



Full wwPDB EM Validation Report ⓘ

May 18, 2024 – 10:24 pm BST

PDB ID : 6RXZ
EMDB ID : EMD-10056
Title : Cryo-EM structure of the 90S pre-ribosome (Kre33-Noc4) from *Chaetomium thermophilum*, state b
Authors : Cheng, J.; Kellner, N.; Griesel, S.; Berninghausen, O.; Beckmann, R.; Hurt, E.
Deposited on : 2019-06-10
Resolution : 4.40 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

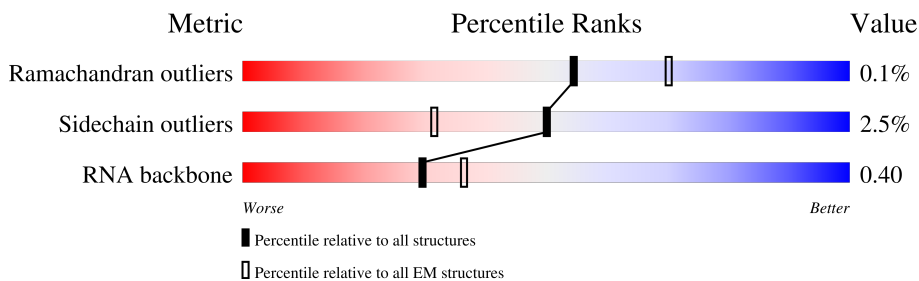
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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.



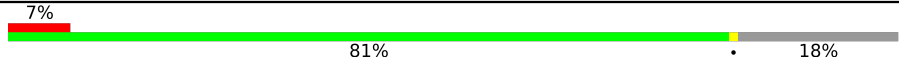
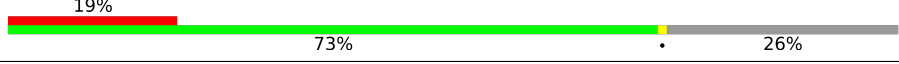
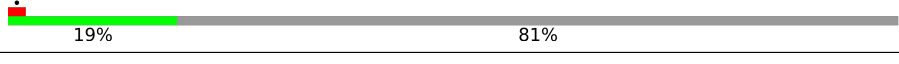
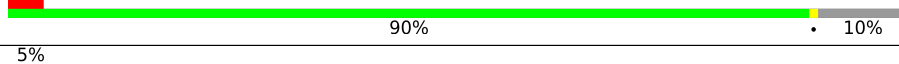

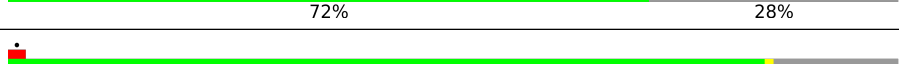
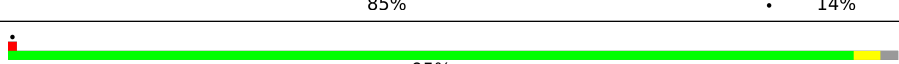
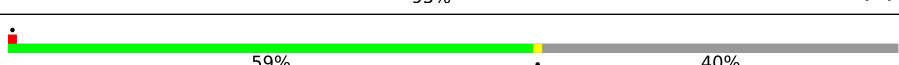
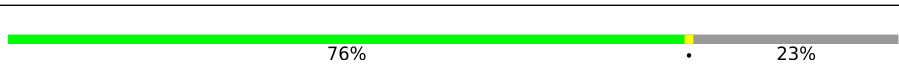


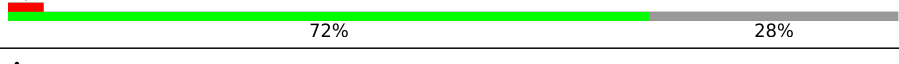
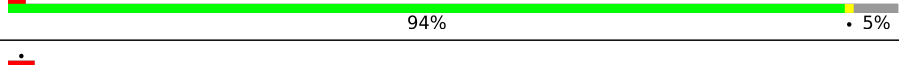
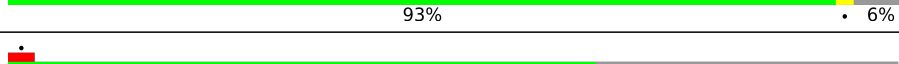
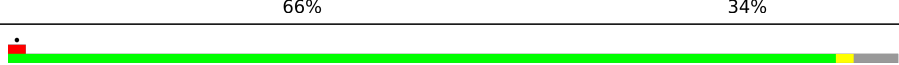
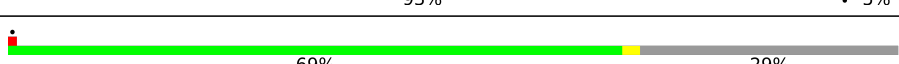
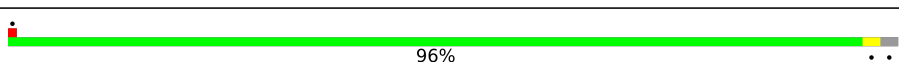
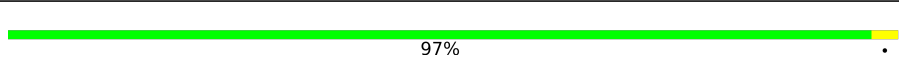

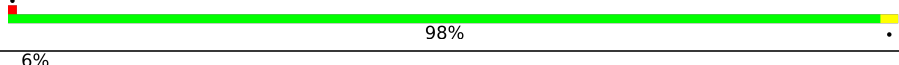
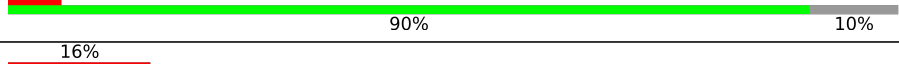




Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	UA	904	
2	UB	907	
3	UC	648	
4	UD	884	
5	UF	414	
6	UG	558	
7	UJ	1802	
8	UK	270	

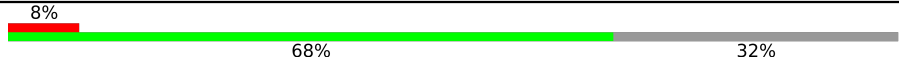
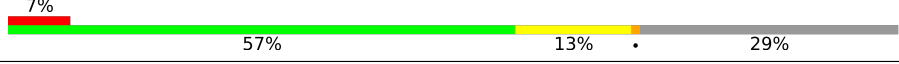
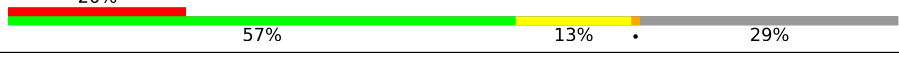

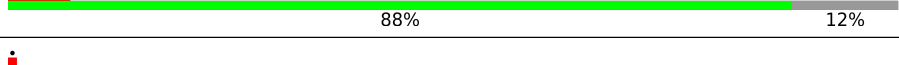
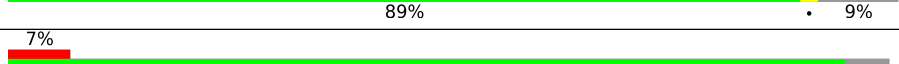
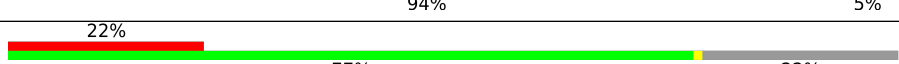
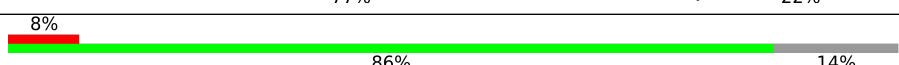
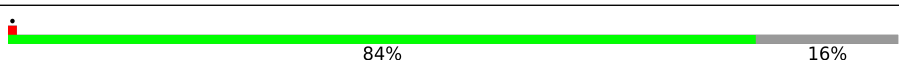


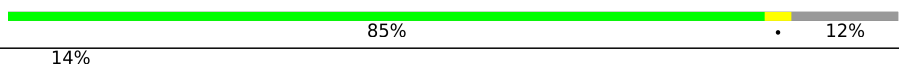
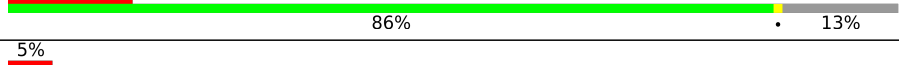
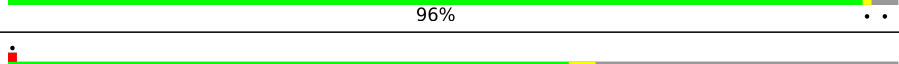
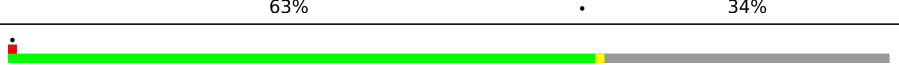

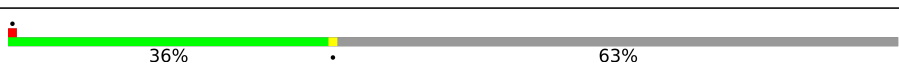
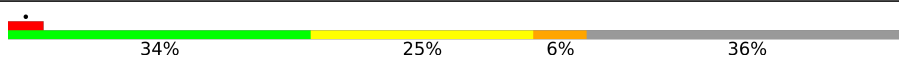
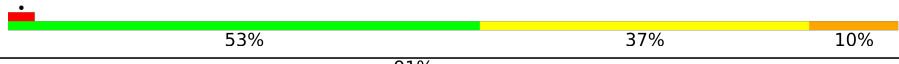
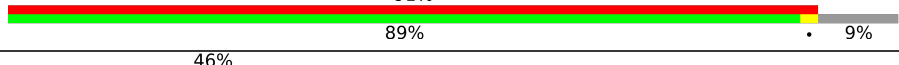





Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	UL	962	
10	UM	912	
11	UN	938	
12	UO	557	
13	UQ	960	
14	UR	618	
15	UU	1049	
16	UX	193	
17	UZ	391	
18	CA	313	
18	CB	313	
19	CC	523	
20	CD	582	
21	CE	127	
21	CF	127	
22	CG	630	
23	CH	411	
24	CI	1163	
25	CJ	183	
26	CK	297	
27	CL	785	
28	CM	446	
29	CN	252	
29	CO	252	
30	CP	322	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
31	CQ	259	
32	CR	1073	
32	CS	1073	
33	CT	203	
34	Cb	264	
35	Cc	212	
36	Cd	239	
37	Ce	203	
38	Cf	202	
39	Cg	190	
40	Ch	151	
41	Ci	150	
42	Cj	143	
43	Ck	161	
44	Cm	130	
45	Cn	145	
46	Co	136	
47	Cp	68	
48	CU	311	
49	C1	2323	
50	C2	230	
51	UV	1171	
52	CV	322	
53	CW	668	
54	UT	2612	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
55	UH	930	
56	UE	410	
56	UI	410	
57	US	549	
58	CI	156	
59	CX	480	
60	CY	381	
61	CZ	609	
62	UP	364	
63	Cz	1796	

2 Entry composition [i](#)

There are 64 unique types of molecules in this entry. The entry contains 218474 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 protein called Periodic tryptophan protein 2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	UA	839	6366	4101	1136	1105	24	0	0

- Molecule 2 is a protein called Utp2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	UB	512	4079	2576	781	711	11	0	0

- Molecule 3 is a protein called Utp3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	UC	74	588	371	120	97	0	0

- Molecule 4 is a protein called Utp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	UD	772	6071	3851	1093	1103	24	0	0

- Molecule 5 is a protein called Utp6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	UF	331	2591	1674	504	399	14	0	0

- Molecule 6 is a protein called Utp7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	UG	479	3717	2369	700	636	12	0	0

- Molecule 7 is a protein called UTP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	UJ	1090	8416	5408	1452	1525	31	0	0

- Molecule 8 is a protein called U3 small nucleolar RNA-associated protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	UK	217	1687	1062	351	269	5	0	0

- Molecule 9 is a protein called Utp12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	UL	785	6175	3940	1088	1130	17	0	0

- Molecule 10 is a protein called Utp13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	UM	679	5273	3351	924	986	12	0	0

- Molecule 11 is a protein called Utp14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	UN	177	1401	892	263	239	7	0	0

- Molecule 12 is a protein called Utp15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	UO	504	3819	2422	699	684	14	0	0

- Molecule 13 is a protein called Utp17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	UQ	789	6008	3831	1037	1119	21	0	0

- Molecule 14 is a protein called Utp18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	UR	447	3491	2209	656	616	10	0	0

- Molecule 15 is a protein called Putative U3 snoRNP protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	UU	902	6734	4336	1236	1136	26	0	0

- Molecule 16 is a protein called Utp24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	UX	190	1470	932	282	246	10	0	0

- Molecule 17 is a protein called Utp30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	UZ	235	1815	1184	330	298	3	0	0

- Molecule 18 is a protein called Nop1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	CA	242	1778	1149	327	293	9	0	0
18	CB	237	1816	1154	318	335	9	0	0

- Molecule 19 is a protein called Putative nucleolar protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	CC	387	2866	1836	527	492	11	0	0

- Molecule 20 is a protein called Nop58.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	CD	420	3150	2023	560	557	10	0	0

- Molecule 21 is a protein called Snu13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	CE	121	Total	C	N	O	S	0	0
			879	557	165	154	3		
21	CF	120	Total	C	N	O	S	0	0
			864	550	161	150	3		

- Molecule 22 is a protein called Rrp9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	CG	416	Total	C	N	O	S	0	0
			3245	2065	587	580	13		

- Molecule 23 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	CH	389	Total	C	N	O	S	0	0
			2888	1827	526	525	10		

- Molecule 24 is a protein called Bms1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	CI	822	Total	C	N	O	S	0	0
			6486	4169	1213	1077	27		

- Molecule 25 is a protein called Imp3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	CJ	179	Total	C	N	O	S	0	0
			1434	918	283	226	7		

- Molecule 26 is a protein called Putative U3 small nucleolar ribonucleoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	CK	297	Total	C	N	O	S	0	0
			2329	1476	445	400	8		

- Molecule 27 is a protein called Putative U3 small nucleolar ribonucleoprotein protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	CL	231	Total	C	N	O	S	0	0
			1786	1114	339	327	6		

- Molecule 28 is a protein called Sof1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	CM	445	3501	2195	672	619	15	0	0

- Molecule 29 is a protein called Emg1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	CN	226	1762	1119	306	327	10	0	0
29	CO	215	1683	1067	293	313	10	0	0

- Molecule 30 is a protein called KRR1 small subunit processome component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	CP	187	1504	961	269	265	9	0	0

- Molecule 31 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	CQ	175	1361	862	250	242	7	0	0

- Molecule 32 is a protein called Kre33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	CR	760	5989	3851	1024	1087	27	0	0
32	CS	760	5989	3851	1024	1087	27	0	0

- Molecule 33 is a protein called Fcf2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	CT	131	1035	656	197	178	4	0	0

- Molecule 34 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Cb	232	1851	1179	340	325	7	0	0

- Molecule 35 is a protein called 40S ribosomal protein s5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	Cc	192	1464	926	278	253	7	0	0

- Molecule 36 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	Cd	226	1819	1138	363	313	5	0	0

- Molecule 37 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
37	Ce	159	1279	810	237	232	0	0

- Molecule 38 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	Cf	174	1398	872	283	242	1	0	0

- Molecule 39 is a protein called 40S ribosomal protein s9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	Cg	159	1242	801	255	184	2	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
40	Ch	49	406	265	79	62	0	0

- Molecule 41 is a protein called 40S ribosomal protein S14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	Ci	115	791	492	154	141	4	0	0

