.94	0.37	58,58,58,58	4
86	OHX	1	4055	7/7	0.94	0.28	81,81,81,81	5
86	OHX	2	2045	7/7	0.94	0.25	95,95,95,95	4
85	MG	5	3737	1/1	0.94	0.61	40,40,40,40	0
85	MG	1	3749	1/1	0.94	0.56	17,17,17,17	0
85	MG	5	3740	1/1	0.94	0.33	45,45,45,45	0
86	OHX	2	2057	7/7	0.94	0.29	79,79,79,79	1
86	OHX	5	4053	7/7	0.94	0.19	65,65,65,65	5
86	OHX	2	2059	7/7	0.94	0.25	101,101,101,101	4
85	MG	1	3694	1/1	0.94	0.21	46,46,46,46	0
86	OHX	5	4057	7/7	0.94	0.26	50,50,50,50	2
86	OHX	5	4058	7/7	0.94	0.25	36,36,36,36	6
86	OHX	5	4059	7/7	0.94	0.24	47,47,47,47	3
85	MG	1	3621	1/1	0.94	0.41	52,52,52,52	0
85	MG	1	3542	1/1	0.94	0.42	50,50,50,50	0
85	MG	5	3493	1/1	0.94	0.71	42,42,42,42	0
86	OHX	1	4072	7/7	0.94	0.30	47,47,47,47	3
86	OHX	5	4076	7/7	0.94	0.19	43,43,43,43	3
85	MG	5	3747	1/1	0.94	0.66	51,51,51,51	0
86	OHX	5	4079	7/7	0.94	0.29	54,54,54,54	5
86	OHX	5	4080	7/7	0.94	0.28	55,55,55,55	3
86	OHX	5	4081	7/7	0.94	0.42	35,35,35,35	3
85	MG	1	3445	1/1	0.94	0.78	57,57,57,57	0
85	MG	6	1959	1/1	0.94	0.36	98,98,98,98	0
85	MG	5	3751	1/1	0.94	0.73	53,53,53,53	0
85	MG	5	3752	1/1	0.94	0.34	40,40,40,40	0
85	MG	5	3498	1/1	0.94	0.53	32,32,32,32	0
86	OHX	2	2096	7/7	0.94	0.18	108,108,108,108	6
86	OHX	5	4097	7/7	0.94	0.19	75,75,75,75	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	1	3699	1/1	0.94	0.27	49,49,49,49	0
85	MG	1	3624	1/1	0.94	0.35	33,33,33,33	0
85	MG	1	3594	1/1	0.94	0.46	48,48,48,48	0
86	OHX	5	4102	7/7	0.94	0.21	45,45,45,45	5
85	MG	5	3758	1/1	0.94	0.31	36,36,36,36	0
86	OHX	1	4084	7/7	0.94	0.23	42,42,42,42	5
85	MG	1	3628	1/1	0.94	0.62	41,41,41,41	0
85	MG	5	3505	1/1	0.94	0.83	25,25,25,25	0
85	MG	1	3411	1/1	0.94	0.55	43,43,43,43	0
86	OHX	5	4112	7/7	0.94	0.20	51,51,51,51	6
85	MG	5	3507	1/1	0.94	0.40	38,38,38,38	0
86	OHX	1	4091	7/7	0.94	0.36	42,42,42,42	4
86	OHX	5	4117	7/7	0.94	0.30	40,40,40,40	5
85	MG	5	3765	1/1	0.94	0.14	39,39,39,39	0
85	MG	1	3510	1/1	0.94	0.31	39,39,39,39	0
85	MG	5	3511	1/1	0.94	0.26	43,43,43,43	0
86	OHX	2	2115	7/7	0.94	0.22	91,91,91,91	6
86	OHX	5	4124	7/7	0.94	0.31	51,51,51,51	6
85	MG	5	3514	1/1	0.94	0.57	35,35,35,35	0
85	MG	5	3415	1/1	0.94	0.29	44,44,44,44	0
86	OHX	2	2118	7/7	0.94	0.15	143,143,143,143	7
86	OHX	2	2119	7/7	0.94	0.35	62,62,62,62	3
85	MG	5	3516	1/1	0.94	0.56	21,21,21,21	0
85	MG	5	3416	1/1	0.94	0.63	31,31,31,31	0
85	MG	2	1954	1/1	0.94	0.27	105,105,105,105	0
85	MG	5	3520	1/1	0.94	0.40	30,30,30,30	0
85	MG	1	3515	1/1	0.94	0.39	28,28,28,28	0
86	OHX	1	4105	7/7	0.94	0.27	46,46,46,46	5
86	OHX	2	2126	7/7	0.94	0.48	64,64,64,64	4
85	MG	5	3419	1/1	0.94	0.23	36,36,36,36	0
85	MG	1	3482	1/1	0.94	0.49	33,33,33,33	0
86	OHX	1	4109	7/7	0.94	0.20	48,48,48,48	4
85	MG	1	3559	1/1	0.94	0.49	22,22,22,22	0
86	OHX	2	2131	7/7	0.94	0.11	109,109,109,109	5
85	MG	1	3562	1/1	0.94	0.91	33,33,33,33	0
86	OHX	3	218	7/7	0.94	0.30	54,54,54,54	5
85	MG	1	3712	1/1	0.94	0.51	44,44,44,44	0
85	MG	1	3671	1/1	0.94	0.50	47,47,47,47	0
85	MG	5	3542	1/1	0.94	0.64	46,46,46,46	0
86	OHX	4	233	7/7	0.94	0.24	65,65,65,65	5
85	MG	5	3665	1/1	0.94	0.26	43,43,43,43	0
86	OHX	5	4152	7/7	0.94	0.30	76,76,76,76	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	M0	303	7/7	0.94	0.39	55,55,55,55	4
85	MG	6	1912	1/1	0.94	0.69	39,39,39,39	0
85	MG	5	3430	1/1	0.94	0.34	36,36,36,36	0
86	OHX	M8	201	7/7	0.94	0.25	47,47,47,47	3
85	MG	1	3464	1/1	0.94	0.52	38,38,38,38	0
85	MG	5	3793	1/1	0.94	0.68	37,37,37,37	0
85	MG	2	1962	1/1	0.94	0.35	88,88,88,88	0
85	MG	5	3671	1/1	0.94	0.27	84,84,84,84	0
85	MG	5	3433	1/1	0.94	0.33	37,37,37,37	0
86	OHX	6	2065	7/7	0.94	0.18	138,138,138,138	5
86	OHX	5	4163	7/7	0.94	0.31	36,36,36,36	4
86	OHX	6	2066	7/7	0.94	0.16	162,162,162,162	3
85	MG	2	1924	1/1	0.94	0.61	100,100,100,100	0
86	OHX	6	2077	7/7	0.94	0.24	98,98,98,98	5
85	MG	1	3468	1/1	0.94	0.72	39,39,39,39	0
85	MG	5	3675	1/1	0.94	0.46	34,34,34,34	1
85	MG	1	3676	1/1	0.94	0.24	52,52,52,52	0
85	MG	1	3490	1/1	0.94	0.66	34,34,34,34	0
85	MG	5	3557	1/1	0.94	0.78	29,29,29,29	0
85	MG	5	3810	1/1	0.94	0.32	50,50,50,50	0
86	OHX	6	2104	7/7	0.94	0.17	91,91,91,91	5
85	MG	1	3610	1/1	0.94	0.41	45,45,45,45	0
86	OHX	8	226	7/7	0.94	0.29	47,47,47,47	3
85	MG	1	3469	1/1	0.94	0.56	41,41,41,41	0
86	OHX	6	2111	7/7	0.94	0.22	73,73,73,73	5
85	MG	4	208	1/1	0.94	0.45	37,37,37,37	0
86	OHX	1	3825	7/7	0.94	0.28	91,91,91,91	5
86	OHX	1	3849	7/7	0.94	0.28	48,48,48,48	5
85	MG	4	209	1/1	0.94	0.39	51,51,51,51	0
85	MG	5	3571	1/1	0.94	0.53	34,34,34,34	0
85	MG	7	202	1/1	0.94	0.78	19,19,19,19	0
86	OHX	6	2127	7/7	0.94	0.36	58,58,58,58	5
85	MG	7	204	1/1	0.94	0.70	44,44,44,44	0
86	OHX	1	3893	7/7	0.94	0.17	155,155,155,155	6
85	MG	1	3424	1/1	0.94	0.48	59,59,59,59	0
86	OHX	1	3904	7/7	0.94	0.44	59,59,59,59	3
86	OHX	1	3908	7/7	0.94	0.19	91,91,91,91	3
87	ZN	e1	501	1/1	0.94	0.04	173,173,173,173	0
89	PRO	1	4114	7/8	0.94	0.20	41,41,51,51	0
85	MG	6	1940	1/1	0.95	0.51	36,36,36,36	0
85	MG	5	3688	1/1	0.95	0.18	47,47,47,47	0
85	MG	5	3428	1/1	0.95	0.53	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	2	2106	7/7	0.95	0.38	78,78,78,78	3
85	MG	5	3429	1/1	0.95	0.41	31,31,31,31	0
85	MG	5	3607	1/1	0.95	0.25	36,36,36,36	0
86	OHX	1	4045	7/7	0.95	0.32	54,54,54,54	1
86	OHX	2	2110	7/7	0.95	0.15	112,112,112,112	5
85	MG	2	1961	1/1	0.95	0.52	86,86,86,86	0
86	OHX	6	2180	7/7	0.95	0.14	97,97,97,97	6
85	MG	5	3609	1/1	0.95	0.18	35,35,35,35	0
85	MG	1	3496	1/1	0.95	0.49	41,41,41,41	0
85	MG	5	3611	1/1	0.95	0.39	38,38,38,38	0
86	OHX	1	4053	7/7	0.95	0.18	43,43,43,43	3
86	OHX	s4	602	7/7	0.95	0.20	76,76,76,76	3
86	OHX	1	4054	7/7	0.95	0.21	77,77,77,77	6
85	MG	1	3527	1/1	0.95	0.67	31,31,31,31	0
86	OHX	1	4057	7/7	0.95	0.10	109,109,109,109	5
85	MG	1	3446	1/1	0.95	0.41	41,41,41,41	0
85	MG	5	3614	1/1	0.95	0.58	41,41,41,41	0
86	OHX	c8	203	7/7	0.95	0.22	99,99,99,99	5
85	MG	5	3699	1/1	0.95	0.33	39,39,39,39	0
85	MG	5	3508	1/1	0.95	0.73	31,31,31,31	0
86	OHX	sR	401	7/7	0.95	0.13	129,129,129,129	6
86	OHX	5	3869	7/7	0.95	0.32	35,35,35,35	4
86	OHX	5	3889	7/7	0.95	0.46	42,42,42,42	3
85	MG	5	3701	1/1	0.95	0.34	38,38,38,38	0
86	OHX	5	3919	7/7	0.95	0.29	73,73,73,73	3
86	OHX	5	3922	7/7	0.95	0.14	119,119,119,119	6
86	OHX	2	2121	7/7	0.95	0.58	94,94,94,94	4
85	MG	5	3808	1/1	0.95	0.24	36,36,36,36	0
85	MG	6	1997	1/1	0.95	0.42	53,53,53,53	0
85	MG	5	3617	1/1	0.95	0.83	35,35,35,35	0
85	MG	6	1945	1/1	0.95	0.54	51,51,51,51	0
86	OHX	1	4071	7/7	0.95	0.30	42,42,42,42	3
86	OHX	5	3949	7/7	0.95	0.22	56,56,56,56	4
86	OHX	5	3950	7/7	0.95	0.20	95,95,95,95	4
86	OHX	5	3957	7/7	0.95	0.39	46,46,46,46	3
86	OHX	5	3963	7/7	0.95	0.30	62,62,62,62	5
86	OHX	5	3970	7/7	0.95	0.22	80,80,80,80	3
85	MG	1	3432	1/1	0.95	0.37	49,49,49,49	0
86	OHX	5	3974	7/7	0.95	0.29	53,53,53,53	4
85	MG	1	3735	1/1	0.95	0.35	49,49,49,49	0
86	OHX	5	3978	7/7	0.95	0.18	69,69,69,69	4