- Molecule 42 is a protein called 40S ribosomal protein S16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	Cj	126	943	613	177	151	2	0	0

- Molecule 43 is a protein called 40S ribosomal protein S11-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	Ck	140	1163	750	224	184	5	0	0

- Molecule 44 is a protein called 40S ribosomal protein S22-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	Cm	126	985	632	184	164	5	0	0

- Molecule 45 is a protein called 40S ribosomal protein s23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	Cn	96	702	456	134	110	2	0	0

- Molecule 46 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	Co	92	741	474	139	126	2	0	0

- Molecule 47 is a protein called 40S ribosomal protein S28-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
47	Cp	61	455	284	97	74	0	0

- Molecule 48 is a protein called Faf1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	CU	114	882	544	178	154	6	0	0

- Molecule 49 is a RNA chain called 35S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
49	C1	1487	31732	14158	5691	10396	1487	0	0

- Molecule 50 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
50	C2	230	4891	2182	856	1623	230	0	0

- Molecule 51 is a protein called U3 small nucleolar RNA-associated protein 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	UV	1061	8424	5399	1480	1523	22	0	0

- Molecule 52 is a protein called Rrp7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	CV	148	1145	729	198	216	2	0	0

- Molecule 53 is a protein called Ribosome biogenesis protein ENP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	CW	382	2924	1857	530	524	13	0	0

- Molecule 54 is a protein called Utp20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	UT	2028	16000	10303	2813	2816	68	0	0

- Molecule 55 is a protein called Utp8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	UH	359	2809	1773	496	527	13	0	0

- Molecule 56 is a protein called Utp5.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	UE	125	Total	C	N	O	S	0	0
			972	608	183	175	6		
56	UI	125	Total	C	N	O	S	0	0
			972	608	183	175	6		

- Molecule 57 is a protein called Noc4.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	US	451	Total	C	N	O	S	0	0
			3672	2389	608	660	15		

- Molecule 58 is a protein called Rps18.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Cl	80	Total	C	N	O	S	0	0
			633	400	115	117	1		

- Molecule 59 is a protein called Enp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	CX	267	Total	C	N	O	S	0	0
			2122	1380	374	358	10		

- Molecule 60 is a protein called U3 small nucleolar ribonucleoprotein protein lcp5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	CY	122	Total	C	N	O	S	0	0
			975	590	194	188	3		

- Molecule 61 is a protein called Bfr2.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	CZ	42	Total	C	N	O	S	0	0
			354	223	68	62	1		

- Molecule 62 is a protein called Utp16.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	UP	54	Total	C	N	O	0	0
			422	264	88	70		

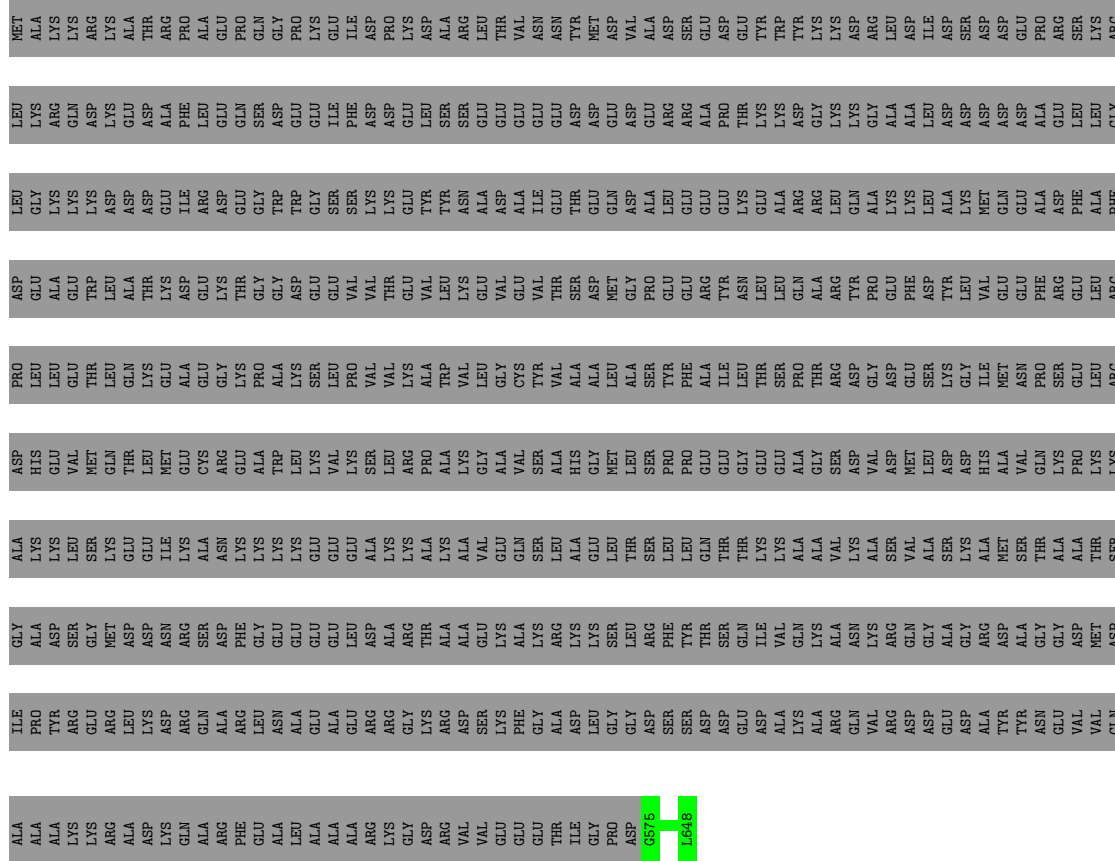
- Molecule 63 is a protein called Rrp5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	Cz	275	2259	1435	401	420	3	0	0

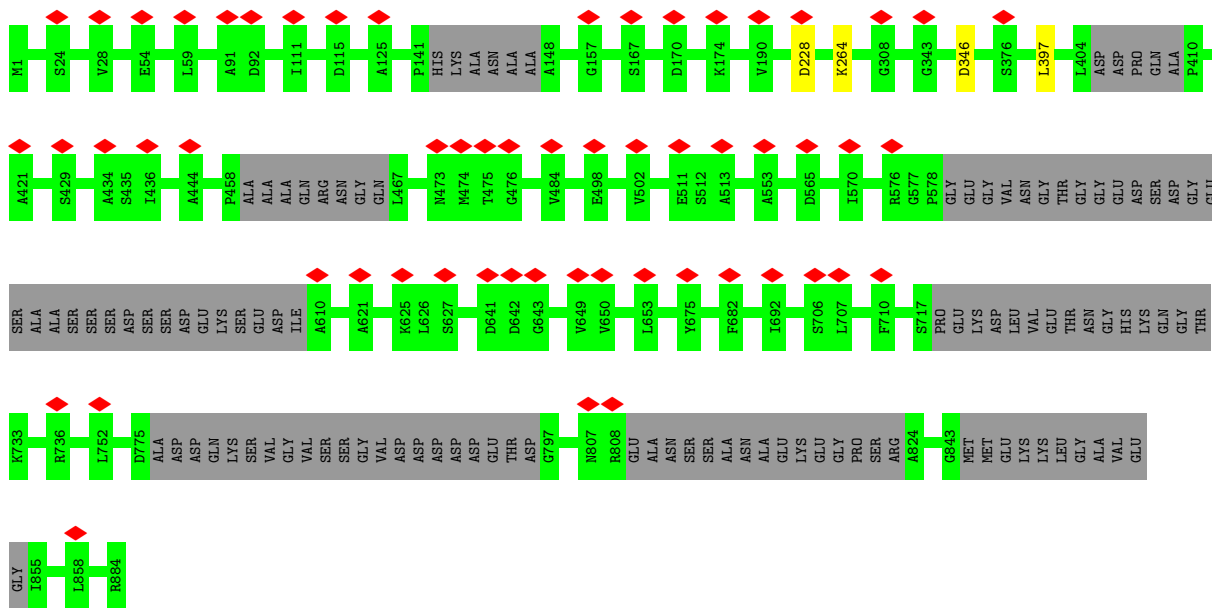
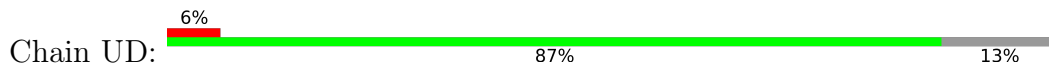
- Molecule 64 is ZINC ION (three-letter code: ZN) (formula: Zn).

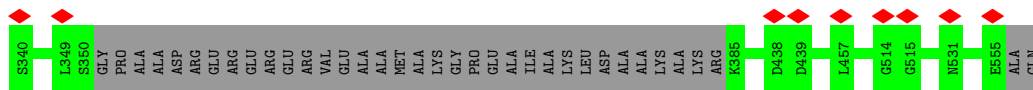
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
64	UX	1	1	1	0

● Molecule 3: Utp3

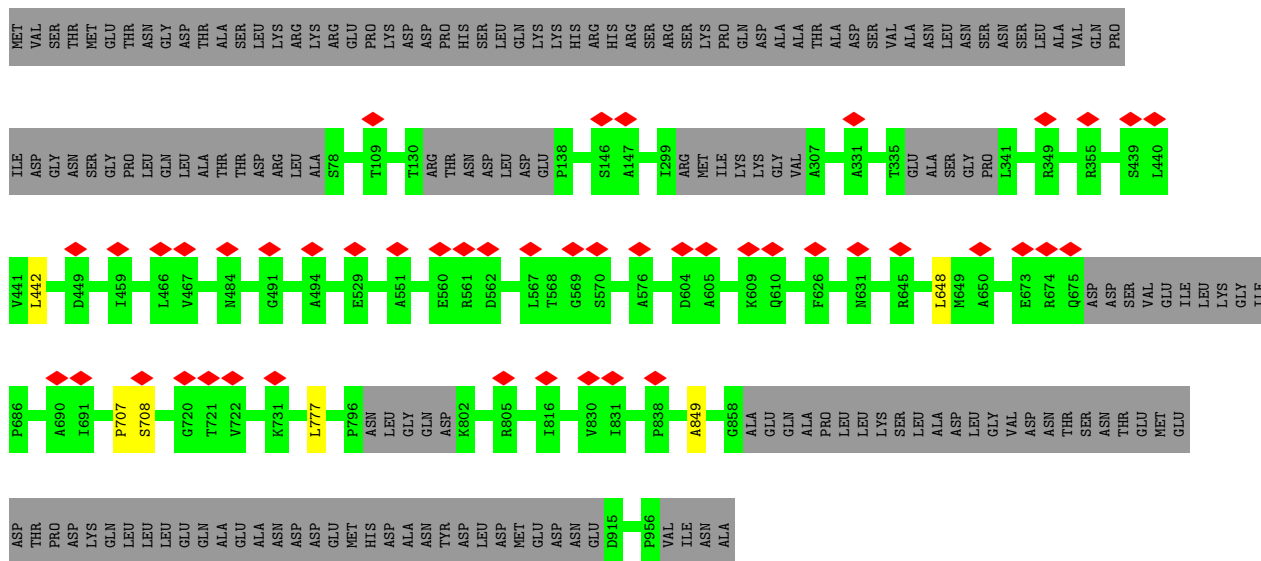
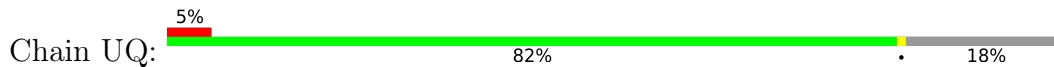


● Molecule 4: Utp4

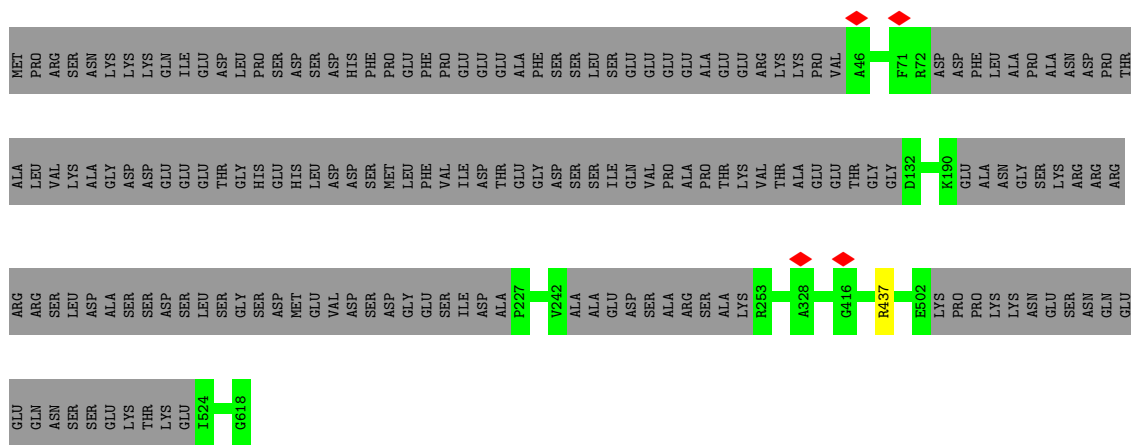
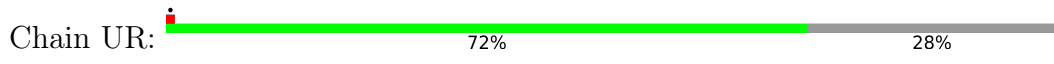




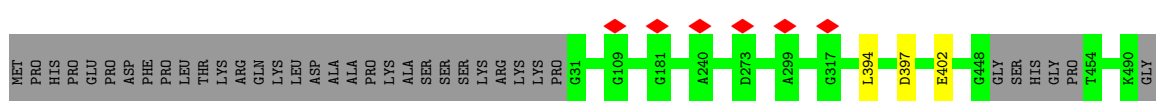
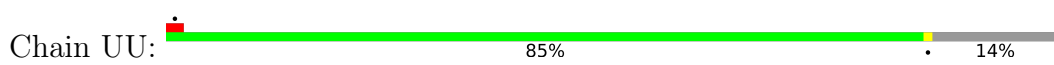
• Molecule 13: Utp17

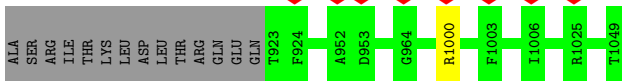
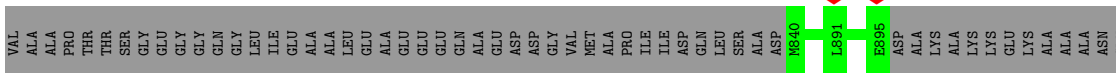
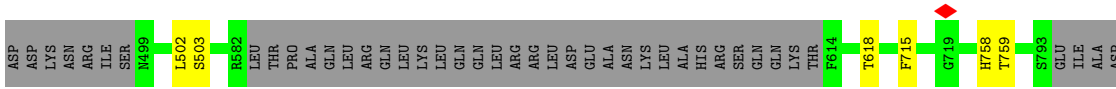


• Molecule 14: Utp18

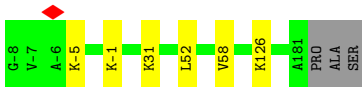


• Molecule 15: Putative U3 snoRNP protein

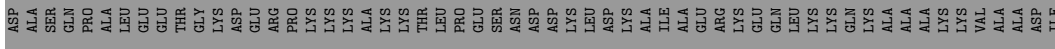
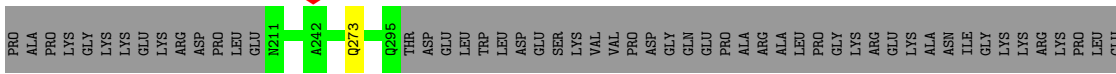
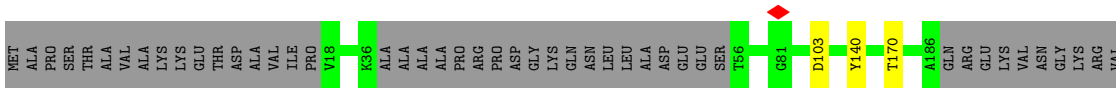




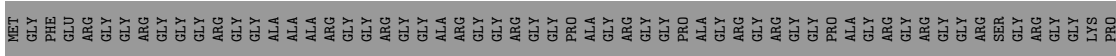
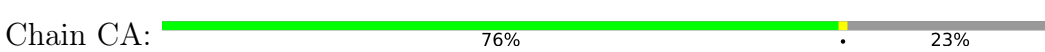
• Molecule 16: Utp24



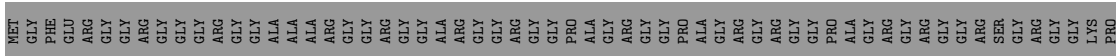
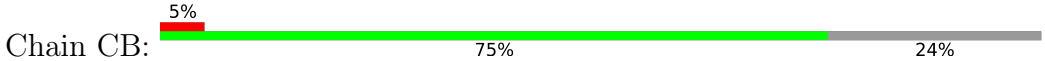
• Molecule 17: Utp30

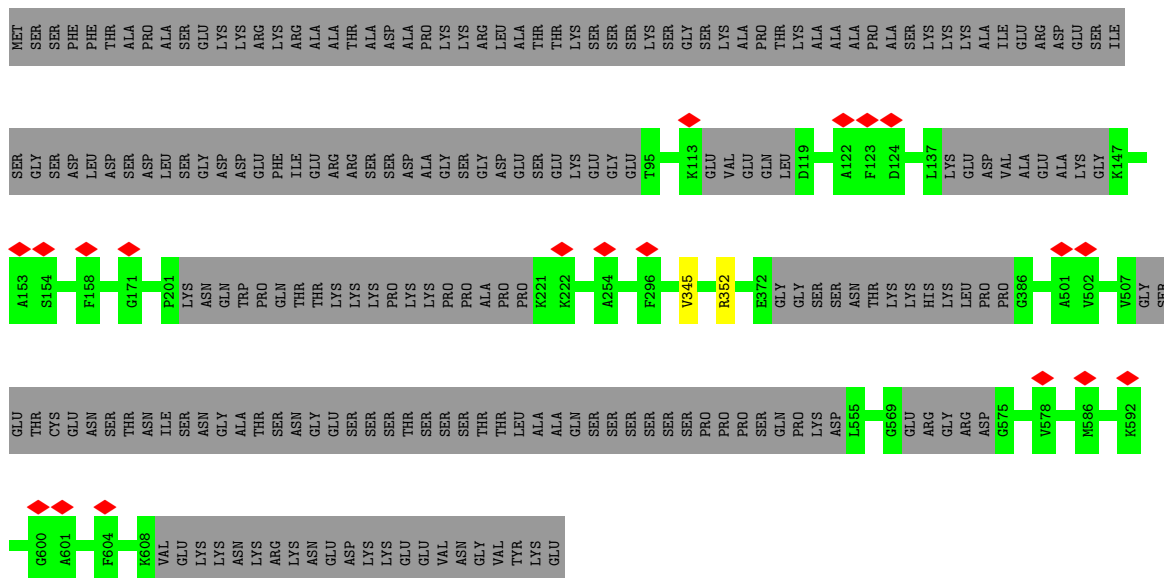


• Molecule 18: Nop1

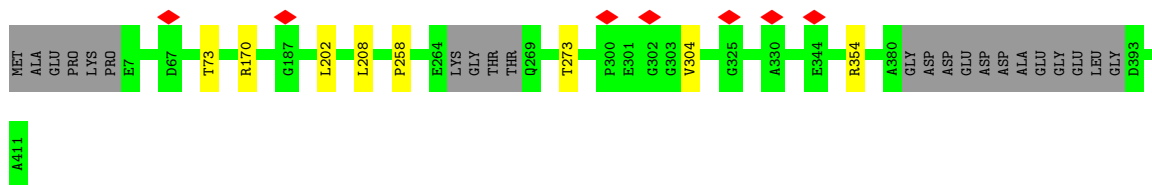


• Molecule 18: Nop1

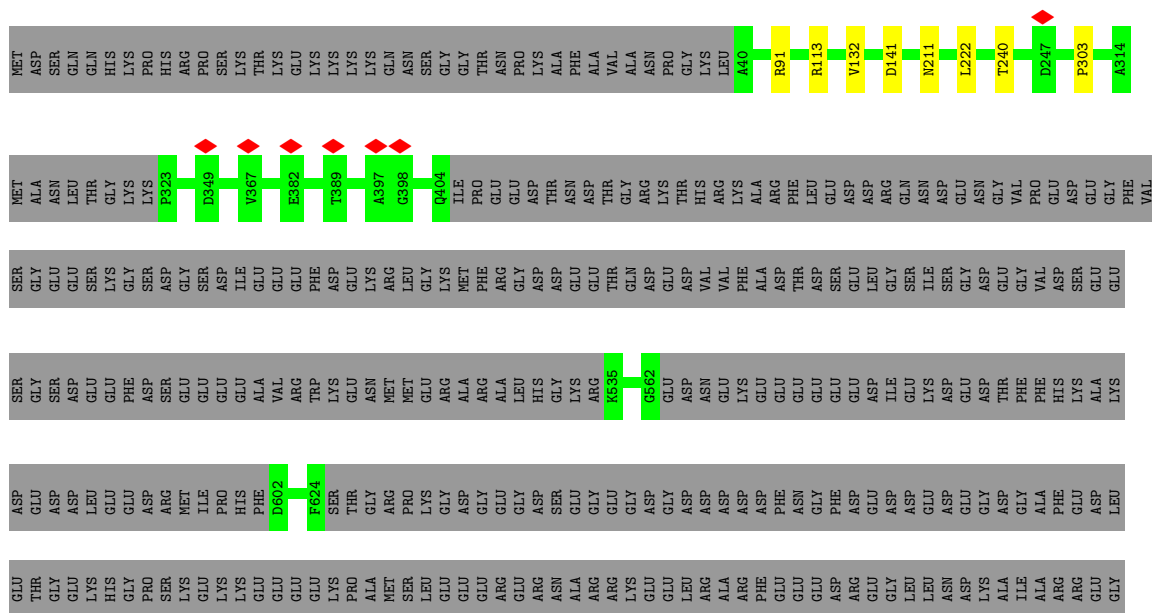




• Molecule 23: RNA 3'-terminal phosphate cyclase-like protein



• Molecule 24: Bms1





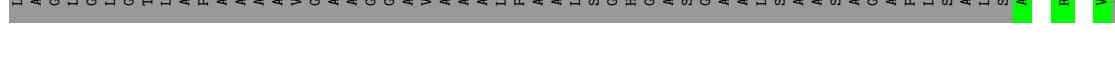
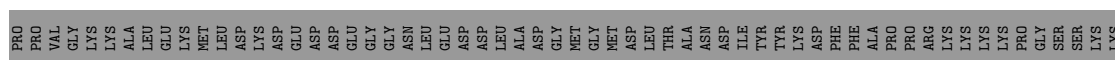
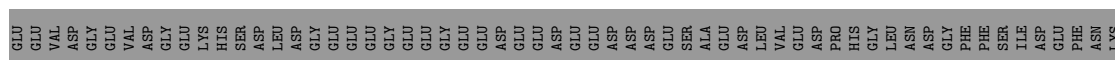
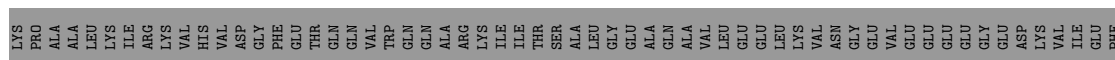
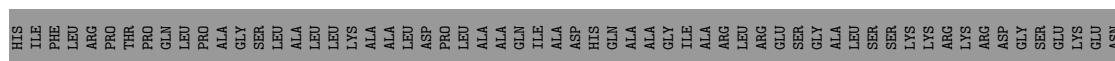
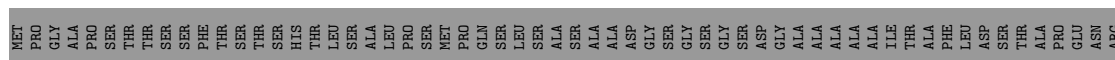
● Molecule 25: Imp3



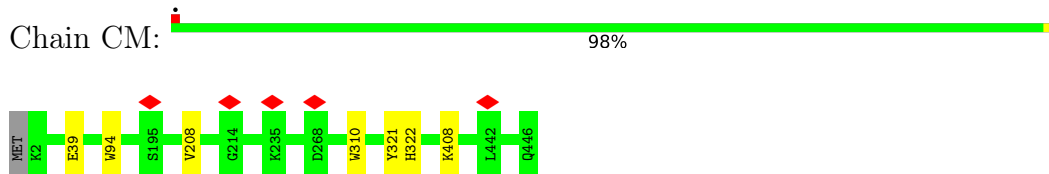
● Molecule 26: Putative U3 small nucleolar ribonucleoprotein



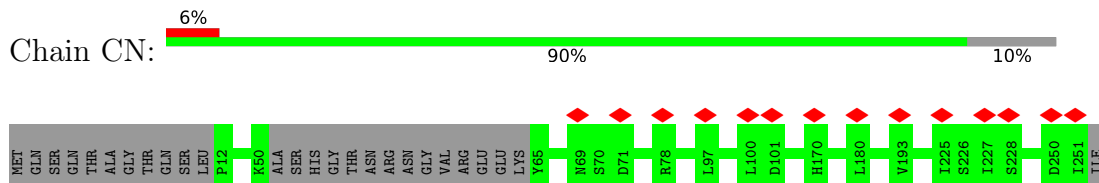
● Molecule 27: Putative U3 small nucleolar ribonucleoprotein protein