86	OHX	5	3982	7/7	0.95	0.20	58,58,58,58	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	5	3983	7/7	0.95	0.35	46,46,46,46	3
86	OHX	2	2128	7/7	0.95	0.11	115,115,115,115	7
85	MG	1	3736	1/1	0.95	0.12	50,50,50,50	0
85	MG	5	3441	1/1	0.95	0.47	30,30,30,30	0
85	MG	6	1949	1/1	0.95	0.25	77,77,77,77	0
86	OHX	5	3995	7/7	0.95	0.24	88,88,88,88	5
86	OHX	5	4005	7/7	0.95	0.20	82,82,82,82	3
85	MG	1	3698	1/1	0.95	0.24	42,42,42,42	0
85	MG	1	3481	1/1	0.95	0.36	40,40,40,40	0
85	MG	6	1952	1/1	0.95	0.65	53,53,53,53	0
86	OHX	5	4012	7/7	0.95	0.26	41,41,41,41	4
85	MG	2	1915	1/1	0.95	0.69	57,57,57,57	0
86	OHX	5	4016	7/7	0.95	0.19	62,62,62,62	7
85	MG	5	3524	1/1	0.95	0.15	48,48,48,48	0
85	MG	5	3720	1/1	0.95	0.42	34,34,34,34	0
85	MG	1	3504	1/1	0.95	0.65	42,42,42,42	0
85	MG	8	202	1/1	0.95	0.31	42,42,42,42	0
86	OHX	5	4032	7/7	0.95	0.19	71,71,71,71	4
86	OHX	1	4086	7/7	0.95	0.16	65,65,65,65	4
86	OHX	1	4087	7/7	0.95	0.24	44,44,44,44	6
86	OHX	5	4036	7/7	0.95	0.31	38,38,38,38	5
85	MG	5	3722	1/1	0.95	0.66	41,41,41,41	0
85	MG	2	1926	1/1	0.95	0.30	76,76,76,76	0
85	MG	5	3724	1/1	0.95	0.36	35,35,35,35	0
85	MG	6	1957	1/1	0.95	0.14	94,94,94,94	0
85	MG	5	3452	1/1	0.95	0.40	29,29,29,29	0
85	MG	5	3636	1/1	0.95	0.52	43,43,43,43	0
86	OHX	5	4049	7/7	0.95	0.24	37,37,37,37	3
85	MG	1	3744	1/1	0.95	0.33	44,44,44,44	0
85	MG	1	3536	1/1	0.95	0.59	29,29,29,29	0
85	MG	5	3544	1/1	0.95	0.63	48,48,48,48	0
85	MG	5	3733	1/1	0.95	0.12	50,50,50,50	0
85	MG	2	1937	1/1	0.95	0.47	80,80,80,80	0
85	MG	6	1962	1/1	0.95	0.13	93,93,93,93	0
85	MG	5	3547	1/1	0.95	0.38	53,53,53,53	0
86	OHX	S9	201	7/7	0.95	0.22	94,94,94,94	6
86	OHX	5	4060	7/7	0.95	0.39	45,45,45,45	5
85	MG	1	3616	1/1	0.95	0.11	58,58,58,58	0
86	OHX	D9	102	7/7	0.95	0.13	97,97,97,97	6
86	OHX	5	4063	7/7	0.95	0.33	39,39,39,39	3
86	OHX	5	4067	7/7	0.95	0.36	34,34,34,34	4
85	MG	5	3739	1/1	0.95	0.49	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	1	3538	1/1	0.95	0.64	39,39,39,39	0
85	MG	1	3584	1/1	0.95	0.74	33,33,33,33	0
85	MG	m7	201	1/1	0.95	0.36	36,36,36,36	0
86	OHX	1	3870	7/7	0.95	0.29	67,67,67,67	3
85	MG	m7	203	1/1	0.95	0.35	34,34,34,34	0
86	OHX	1	3883	7/7	0.95	0.26	71,71,71,71	1
86	OHX	1	3886	7/7	0.95	0.23	56,56,56,56	4
86	OHX	3	213	7/7	0.95	0.19	82,82,82,82	5
86	OHX	5	4085	7/7	0.95	0.12	143,143,143,143	7
86	OHX	1	3887	7/7	0.95	0.20	131,131,131,131	5
86	OHX	1	3890	7/7	0.95	0.30	48,48,48,48	3
86	OHX	5	4089	7/7	0.95	0.26	47,47,47,47	3
86	OHX	5	4090	7/7	0.95	0.26	51,51,51,51	4
85	MG	5	3648	1/1	0.95	0.34	37,37,37,37	0
86	OHX	5	4092	7/7	0.95	0.45	33,33,33,33	2
86	OHX	4	222	7/7	0.95	0.19	61,61,61,61	3
86	OHX	4	226	7/7	0.95	0.18	106,106,106,106	5
85	MG	2	1988	1/1	0.95	0.15	88,88,88,88	0
86	OHX	4	230	7/7	0.95	0.23	45,45,45,45	3
86	OHX	4	231	7/7	0.95	0.22	75,75,75,75	5
85	MG	5	3745	1/1	0.95	0.48	34,34,34,34	0
85	MG	1	3470	1/1	0.95	0.63	46,46,46,46	0
85	MG	2	1971	1/1	0.95	0.20	81,81,81,81	0
86	OHX	1	3910	7/7	0.95	0.17	81,81,81,81	4
85	MG	1	3681	1/1	0.95	0.90	37,37,37,37	0
86	OHX	5	4108	7/7	0.95	0.18	66,66,66,66	3
85	MG	5	3656	1/1	0.95	0.58	41,41,41,41	0
86	OHX	5	4111	7/7	0.95	0.24	74,74,74,74	7
85	MG	1	3426	1/1	0.95	0.47	52,52,52,52	0
86	OHX	1	3919	7/7	0.95	0.13	106,106,106,106	3
86	OHX	1	3920	7/7	0.95	0.37	43,43,43,43	3
85	MG	M0	301	1/1	0.95	0.34	41,41,41,41	0
86	OHX	1	3925	7/7	0.95	0.21	96,96,96,96	5
86	OHX	6	2039	7/7	0.95	0.12	126,126,126,126	5
86	OHX	6	2043	7/7	0.95	0.31	90,90,90,90	5
85	MG	6	1975	1/1	0.95	0.21	90,90,90,90	0
86	OHX	6	2060	7/7	0.95	0.20	96,96,96,96	1
85	MG	6	1976	1/1	0.95	0.21	32,32,32,32	0
86	OHX	1	3937	7/7	0.95	0.10	110,110,110,110	6
86	OHX	1	3939	7/7	0.95	0.25	54,54,54,54	3
86	OHX	6	2072	7/7	0.95	0.29	76,76,76,76	3
86	OHX	5	4129	7/7	0.95	0.31	37,37,37,37	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	2	2010	7/7	0.95	0.28	101,101,101,101	4
85	MG	1	3517	1/1	0.95	0.41	46,46,46,46	0
86	OHX	6	2084	7/7	0.95	0.21	104,104,104,104	5
86	OHX	2	2026	7/7	0.95	0.22	103,103,103,103	4
86	OHX	2	2034	7/7	0.95	0.17	119,119,119,119	4
86	OHX	1	3958	7/7	0.95	0.30	45,45,45,45	4
86	OHX	6	2095	7/7	0.95	0.22	99,99,99,99	3
86	OHX	1	3960	7/7	0.95	0.20	42,42,42,42	4
85	MG	5	3474	1/1	0.95	0.31	63,63,63,63	0
85	MG	5	3478	1/1	0.95	0.83	21,21,21,21	0
86	OHX	6	2105	7/7	0.95	0.17	81,81,81,81	4
85	MG	5	3479	1/1	0.95	0.12	70,70,70,70	0
85	MG	1	3546	1/1	0.95	0.63	36,36,36,36	0
85	MG	1	3518	1/1	0.95	0.67	31,31,31,31	0
86	OHX	5	4146	7/7	0.95	0.18	71,71,71,71	5
86	OHX	2	2047	7/7	0.95	0.22	80,80,80,80	4
85	MG	5	3482	1/1	0.95	0.72	37,37,37,37	0
85	MG	1	3720	1/1	0.95	0.49	48,48,48,48	0
86	OHX	2	2051	7/7	0.95	0.25	101,101,101,101	5
86	OHX	6	2122	7/7	0.95	0.34	77,77,77,77	4
86	OHX	2	2053	7/7	0.95	0.24	107,107,107,107	4
85	MG	5	3766	1/1	0.95	0.45	27,27,27,27	0
86	OHX	6	2126	7/7	0.95	0.29	53,53,53,53	3
85	MG	1	3519	1/1	0.95	0.88	49,49,49,49	0
86	OHX	1	3988	7/7	0.95	0.17	87,87,87,87	5
86	OHX	2	2058	7/7	0.95	0.33	67,67,67,67	4
86	OHX	6	2132	7/7	0.95	0.23	94,94,94,94	6
86	OHX	1	3993	7/7	0.95	0.23	94,94,94,94	7
85	MG	2	1990	1/1	0.95	0.54	49,49,49,49	0
86	OHX	1	3996	7/7	0.95	0.25	64,64,64,64	5
86	OHX	1	3997	7/7	0.95	0.23	55,55,55,55	5
86	OHX	2	2062	7/7	0.95	0.19	109,109,109,109	6
85	MG	2	1920	1/1	0.95	0.60	76,76,76,76	0
85	MG	3	201	1/1	0.95	0.17	80,80,80,80	0
86	OHX	1	4006	7/7	0.95	0.23	48,48,48,48	5
86	OHX	6	2142	7/7	0.95	0.22	95,95,95,95	7
85	MG	1	3561	1/1	0.95	0.77	22,22,22,22	0
86	OHX	1	4010	7/7	0.95	0.26	44,44,44,44	5
86	OHX	1	4011	7/7	0.95	0.16	62,62,62,62	3
86	OHX	7	222	7/7	0.95	0.41	38,38,38,38	4
86	OHX	1	4012	7/7	0.95	0.26	64,64,64,64	1
86	OHX	6	2148	7/7	0.95	0.28	54,54,54,54	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	8	217	7/7	0.95	0.24	78,78,78,78	5
86	OHX	2	2069	7/7	0.95	0.20	115,115,115,115	4
86	OHX	8	222	7/7	0.95	0.15	100,100,100,100	5
85	MG	5	3677	1/1	0.95	0.30	29,29,29,29	0
85	MG	5	3678	1/1	0.95	0.60	37,37,37,37	0
85	MG	5	3490	1/1	0.95	0.34	40,40,40,40	0
85	MG	6	1936	1/1	0.95	0.37	76,76,76,76	0
86	OHX	2	2081	7/7	0.95	0.21	120,120,120,120	6
86	OHX	2	2083	7/7	0.95	0.43	87,87,87,87	2
85	MG	5	3780	1/1	0.95	0.29	30,30,30,30	0
86	OHX	1	4023	7/7	0.95	0.42	73,73,73,73	3
86	OHX	l5	303	7/7	0.95	0.18	90,90,90,90	6
86	OHX	2	2088	7/7	0.95	0.18	91,91,91,91	6
86	OHX	m0	302	7/7	0.95	0.41	49,49,49,49	3
86	OHX	m0	303	7/7	0.95	0.23	96,96,96,96	5
86	OHX	2	2089	7/7	0.95	0.13	116,116,116,116	7
85	MG	5	3492	1/1	0.95	0.44	30,30,30,30	0
86	OHX	m8	201	7/7	0.95	0.31	47,47,47,47	3
85	MG	1	3494	1/1	0.95	0.44	42,42,42,42	0
85	MG	N8	202	1/1	0.95	0.95	47,47,47,47	0
86	OHX	2	2097	7/7	0.95	0.30	73,73,73,73	5
86	OHX	2	2098	7/7	0.95	0.24	111,111,111,111	6
85	MG	3	204	1/1	0.95	0.57	33,33,33,33	0
85	MG	5	3425	1/1	0.95	0.25	41,41,41,41	0