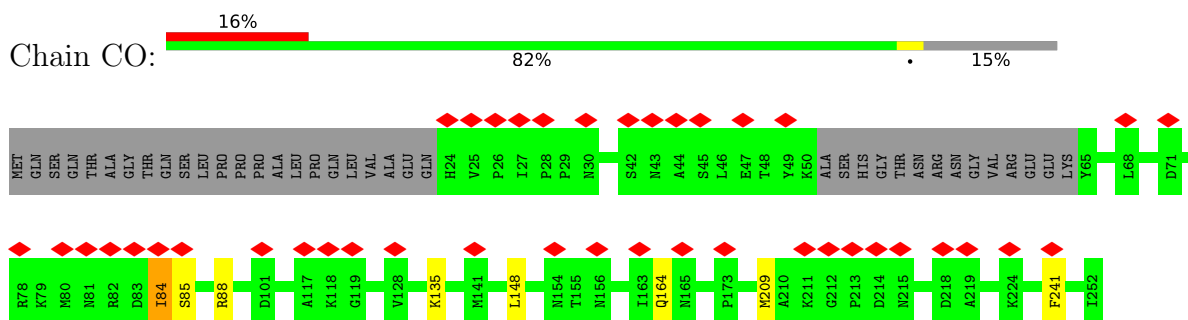
• Molecule 28: Sof1



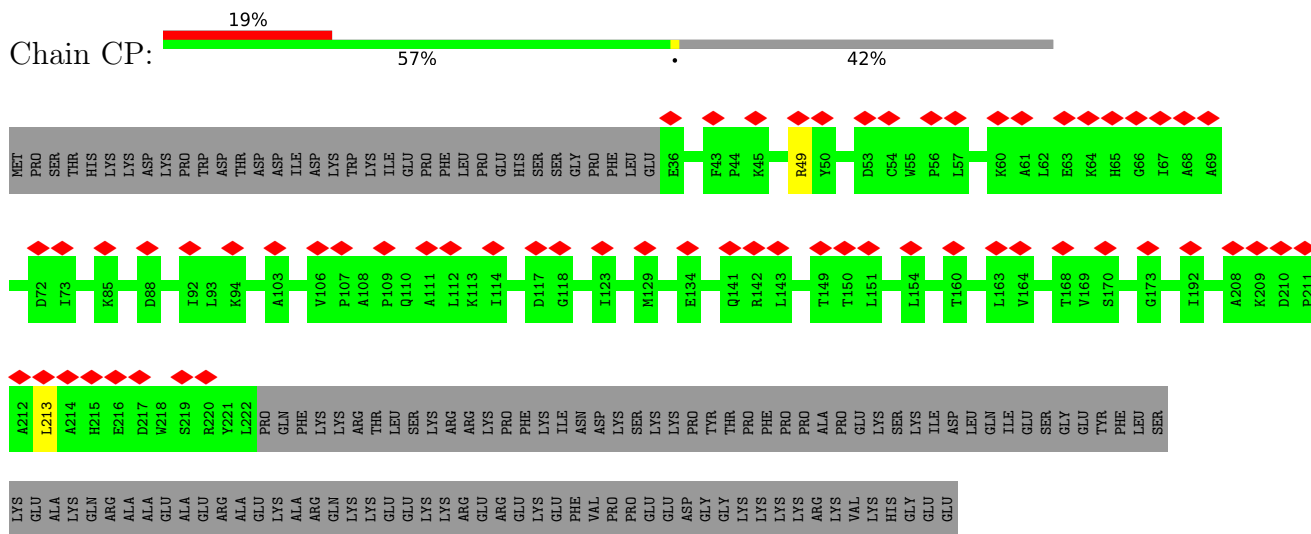
• Molecule 29: Emg1



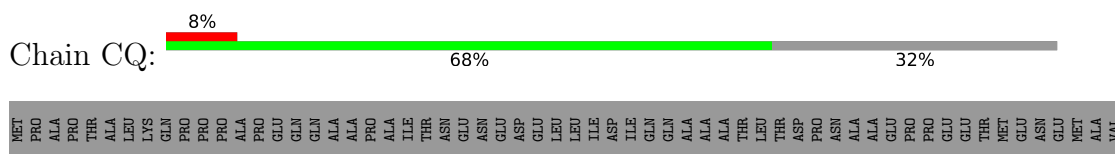
• Molecule 29: Emg1

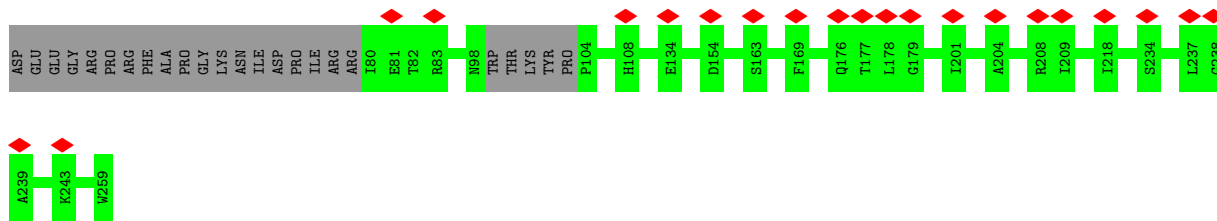


• Molecule 30: KRR1 small subunit processome component

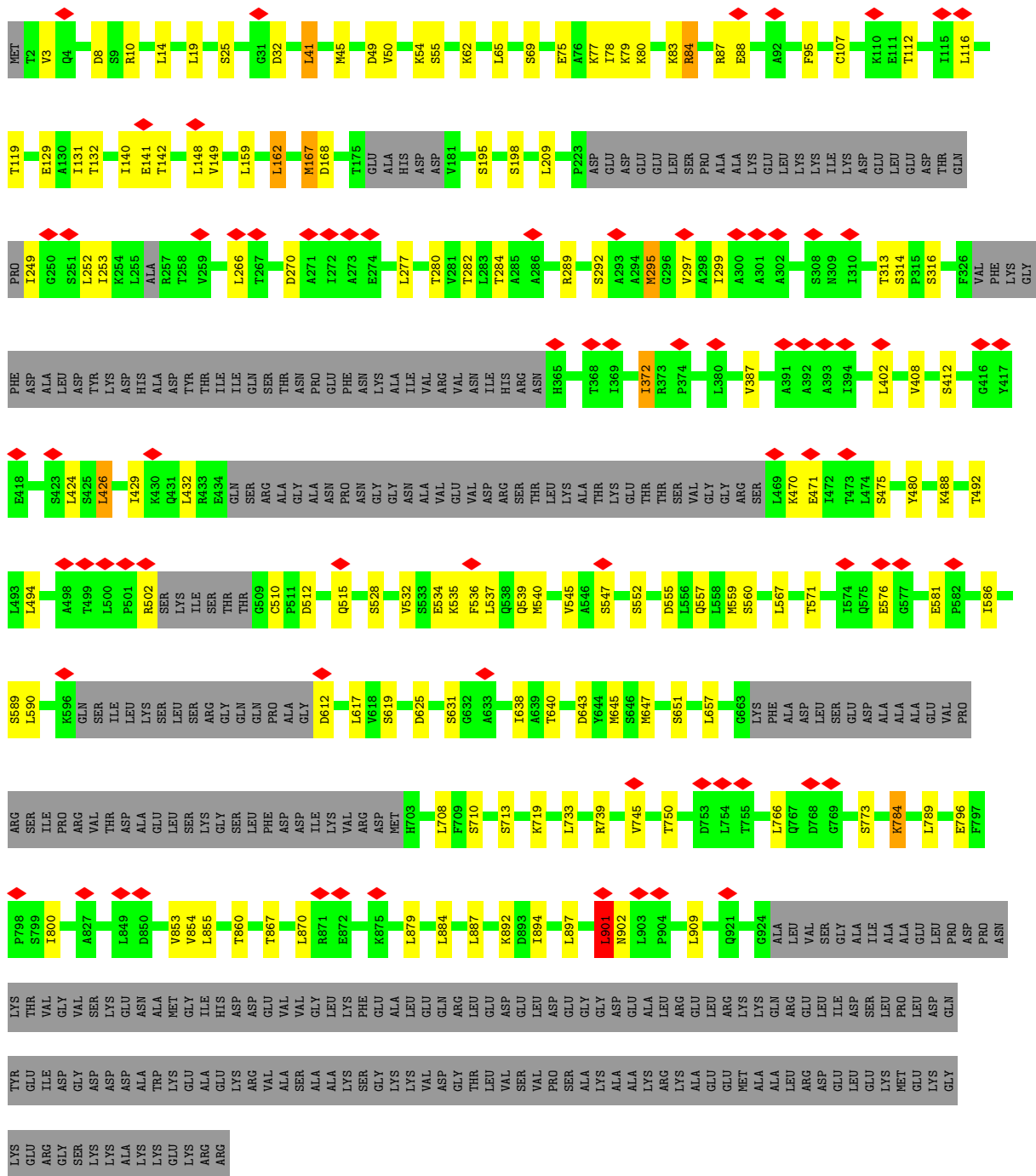


• Molecule 31: Pre-rRNA-processing protein PNO1





• Molecule 32: Kre33




Chain CT:  65% 35%

MET ALA THR LEU GLY LEU PRO ASP GLU ILE ASP ARG LEU ALA ALA ALA ALA ARG LEU ALA GLY SER GLY ASP ALA GLY ALA ILE ALA LEU LYS PRO ALA VAL THR VAL ALA PRO ALA ALA ALA

PRO GLN VAL LYS ALA GLU E88 P77 G77 LYS LYS G82 I141 R202 LYS


- Molecule 34: 40S ribosomal protein S4

Chain Cb:  7% 88% 12%

MET ALA ARG GLY PRO LYS H8 R39 D40 D73 G74 R77 T78 G96 R128 V129 R133 A144 L153 R187 G203 G204 F205 G206 I207 V208 H209 D215 K239 GLY LYS VAL LYS LEU THR ILE ALA GLU ARG ASP GLN ARG ALA ARG

ALA LEU ALA ALA GLY HIS

- Molecule 35: 40S ribosomal protein s5-like protein

Chain Cc:  89% 9%


MET SER GLY GLU VAL GLU VAL Y13 A22 R41 A61 V66 A123 R130 R135 ILE GLY SER SER ALA GLY THR VAL ARG R144 R212

- Molecule 36: 40S ribosomal protein S6

Chain Cd:  7% 94% 5%

MH G11 D29 K30 R31 M32 E35 I68 S78 E79 G80 D89 G90 L111 S112 I113 V114 E118 G123 V157 I158 K226 ALA ASP LEU ARG LYS ARG ARG ALA SER SER HIS LYS


- Molecule 37: 40S ribosomal protein S7

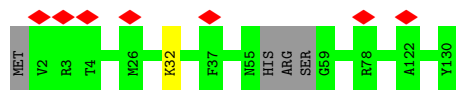
Chain Ce:  22% 77% 22%

MET SER ALA PRO SER LEU ASN ILE ALA ALA ASN SER PRO S15 D32 L33 M36 T37 A38 D39 L40 K41 A42 A43 L44 R45 V57 G58 H77 R78 V79 Q80 Q81 R82 R85 E86 K89 K90 D93 R94 H95 V96 L97 A100 A101 R102 R103 ILE LEU PRO LYS

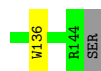
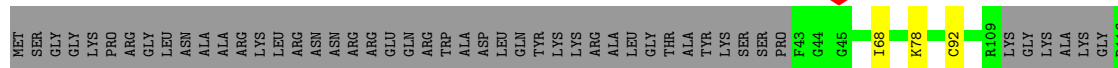
PRO LYS ARG SER ALA ARG SER ARG ASN THR LEU LYS ARG PRO THR L128 T129 A130 D133 P142 V143 E144 I145 V146 G147 E166 K167 E168 R169 G170 D173 R184 R185 L186 R189 Q197 THR THR ILE THR ASP TYR

- Molecule 38: 40S ribosomal protein S8

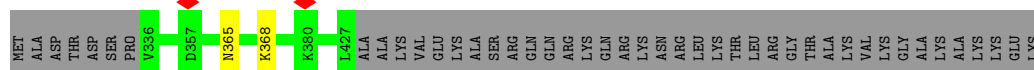
Chain Cf:  8% 86% 14%



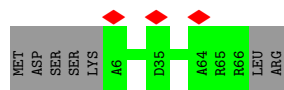
• Molecule 45: 40S ribosomal protein s23-like protein



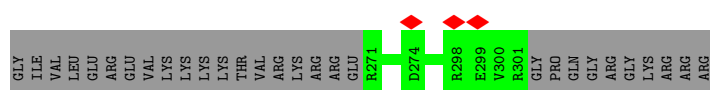
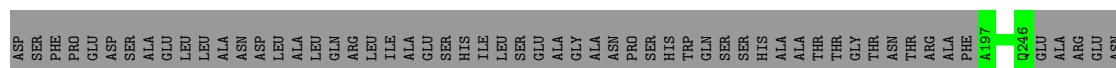
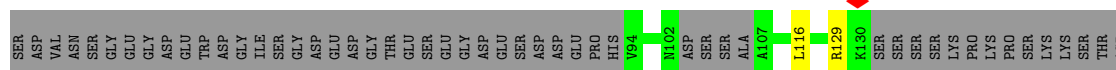
• Molecule 46: 40S ribosomal protein S24



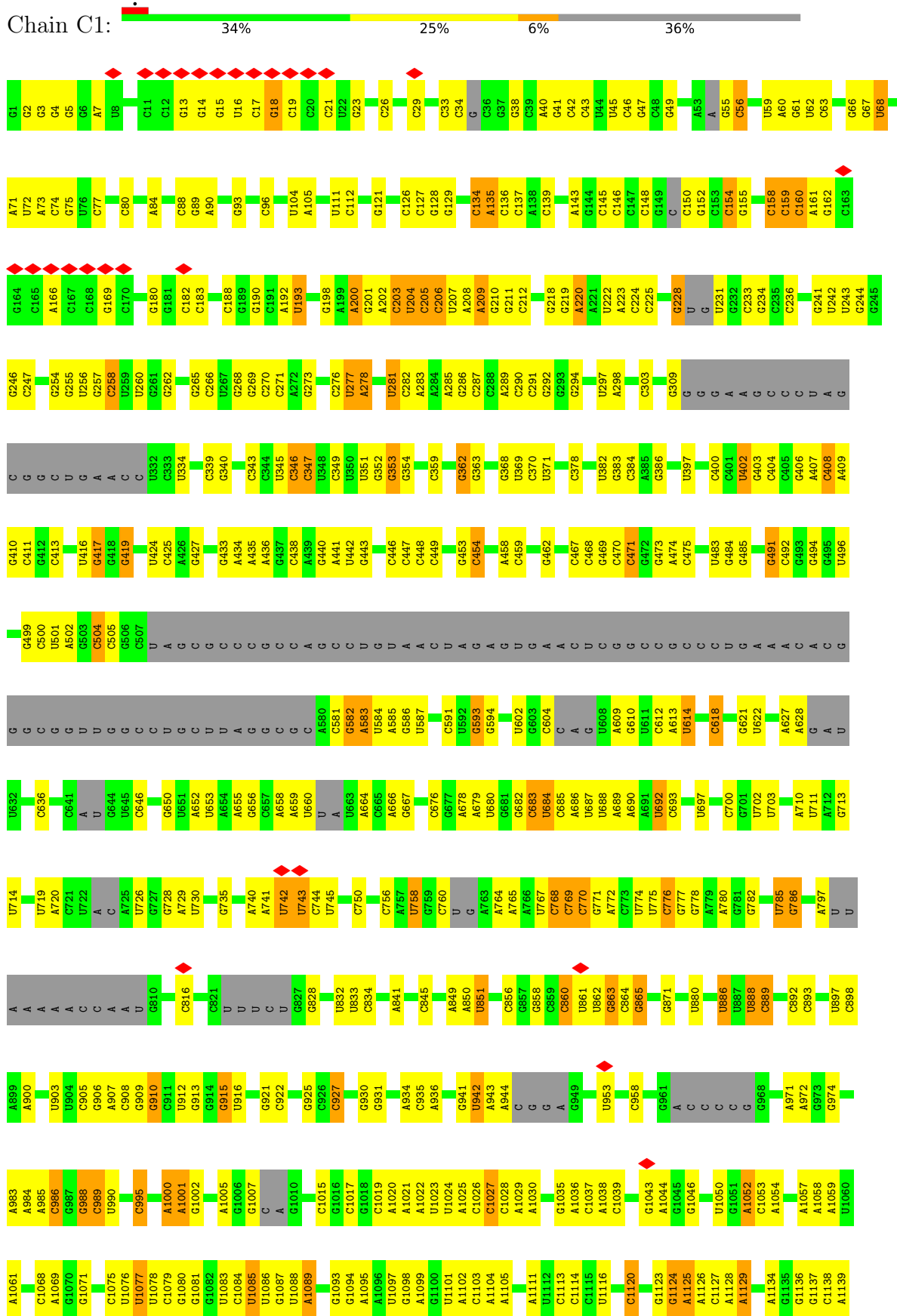
• Molecule 47: 40S ribosomal protein S28-like protein

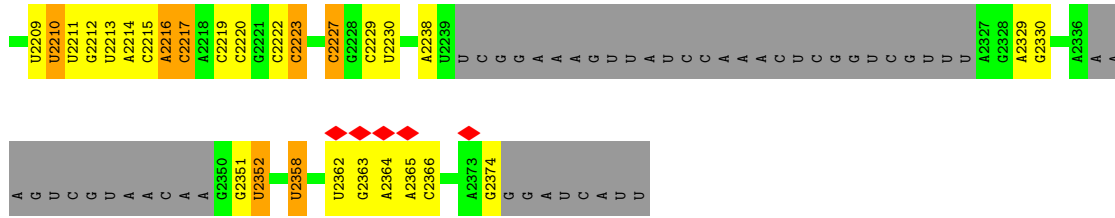


• Molecule 48: Faf1

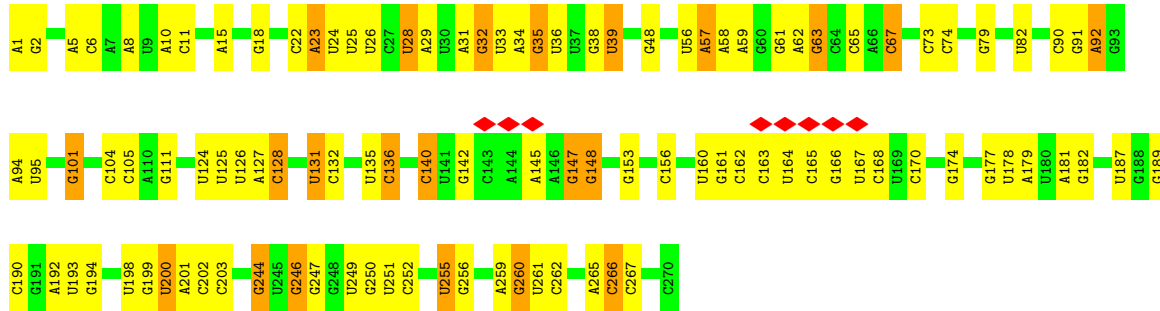


• Molecule 49: 35S ribosomal RNA

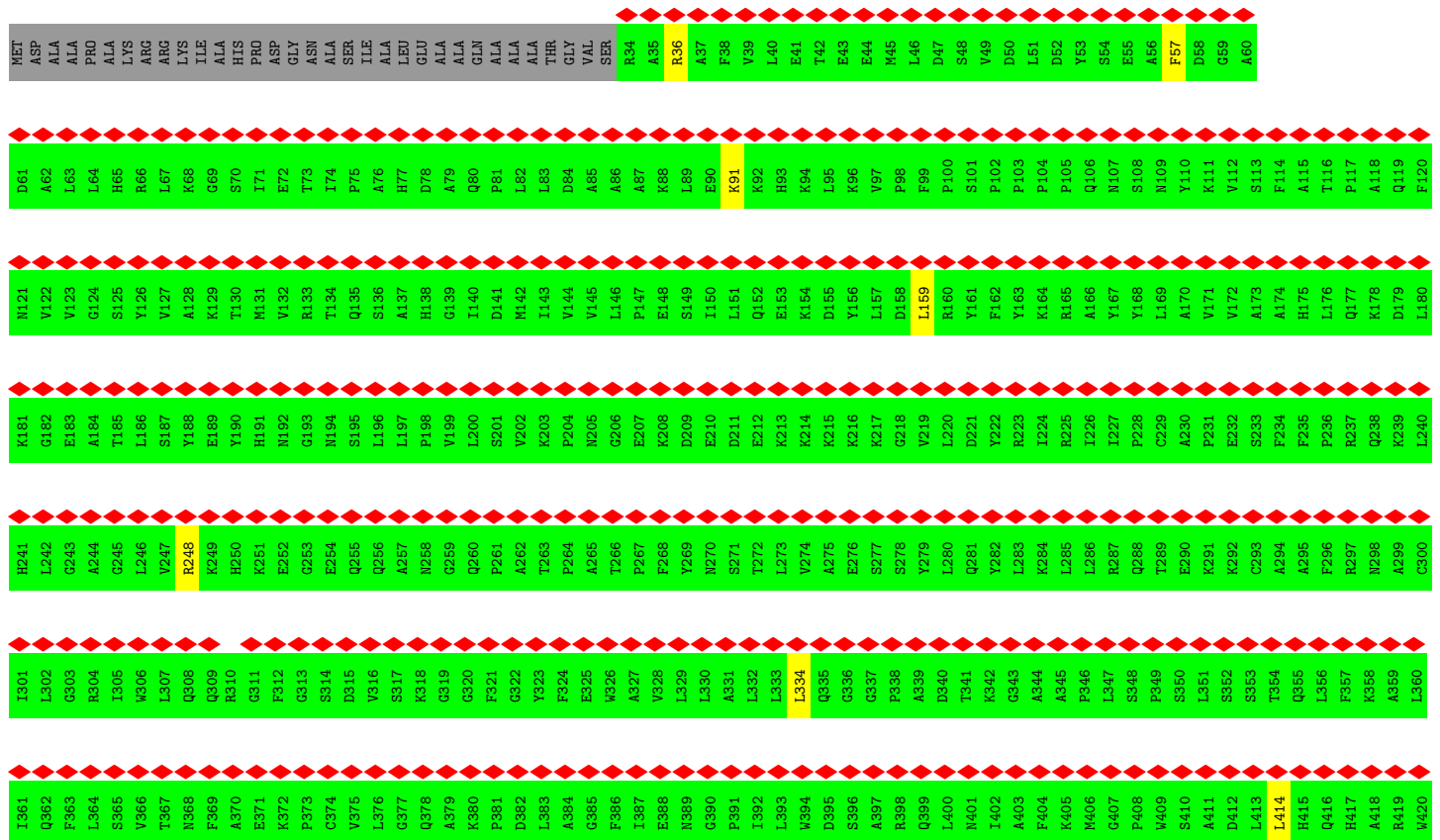
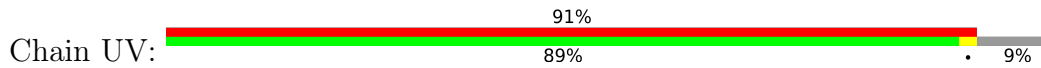




• Molecule 50: U3 snoRNA

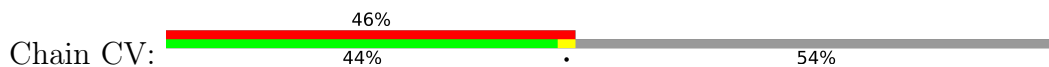


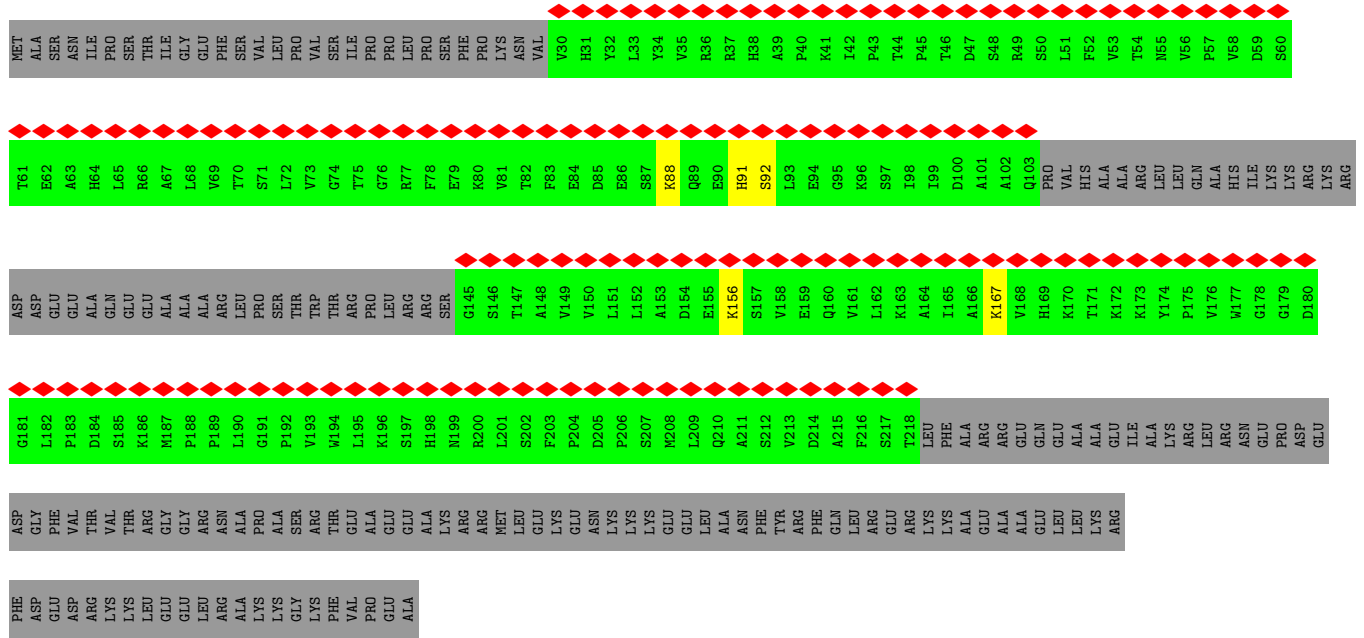
• Molecule 51: U3 small nucleolar RNA-associated protein 22



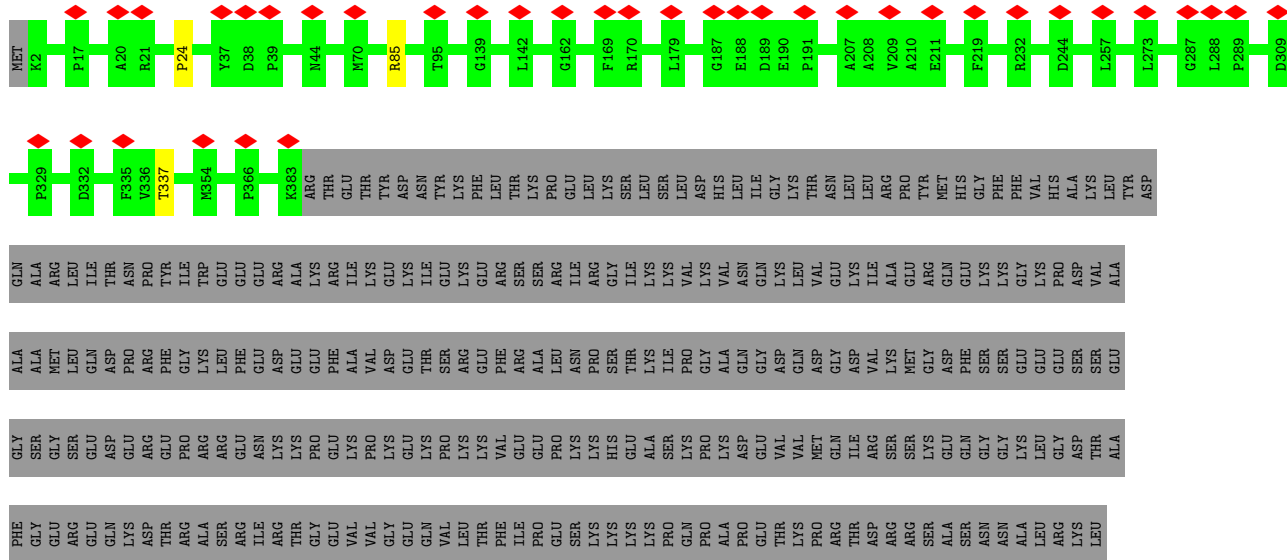
ARG	E1081	T961	G1021	H841	R781	F721	L661	E601	L541	K481	T421
VAL	E1082	A962	K1022	K842	Q782	L722	P662	I602	N542	V482	R422
GLU	E1083	A963	K1023	L843	T783	L723	L663	M603	M543	Y483	K423
GLU	D1084	A964	Q1024	S844	K784	M724	R664	R604	A544	R484	L424
VAL	K1085	K965	E1025	M845	D785	I725	I665	Y605	A544	I485	L425
ASN	K1086	S966	I1026	H846	K786	G726	R666	I606	T546	I486	A426
ARG	T1087	A967	I1027	F847	T787	R727	H667	L607	V547	R487	D427
GLY	G1088	A968	F1028	P848	T788	L728	V668	G608	D548	R488	G428
ILE	A1089	R969	I1029	P849	E789	L729	N669	L609	R499	A489	A429
LEU	V1090	R970	M1030	E850	Q790	E730	P670	H610	G550	L490	V430
ALA	W1091	I971	L1031	L851	Y791	R731	I671	L611	P551	S491	D431
GLU	N1092	R972	A1032	L852	L792	F732	C672	R612	S552	D492	Q432
VAL	P1093	E973	P1033	E853	R793	K733	P673	V613	A553	K493	F433
ALA	T1094	Q974	E1034	L854	Q794	P734	E674	G614	G554	M494	Q434
ILE	L1095	G975	T1035	F855	R795	G735	L875	Q615	P555	M495	P435
GLY	V1096	V976	V1036	V856	A796	E736	R676	L616	S556	E496	T436
GLU	K1097	D977	E1037	L857	S797	I737	H677	Q617	A557	G497	F437
VAL	X1098	L978	P1038	H858	T798	R738	S678	D618	E558	G498	I438
ARG	W1100	D979	P1039	T859	Q799	T739	S679	D619	E559	E499	L439
ILE	R1101	V980	L1040	F860	L800	H740	L680	I620	K560	R500	K440
GLU	V1102	R981	P1041	L861	A601	V741	K681	V621	E561	A501	A441
LYS	N1103	R982	V1042	A862	S802	G742	T682	F622	T562	R502	D442
LEU	L1104	L983	A1043	P863	F803	L743	P683	Y623	C563	L503	L443
P1105	P1105	F984	Q1044	Y864	R804	D744	S684	G624	E564	I504	P444
T1106	T1106	V985	H1045	P865	R605	D745	F865	R625	K565	H505	T445
S1107	S1107	R986	P1046	V866	T806	A746	G866	S626	F566	L506	H446
Y1108	Y1108	S987	V1047	D867	F807	R747	P867	L627	R567	K507	T447
X1109	X1109	L888	D1048	V668	V608	Y748	S688	P628	R568	V508	Y448
P1110	P1110	K989	V1049	P869	H609	E749	K689	A629	F569	S509	D449
V1111	V1111	E990	L1050	S870	L810	T750	S690	L630	W570	P510	L450
ALA	GLY	Y991	L1051	S871	P611	E751	G691	L631	G571	G511	V451
GLY	GLY	D992	K1052	P872	L812	N752	P692	S632	E572	F512	A452
LYS	LYS	V993	G1053	T873	H613	L753	R693	I633	K573	S513	R453
ASP	ASP	L994	L1054	T874	T814	A754	P694	K634	S574	S514	M454
GLU	GLU	L995	S1055	G875	Q615	F755	M695	P635	E575	S515	D455
SER	SER	Y996	A1056	F876	V616	L756	E696	S636	E576	S516	P456
GLU	GLU	L997	Y1057	L877	I617	D757	V697	D637	L576	W517	E457
ASP	ASP	T941	Y1058	R878	T618	V758	V698	T638	R577	W517	E457
GLU	GLU	H942	D1059	T879	T619	I759	I699	A639	R578	S518	K458
ASP	ASP	W943	S1060	L880	A820	V760	S700	L640	F579	L519	V459
ASP	ASP	T944	A1061	L881	T621	A761	F701	F641	G581	N520	S460
GLU	GLU	S945	L1002	F882	T622	S762	E702	N642	G582	E521	E461
ASP	ASP	V946	K1003	L883	R623	G763	A703	V643	T583	P523	A462
ASP	ASP	D947	S1004	A884	F824	A764	S704	A644	I584	Q524	P464
GLY	GLY	G948	A1005	R885	P625	C765	G705	R645	R585	P525	D465
SER	SER	H949	L1006	V886	A826	F766	K706	K646	E586	Q526	D466
GLU	GLU	P950	T1007	D887	L627	R767	W707	T647	T587	K527	V467
ARG	ARG	R951	G1008	W888	S828	V768	P708	F648	L588	A528	A468
GLU	GLU	P952	T1009	R889	P629	R769	E709	T649	V589	G529	H469
LYS	LYS	S953	L1070	T890	T630	I770	S710	S650	W590	T530	E470
ARG	ARG	K954	T1011	D891	I631	Q771	L711	F651	S991	P531	A471
GLY	GLY	V955	F1012	P892	R832	A772	I712	E652	A992	I532	R472
GLU	GLU	V956	D1013	L893	L633	D773	A713	R653	Q593	E533	G473
GLY	GLY	A957	R1014	T894	V634	L774	I714	D654	T594	I534	R474
ASP	ASP	A958	A1015	I895	E775	E775	Q715	L655	P595	G535	H475
GLU	GLU	R959	T1016	D896	H636	E776	R716	R656	F596	V536	W476
GLY	GLY	H960	E1017	T897	W637	S777	T717	D657	D597	L537	Q477
GLY	GLY	SER	LEU	ASN	F838	L778	K718	L658	L598	F538	V478
GLY	GLY	ASN	G1020	S839	S839	L779	I719	E559	C599	D539	G479
GLY	GLY					E780	A720	D660	E600	P540	H480

• Molecule 52: Rrp7

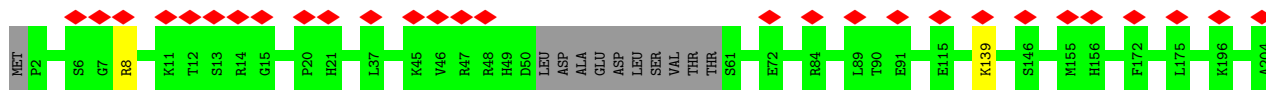
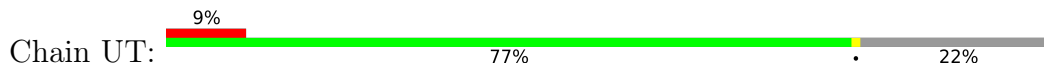