88	SPS	5	3403	23/23	0.95	0.34	35,38,52,54	23
86	OHX	2	2102	7/7	0.95	0.20	118,118,118,118	5
89	PRO	5	4173	7/8	0.95	0.16	35,35,45,45	0
86	OHX	2	2060	7/7	0.96	0.27	89,89,89,89	6
85	MG	5	3800	1/1	0.96	0.30	70,70,70,70	0
86	OHX	5	3938	7/7	0.96	0.20	50,50,50,50	3
86	OHX	1	3913	7/7	0.96	0.21	54,54,54,54	3
86	OHX	2	2063	7/7	0.96	0.10	153,153,153,153	7
86	OHX	5	3945	7/7	0.96	0.25	46,46,46,46	3
85	MG	1	3513	1/1	0.96	0.31	34,34,34,34	0
86	OHX	1	3916	7/7	0.96	0.41	54,54,54,54	4
85	MG	1	3560	1/1	0.96	0.71	46,46,46,46	0
86	OHX	5	3951	7/7	0.96	0.41	67,67,67,67	5
86	OHX	5	3952	7/7	0.96	0.12	100,100,100,100	2
86	OHX	5	3955	7/7	0.96	0.12	149,149,149,149	4
85	MG	5	3581	1/1	0.96	0.60	24,24,24,24	0
86	OHX	5	3962	7/7	0.96	0.25	47,47,47,47	4
85	MG	5	3584	1/1	0.96	0.45	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	5	3969	7/7	0.96	0.20	105,105,105,105	5
86	OHX	2	2070	7/7	0.96	0.10	108,108,108,108	5
85	MG	5	3805	1/1	0.96	0.25	37,37,37,37	0
86	OHX	5	3972	7/7	0.96	0.20	89,89,89,89	1
85	MG	5	3806	1/1	0.96	0.60	37,37,37,37	0
86	OHX	1	3930	7/7	0.96	0.35	118,118,118,118	2
86	OHX	5	3976	7/7	0.96	0.16	115,115,115,115	3
86	OHX	5	3977	7/7	0.96	0.23	58,58,58,58	4
86	OHX	2	2075	7/7	0.96	0.21	80,80,80,80	6
85	MG	5	3458	1/1	0.96	0.73	28,28,28,28	0
86	OHX	1	3940	7/7	0.96	0.20	77,77,77,77	5
86	OHX	5	3985	7/7	0.96	0.18	55,55,55,55	2
86	OHX	1	3942	7/7	0.96	0.12	94,94,94,94	4
85	MG	5	3725	1/1	0.96	0.27	51,51,51,51	0
86	OHX	1	3946	7/7	0.96	0.22	69,69,69,69	3
86	OHX	3	211	7/7	0.96	0.33	64,64,64,64	3
86	OHX	5	3994	7/7	0.96	0.25	42,42,42,42	4
86	OHX	1	3947	7/7	0.96	0.28	80,80,80,80	3
86	OHX	5	3997	7/7	0.96	0.16	62,62,62,62	5
86	OHX	5	4001	7/7	0.96	0.20	41,41,41,41	4
86	OHX	3	215	7/7	0.96	0.15	90,90,90,90	3
85	MG	5	3509	1/1	0.96	0.55	25,25,25,25	0
85	MG	5	3587	1/1	0.96	0.48	30,30,30,30	0
86	OHX	5	4009	7/7	0.96	0.37	41,41,41,41	3
86	OHX	5	4010	7/7	0.96	0.16	72,72,72,72	5
86	OHX	2	2084	7/7	0.96	0.18	95,95,95,95	5
86	OHX	2	2085	7/7	0.96	0.14	103,103,103,103	4
86	OHX	4	223	7/7	0.96	0.22	61,61,61,61	3
86	OHX	5	4015	7/7	0.96	0.25	36,36,36,36	4
86	OHX	4	225	7/7	0.96	0.25	44,44,44,44	3
85	MG	5	3812	1/1	0.96	0.40	32,32,32,32	0
86	OHX	5	4019	7/7	0.96	0.18	76,76,76,76	6
86	OHX	1	3961	7/7	0.96	0.31	45,45,45,45	5
86	OHX	2	2087	7/7	0.96	0.14	89,89,89,89	5
86	OHX	5	4028	7/7	0.96	0.25	72,72,72,72	4
85	MG	5	3588	1/1	0.96	0.66	29,29,29,29	0
85	MG	2	1980	1/1	0.96	0.12	104,104,104,104	0
85	MG	1	3597	1/1	0.96	0.37	47,47,47,47	0
85	MG	5	3591	1/1	0.96	0.39	42,42,42,42	0
86	OHX	L4	401	7/7	0.96	0.15	67,67,67,67	7
86	OHX	L5	301	7/7	0.96	0.17	88,88,88,88	6
86	OHX	5	4038	7/7	0.96	0.17	106,106,106,106	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	1	3968	7/7	0.96	0.26	72,72,72,72	3
86	OHX	5	4041	7/7	0.96	0.22	73,73,73,73	4
86	OHX	1	3970	7/7	0.96	0.15	68,68,68,68	1
86	OHX	5	4044	7/7	0.96	0.21	51,51,51,51	3
86	OHX	5	4045	7/7	0.96	0.43	48,48,48,48	2
85	MG	5	3513	1/1	0.96	0.36	37,37,37,37	0
86	OHX	1	3973	7/7	0.96	0.17	63,63,63,63	5
85	MG	6	1991	1/1	0.96	0.15	77,77,77,77	0
85	MG	7	203	1/1	0.96	0.51	54,54,54,54	0
86	OHX	O1	201	7/7	0.96	0.19	93,93,93,93	3
86	OHX	1	3976	7/7	0.96	0.24	41,41,41,41	4
86	OHX	1	3978	7/7	0.96	0.16	77,77,77,77	3
86	OHX	6	2029	7/7	0.96	0.23	68,68,68,68	2
85	MG	5	3735	1/1	0.96	0.23	37,37,37,37	0
85	MG	1	3431	1/1	0.96	0.34	47,47,47,47	0
86	OHX	6	2044	7/7	0.96	0.25	46,46,46,46	2
86	OHX	1	3981	7/7	0.96	0.37	53,53,53,53	3
86	OHX	6	2057	7/7	0.96	0.22	58,58,58,58	2
85	MG	5	3666	1/1	0.96	0.46	54,54,54,54	0
86	OHX	6	2064	7/7	0.96	0.21	98,98,98,98	5
86	OHX	1	3984	7/7	0.96	0.12	127,127,127,127	7
86	OHX	5	4066	7/7	0.96	0.27	38,38,38,38	4
85	MG	7	209	1/1	0.96	0.13	54,54,54,54	0
86	OHX	1	3987	7/7	0.96	0.20	73,73,73,73	5
86	OHX	5	4070	7/7	0.96	0.20	73,73,73,73	3
86	OHX	5	4071	7/7	0.96	0.25	45,45,45,45	3
86	OHX	5	4072	7/7	0.96	0.30	40,40,40,40	4
86	OHX	5	4073	7/7	0.96	0.32	44,44,44,44	4
86	OHX	5	4074	7/7	0.96	0.17	77,77,77,77	6
85	MG	2	1981	1/1	0.96	0.40	79,79,79,79	0
86	OHX	6	2073	7/7	0.96	0.30	69,69,69,69	5
86	OHX	1	3989	7/7	0.96	0.18	94,94,94,94	5
86	OHX	6	2078	7/7	0.96	0.22	60,60,60,60	5
85	MG	2	1984	1/1	0.96	0.37	67,67,67,67	0
86	OHX	6	2083	7/7	0.96	0.23	94,94,94,94	7
85	MG	5	3466	1/1	0.96	0.43	37,37,37,37	0
85	MG	7	213	1/1	0.96	0.18	49,49,49,49	0
86	OHX	5	4084	7/7	0.96	0.27	35,35,35,35	6
86	OHX	2	2108	7/7	0.96	0.24	79,79,79,79	5
85	MG	1	3655	1/1	0.96	0.82	44,44,44,44	0
86	OHX	6	2089	7/7	0.96	0.23	56,56,56,56	4
86	OHX	6	2090	7/7	0.96	0.17	91,91,91,91	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
85	MG	1	3716	1/1	0.96	0.32	65,65,65,65	0
86	OHX	6	2098	7/7	0.96	0.23	87,87,87,87	5
86	OHX	6	2099	7/7	0.96	0.19	81,81,81,81	5
86	OHX	5	4093	7/7	0.96	0.18	55,55,55,55	6
86	OHX	5	4094	7/7	0.96	0.29	36,36,36,36	3
85	MG	5	3743	1/1	0.96	0.46	32,32,32,32	0
86	OHX	1	4002	7/7	0.96	0.34	65,65,65,65	7
86	OHX	1	4003	7/7	0.96	0.18	63,63,63,63	3
85	MG	1	3684	1/1	0.96	0.36	52,52,52,52	0
86	OHX	6	2106	7/7	0.96	0.25	85,85,85,85	4
85	MG	1	3627	1/1	0.96	0.79	41,41,41,41	0
86	OHX	5	4103	7/7	0.96	0.19	40,40,40,40	5
86	OHX	6	2108	7/7	0.96	0.15	109,109,109,109	6
86	OHX	1	4008	7/7	0.96	0.27	47,47,47,47	5
85	MG	2	1931	1/1	0.96	0.43	65,65,65,65	0
85	MG	5	3605	1/1	0.96	0.45	33,33,33,33	0
86	OHX	6	2115	7/7	0.96	0.18	58,58,58,58	2
86	OHX	5	4109	7/7	0.96	0.18	53,53,53,53	5
86	OHX	6	2117	7/7	0.96	0.20	65,65,65,65	3
85	MG	5	3606	1/1	0.96	0.17	39,39,39,39	1
86	OHX	6	2119	7/7	0.96	0.24	60,60,60,60	3
86	OHX	5	4113	7/7	0.96	0.27	52,52,52,52	6
86	OHX	5	4114	7/7	0.96	0.18	55,55,55,55	4
85	MG	5	3528	1/1	0.96	0.74	21,21,21,21	0
85	MG	12	301	1/1	0.96	0.58	37,37,37,37	0
85	MG	1	3500	1/1	0.96	0.84	30,30,30,30	0
85	MG	5	3530	1/1	0.96	0.48	31,31,31,31	0
86	OHX	6	2124	7/7	0.96	0.11	103,103,103,103	6
85	MG	1	3522	1/1	0.96	0.52	31,31,31,31	0
85	MG	5	3533	1/1	0.96	0.73	28,28,28,28	0
85	MG	5	3475	1/1	0.96	0.62	51,51,51,51	0
86	OHX	1	4020	7/7	0.96	0.29	47,47,47,47	3
85	MG	1	3722	1/1	0.96	0.17	43,43,43,43	0
85	MG	M5	301	1/1	0.96	0.28	42,42,42,42	0
85	MG	1	3689	1/1	0.96	0.32	44,44,44,44	0
85	MG	1	3569	1/1	0.96	0.70	39,39,39,39	0
86	OHX	1	4025	7/7	0.96	0.22	56,56,56,56	3
85	MG	5	3761	1/1	0.96	0.19	38,38,38,38	0
85	MG	1	3541	1/1	0.96	0.64	28,28,28,28	0
85	MG	m7	202	1/1	0.96	0.57	33,33,33,33	0
85	MG	1	3401	1/1	0.96	0.34	43,43,43,43	0
86	OHX	2	2132	7/7	0.96	0.28	87,87,87,87	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
85	MG	5	3484	1/1	0.96	0.62	28,28,28,28	0
85	MG	2	1934	1/1	0.96	0.23	80,80,80,80	0
86	OHX	5	4138	7/7	0.96	0.28	44,44,44,44	5
86	OHX	6	2144	7/7	0.96	0.17	85,85,85,85	7
85	MG	M7	202	1/1	0.96	0.85	40,40,40,40	0
86	OHX	1	4035	7/7	0.96	0.15	65,65,65,65	4
85	MG	5	3550	1/1	0.96	0.84	44,44,44,44	0