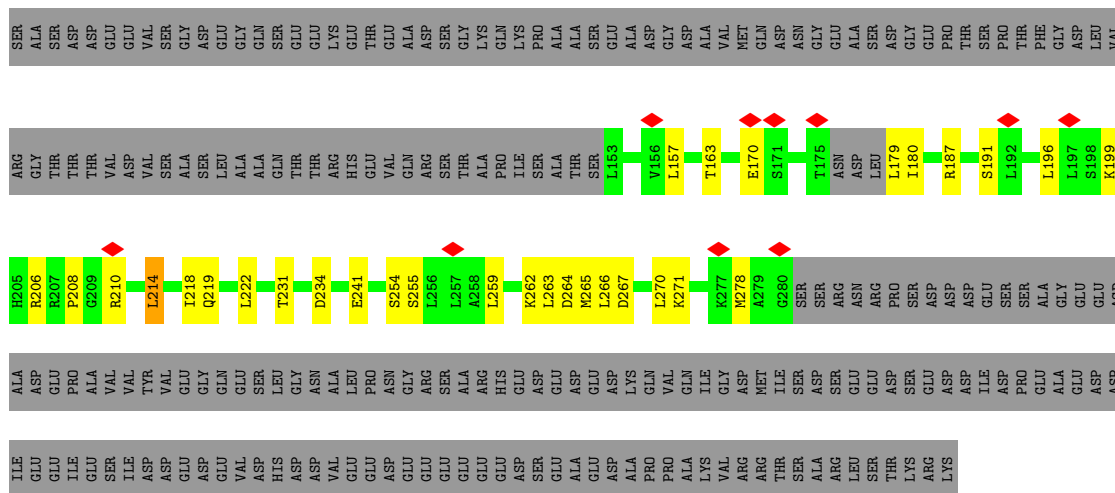


• Molecule 53: Ribosome biogenesis protein ENP2

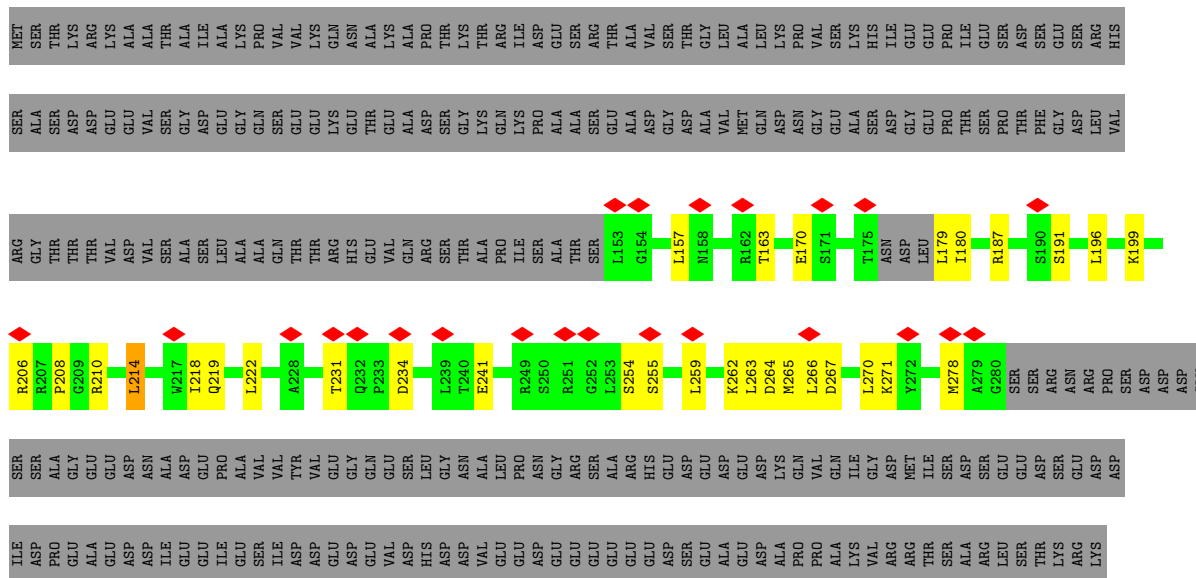


• Molecule 54: Utp20

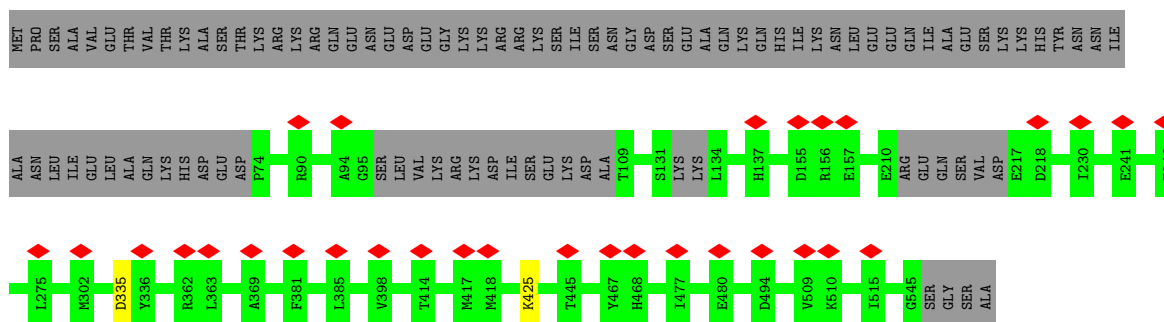
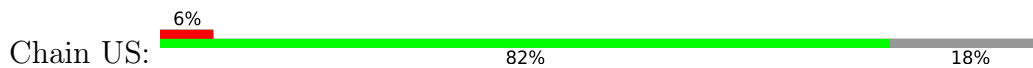




• Molecule 56: Utp5



• Molecule 57: Noc4



• Molecule 58: Rps18

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24283	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.834	Depositor
Minimum map value	-0.505	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	520.32, 520.32, 520.32	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	Depositor

5 Model quality i

5.1 Standard geometry i

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

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	UA	0.55	2/6521 (0.0%)	0.71	2/8867 (0.0%)
2	UB	0.37	0/4154	0.56	1/5583 (0.0%)
3	UC	0.59	0/595	0.65	0/786
4	UD	0.33	0/6211	0.58	1/8408 (0.0%)
5	UF	0.34	0/2657	0.53	0/3596
6	UG	0.49	0/3790	0.65	1/5120 (0.0%)
7	UJ	0.33	0/8567	0.59	2/11619 (0.0%)
8	UK	0.64	2/1701 (0.1%)	0.67	1/2251 (0.0%)
9	UL	0.34	0/6299	0.63	2/8531 (0.0%)
10	UM	0.30	0/5366	0.59	2/7282 (0.0%)
11	UN	0.38	0/1425	0.57	1/1913 (0.1%)
12	UO	0.36	0/3903	0.61	1/5312 (0.0%)
13	UQ	0.32	0/6136	0.59	3/8348 (0.0%)
14	UR	0.40	0/3564	0.61	0/4816
15	UU	0.43	0/6903	0.63	2/9392 (0.0%)
16	UX	0.61	0/1493	0.70	1/2011 (0.0%)
17	UZ	0.40	0/1857	0.62	0/2526
18	CA	0.53	0/1814	0.65	1/2456 (0.0%)
18	CB	0.36	0/1853	0.59	0/2511
19	CC	0.38	0/2911	0.58	1/3937 (0.0%)
20	CD	0.37	0/3205	0.62	1/4338 (0.0%)
21	CE	0.46	0/891	0.60	0/1214
21	CF	0.40	0/876	0.66	0/1195
22	CG	0.34	0/3307	0.60	0/4462
23	CH	0.42	0/2939	0.64	1/3988 (0.0%)
24	CI	0.59	3/6631 (0.0%)	0.70	4/8943 (0.0%)
25	CJ	0.74	1/1462 (0.1%)	0.76	0/1967
26	CK	0.71	1/2376 (0.0%)	0.81	3/3214 (0.1%)
27	CL	0.48	0/1812	0.59	0/2437
28	CM	0.56	3/3573 (0.1%)	0.69	1/4829 (0.0%)
29	CN	0.33	0/1797	0.60	0/2443
29	CO	0.32	0/1714	0.60	2/2325 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	CP	0.30	0/1528	0.63	1/2057 (0.0%)
31	CQ	0.29	0/1379	0.57	0/1850
32	CR	0.37	1/6108 (0.0%)	0.74	13/8266 (0.2%)
32	CS	0.37	1/6108 (0.0%)	0.74	13/8266 (0.2%)
33	CT	0.53	0/1053	0.62	0/1413
34	Cb	0.31	0/1890	0.59	0/2548
35	Cc	0.44	0/1485	0.59	0/2008
36	Cd	0.32	0/1850	0.58	0/2474
37	Ce	0.35	0/1298	0.67	1/1750 (0.1%)
38	Cf	0.30	0/1429	0.56	0/1915
39	Cg	0.46	0/1259	0.60	0/1687
40	Ch	0.28	0/412	0.57	0/549
41	Ci	0.31	0/801	0.60	0/1087
42	Cj	0.58	0/958	0.72	0/1293
43	Ck	0.31	0/1190	0.53	0/1592
44	Cm	0.40	0/1001	0.59	0/1345
45	Cn	0.81	2/712 (0.3%)	0.79	0/954
46	Co	0.34	0/754	0.59	0/1011
47	Cp	0.34	0/458	0.65	0/617
48	CU	0.35	0/887	0.61	1/1178 (0.1%)
49	C1	0.83	45/35454 (0.1%)	1.37	556/55209 (1.0%)
50	C2	0.88	3/5459 (0.1%)	1.47	88/8498 (1.0%)
51	UV	0.33	0/8638	0.66	6/11725 (0.1%)
52	CV	0.34	0/1172	0.71	0/1592
53	CW	0.32	0/2996	0.63	1/4075 (0.0%)
54	UT	0.31	0/16314	0.57	4/22075 (0.0%)
55	UH	0.34	0/2852	0.60	3/3846 (0.1%)
56	UE	0.38	0/980	0.78	2/1316 (0.2%)
56	UI	0.38	0/980	0.78	2/1316 (0.2%)
57	US	0.33	0/3765	0.56	1/5100 (0.0%)
58	CI	0.32	0/638	0.65	0/857
59	CX	0.27	0/2172	0.51	0/2946
60	CY	0.36	0/982	0.61	0/1298
61	CZ	0.33	0/362	0.73	1/483 (0.2%)
62	UP	0.33	0/428	0.57	0/570
63	Cz	0.31	0/2310	0.54	0/3120
All	All	0.51	64/226365 (0.0%)	0.84	727/314506 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	UA	0	10
5	UF	0	1
6	UG	0	2
8	UK	0	2
9	UL	0	2
10	UM	0	4
11	UN	0	1
12	UO	0	1
13	UQ	0	2
15	UU	0	4
16	UX	0	2
17	UZ	0	2
18	CB	0	1
21	CE	0	1
21	CF	0	2
23	CH	0	1
24	CI	0	6
25	CJ	0	2
26	CK	0	1
28	CM	0	1
29	CO	0	2
32	CR	0	1
32	CS	0	1
37	Ce	0	1
41	Ci	0	1
42	Cj	0	3
45	Cn	0	1
46	Co	0	1
51	UV	0	4
52	CV	0	2
54	UT	0	5
55	UH	0	1
58	Cl	0	1
60	CY	0	1
63	Cz	0	1
All	All	0	74

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	UA	488	TRP	CB-CG	-8.05	1.35	1.50
50	C2	57	A	N7-C5	-7.73	1.34	1.39
32	CS	515	GLN	CA-CB	7.33	1.70	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	CR	515	GLN	CA-CB	7.33	1.70	1.53
49	C1	1154	A	N9-C4	-6.99	1.33	1.37
28	CM	321	TYR	CD2-CE2	-6.89	1.29	1.39
49	C1	1140	A	N7-C5	-6.78	1.35	1.39
49	C1	1129	A	N9-C4	-6.78	1.33	1.37
49	C1	2066	A	N9-C4	-6.78	1.33	1.37
28	CM	94	TRP	CB-CG	-6.71	1.38	1.50
49	C1	255	G	N3-C4	-6.67	1.30	1.35
49	C1	1137	G	N7-C5	-6.61	1.35	1.39
45	Cn	136	TRP	CB-CG	-6.30	1.39	1.50
49	C1	1158	G	N9-C4	-6.30	1.32	1.38
49	C1	2071	G	C6-N1	-6.29	1.35	1.39
49	C1	1140	A	C5-C6	-6.21	1.35	1.41
49	C1	1138	C	N1-C6	-6.11	1.33	1.37
49	C1	2173	G	N7-C5	-6.01	1.35	1.39
49	C1	2172	C	N1-C6	-5.96	1.33	1.37
49	C1	1140	A	N3-C4	-5.95	1.31	1.34
49	C1	2176	A	N3-C4	-5.91	1.31	1.34
49	C1	407	A	N7-C5	-5.91	1.35	1.39
49	C1	2179	C	N3-C4	-5.91	1.29	1.33
49	C1	2177	G	C6-N1	-5.90	1.35	1.39
49	C1	1155	G	C5-C6	-5.88	1.36	1.42
24	CI	987	VAL	CB-CG1	-5.88	1.40	1.52
49	C1	1145	G	C6-N1	-5.86	1.35	1.39
49	C1	2174	C	N1-C6	-5.76	1.33	1.37
24	CI	977	PHE	CB-CG	-5.69	1.41	1.51
1	UA	488	TRP	CA-C	-5.65	1.38	1.52
49	C1	1158	G	C5-C4	-5.63	1.34	1.38
49	C1	2180	A	N7-C5	-5.59	1.35	1.39
49	C1	2180	A	C5-C6	-5.59	1.36	1.41
45	Cn	92	CYS	CB-SG	-5.58	1.72	1.81
49	C1	1138	C	N3-C4	-5.54	1.30	1.33
49	C1	2188	G	N7-C5	-5.51	1.35	1.39
49	C1	2190	G	N7-C5	-5.50	1.35	1.39
49	C1	1156	C	N1-C6	-5.49	1.33	1.37
49	C1	1179	G	C6-N1	-5.47	1.35	1.39
26	CK	287	TYR	CD1-CE1	-5.47	1.31	1.39
49	C1	1146	G	N7-C5	-5.43	1.35	1.39
49	C1	2071	G	N1-C2	-5.42	1.33	1.37
49	C1	1148	G	N9-C4	-5.32	1.33	1.38
24	CI	851	TRP	CB-CG	-5.29	1.40	1.50
49	C1	1148	G	C5-C6	-5.29	1.37	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	C1	1175	A	N7-C5	-5.28	1.36	1.39
49	C1	2177	G	N3-C4	-5.27	1.31	1.35
49	C1	2177	G	N7-C5	-5.24	1.36	1.39
49	C1	363	G	C6-N1	-5.22	1.35	1.39
8	UK	34	TYR	CD1-CE1	-5.21	1.31	1.39
8	UK	34	TYR	CD2-CE2	-5.21	1.31	1.39
49	C1	1140	A	C5-C4	-5.19	1.35	1.38
49	C1	2175	A	C6-N1	-5.16	1.31	1.35
50	C2	32	G	N7-C5	-5.15	1.36	1.39
49	C1	1138	C	C4-C5	-5.13	1.38	1.43
49	C1	1155	G	C5-C4	-5.12	1.34	1.38
49	C1	407	A	N3-C4	-5.10	1.31	1.34
50	C2	59	A	N7-C5	-5.10	1.36	1.39
49	C1	1145	G	C5-C6	-5.10	1.37	1.42
49	C1	353	G	N9-C8	-5.08	1.34	1.37
49	C1	1139	A	N7-C5	-5.07	1.36	1.39
25	CJ	113	VAL	CB-CG2	-5.07	1.42	1.52
49	C1	1146	G	C5-C4	-5.02	1.34	1.38
28	CM	310	TRP	CB-CG	-5.01	1.41	1.50

All (727) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	C2	2	G	O5'-P-OP1	-32.38	71.84	110.70
50	C2	2	G	OP1-P-OP2	-26.27	80.19	119.60
24	CI	995	VAL	C-N-CA	19.84	171.29	121.70
50	C2	2	G	O5'-P-OP2	17.99	132.29	110.70
49	C1	2074	C	N1-C2-O2	16.01	128.50	118.90
50	C2	1	A	OP2-P-O3'	-13.64	75.20	105.20
49	C1	1138	C	N3-C2-O2	-13.20	112.66	121.90
49	C1	1155	G	C5-C6-O6	-13.06	120.76	128.60
50	C2	1	A	OP1-P-O3'	13.01	133.82	105.20
49	C1	2168	U	N1-C2-O2	12.86	131.80	122.80
49	C1	1138	C	C2-N1-C1'	12.57	132.63	118.80
49	C1	2168	U	N3-C2-O2	-12.51	113.44	122.20
49	C1	942	U	N3-C2-O2	-12.29	113.60	122.20
49	C1	55	G	OP1-P-O3'	-11.86	79.11	105.20
49	C1	45	U	OP1-P-O3'	-11.29	80.37	105.20
49	C1	2217	C	C2-N1-C1'	11.14	131.05	118.80
49	C1	2217	C	N1-C2-O2	11.00	125.50	118.90
49	C1	2069	G	C8-N9-C4	-10.83	102.07	106.40
32	CR	426	LEU	CA-CB-CG	10.81	140.16	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	CS	426	LEU	CA-CB-CG	10.81	140.16	115.30
49	C1	758	U	N3-C2-O2	-10.75	114.67	122.20
49	C1	2074	C	C2-N1-C1'	10.75	130.62	118.80
49	C1	618	C	N1-C2-O2	10.68	125.31	118.90
49	C1	2074	C	N3-C2-O2	-10.63	114.46	121.90
49	C1	160	C	C6-N1-C2	-10.44	116.12	120.30
49	C1	1547	C	N1-C2-O2	10.40	125.14	118.90
49	C1	160	C	N3-C2-O2	-10.12	114.82	121.90
49	C1	2168	U	C2-N1-C1'	10.10	129.81	117.70
49	C1	785	U	OP1-P-O3'	-10.04	83.10	105.20
49	C1	1155	G	N1-C6-O6	10.03	125.92	119.90
49	C1	1662	C	N3-C2-O2	-9.94	114.94	121.90
49	C1	258	C	N1-C2-O2	9.81	124.78	118.90
49	C1	786	G	OP1-P-OP2	9.79	134.29	119.60
49	C1	1138	C	N1-C2-O2	9.67	124.70	118.90
49	C1	2074	C	C6-N1-C1'	-9.64	109.24	120.80
49	C1	203	C	N1-C2-O2	9.59	124.65	118.90
57	US	335	ASP	C-N-CA	9.57	145.62	121.70
49	C1	505	C	N3-C2-O2	-9.55	115.22	121.90
50	C2	39	U	N3-C2-O2	-9.54	115.52	122.20
26	CK	235	ASP	CB-CG-OD1	9.39	126.75	118.30
32	CS	372	ILE	C-N-CA	9.38	145.15	121.70
32	CR	372	ILE	C-N-CA	9.37	145.12	121.70
49	C1	1138	C	C6-N1-C1'	-9.32	109.62	120.80
49	C1	45	U	OP2-P-O3'	-9.30	84.74	105.20
49	C1	258	C	C2-N1-C1'	9.27	129.00	118.80
50	C2	140	C	N3-C2-O2	-9.14	115.50	121.90
49	C1	758	U	C2-N1-C1'	9.02	128.52	117.70
32	CR	41	LEU	CA-CB-CG	9.00	135.99	115.30
32	CS	41	LEU	CA-CB-CG	8.99	135.98	115.30
49	C1	255	G	C8-N9-C4	-8.99	102.81	106.40
49	C1	255	G	C2-N3-C4	-8.89	107.45	111.90
49	C1	942	U	N1-C2-O2	8.79	128.96	122.80
49	C1	1167	C	N1-C2-O2	8.64	124.08	118.90
49	C1	134	C	C6-N1-C2	-8.64	116.85	120.30
49	C1	618	C	N3-C2-O2	-8.60	115.88	121.90
49	C1	1155	G	C4-C5-N7	8.52	114.21	110.80
49	C1	1550	U	C2-N1-C1'	8.51	127.92	117.70
49	C1	2217	C	C6-N1-C1'	-8.51	110.59	120.80
49	C1	618	C	C2-N1-C1'	8.49	128.14	118.80
49	C1	2181	U	N3-C2-O2	-8.48	116.27	122.20
49	C1	927	C	N3-C2-O2	-8.43	116.00	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	C1	1547	C	C2-N1-C1'	8.38	128.02	118.80
49	C1	1148	G	C4-C5-N7	8.38	114.15	110.80
49	C1	255	G	N3-C2-N2	-8.36	114.05	119.90
49	C1	2173	G	C8-N9-C4	-8.33	103.07	106.40
49	C1	750	C	N1-C2-O2	8.32	123.89	118.90
49	C1	1077	U	N1-C2-O2	8.31	128.62	122.80
49	C1	768	C	C2-N1-C1'	8.29	127.92	118.80
49	C1	2106	U	C2-N1-C1'	8.29	127.65	117.70
49	C1	255	G	N1-C2-N3	8.29	128.87	123.90
49	C1	370	C	N1-C2-O2	8.28	123.87	118.90
49	C1	785	U	OP2-P-O3'	-8.27	87.00	105.20
32	CS	84	ARG	NE-CZ-NH1	8.26	124.43	120.30
53	CW	24	PRO	CA-N-CD	-8.25	99.95	111.50
49	C1	2084	C	N3-C2-O2	-8.24	116.13	121.90
32	CR	84	ARG	NE-CZ-NH1	8.22	124.41	120.30
49	C1	1167	C	C6-N1-C2	-8.19	117.02	120.30
49	C1	159	C	C6-N1-C2	-8.18	117.03	120.30
49	C1	471	C	N3-C2-O2	-8.13	116.21	121.90
50	C2	267	C	N3-C2-O2	-8.13	116.21	121.90
49	C1	413	C	C6-N1-C2	-8.05	117.08	120.30
49	C1	2202	C	N1-C2-O2	8.05	123.73	118.90
49	C1	1747	A	C6-N1-C2	-8.03	113.78	118.60
49	C1	471	C	C6-N1-C2	-7.98	117.11	120.30
49	C1	233	C	C2-N1-C1'	7.97	127.57	118.80
32	CS	162	LEU	CA-CB-CG	7.94	133.56	115.30
32	CR	162	LEU	CA-CB-CG	7.94	133.55	115.30
49	C1	408	C	C5-C6-N1	7.92	124.96	121.00
49	C1	1486	G	C8-N9-C4	-7.92	103.23	106.40
49	C1	1761	C	C6-N1-C2	-7.91	117.14	120.30
49	C1	34	C	N1-C2-O2	7.89	123.64	118.90
49	C1	2182	C	C6-N1-C2	-7.88	117.15	120.30
49	C1	1486	G	N3-C4-C5	-7.87	124.66	128.60
49	C1	68	U	C2-N1-C1'	7.86	127.14	117.70
49	C1	1145	G	C4-C5-N7	7.86	113.94	110.80
49	C1	112	C	N1-C2-O2	7.85	123.61	118.90
49	C1	80	C	N3-C2-O2	-7.85	116.41	121.90
49	C1	408	C	C2-N1-C1'	7.84	127.43	118.80
49	C1	218	G	N3-C4-N9	7.82	130.69	126.00
49	C1	582	G	OP1-P-O3'	7.82	122.39	105.20
49	C1	1145	G	C6-C5-N7	-7.81	125.71	130.40
49	C1	1077	U	N3-C2-O2	-7.80	116.74	122.20
49	C1	1145	G	N3-C4-N9	7.80	130.68	126.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	C1	1167	C	N3-C2-O2	-7.74	116.48	121.90
49	C1	470	C	N1-C2-O2	7.73	123.54	118.90
54	UT	854	LEU	CA-CB-CG	7.72	133.07	115.30
49	C1	148	C	C6-N1-C2	-7.71	117.22	120.30
49	C1	1027	C	N3-C2-O2	-7.68	116.52	121.90
49	C1	2069	G	N3-C4-C5	-7.66	124.77	128.60
49	C1	2202	C	N3-C2-O2	-7.63	116.56	121.90
49	C1	1138	C	C6-N1-C2	-7.61	117.25	120.30
49	C1	449	C	N3-C2-O2	-7.50	116.65	121.90
49	C1	159	C	N3-C2-O2	-7.49	116.66	121.90
49	C1	692	U	N1-C2-O2	7.48	128.04	122.80
49	C1	2069	G	N7-C8-N9	7.47	116.84	113.10
49	C1	134	C	P-O3'-C3'	7.47	128.66	119.70
49	C1	68	U	N1-C2-O2	7.46	128.02	122.80
49	C1	255	G	N3-C4-N9	-7.45	121.53	126.00
30	CP	213	LEU	CA-CB-CG	7.41	132.35	115.30
49	C1	2179	C	N3-C2-O2	-7.41	116.71	121.90
49	C1	34	C	N3-C2-O2	-7.41	116.71	121.90
50	C2	246	G	C4-N9-C1'	7.41	136.13	126.50
49	C1	134	C	C2-N1-C1'	7.40	126.94	118.80
49	C1	370	C	N3-C2-O2	-7.40	116.72	121.90
49	C1	2217	C	N3-C2-O2	-7.39	116.73	121.90
49	C1	1760	G	N3-C4-N9	7.39	130.43	126.00
51	UV	1058	TYR	CA-CB-CG	7.38	127.41	113.40
50	C2	79	G	C4-C5-N7	7.37	113.75	110.80
49	C1	1662	C	N1-C2-O2	7.35	123.31	118.90
49	C1	2106	U	N1-C2-O2	7.35	127.95	122.80
49	C1	2168	U	C6-N1-C1'	-7.35	110.91	121.20
49	C1	148	C	N3-C2-O2	-7.34	116.76	121.90
15	UU	502	LEU	CA-CB-CG	7.32	132.14	115.30
49	C1	362	G	C8-N9-C4	-7.32	103.47	106.40
49	C1	408	C	C6-N1-C2	-7.32	117.37	120.30
49	C1	989	C	C2-N1-C1'	7.31	126.84	118.80
50	C2	203	C	N3-C2-O2	-7.30	116.79	121.90
49	C1	1145	G	C8-N9-C1'	-7.28	117.53	127.00
49	C1	1758	C	C2-N3-C4	-7.27	116.26	119.90
49	C1	1222	C	N1-C2-O2	7.26	123.26	118.90
49	C1	1114	C	N1-C2-O2	7.26	123.25	118.90
49	C1	137	C	N1-C2-O2	7.22	123.23	118.90
49	C1	995	C	C2-N1-C1'	7.21	126.74	118.80
49	C1	2202	C	C2-N1-C1'	7.21	126.73	118.80
49	C1	1180	C	C6-N1-C2	-7.21	117.42	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	C1	454	C	C2-N1-C1'	7.20	126.72	118.80
49	C1	1167	C	C2-N1-C1'	7.20	126.72	118.80
49	C1	2071	G	C5-C6-N1	7.20	115.10	111.50
50	C2	92	A	C2-N3-C4	7.20	114.20	110.60
49	C1	2182	C	C5-C6-N1	7.19	124.59	121.00
49	C1	1174	C	C6-N1-C2	-7.16	117.44	120.30
49	C1	258	C	C5-C6-N1	7.14	124.57	121.00
49	C1	56	C	OP1-P-OP2	7.12	130.28	119.60
49	C1	1550	U	N1-C2-O2	7.12	127.78	122.80
49	C1	2188	G	C4-N9-C1'	7.11	135.74	126.50
49	C1	158	C	N1-C2-O2	7.11	123.16	118.90
49	C1	346	C	N3-C2-O2	-7.10	116.93	121.90
49	C1	2173	G	N7-C8-N9	7.10	116.65	113.10
50	C2	79	G	N3-C4-N9	7.03	130.22	126.00
49	C1	1486	G	C4-N9-C1'	7.02	135.63	126.50
49	C1	618	C	C6-N1-C2	-7.01	117.50	120.30
49	C1	505	C	N1-C2-O2	6.99	123.09	118.90
49	C1	278	A	O5'-P-OP1	-6.99	99.41	105.70
49	C1	851	U	N3-C2-O2	-6.96	117.33	122.20
49	C1	1081	G	C5-C6-O6	6.96	132.78	128.60
49	C1	1171	C	N1-C2-O2	6.96	123.08	118.90
49	C1	1145	G	C4-N9-C1'	6.95	135.54	126.50
49	C1	258	C	C6-N1-C1'	-6.95	112.46	120.80
49	C1	413	C	C2-N1-C1'	6.95	126.44	118.80
49	C1	886	U	N1-C2-O2	6.94	127.66	122.80
49	C1	1077	U	C2-N1-C1'	6.94	126.03	117.70
49	C1	758	U	N1-C2-O2	6.93	127.65	122.80
50	C2	200	U	N1-C2-O2	6.92	127.64	122.80
50	C2	23	A	C6-N1-C2	-6.90	114.46	118.60
49	C1	400	C	C6-N1-C2	-6.90	117.54	120.30
49	C1	1222	C	C2-N1-C1'	6.89	126.39	118.80
49	C1	1645	U	C2-N1-C1'	6.89	125.97	117.70
50	C2	128	C	O4'-C1'-N1	6.89	113.71	108.20
49	C1	1486	G	N7-C8-N9	6.89	116.54	113.10
50	C2	57	A	N1-C6-N6	6.88	122.73	118.60
50	C2	74	C	N3-C2-O2	-6.87	117.09	121.90
49	C1	1163	A	P-O3'-C3'	6.86	127.93	119.70
49	C1	134	C	N3-C2-O2	-6.85	117.10	121.90
49	C1	345	U	N3-C2-O2	-6.84	117.41	122.20
49	C1	400	C	C2-N1-C1'	6.84	126.33	118.80
49	C1	1626	G	C8-N9-C4	-6.84	103.66	106.40
49	C1	1655	U	N3-C2-O2	-6.84	117.41	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	C2	61	G	C8-N9-C1'	6.84	135.89	127.00
49	C1	2173	G	C6-C5-N7	-6.83	126.30	130.40
49	C1	46	C	OP1-P-OP2	6.83	129.84	119.60
50	C2	147	G	N3-C4-N9	6.81	130.09	126.00
49	C1	56	C	C2-N1-C1'	6.80	126.28	118.80
49	C1	255	G	N9-C4-C5	6.79	108.12	105.40
49	C1	1084	C	N3-C2-O2	-6.79	117.15	121.90
49	C1	2180	A	C4-C5-N7	6.79	114.09	110.70
49	C1	203	C	C2-N1-C1'	6.79	126.26	118.80
49	C1	404	C	C2-N1-C1'	6.79	126.26	118.80
49	C1	270	C	N3-C2-O2	-6.78	117.15	121.90
55	UH	832	LEU	CA-CB-CG	-6.77	99.72	115.30
15	UU	715	PHE	C-N-CA	6.77	138.63	121.70
49	C1	692	U	N3-C2-O2	-6.77	117.46	122.20
50	C2	140	C	N1-C2-O2	6.77	122.96	118.90
49	C1	1757	C	N3-C2-O2	-6.76	117.17	121.90
49	C1	218	G	C8-N9-C1'	-6.76	118.22	127.00
49	C1	1145	G	N9-C4-C5	-6.75	102.70	105.40
49	C1	408	C	N1-C2-O2	6.74	122.94	118.90
50	C2	246	G	C8-N9-C1'	-6.74	118.24	127.00
49	C1	491	G	C4-N9-C1'	6.74	135.26	126.50
49	C1	1736	A	N7-C8-N9	6.73	117.17	113.80
50	C2	200	U	C2-N1-C1'	6.72	125.77	117.70
49	C1	2180	A	C6-C5-N7	-6.72	127.59	132.30
50	C2	35	G	C6-C5-N7	-6.72	126.37	130.40