85	MG	5	3624	1/1	0.96	0.33	31,31,31,31	0
85	MG	1	3609	1/1	0.96	0.50	44,44,44,44	0
86	OHX	5	4145	7/7	0.96	0.19	70,70,70,70	7
85	MG	6	1929	1/1	0.96	0.30	49,49,49,49	0
86	OHX	6	2151	7/7	0.96	0.23	65,65,65,65	4
85	MG	6	1930	1/1	0.96	0.72	45,45,45,45	0
85	MG	q1	101	1/1	0.96	0.28	50,50,50,50	0
85	MG	1	3439	1/1	0.96	0.35	60,60,60,60	0
85	MG	q3	502	1/1	0.96	0.53	48,48,48,48	0
85	MG	1	3414	1/1	0.96	0.72	43,43,43,43	0
85	MG	N3	201	1/1	0.96	0.63	36,36,36,36	0
86	OHX	2	1999	7/7	0.96	0.16	113,113,113,113	2
86	OHX	2	2004	7/7	0.96	0.12	135,135,135,135	5
86	OHX	2	2007	7/7	0.96	0.20	94,94,94,94	5
85	MG	5	3779	1/1	0.96	0.61	35,35,35,35	0
85	MG	2	1947	1/1	0.96	0.19	76,76,76,76	0
86	OHX	2	2020	7/7	0.96	0.13	117,117,117,117	3
86	OHX	1	4056	7/7	0.96	0.15	85,85,85,85	5
86	OHX	S1	301	7/7	0.96	0.17	121,121,121,121	2
86	OHX	2	2022	7/7	0.96	0.34	78,78,78,78	4
86	OHX	1	4059	7/7	0.96	0.29	72,72,72,72	4
85	MG	1	3734	1/1	0.96	0.58	35,35,35,35	1
86	OHX	6	2170	7/7	0.96	0.15	83,83,83,83	7
86	OHX	2	2027	7/7	0.96	0.26	75,75,75,75	4
86	OHX	5	4167	7/7	0.96	0.29	38,38,38,38	3
85	MG	5	3564	1/1	0.96	0.67	27,27,27,27	0
86	OHX	C5	201	7/7	0.96	0.10	122,122,122,122	7
85	MG	5	3565	1/1	0.96	0.34	32,32,32,32	0
86	OHX	SR	401	7/7	0.96	0.10	144,144,144,144	6
86	OHX	7	221	7/7	0.96	0.29	50,50,50,50	4
86	OHX	1	3821	7/7	0.96	0.28	66,66,66,66	5
85	MG	1	3640	1/1	0.96	0.44	62,62,62,62	0
85	MG	1	3547	1/1	0.96	0.91	32,32,32,32	0
86	OHX	1	3853	7/7	0.96	0.33	54,54,54,54	3
85	MG	2	1968	1/1	0.96	0.15	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	8	219	7/7	0.96	0.22	80,80,80,80	2
86	OHX	1	3859	7/7	0.96	0.28	53,53,53,53	2
86	OHX	1	3862	7/7	0.96	0.19	83,83,83,83	3
86	OHX	8	224	7/7	0.96	0.14	95,95,95,95	7
85	MG	5	3639	1/1	0.96	0.30	36,36,36,36	0
86	OHX	2	2046	7/7	0.96	0.20	83,83,83,83	7
85	MG	1	3553	1/1	0.96	0.55	24,24,24,24	0
85	MG	1	3554	1/1	0.96	0.37	37,37,37,37	0
85	MG	2	1944	1/1	0.96	0.13	102,102,102,102	0
85	MG	5	3576	1/1	0.96	0.47	28,28,28,28	0
85	MG	1	3530	1/1	0.96	0.61	41,41,41,41	0
85	MG	5	3717	1/1	0.96	0.67	16,16,16,16	0
86	OHX	1	3892	7/7	0.96	0.22	65,65,65,65	3
86	OHX	2	2055	7/7	0.96	0.16	63,63,63,63	5
86	OHX	1	3897	7/7	0.96	0.31	49,49,49,49	5
86	OHX	1	3898	7/7	0.96	0.21	89,89,89,89	5
86	OHX	m4	201	7/7	0.96	0.63	108,108,108,108	7
85	MG	5	3718	1/1	0.96	0.52	26,26,26,26	1
86	OHX	5	3871	7/7	0.96	0.24	72,72,72,72	2
86	OHX	5	3876	7/7	0.96	0.34	43,43,43,43	3
86	OHX	1	3900	7/7	0.96	0.24	57,57,57,57	3
86	OHX	5	3914	7/7	0.96	0.22	74,74,74,74	4
86	OHX	5	3916	7/7	0.96	0.32	77,77,77,77	3
85	MG	5	3797	1/1	0.96	0.36	39,39,39,39	0
86	OHX	1	3906	7/7	0.96	0.31	65,65,65,65	4
86	OHX	1	3907	7/7	0.96	0.24	71,71,71,71	3
85	MG	5	3578	1/1	0.96	0.44	35,35,35,35	0
86	OHX	5	3928	7/7	0.96	0.13	146,146,146,146	3
89	PRO	B	101	7/8	0.96	0.24	32,32,56,56	0
85	MG	1	3451	1/1	0.97	0.46	53,53,53,53	0
85	MG	1	3564	1/1	0.97	0.40	30,30,30,30	0
86	OHX	3	210	7/7	0.97	0.33	51,51,51,51	5
85	MG	1	3651	1/1	0.97	0.25	49,49,49,49	0
86	OHX	3	212	7/7	0.97	0.25	86,86,86,86	3
86	OHX	2	2100	7/7	0.97	0.14	83,83,83,83	4
86	OHX	3	214	7/7	0.97	0.23	83,83,83,83	4
86	OHX	1	3950	7/7	0.97	0.17	41,41,41,41	4
86	OHX	5	3964	7/7	0.97	0.10	107,107,107,107	2
86	OHX	5	3965	7/7	0.97	0.20	49,49,49,49	4
86	OHX	5	3966	7/7	0.97	0.23	50,50,50,50	4
86	OHX	5	3967	7/7	0.97	0.23	49,49,49,49	5
86	OHX	3	216	7/7	0.97	0.20	49,49,49,49	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	1	3951	7/7	0.97	0.15	159,159,159,159	7
85	MG	l3	402	1/1	0.97	0.45	39,39,39,39	1
86	OHX	1	3954	7/7	0.97	0.22	122,122,122,122	3
86	OHX	4	220	7/7	0.97	0.19	81,81,81,81	2
86	OHX	4	221	7/7	0.97	0.17	84,84,84,84	3
85	MG	5	3619	1/1	0.97	0.32	47,47,47,47	0
86	OHX	1	3956	7/7	0.97	0.16	57,57,57,57	5
86	OHX	4	224	7/7	0.97	0.17	86,86,86,86	3
86	OHX	1	3957	7/7	0.97	0.26	49,49,49,49	5
85	MG	5	3551	1/1	0.97	0.45	32,32,32,32	0
86	OHX	5	3984	7/7	0.97	0.27	56,56,56,56	4
86	OHX	4	227	7/7	0.97	0.14	103,103,103,103	6
86	OHX	5	3986	7/7	0.97	0.27	58,58,58,58	5
85	MG	2	1983	1/1	0.97	0.17	84,84,84,84	0
85	MG	5	3764	1/1	0.97	0.28	43,43,43,43	0
86	OHX	5	3990	7/7	0.97	0.23	44,44,44,44	4
86	OHX	1	3962	7/7	0.97	0.35	59,59,59,59	2
86	OHX	5	3992	7/7	0.97	0.17	80,80,80,80	5
85	MG	m0	301	1/1	0.97	0.44	33,33,33,33	0
85	MG	6	1934	1/1	0.97	0.35	43,43,43,43	0
86	OHX	L3	403	7/7	0.97	0.15	72,72,72,72	5
85	MG	1	3477	1/1	0.97	0.61	41,41,41,41	0
86	OHX	5	3999	7/7	0.97	0.29	38,38,38,38	5
85	MG	1	3511	1/1	0.97	0.51	36,36,36,36	0
86	OHX	5	4002	7/7	0.97	0.19	70,70,70,70	4
86	OHX	5	4003	7/7	0.97	0.18	54,54,54,54	3
85	MG	5	3556	1/1	0.97	0.38	33,33,33,33	0
85	MG	6	1977	1/1	0.97	0.12	57,57,57,57	0
85	MG	5	3497	1/1	0.97	0.45	36,36,36,36	0
85	MG	1	3454	1/1	0.97	0.90	31,31,31,31	0
86	OHX	1	3972	7/7	0.97	0.21	55,55,55,55	4
85	MG	1	3715	1/1	0.97	0.48	46,46,46,46	0
85	MG	1	3455	1/1	0.97	0.52	29,29,29,29	0
85	MG	5	3776	1/1	0.97	0.10	75,75,75,75	0
86	OHX	5	4014	7/7	0.97	0.18	48,48,48,48	3
85	MG	1	3514	1/1	0.97	0.43	35,35,35,35	0
86	OHX	O7	104	7/7	0.97	0.19	78,78,78,78	4
86	OHX	1	3977	7/7	0.97	0.15	72,72,72,72	7
86	OHX	6	2020	7/7	0.97	0.22	100,100,100,100	4
86	OHX	5	4023	7/7	0.97	0.23	39,39,39,39	2
86	OHX	6	2025	7/7	0.97	0.33	62,62,62,62	2
86	OHX	5	4025	7/7	0.97	0.29	50,50,50,50	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	5	3566	1/1	0.97	0.67	31,31,31,31	0
86	OHX	5	4027	7/7	0.97	0.18	49,49,49,49	3
85	MG	5	3704	1/1	0.97	0.69	2,2,2,2	0
86	OHX	5	4029	7/7	0.97	0.13	76,76,76,76	4
86	OHX	5	4030	7/7	0.97	0.15	70,70,70,70	5
85	MG	5	3567	1/1	0.97	0.39	37,37,37,37	0
85	MG	5	3568	1/1	0.97	0.63	22,22,22,22	0
86	OHX	6	2045	7/7	0.97	0.23	91,91,91,91	5
86	OHX	6	2050	7/7	0.97	0.18	87,87,87,87	5
86	OHX	5	4035	7/7	0.97	0.28	40,40,40,40	3
86	OHX	1	3982	7/7	0.97	0.20	47,47,47,47	5
86	OHX	6	2053	7/7	0.97	0.17	92,92,92,92	5
85	MG	1	3550	1/1	0.97	0.67	33,33,33,33	0
86	OHX	5	4039	7/7	0.97	0.19	72,72,72,72	4
85	MG	5	3504	1/1	0.97	0.53	28,28,28,28	0
86	OHX	6	2061	7/7	0.97	0.24	86,86,86,86	4
86	OHX	5	4042	7/7	0.97	0.32	43,43,43,43	3
86	OHX	6	2062	7/7	0.97	0.14	117,117,117,117	4
86	OHX	1	3985	7/7	0.97	0.38	38,38,38,38	2
85	MG	1	3631	1/1	0.97	0.23	42,42,42,42	0
85	MG	5	3455	1/1	0.97	0.55	31,31,31,31	0
86	OHX	6	2069	7/7	0.97	0.17	73,73,73,73	4
85	MG	1	3531	1/1	0.97	0.58	40,40,40,40	0
86	OHX	2	1996	7/7	0.97	0.24	101,101,101,101	5
86	OHX	2	1998	7/7	0.97	0.20	116,116,116,116	2
86	OHX	6	2074	7/7	0.97	0.15	70,70,70,70	2
86	OHX	1	3991	7/7	0.97	0.26	57,57,57,57	3
86	OHX	1	3992	7/7	0.97	0.28	52,52,52,52	3
85	MG	L2	302	1/1	0.97	0.29	41,41,41,41	0
86	OHX	5	4056	7/7	0.97	0.22	40,40,40,40	6
86	OHX	6	2081	7/7	0.97	0.18	74,74,74,74	6
86	OHX	6	2082	7/7	0.97	0.15	99,99,99,99	5
86	OHX	1	3994	7/7	0.97	0.23	54,54,54,54	5
86	OHX	2	2002	7/7	0.97	0.24	101,101,101,101	3
85	MG	1	3552	1/1	0.97	0.74	37,37,37,37	0
86	OHX	2	2005	7/7	0.97	0.17	99,99,99,99	3
86	OHX	1	3998	7/7	0.97	0.28	107,107,107,107	4
86	OHX	5	4064	7/7	0.97	0.33	52,52,52,52	3
85	MG	5	3459	1/1	0.97	0.47	34,34,34,34	0
85	MG	1	3606	1/1	0.97	0.21	43,43,43,43	0
86	OHX	6	2091	7/7	0.97	0.25	83,83,83,83	3
86	OHX	6	2092	7/7	0.97	0.25	69,69,69,69	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	6	2093	7/7	0.97	0.21	45,45,45,45	2
86	OHX	1	4001	7/7	0.97	0.15	61,61,61,61	4
86	OHX	6	2096	7/7	0.97	0.14	94,94,94,94	5
86	OHX	6	2097	7/7	0.97	0.54	49,49,49,49	1
85	MG	5	3716	1/1	0.97	0.33	34,34,34,34	0
86	OHX	2	2136	7/7	0.97	0.20	74,74,74,74	6
86	OHX	5	4077	7/7	0.97	0.36	32,32,32,32	3
86	OHX	2	2017	7/7	0.97	0.36	74,74,74,74	4
86	OHX	1	4005	7/7	0.97	0.34	40,40,40,40	4
86	OHX	2	2019	7/7	0.97	0.23	81,81,81,81	3
85	MG	5	3512	1/1	0.97	0.58	28,28,28,28	0
86	OHX	2	2021	7/7	0.97	0.18	99,99,99,99	5
85	MG	1	3427	1/1	0.97	0.87	42,42,42,42	0
86	OHX	2	2023	7/7	0.97	0.11	106,106,106,106	4
86	OHX	2	2024	7/7	0.97	0.23	100,100,100,100	6
86	OHX	2	2025	7/7	0.97	0.20	79,79,79,79	5
86	OHX	6	2112	7/7	0.97	0.27	66,66,66,66	4
86	OHX	6	2113	7/7	0.97	0.26	67,67,67,67	3
85	MG	1	3724	1/1	0.97	0.34	55,55,55,55	0
86	OHX	1	4015	7/7	0.97	0.27	47,47,47,47	2
85	MG	5	3796	1/1	0.97	0.44	42,42,42,42	0
86	OHX	2	2029	7/7	0.97	0.13	98,98,98,98	5
86	OHX	2	2030	7/7	0.97	0.20	98,98,98,98	5
86	OHX	2	2032	7/7	0.97	0.20	102,102,102,102	6
86	OHX	5	4096	7/7	0.97	0.12	119,119,119,119	7
85	MG	5	3582	1/1	0.97	0.56	31,31,31,31	0
85	MG	2	1928	1/1	0.97	0.34	71,71,71,71	0
85	MG	5	3799	1/1	0.97	0.42	42,42,42,42	0
86	OHX	2	2037	7/7	0.97	0.25	73,73,73,73	4
86	OHX	2	2041	7/7	0.97	0.09	141,141,141,141	6
85	MG	1	3555	1/1	0.97	0.61	26,26,26,26	0
85	MG	5	3653	1/1	0.97	0.27	47,47,47,47	0
86	OHX	6	2128	7/7	0.97	0.36	53,53,53,53	4
85	MG	5	3654	1/1	0.97	0.56	31,31,31,31	0
85	MG	6	1916	1/1	0.97	0.61	66,66,66,66	0
86	OHX	C8	201	7/7	0.97	0.19	111,111,111,111	4
85	MG	1	3580	1/1	0.97	0.69	35,35,35,35	0
85	MG	5	3657	1/1	0.97	0.53	33,33,33,33	0
86	OHX	1	3787	7/7	0.97	0.21	72,72,72,72	3
86	OHX	1	3807	7/7	0.97	0.33	73,73,73,73	2
86	OHX	1	4034	7/7	0.97	0.28	75,75,75,75	3
86	OHX	1	3820	7/7	0.97	0.37	47,47,47,47	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	6	2139	7/7	0.97	0.21	86,86,86,86	3
85	MG	1	3581	1/1	0.97	0.81	29,29,29,29	0
85	MG	1	3583	1/1	0.97	0.64	31,31,31,31	0
86	OHX	5	4118	7/7	0.97	0.27	49,49,49,49	4
86	OHX	1	3829	7/7	0.97	0.23	59,59,59,59	2
86	OHX	5	4120	7/7	0.97	0.21	64,64,64,64	5
86	OHX	1	3832	7/7	0.97	0.20	80,80,80,80	3
86	OHX	1	4040	7/7	0.97	0.27	52,52,52,52	4
86	OHX	1	3834	7/7	0.97	0.26	62,62,62,62	3
86	OHX	1	3841	7/7	0.97	0.21	70,70,70,70	3
86	OHX	1	3845	7/7	0.97	0.15	123,123,123,123	3
86	OHX	1	3848	7/7	0.97	0.21	76,76,76,76	3
86	OHX	2	2052	7/7	0.97	0.15	90,90,90,90	5
85	MG	5	3660	1/1	0.97	0.58	46,46,46,46	0
86	OHX	1	3855	7/7	0.97	0.29	87,87,87,87	3
86	OHX	1	4049	7/7	0.97	0.15	61,61,61,61	5
85	MG	1	3447	1/1	0.97	0.48	51,51,51,51	0
86	OHX	1	4051	7/7	0.97	0.18	58,58,58,58	3
86	OHX	1	3858	7/7	0.97	0.14	98,98,98,98	4
85	MG	5	3732	1/1	0.97	0.32	30,30,30,30	0
85	MG	1	3585	1/1	0.97	0.81	20,20,20,20	0
86	OHX	1	3866	7/7	0.97	0.19	69,69,69,69	3
85	MG	6	1922	1/1	0.97	0.19	55,55,55,55	0
86	OHX	6	2160	7/7	0.97	0.19	69,69,69,69	5
85	MG	5	3525	1/1	0.97	0.64	31,31,31,31	0
85	MG	5	3526	1/1	0.97	0.46	29,29,29,29	0
86	OHX	1	3874	7/7	0.97	0.26	50,50,50,50	3
86	OHX	1	3875	7/7	0.97	0.52	53,53,53,53	3
86	OHX	1	3877	7/7	0.97	0.12	95,95,95,95	2
86	OHX	1	3879	7/7	0.97	0.36	44,44,44,44	2
86	OHX	1	4064	7/7	0.97	0.38	39,39,39,39	3
85	MG	5	3527	1/1	0.97	0.42	32,32,32,32	0
86	OHX	1	3884	7/7	0.97	0.20	74,74,74,74	4
85	MG	1	3441	1/1	0.97	0.41	52,52,52,52	0
85	MG	1	3587	1/1	0.97	0.61	35,35,35,35	0
85	MG	5	3427	1/1	0.97	0.51	40,40,40,40	0
86	OHX	2	2066	7/7	0.97	0.12	160,160,160,160	7
86	OHX	2	2067	7/7	0.97	0.17	132,132,132,132	4
85	MG	1	3472	1/1	0.97	0.39	42,42,42,42	0
86	OHX	1	3895	7/7	0.97	0.16	57,57,57,57	4
85	MG	7	205	1/1	0.97	0.53	26,26,26,26	0
85	MG	1	3502	1/1	0.97	0.90	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
85	MG	5	3534	1/1	0.97	0.54	25,25,25,25	0
86	OHX	2	2073	7/7	0.97	0.20	63,63,63,63	6
86	OHX	1	3902	7/7	0.97	0.25	53,53,53,53	3
85	MG	6	2003	1/1	0.97	0.12	96,96,96,96	0
86	OHX	1	3905	7/7	0.97	0.23	57,57,57,57	1
85	MG	5	3536	1/1	0.97	0.81	29,29,29,29	0
85	MG	5	3537	1/1	0.97	0.62	26,26,26,26	0
85	MG	5	3538	1/1	0.97	0.65	32,32,32,32	0
86	OHX	2	2078	7/7	0.97	0.14	115,115,115,115	7
86	OHX	1	3911	7/7	0.97	0.22	61,61,61,61	3
86	OHX	2	2080	7/7	0.97	0.13	91,91,91,91	4
85	MG	5	3539	1/1	0.97	0.54	33,33,33,33	0
86	OHX	2	2082	7/7	0.97	0.15	90,90,90,90	5
86	OHX	5	4170	7/7	0.97	0.33	71,71,71,71	3
85	MG	5	3749	1/1	0.97	0.56	30,30,30,30	0
85	MG	2	1982	1/1	0.97	0.76	46,46,46,46	0
86	OHX	7	216	7/7	0.97	0.34	62,62,62,62	3
86	OHX	7	220	7/7	0.97	0.36	73,73,73,73	1
85	MG	1	3738	1/1	0.97	0.29	41,41,41,41	0
86	OHX	5	3866	7/7	0.97	0.25	60,60,60,60	3
85	MG	6	1966	1/1	0.97	0.43	56,56,56,56	0
85	MG	5	3753	1/1	0.97	0.62	30,30,30,30	0
86	OHX	5	3872	7/7	0.97	0.27	82,82,82,82	3
86	OHX	5	3874	7/7	0.97	0.23	62,62,62,62	3
85	MG	8	206	1/1	0.97	0.30	47,47,47,47	0
86	OHX	8	221	7/7	0.97	0.25	62,62,62,62	3
86	OHX	5	3882	7/7	0.97	0.19	89,89,89,89	3
85	MG	1	3412	1/1	0.97	0.21	68,68,68,68	0
86	OHX	5	3890	7/7	0.97	0.20	69,69,69,69	3
86	OHX	8	225	7/7	0.97	0.24	40,40,40,40	3
86	OHX	5	3891	7/7	0.97	0.26	66,66,66,66	4
86	OHX	8	227	7/7	0.97	0.20	59,59,59,59	3
86	OHX	5	3895	7/7	0.97	0.22	63,63,63,63	3
86	OHX	5	3900	7/7	0.97	0.26	52,52,52,52	3
86	OHX	5	3902	7/7	0.97	0.22	72,72,72,72	3
86	OHX	5	3909	7/7	0.97	0.19	77,77,77,77	4
86	OHX	5	3910	7/7	0.97	0.27	57,57,57,57	3
86	OHX	14	402	7/7	0.97	0.20	69,69,69,69	5
86	OHX	14	403	7/7	0.97	0.13	51,51,51,51	7
86	OHX	2	2091	7/7	0.97	0.23	89,89,89,89	5
86	OHX	5	3915	7/7	0.97	0.27	39,39,39,39	4
86	OHX	1	3929	7/7	0.97	0.19	53,53,53,53	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
85	MG	6	1968	1/1	0.97	0.25	48,48,48,48	0
86	OHX	1	3932	7/7	0.97	0.24	57,57,57,57	5
86	OHX	1	3933	7/7	0.97	0.14	91,91,91,91	4
86	OHX	5	3924	7/7	0.97	0.29	43,43,43,43	5
86	OHX	1	3934	7/7	0.97	0.19	54,54,54,54	3
86	OHX	1	3935	7/7	0.97	0.15	71,71,71,71	2
86	OHX	1	3936	7/7	0.97	0.34	54,54,54,54	3
86	OHX	n3	202	7/7	0.97	0.20	60,60,60,60	3
85	MG	5	3437	1/1	0.97	0.29	34,34,34,34	0
86	OHX	1	3938	7/7	0.97	0.23	53,53,53,53	3
86	OHX	5	3939	7/7	0.97	0.17	92,92,92,92	2
87	ZN	E1	501	1/1	0.97	0.05	145,145,145,145	0
86	OHX	5	3940	7/7	0.97	0.25	62,62,62,62	2
86	OHX	2	2094	7/7	0.97	0.19	87,87,87,87	5
87	ZN	q2	202	1/1	0.97	0.07	71,71,71,71	0
88	SPS	1	4113	23/23	0.97	0.21	39,42,55,58	0
86	OHX	2	2095	7/7	0.97	0.28	75,75,75,75	5
86	OHX	5	3943	7/7	0.97	0.27	44,44,44,44	2
86	OHX	1	3941	7/7	0.97	0.16	51,51,51,51	3
85	MG	6	1969	1/1	0.97	0.42	55,55,55,55	0
89	PRO	C	101	7/8	0.97	0.24	29,29,51,51	0
86	OHX	6	2076	7/7	0.98	0.18	52,52,52,52	5
86	OHX	2	2042	7/7	0.98	0.18	68,68,68,68	5
85	MG	5	3473	1/1	0.98	0.51	30,30,30,30	0
86	OHX	6	2079	7/7	0.98	0.22	51,51,51,51	3
85	MG	1	3548	1/1	0.98	0.65	30,30,30,30	0
85	MG	1	3484	1/1	0.98	0.12	52,52,52,52	0
85	MG	5	3476	1/1	0.98	0.29	42,42,42,42	0
85	MG	5	3477	1/1	0.98	0.41	27,27,27,27	0
86	OHX	1	3903	7/7	0.98	0.20	53,53,53,53	3
86	OHX	2	2048	7/7	0.98	0.12	141,141,141,141	5
85	MG	5	3644	1/1	0.98	0.52	34,34,34,34	0
86	OHX	5	3996	7/7	0.98	0.24	52,52,52,52	3
85	MG	5	3443	1/1	0.98	0.59	44,44,44,44	0
86	OHX	5	3998	7/7	0.98	0.18	43,43,43,43	5
86	OHX	1	4043	7/7	0.98	0.29	39,39,39,39	2
85	MG	1	3579	1/1	0.98	0.57	35,35,35,35	0
85	MG	5	3601	1/1	0.98	0.72	26,26,26,26	0
86	OHX	1	3909	7/7	0.98	0.33	73,73,73,73	4
86	OHX	5	4004	7/7	0.98	0.15	55,55,55,55	2
85	MG	2	1935	1/1	0.98	0.29	70,70,70,70	0
86	OHX	6	2094	7/7	0.98	0.15	109,109,109,109	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	5	4007	7/7	0.98	0.23	40,40,40,40	3
85	MG	1	3479	1/1	0.98	0.31	45,45,45,45	0
85	MG	5	3519	1/1	0.98	0.64	35,35,35,35	0
86	OHX	2	2056	7/7	0.98	0.25	99,99,99,99	4
85	MG	5	3559	1/1	0.98	0.60	22,22,22,22	0
85	MG	5	3652	1/1	0.98	0.43	35,35,35,35	0
86	OHX	6	2101	7/7	0.98	0.18	62,62,62,62	2
85	MG	5	3447	1/1	0.98	0.38	31,31,31,31	0
86	OHX	1	3917	7/7	0.98	0.21	54,54,54,54	4
86	OHX	1	3918	7/7	0.98	0.15	91,91,91,91	5
85	MG	5	3562	1/1	0.98	0.31	27,27,27,27	0
86	OHX	5	4018	7/7	0.98	0.25	48,48,48,48	4
86	OHX	2	2061	7/7	0.98	0.20	88,88,88,88	5
86	OHX	5	4020	7/7	0.98	0.39	47,47,47,47	1
86	OHX	5	4021	7/7	0.98	0.21	36,36,36,36	2
86	OHX	5	4022	7/7	0.98	0.24	37,37,37,37	1
86	OHX	1	3921	7/7	0.98	0.14	82,82,82,82	3
86	OHX	1	3922	7/7	0.98	0.21	82,82,82,82	3
86	OHX	6	2109	7/7	0.98	0.12	99,99,99,99	6
86	OHX	1	4060	7/7	0.98	0.27	65,65,65,65	4
86	OHX	1	3923	7/7	0.98	0.23	40,40,40,40	3
85	MG	5	3703	1/1	0.98	0.09	58,58,58,58	0
85	MG	1	3582	1/1	0.98	0.76	27,27,27,27	0
86	OHX	1	3926	7/7	0.98	0.18	57,57,57,57	4
85	MG	1	3488	1/1	0.98	0.55	37,37,37,37	0
86	OHX	6	2116	7/7	0.98	0.23	61,61,61,61	2
85	MG	1	3705	1/1	0.98	0.45	33,33,33,33	0
85	MG	1	3706	1/1	0.98	0.23	38,38,38,38	0
85	MG	4	210	1/1	0.98	0.51	63,63,63,63	0
86	OHX	1	3931	7/7	0.98	0.21	43,43,43,43	4
85	MG	1	3507	1/1	0.98	0.74	30,30,30,30	0
85	MG	5	3811	1/1	0.98	0.16	30,30,30,30	0
85	MG	1	3438	1/1	0.98	0.34	33,33,33,33	0
86	OHX	2	2071	7/7	0.98	0.20	72,72,72,72	6
85	MG	5	3570	1/1	0.98	0.43	29,29,29,29	0
85	MG	B	102	1/1	0.98	0.53	38,38,38,38	0
85	MG	1	3625	1/1	0.98	0.38	41,41,41,41	0
86	OHX	2	1993	7/7	0.98	0.22	96,96,96,96	2
86	OHX	6	2129	7/7	0.98	0.30	58,58,58,58	5
85	MG	1	3556	1/1	0.98	0.40	29,29,29,29	0
85	MG	1	3435	1/1	0.98	0.88	25,25,25,25	0
85	MG	5	3531	1/1	0.98	0.23	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	1	3943	7/7	0.98	0.12	97,97,97,97	6
86	OHX	1	3944	7/7	0.98	0.23	48,48,48,48	4
86	OHX	2	2079	7/7	0.98	0.31	82,82,82,82	3
86	OHX	5	4052	7/7	0.98	0.17	67,67,67,67	5
86	OHX	2	2000	7/7	0.98	0.20	105,105,105,105	3
85	MG	1	3668	1/1	0.98	0.25	38,38,38,38	1
86	OHX	1	3948	7/7	0.98	0.21	37,37,37,37	2
85	MG	6	1901	1/1	0.98	0.56	52,52,52,52	0
85	MG	6	1956	1/1	0.98	0.39	44,44,44,44	0
86	OHX	2	2006	7/7	0.98	0.14	93,93,93,93	3
85	MG	5	3768	1/1	0.98	0.38	34,34,34,34	0
86	OHX	1	3953	7/7	0.98	0.26	58,58,58,58	2
86	OHX	1	3791	7/7	0.98	0.30	41,41,41,41	2
86	OHX	1	3792	7/7	0.98	0.23	74,74,74,74	3
86	OHX	1	3793	7/7	0.98	0.26	68,68,68,68	4
86	OHX	1	3795	7/7	0.98	0.16	85,85,85,85	2
86	OHX	1	3796	7/7	0.98	0.28	57,57,57,57	4
86	OHX	1	3959	7/7	0.98	0.24	112,112,112,112	3
86	OHX	2	2008	7/7	0.98	0.22	89,89,89,89	5
86	OHX	1	3808	7/7	0.98	0.24	74,74,74,74	3
86	OHX	1	3809	7/7	0.98	0.18	80,80,80,80	2
86	OHX	1	3810	7/7	0.98	0.29	62,62,62,62	3
86	OHX	1	3811	7/7	0.98	0.29	79,79,79,79	2
86	OHX	1	3812	7/7	0.98	0.16	88,88,88,88	3
86	OHX	1	3813	7/7	0.98	0.24	52,52,52,52	2
86	OHX	1	3814	7/7	0.98	0.21	76,76,76,76	3
86	OHX	1	3815	7/7	0.98	0.25	85,85,85,85	3
86	OHX	1	3969	7/7	0.98	0.18	65,65,65,65	4
86	OHX	1	3816	7/7	0.98	0.28	62,62,62,62	5
86	OHX	1	3817	7/7	0.98	0.19	109,109,109,109	5
86	OHX	1	3819	7/7	0.98	0.28	81,81,81,81	3
86	OHX	2	2009	7/7	0.98	0.19	89,89,89,89	4
85	MG	7	206	1/1	0.98	0.42	34,34,34,34	0
85	MG	1	3571	1/1	0.98	0.31	53,53,53,53	0
86	OHX	1	3826	7/7	0.98	0.19	84,84,84,84	4
86	OHX	1	3828	7/7	0.98	0.28	63,63,63,63	2
86	OHX	2	2090	7/7	0.98	0.27	94,94,94,94	6
86	OHX	5	4088	7/7	0.98	0.17	39,39,39,39	4
86	OHX	1	3830	7/7	0.98	0.20	99,99,99,99	3
86	OHX	1	3831	7/7	0.98	0.22	48,48,48,48	3
86	OHX	2	2012	7/7	0.98	0.24	87,87,87,87	3
86	OHX	1	3833	7/7	0.98	0.25	71,71,71,71	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	2	2013	7/7	0.98	0.16	94,94,94,94	4
86	OHX	4	217	7/7	0.98	0.25	61,61,61,61	3
86	OHX	4	218	7/7	0.98	0.23	55,55,55,55	2
86	OHX	4	219	7/7	0.98	0.25	60,60,60,60	4
86	OHX	1	3835	7/7	0.98	0.27	62,62,62,62	1
86	OHX	1	3836	7/7	0.98	0.17	98,98,98,98	3
86	OHX	1	3840	7/7	0.98	0.19	85,85,85,85	3
86	OHX	2	2014	7/7	0.98	0.11	130,130,130,130	7
86	OHX	5	4101	7/7	0.98	0.17	69,69,69,69	3
86	OHX	1	3842	7/7	0.98	0.21	80,80,80,80	3
86	OHX	1	3843	7/7	0.98	0.27	55,55,55,55	2
86	OHX	1	3844	7/7	0.98	0.13	98,98,98,98	5
86	OHX	s1	301	7/7	0.98	0.19	95,95,95,95	2
86	OHX	2	2016	7/7	0.98	0.15	96,96,96,96	4
86	OHX	1	3846	7/7	0.98	0.22	119,119,119,119	3
86	OHX	4	229	7/7	0.98	0.18	60,60,60,60	3
85	MG	5	3770	1/1	0.98	0.27	47,47,47,47	0
86	OHX	2	2018	7/7	0.98	0.16	74,74,74,74	5
86	OHX	1	3850	7/7	0.98	0.27	47,47,47,47	3
86	OHX	1	3852	7/7	0.98	0.28	70,70,70,70	3
86	OHX	L3	402	7/7	0.98	0.20	59,59,59,59	4
85	MG	L3	401	1/1	0.98	0.30	41,41,41,41	0
85	MG	d2	201	1/1	0.98	0.30	59,59,59,59	0
85	MG	1	3589	1/1	0.98	0.29	40,40,40,40	0
86	OHX	5	3843	7/7	0.98	0.20	64,64,64,64	1
86	OHX	5	3846	7/7	0.98	0.26	37,37,37,37	3
86	OHX	5	3850	7/7	0.98	0.26	51,51,51,51	2
86	OHX	5	3855	7/7	0.98	0.22	71,71,71,71	3
86	OHX	5	3856	7/7	0.98	0.25	65,65,65,65	3
86	OHX	5	3858	7/7	0.98	0.22	72,72,72,72	3
86	OHX	5	3860	7/7	0.98	0.21	88,88,88,88	3
86	OHX	5	3862	7/7	0.98	0.27	47,47,47,47	2
86	OHX	5	3863	7/7	0.98	0.21	85,85,85,85	3
86	OHX	5	3865	7/7	0.98	0.17	86,86,86,86	1
86	OHX	1	3857	7/7	0.98	0.27	54,54,54,54	4
86	OHX	5	3868	7/7	0.98	0.25	74,74,74,74	2
85	MG	5	3501	1/1	0.98	0.16	42,42,42,42	0
85	MG	1	3521	1/1	0.98	0.68	43,43,43,43	0
86	OHX	M5	304	7/7	0.98	0.22	72,72,72,72	4
86	OHX	5	3873	7/7	0.98	0.17	58,58,58,58	4
86	OHX	M6	203	7/7	0.98	0.36	43,43,43,43	2
86	OHX	5	3875	7/7	0.98	0.25	49,49,49,49	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
85	MG	5	3541	1/1	0.98	0.50	41,41,41,41	0
86	OHX	5	3879	7/7	0.98	0.26	59,59,59,59	3
86	OHX	5	3881	7/7	0.98	0.19	96,96,96,96	2
86	OHX	1	3864	7/7	0.98	0.32	104,104,104,104	3
86	OHX	5	3884	7/7	0.98	0.17	63,63,63,63	3
86	OHX	5	3885	7/7	0.98	0.17	78,78,78,78	3
86	OHX	5	3888	7/7	0.98	0.22	43,43,43,43	3
85	MG	1	3740	1/1	0.98	0.30	62,62,62,62	0
85	MG	1	3499	1/1	0.98	0.54	37,37,37,37	0
86	OHX	1	4007	7/7	0.98	0.18	43,43,43,43	4
86	OHX	5	3892	7/7	0.98	0.30	63,63,63,63	3
86	OHX	5	3894	7/7	0.98	0.27	50,50,50,50	2
86	OHX	O3	201	7/7	0.98	0.23	52,52,52,52	4
86	OHX	5	3896	7/7	0.98	0.24	42,42,42,42	4
86	OHX	5	3899	7/7	0.98	0.22	49,49,49,49	3
86	OHX	1	3869	7/7	0.98	0.20	92,92,92,92	3
85	MG	5	3679	1/1	0.98	0.42	31,31,31,31	1
86	OHX	5	3904	7/7	0.98	0.28	49,49,49,49	2
86	OHX	5	3905	7/7	0.98	0.26	51,51,51,51	4
86	OHX	5	3907	7/7	0.98	0.19	63,63,63,63	3
85	MG	5	3404	1/1	0.98	0.34	33,33,33,33	0
86	OHX	6	2016	7/7	0.98	0.22	83,83,83,83	4
86	OHX	5	3911	7/7	0.98	0.23	44,44,44,44	4
86	OHX	5	3913	7/7	0.98	0.22	77,77,77,77	3
86	OHX	1	3872	7/7	0.98	0.24	44,44,44,44	4
86	OHX	1	3873	7/7	0.98	0.20	53,53,53,53	5
85	MG	5	3633	1/1	0.98	0.43	34,34,34,34	0
86	OHX	6	2031	7/7	0.98	0.19	80,80,80,80	4
86	OHX	5	3918	7/7	0.98	0.18	36,36,36,36	2
86	OHX	6	2032	7/7	0.98	0.20	117,117,117,117	2
86	OHX	5	3920	7/7	0.98	0.21	36,36,36,36	2
86	OHX	5	3921	7/7	0.98	0.21	57,57,57,57	2
86	OHX	6	2035	7/7	0.98	0.24	82,82,82,82	3
86	OHX	6	2036	7/7	0.98	0.21	58,58,58,58	3
86	OHX	6	2037	7/7	0.98	0.23	101,101,101,101	3
86	OHX	5	3927	7/7	0.98	0.18	64,64,64,64	5
86	OHX	2	2031	7/7	0.98	0.17	81,81,81,81	4
86	OHX	5	3929	7/7	0.98	0.28	41,41,41,41	4
86	OHX	7	215	7/7	0.98	0.19	60,60,60,60	5
86	OHX	5	3930	7/7	0.98	0.17	55,55,55,55	2
86	OHX	7	218	7/7	0.98	0.28	67,67,67,67	3
86	OHX	6	2041	7/7	0.98	0.25	56,56,56,56	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	5	3933	7/7	0.98	0.15	94,94,94,94	4
86	OHX	5	3934	7/7	0.98	0.22	38,38,38,38	2
86	OHX	1	3876	7/7	0.98	0.31	41,41,41,41	2
86	OHX	5	3937	7/7	0.98	0.25	53,53,53,53	2
86	OHX	8	214	7/7	0.98	0.21	62,62,62,62	4
86	OHX	8	215	7/7	0.98	0.28	60,60,60,60	3
86	OHX	8	216	7/7	0.98	0.21	85,85,85,85	3
85	MG	1	3593	1/1	0.98	0.24	50,50,50,50	0
86	OHX	1	3878	7/7	0.98	0.20	58,58,58,58	3
86	OHX	6	2046	7/7	0.98	0.34	60,60,60,60	2
86	OHX	8	220	7/7	0.98	0.23	44,44,44,44	3
86	OHX	6	2047	7/7	0.98	0.21	67,67,67,67	5
86	OHX	6	2048	7/7	0.98	0.18	65,65,65,65	4
86	OHX	6	2049	7/7	0.98	0.19	97,97,97,97	3
86	OHX	5	3944	7/7	0.98	0.22	42,42,42,42	3
86	OHX	2	2033	7/7	0.98	0.23	78,78,78,78	3
86	OHX	5	3946	7/7	0.98	0.18	109,109,109,109	4
86	OHX	5	3947	7/7	0.98	0.27	45,45,45,45	3
86	OHX	1	3880	7/7	0.98	0.22	47,47,47,47	5
86	OHX	6	2052	7/7	0.98	0.18	67,67,67,67	3
86	OHX	1	3881	7/7	0.98	0.17	86,86,86,86	4
86	OHX	6	2054	7/7	0.98	0.12	87,87,87,87	3
86	OHX	6	2056	7/7	0.98	0.20	73,73,73,73	3
85	MG	1	3466	1/1	0.98	0.38	37,37,37,37	0
86	OHX	5	3956	7/7	0.98	0.21	40,40,40,40	2
86	OHX	6	2058	7/7	0.98	0.26	72,72,72,72	2
86	OHX	5	3958	7/7	0.98	0.25	42,42,42,42	2
86	OHX	5	3960	7/7	0.98	0.22	44,44,44,44	3
86	OHX	5	3961	7/7	0.98	0.15	74,74,74,74	1
86	OHX	6	2059	7/7	0.98	0.19	61,61,61,61	3
85	MG	1	3575	1/1	0.98	0.46	32,32,32,32	0
86	OHX	1	3885	7/7	0.98	0.26	53,53,53,53	3
86	OHX	m5	305	7/7	0.98	0.27	54,54,54,54	3
85	MG	2	1918	1/1	0.98	0.36	68,68,68,68	0
86	OHX	6	2063	7/7	0.98	0.08	147,147,147,147	6
85	MG	5	3786	1/1	0.98	0.26	35,35,35,35	0
86	OHX	1	3888	7/7	0.98	0.26	71,71,71,71	3
86	OHX	o3	202	7/7	0.98	0.17	52,52,52,52	3
86	OHX	1	3889	7/7	0.98	0.23	48,48,48,48	2
86	OHX	6	2067	7/7	0.98	0.10	154,154,154,154	3
86	OHX	q2	203	7/7	0.98	0.24	47,47,47,47	2
87	ZN	D6	500	1/1	0.98	0.08	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	6	2068	7/7	0.98	0.13	103,103,103,103	4
86	OHX	2	2038	7/7	0.98	0.09	119,119,119,119	6
87	ZN	Q0	500	1/1	0.98	0.11	54,54,54,54	0
87	ZN	Q2	501	1/1	0.98	0.06	77,77,77,77	0
87	ZN	d6	101	1/1	0.98	0.05	84,84,84,84	0
86	OHX	6	2070	7/7	0.98	0.22	87,87,87,87	3
86	OHX	2	2039	7/7	0.98	0.18	103,103,103,103	7
86	OHX	2	2040	7/7	0.98	0.15	89,89,89,89	3
85	MG	5	3593	1/1	0.98	0.56	22,22,22,22	0
86	OHX	5	3979	7/7	0.98	0.32	67,67,67,67	3
86	OHX	5	3980	7/7	0.98	0.21	55,55,55,55	3
86	OHX	5	3981	7/7	0.98	0.23	69,69,69,69	3
86	OHX	1	3894	7/7	0.98	0.08	132,132,132,132	7
86	OHX	6	2075	7/7	0.98	0.26	76,76,76,76	3
86	OHX	5	4068	7/7	0.99	0.14	49,49,49,49	3
86	OHX	6	2015	7/7	0.99	0.14	78,78,78,78	3
85	MG	5	3583	1/1	0.99	0.60	23,23,23,23	0
86	OHX	5	3906	7/7	0.99	0.19	60,60,60,60	4
86	OHX	6	2017	7/7	0.99	0.23	59,59,59,59	2
86	OHX	5	3908	7/7	0.99	0.20	45,45,45,45	4
86	OHX	6	2018	7/7	0.99	0.19	90,90,90,90	2
86	OHX	6	2019	7/7	0.99	0.23	79,79,79,79	2
85	MG	6	1958	1/1	0.99	0.58	44,44,44,44	0
86	OHX	5	3912	7/7	0.99	0.17	107,107,107,107	2
86	OHX	6	2021	7/7	0.99	0.23	69,69,69,69	3
86	OHX	6	2022	7/7	0.99	0.20	67,67,67,67	2
86	OHX	6	2023	7/7	0.99	0.18	80,80,80,80	3
86	OHX	6	2024	7/7	0.99	0.15	99,99,99,99	3
85	MG	1	3402	1/1	0.99	0.70	36,36,36,36	0
86	OHX	6	2026	7/7	0.99	0.18	66,66,66,66	1
86	OHX	6	2027	7/7	0.99	0.19	76,76,76,76	2
86	OHX	6	2028	7/7	0.99	0.19	63,63,63,63	2
85	MG	1	3733	1/1	0.99	0.28	40,40,40,40	0
86	OHX	6	2030	7/7	0.99	0.19	57,57,57,57	2
86	OHX	5	3923	7/7	0.99	0.24	41,41,41,41	1
86	OHX	2	2015	7/7	0.99	0.13	90,90,90,90	4
86	OHX	5	3925	7/7	0.99	0.19	56,56,56,56	3
85	MG	1	3456	1/1	0.99	0.41	32,32,32,32	0
86	OHX	6	2033	7/7	0.99	0.23	56,56,56,56	5
86	OHX	6	2034	7/7	0.99	0.18	66,66,66,66	5
86	OHX	1	3763	7/7	0.99	0.23	58,58,58,58	2
86	OHX	1	3765	7/7	0.99	0.18	65,65,65,65	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
86	OHX	5	3931	7/7	0.99	0.27	54,54,54,54	4
86	OHX	1	3837	7/7	0.99	0.21	60,60,60,60	2
86	OHX	6	2038	7/7	0.99	0.16	61,61,61,61	5
86	OHX	1	3838	7/7	0.99	0.28	52,52,52,52	3
86	OHX	5	3935	7/7	0.99	0.21	45,45,45,45	1
86	OHX	6	2040	7/7	0.99	0.15	123,123,123,123	5
86	OHX	1	3839	7/7	0.99	0.18	64,64,64,64	3
86	OHX	6	2042	7/7	0.99	0.28	62,62,62,62	3
86	OHX	1	3766	7/7	0.99	0.22	61,61,61,61	2
86	OHX	1	3767	7/7	0.99	0.19	77,77,77,77	2
86	OHX	1	3769	7/7	0.99	0.20	64,64,64,64	2
86	OHX	1	3770	7/7	0.99	0.18	61,61,61,61	2
86	OHX	1	3771	7/7	0.99	0.21	59,59,59,59	2
86	OHX	1	3772	7/7	0.99	0.20	67,67,67,67	2
86	OHX	1	3773	7/7	0.99	0.25	49,49,49,49	2
86	OHX	1	3847	7/7	0.99	0.19	56,56,56,56	3
86	OHX	1	3774	7/7	0.99	0.16	71,71,71,71	3
86	OHX	1	3775	7/7	0.99	0.18	66,66,66,66	2
86	OHX	1	3776	7/7	0.99	0.21	55,55,55,55	1
86	OHX	1	3851	7/7	0.99	0.20	46,46,46,46	3
86	OHX	6	2055	7/7	0.99	0.13	113,113,113,113	4
86	OHX	1	3777	7/7	0.99	0.22	61,61,61,61	3
86	OHX	5	3953	7/7	0.99	0.19	45,45,45,45	3
86	OHX	5	3954	7/7	0.99	0.18	49,49,49,49	2
86	OHX	1	3778	7/7	0.99	0.26	64,64,64,64	1
86	OHX	1	3854	7/7	0.99	0.17	43,43,43,43	4
86	OHX	1	3780	7/7	0.99	0.24	75,75,75,75	1
86	OHX	1	3781	7/7	0.99	0.18	76,76,76,76	2
86	OHX	5	3959	7/7	0.99	0.15	61,61,61,61	4
86	OHX	1	3782	7/7	0.99	0.24	71,71,71,71	4
86	OHX	1	3783	7/7	0.99	0.17	83,83,83,83	2
86	OHX	1	3784	7/7	0.99	0.25	73,73,73,73	2
86	OHX	1	3860	7/7	0.99	0.21	38,38,38,38	2
86	OHX	1	3861	7/7	0.99	0.20	60,60,60,60	3
86	OHX	1	3785	7/7	0.99	0.21	59,59,59,59	2
86	OHX	1	3863	7/7	0.99	0.20	42,42,42,42	3
86	OHX	1	3786	7/7	0.99	0.20	94,94,94,94	3
86	OHX	5	3968	7/7	0.99	0.17	47,47,47,47	4
86	OHX	1	3865	7/7	0.99	0.13	75,75,75,75	2
86	OHX	3	209	7/7	0.99	0.20	76,76,76,76	4
85	MG	c8	201	1/1	0.99	0.11	91,91,91,91	0
86	OHX	1	3788	7/7	0.99	0.20	58,58,58,58	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	5	3973	7/7	0.99	0.25	39,39,39,39	4
86	OHX	1	3868	7/7	0.99	0.17	53,53,53,53	4
86	OHX	1	3789	7/7	0.99	0.19	74,74,74,74	2
86	OHX	1	3790	7/7	0.99	0.22	48,48,48,48	3
85	MG	5	3496	1/1	0.99	0.40	35,35,35,35	0
86	OHX	2	1991	7/7	0.99	0.17	88,88,88,88	0
86	OHX	2	1992	7/7	0.99	0.20	98,98,98,98	1
86	OHX	1	3794	7/7	0.99	0.29	69,69,69,69	2
85	MG	1	3540	1/1	0.99	0.44	41,41,41,41	0
86	OHX	4	216	7/7	0.99	0.20	59,59,59,59	3
86	OHX	2	1994	7/7	0.99	0.14	97,97,97,97	2
86	OHX	1	3798	7/7	0.99	0.21	69,69,69,69	1
86	OHX	1	3799	7/7	0.99	0.22	78,78,78,78	3
86	OHX	6	2085	7/7	0.99	0.32	76,76,76,76	2
86	OHX	5	3987	7/7	0.99	0.26	41,41,41,41	3
86	OHX	1	3800	7/7	0.99	0.27	44,44,44,44	3
86	OHX	1	3801	7/7	0.99	0.18	71,71,71,71	3
86	OHX	5	3817	7/7	0.99	0.19	53,53,53,53	4
86	OHX	5	3818	7/7	0.99	0.17	57,57,57,57	0
86	OHX	5	3819	7/7	0.99	0.25	51,51,51,51	3
86	OHX	5	3821	7/7	0.99	0.18	64,64,64,64	2
86	OHX	5	3823	7/7	0.99	0.23	53,53,53,53	2
86	OHX	5	3825	7/7	0.99	0.18	58,58,58,58	1
86	OHX	5	3827	7/7	0.99	0.21	80,80,80,80	1
86	OHX	5	3828	7/7	0.99	0.19	50,50,50,50	3
86	OHX	5	3829	7/7	0.99	0.21	44,44,44,44	5
86	OHX	5	3830	7/7	0.99	0.17	67,67,67,67	0
86	OHX	5	4000	7/7	0.99	0.16	45,45,45,45	2
86	OHX	5	3832	7/7	0.99	0.23	56,56,56,56	2
86	OHX	5	3834	7/7	0.99	0.26	51,51,51,51	1
86	OHX	5	3835	7/7	0.99	0.19	54,54,54,54	1
86	OHX	5	3836	7/7	0.99	0.19	65,65,65,65	3
86	OHX	5	3840	7/7	0.99	0.23	65,65,65,65	2
86	OHX	5	3842	7/7	0.99	0.20	38,38,38,38	3
86	OHX	1	3802	7/7	0.99	0.18	60,60,60,60	2
86	OHX	7	214	7/7	0.99	0.28	70,70,70,70	1
86	OHX	5	3845	7/7	0.99	0.25	48,48,48,48	2
86	OHX	1	3882	7/7	0.99	0.22	64,64,64,64	3
86	OHX	7	217	7/7	0.99	0.20	40,40,40,40	1
86	OHX	5	3847	7/7	0.99	0.20	48,48,48,48	1
86	OHX	7	219	7/7	0.99	0.22	67,67,67,67	2
86	OHX	5	3848	7/7	0.99	0.21	54,54,54,54	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	5	3849	7/7	0.99	0.17	100,100,100,100	3
86	OHX	1	3803	7/7	0.99	0.18	73,73,73,73	3
86	OHX	5	3851	7/7	0.99	0.17	55,55,55,55	4
86	OHX	5	3852	7/7	0.99	0.27	55,55,55,55	2
86	OHX	8	212	7/7	0.99	0.23	57,57,57,57	3
86	OHX	8	213	7/7	0.99	0.17	57,57,57,57	2
86	OHX	5	3853	7/7	0.99	0.18	56,56,56,56	3
86	OHX	5	3854	7/7	0.99	0.14	78,78,78,78	2
86	OHX	1	3804	7/7	0.99	0.20	62,62,62,62	1
86	OHX	1	3805	7/7	0.99	0.16	93,93,93,93	4
86	OHX	5	3857	7/7	0.99	0.19	54,54,54,54	1
86	OHX	1	3806	7/7	0.99	0.24	52,52,52,52	2
86	OHX	5	3859	7/7	0.99	0.23	55,55,55,55	1
86	OHX	2	1995	7/7	0.99	0.28	76,76,76,76	2
86	OHX	5	3861	7/7	0.99	0.20	46,46,46,46	3
85	MG	5	3413	1/1	0.99	0.42	36,36,36,36	0
86	OHX	2	1997	7/7	0.99	0.11	107,107,107,107	5
86	OHX	5	3864	7/7	0.99	0.16	88,88,88,88	3
85	MG	1	3549	1/1	0.99	0.20	59,59,59,59	0
85	MG	1	3453	1/1	0.99	0.79	39,39,39,39	0
86	OHX	5	3867	7/7	0.99	0.10	126,126,126,126	2
86	OHX	2	2028	7/7	0.99	0.14	108,108,108,108	5
86	OHX	6	2100	7/7	0.99	0.13	71,71,71,71	3
86	OHX	5	3870	7/7	0.99	0.19	76,76,76,76	5
86	OHX	13	403	7/7	0.99	0.14	50,50,50,50	3
85	MG	1	3506	1/1	0.99	0.61	32,32,32,32	0
86	OHX	2	2001	7/7	0.99	0.13	120,120,120,120	2
85	MG	6	2005	1/1	0.99	0.32	88,88,88,88	0
86	OHX	1	3896	7/7	0.99	0.29	49,49,49,49	2
86	OHX	2	2003	7/7	0.99	0.23	76,76,76,76	5
85	MG	5	3434	1/1	0.99	0.51	33,33,33,33	0
86	OHX	5	3877	7/7	0.99	0.17	62,62,62,62	3
86	OHX	5	3878	7/7	0.99	0.20	73,73,73,73	3
86	OHX	1	3818	7/7	0.99	0.23	62,62,62,62	2
86	OHX	5	3880	7/7	0.99	0.18	47,47,47,47	3
86	OHX	M5	303	7/7	0.99	0.20	61,61,61,61	2
86	OHX	m5	306	7/7	0.99	0.16	76,76,76,76	3
86	OHX	m6	201	7/7	0.99	0.28	36,36,36,36	3
85	MG	1	3486	1/1	0.99	0.61	39,39,39,39	0
86	OHX	5	3883	7/7	0.99	0.23	53,53,53,53	1
86	OHX	1	3901	7/7	0.99	0.19	62,62,62,62	4
85	MG	N8	201	1/1	0.99	0.38	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
86	OHX	n9	101	7/7	0.99	0.19	62,62,62,62	2
86	OHX	5	3886	7/7	0.99	0.18	79,79,79,79	3
86	OHX	5	3887	7/7	0.99	0.21	44,44,44,44	2
85	MG	5	3560	1/1	0.99	0.69	27,27,27,27	0
86	OHX	o7	503	7/7	0.99	0.28	62,62,62,62	1
86	OHX	1	3822	7/7	0.99	0.21	50,50,50,50	4
86	OHX	1	3823	7/7	0.99	0.10	111,111,111,111	4
86	OHX	1	3824	7/7	0.99	0.16	68,68,68,68	3
87	ZN	D9	101	1/1	0.99	0.07	89,89,89,89	0
85	MG	1	3425	1/1	0.99	0.90	27,27,27,27	0
87	ZN	O7	102	1/1	0.99	0.15	47,47,47,47	0
86	OHX	5	3893	7/7	0.99	0.23	59,59,59,59	2
85	MG	1	3590	1/1	0.99	0.32	43,43,43,43	0
87	ZN	Q3	501	1/1	0.99	0.10	78,78,78,78	0
86	OHX	1	3827	7/7	0.99	0.24	45,45,45,45	4
85	MG	1	3509	1/1	0.99	0.63	33,33,33,33	0
87	ZN	d9	101	1/1	0.99	0.10	91,91,91,91	0
86	OHX	5	3897	7/7	0.99	0.22	46,46,46,46	5
87	ZN	o7	501	1/1	0.99	0.17	45,45,45,45	0
87	ZN	q0	500	1/1	0.99	0.13	42,42,42,42	0
86	OHX	5	3898	7/7	0.99	0.16	58,58,58,58	4
86	OHX	Q2	503	7/7	0.99	0.20	46,46,46,46	2
86	OHX	6	2013	7/7	0.99	0.18	87,87,87,87	2
86	OHX	5	3901	7/7	0.99	0.26	43,43,43,43	3
86	OHX	5	4065	7/7	0.99	0.21	39,39,39,39	3
86	OHX	6	2014	7/7	0.99	0.25	76,76,76,76	3
86	OHX	5	3903	7/7	0.99	0.31	91,91,91,91	2
86	OHX	1	3761	7/7	1.00	0.19	57,57,57,57	1
86	OHX	1	3779	7/7	1.00	0.18	49,49,49,49	4
86	OHX	6	2012	7/7	1.00	0.20	70,70,70,70	3
86	OHX	N9	101	7/7	1.00	0.22	64,64,64,64	1
86	OHX	5	3831	7/7	1.00	0.20	61,61,61,61	1
86	OHX	1	3764	7/7	1.00	0.17	65,65,65,65	2
86	OHX	5	3833	7/7	1.00	0.20	59,59,59,59	2
86	OHX	m5	304	7/7	1.00	0.19	61,61,61,61	2
86	OHX	5	3820	7/7	1.00	0.19	52,52,52,52	3
86	OHX	1	3768	7/7	1.00	0.22	52,52,52,52	2
86	OHX	5	3822	7/7	1.00	0.20	61,61,61,61	2
86	OHX	5	3837	7/7	1.00	0.17	71,71,71,71	0
86	OHX	5	3838	7/7	1.00	0.16	58,58,58,58	2
86	OHX	5	3839	7/7	1.00	0.16	64,64,64,64	2
86	OHX	1	3797	7/7	1.00	0.17	54,54,54,54	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
87	ZN	q3	501	1/1	1.00	0.16	62,62,62,62	0
86	OHX	5	3841	7/7	1.00	0.19	51,51,51,51	1
86	OHX	8	211	7/7	1.00	0.18	64,64,64,64	1
86	OHX	5	3824	7/7	1.00	0.19	62,62,62,62	2
86	OHX	1	3762	7/7	1.00	0.19	55,55,55,55	3
86	OHX	5	3844	7/7	1.00	0.22	62,62,62,62	2
86	OHX	5	3826	7/7	1.00	0.20	46,46,46,46	1

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.