50	C2	260	G	N3-C4-N9	6.71	130.03	126.00
49	C1	1165	U	C2-N1-C1'	6.71	125.75	117.70
49	C1	583	A	O5'-P-OP1	-6.70	99.67	105.70
49	C1	2191	U	C6-N1-C2	-6.70	116.98	121.00
49	C1	55	G	OP2-P-O3'	-6.69	90.49	105.20
49	C1	135	A	C8-N9-C4	-6.68	103.13	105.80
49	C1	1046	G	N1-C6-O6	-6.67	115.90	119.90
55	UH	726	LEU	CA-CB-CG	6.67	130.65	115.30
49	C1	851	U	N1-C2-O2	6.67	127.47	122.80
49	C1	1486	G	C2-N3-C4	6.66	115.23	111.90
50	C2	39	U	N1-C2-O2	6.66	127.46	122.80
49	C1	2229	C	C5-C6-N1	6.65	124.33	121.00
49	C1	1741	A	C8-N9-C4	-6.64	103.14	105.80
24	CI	974	ARG	NE-CZ-NH2	-6.63	116.98	120.30
49	C1	986	C	C2-N1-C1'	6.63	126.09	118.80
49	C1	2071	G	N3-C4-N9	6.63	129.98	126.00
49	C1	915	G	N1-C6-O6	-6.62	115.93	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	C1	218	G	C4-N9-C1'	6.61	135.09	126.50
49	C1	2071	G	N1-C2-N2	-6.61	110.25	116.20
49	C1	2195	U	C2-N1-C1'	6.60	125.62	117.70
49	C1	160	C	N1-C2-O2	6.60	122.86	118.90
49	C1	2047	G	C5-C6-O6	6.57	132.54	128.60
49	C1	449	C	C6-N1-C2	-6.57	117.67	120.30
49	C1	1075	C	N3-C2-O2	-6.56	117.31	121.90
32	CR	167	MET	CA-CB-CG	6.55	124.44	113.30
32	CS	167	MET	CA-CB-CG	6.55	124.43	113.30
49	C1	2047	G	C4-N9-C1'	-6.55	117.99	126.50
49	C1	470	C	C2-N1-C1'	6.53	125.98	118.80
49	C1	2116	C	N3-C2-O2	-6.52	117.33	121.90
49	C1	1471	U	C2-N1-C1'	6.52	125.53	117.70
50	C2	61	G	N3-C4-N9	-6.52	122.09	126.00
49	C1	2176	A	C8-N9-C4	-6.51	103.19	105.80
49	C1	447	C	N3-C2-O2	-6.51	117.34	121.90
49	C1	1758	C	C2-N1-C1'	-6.50	111.65	118.80
49	C1	209	A	P-O3'-C3'	6.50	127.50	119.70
49	C1	2116	C	N1-C2-O2	6.50	122.80	118.90
49	C1	1155	G	C6-C5-N7	-6.50	126.50	130.40
49	C1	2172	C	N3-C2-O2	-6.50	117.35	121.90
49	C1	203	C	N3-C2-O2	-6.50	117.35	121.90
51	UV	159	LEU	CA-CB-CG	6.49	130.23	115.30
49	C1	1747	A	N1-C2-N3	6.49	132.54	129.30
49	C1	1179	G	N9-C4-C5	-6.47	102.81	105.40
50	C2	260	G	C8-N9-C1'	-6.46	118.60	127.00
49	C1	2106	U	N3-C2-O2	-6.46	117.68	122.20
49	C1	2227	C	C2-N1-C1'	6.45	125.90	118.80
49	C1	1736	A	C5-N7-C8	-6.45	100.67	103.90
49	C1	1171	C	N3-C2-O2	-6.44	117.39	121.90
50	C2	56	U	N3-C2-O2	-6.43	117.70	122.20
50	C2	56	U	N1-C2-O2	6.42	127.30	122.80
11	UN	901	LEU	CA-CB-CG	6.42	130.06	115.30
50	C2	57	A	C6-C5-N7	-6.42	127.81	132.30
49	C1	1645	U	N1-C2-O2	6.41	127.29	122.80
49	C1	21	C	N3-C2-O2	-6.41	117.41	121.90
49	C1	2047	G	N3-C4-N9	-6.41	122.15	126.00
49	C1	886	U	N3-C2-O2	-6.41	117.71	122.20
49	C1	2071	G	C6-N1-C2	-6.40	121.26	125.10
50	C2	202	C	N3-C2-O2	-6.40	117.42	121.90
50	C2	128	C	C6-N1-C2	-6.40	117.74	120.30
49	C1	2179	C	N1-C2-O2	6.39	122.73	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	C1	419	G	C8-N9-C1'	-6.38	118.70	127.00
49	C1	419	G	C4-N9-C1'	6.38	134.79	126.50
49	C1	1757	C	N1-C2-O2	6.38	122.73	118.90
50	C2	90	C	O4'-C1'-N1	6.38	113.30	108.20
49	C1	206	C	C2-N1-C1'	6.37	125.81	118.80
49	C1	910	G	C5-C6-O6	6.37	132.42	128.60
49	C1	193	U	N1-C2-O2	6.36	127.25	122.80
49	C1	454	C	N1-C2-O2	6.36	122.72	118.90
49	C1	1166	U	C2-N1-C1'	6.35	125.32	117.70
19	CC	78	LEU	CA-CB-CG	6.34	129.88	115.30
49	C1	2209	U	N3-C2-O2	-6.33	117.77	122.20
49	C1	1156	C	C6-N1-C2	6.33	122.83	120.30
50	C2	267	C	C6-N1-C2	-6.33	117.77	120.30
50	C2	266	C	C2-N1-C1'	6.32	125.75	118.80
49	C1	347	C	C2-N1-C1'	6.31	125.74	118.80
50	C2	260	G	C4-N9-C1'	6.30	134.69	126.50
49	C1	2203	C	N1-C2-O2	6.30	122.68	118.90
49	C1	683	C	C2-N1-C1'	6.30	125.73	118.80
54	UT	698	LEU	CA-CB-CG	6.29	129.78	115.30
49	C1	750	C	N3-C2-O2	-6.29	117.50	121.90
50	C2	266	C	N1-C2-O2	6.28	122.67	118.90
49	C1	190	G	C5-C6-O6	6.28	132.37	128.60
49	C1	1167	C	C5-C6-N1	6.28	124.14	121.00
49	C1	2189	C	N1-C2-O2	6.27	122.66	118.90
49	C1	504	C	N1-C2-O2	6.25	122.65	118.90
49	C1	1145	G	C5-C6-O6	-6.24	124.85	128.60
49	C1	768	C	C6-N1-C1'	-6.24	113.31	120.80
49	C1	255	G	N7-C8-N9	6.24	116.22	113.10
49	C1	370	C	C2-N1-C1'	6.24	125.66	118.80
49	C1	1154	A	C2-N3-C4	-6.24	107.48	110.60
49	C1	129	G	N3-C4-N9	-6.24	122.26	126.00
49	C1	402	U	N1-C2-O2	6.22	127.16	122.80
50	C2	131	U	C2-N1-C1'	6.22	125.17	117.70
49	C1	1550	U	N3-C2-O2	-6.22	117.85	122.20
49	C1	447	C	C6-N1-C2	-6.21	117.81	120.30
49	C1	2217	C	C5-C6-N1	6.21	124.11	121.00
49	C1	233	C	C6-N1-C1'	-6.20	113.36	120.80
49	C1	1148	G	C5-N7-C8	-6.20	101.20	104.30
49	C1	915	G	C5-C6-O6	6.20	132.32	128.60
49	C1	1645	U	N3-C2-O2	-6.20	117.86	122.20
49	C1	618	C	C5-C6-N1	6.18	124.09	121.00
49	C1	1027	C	C6-N1-C2	-6.17	117.83	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	C1	419	G	N3-C4-N9	6.17	129.70	126.00
49	C1	860	C	C2-N1-C1'	-6.17	112.02	118.80
49	C1	1165	U	N1-C2-O2	6.17	127.11	122.80
49	C1	776	C	N1-C2-O2	6.16	122.60	118.90
49	C1	1625	G	N3-C4-N9	6.16	129.70	126.00
49	C1	1046	G	C5-C6-O6	6.15	132.29	128.60
49	C1	1547	C	C5-C6-N1	6.14	124.07	121.00
49	C1	303	C	C5-C6-N1	6.14	124.07	121.00
49	C1	281	U	P-O3'-C3'	6.14	127.06	119.70
32	CR	901	LEU	CA-CB-CG	6.13	129.41	115.30
1	UA	426	LEU	CA-CB-CG	6.13	129.41	115.30
50	C2	82	U	N1-C2-O2	6.13	127.09	122.80
8	UK	51	LEU	CB-CG-CD2	-6.13	100.58	111.00
32	CS	901	LEU	CA-CB-CG	6.13	129.39	115.30
49	C1	2230	U	N3-C2-O2	-6.12	117.91	122.20
7	UJ	488	LEU	CA-CB-CG	6.12	129.38	115.30
49	C1	33	C	N3-C2-O2	-6.12	117.61	121.90
49	C1	1630	C	N3-C2-O2	-6.12	117.61	121.90
49	C1	2047	G	N1-C6-O6	-6.12	116.23	119.90
49	C1	371	U	C2-N1-C1'	6.11	125.03	117.70
49	C1	1120	C	C2-N1-C1'	6.11	125.52	118.80
50	C2	128	C	C5-C6-N1	6.11	124.05	121.00
49	C1	190	G	N3-C4-N9	-6.10	122.34	126.00
49	C1	1113	C	N1-C2-O2	6.08	122.55	118.90
49	C1	1157	C	C2-N1-C1'	6.08	125.49	118.80
49	C1	1179	G	C4-C5-N7	6.07	113.23	110.80
49	C1	277	U	P-O3'-C3'	6.07	126.98	119.70
49	C1	417	G	C6-C5-N7	-6.06	126.77	130.40
50	C2	202	C	N1-C2-O2	6.06	122.53	118.90
49	C1	1147	U	OP2-P-O3'	6.04	118.49	105.20
49	C1	1001	A	OP2-P-O3'	6.04	118.48	105.20
1	UA	656	LEU	CA-CB-CG	-6.04	101.42	115.30
55	UH	730	PHE	C-N-CA	6.03	136.78	121.70
50	C2	57	A	C4-C5-C6	6.03	120.02	117.00
49	C1	1760	G	C8-N9-C1'	-6.03	119.16	127.00
50	C2	23	A	C5-C6-N1	6.03	120.72	117.70
49	C1	622	U	N3-C2-O2	-6.03	117.98	122.20
49	C1	1549	U	N3-C4-C5	6.02	118.21	114.60
49	C1	2071	G	N3-C4-C5	-6.01	125.59	128.60
12	UO	239	LEU	CA-CB-CG	6.01	129.12	115.30
49	C1	2089	G	N3-C4-N9	6.01	129.61	126.00
49	C1	908	C	C5-C6-N1	6.00	124.00	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	C2	79	G	C6-C5-N7	-5.99	126.81	130.40
49	C1	2075	U	O5'-P-OP2	-5.99	100.31	105.70
49	C1	683	C	N1-C2-O2	5.98	122.49	118.90
29	CO	164	GLN	C-N-CA	5.98	136.65	121.70
49	C1	258	C	N3-C2-O2	-5.97	117.72	121.90
50	C2	5	A	C8-N9-C4	5.97	108.19	105.80
49	C1	2196	U	N3-C2-O2	-5.96	118.03	122.20
49	C1	1120	C	N1-C2-O2	5.96	122.47	118.90
49	C1	1473	U	C5-C6-N1	5.95	125.67	122.70
26	CK	89	LEU	CB-CG-CD2	-5.95	100.89	111.00
50	C2	61	G	C4-N9-C1'	-5.95	118.77	126.50
49	C1	2069	G	N9-C4-C5	5.94	107.78	105.40
50	C2	63	G	C4-N9-C1'	5.94	134.22	126.50
49	C1	3	G	N3-C4-N9	-5.94	122.44	126.00
49	C1	1141	G	C4-C5-N7	5.93	113.17	110.80
49	C1	1547	C	N3-C2-O2	-5.93	117.75	121.90
49	C1	769	C	C2-N1-C1'	5.92	125.31	118.80
50	C2	252	C	N3-C2-O2	-5.92	117.75	121.90
50	C2	140	C	C6-N1-C2	-5.92	117.93	120.30
49	C1	1735	A	N3-C4-N9	5.91	132.13	127.40
49	C1	1625	G	N3-C4-C5	-5.91	125.64	128.60
49	C1	2047	G	C8-N9-C1'	5.90	134.67	127.00
49	C1	2090	G	C2-N3-C4	-5.90	108.95	111.90
49	C1	1222	C	N3-C2-O2	-5.89	117.78	121.90
49	C1	1138	C	C4-C5-C6	5.88	120.34	117.40
49	C1	1001	A	P-O3'-C3'	5.88	126.75	119.70
49	C1	1760	G	C4-N9-C1'	5.87	134.14	126.50
50	C2	255	U	P-O3'-C3'	5.87	126.74	119.70
48	CU	116	LEU	CA-CB-CG	5.87	128.79	115.30
49	C1	1560	C	N3-C2-O2	-5.86	117.80	121.90
49	C1	80	C	C6-N1-C2	-5.86	117.96	120.30
49	C1	247	C	C6-N1-C2	-5.85	117.96	120.30
49	C1	1758	C	C6-N1-C1'	5.85	127.82	120.80
49	C1	148	C	N1-C2-N3	5.85	123.30	119.20
49	C1	112	C	N3-C2-O2	-5.85	117.81	121.90
49	C1	68	U	C6-N1-C1'	-5.84	113.02	121.20
54	UT	2116	LEU	CA-CB-CG	-5.84	101.87	115.30
49	C1	2180	A	C5-N7-C8	-5.84	100.98	103.90
49	C1	491	G	C8-N9-C1'	-5.83	119.42	127.00
49	C1	910	G	N3-C4-N9	-5.83	122.50	126.00
49	C1	1547	C	C6-N1-C1'	-5.82	113.81	120.80
49	C1	1550	U	C6-N1-C1'	-5.82	113.05	121.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	C1	2173	G	C4-C5-N7	5.82	113.13	110.80
49	C1	2188	G	C8-N9-C1'	-5.82	119.44	127.00
49	C1	347	C	C6-N1-C2	-5.81	117.97	120.30
49	C1	419	G	C6-C5-N7	-5.81	126.91	130.40
49	C1	989	C	N1-C2-O2	5.81	122.39	118.90
49	C1	2049	G	C6-N1-C2	-5.81	121.62	125.10
49	C1	1736	A	C4-C5-N7	5.80	113.60	110.70
49	C1	1175	A	C6-N1-C2	-5.80	115.12	118.60
49	C1	1560	C	N1-C2-O2	5.80	122.38	118.90
56	UI	179	LEU	CA-CB-CG	5.79	128.62	115.30
50	C2	101	G	N3-C4-N9	-5.78	122.53	126.00
49	C1	496	U	N3-C2-O2	-5.78	118.15	122.20
49	C1	886	U	C2-N1-C1'	5.78	124.64	117.70
49	C1	1472	A	N7-C8-N9	5.78	116.69	113.80
49	C1	2177	G	C8-N9-C4	-5.77	104.09	106.40
56	UE	179	LEU	CA-CB-CG	5.77	128.58	115.30
50	C2	136	C	N1-C2-O2	5.77	122.36	118.90
49	C1	470	C	N3-C2-O2	-5.76	117.87	121.90
49	C1	287	C	C5-C6-N1	5.76	123.88	121.00
49	C1	922	C	N3-C2-O2	-5.76	117.87	121.90
49	C1	2223	C	C2-N1-C1'	5.75	125.13	118.80
49	C1	1655	U	N1-C2-N3	5.75	118.35	114.90
50	C2	200	U	N3-C2-O2	-5.74	118.18	122.20
51	UV	1054	LEU	CA-CB-CG	5.74	128.51	115.30
49	C1	2181	U	N1-C2-O2	5.74	126.82	122.80
49	C1	56	C	N1-C2-O2	5.74	122.34	118.90
49	C1	413	C	C5-C6-N1	5.74	123.87	121.00
49	C1	2165	U	C5-C6-N1	5.73	125.57	122.70
49	C1	343	C	C2-N1-C1'	5.73	125.10	118.80
49	C1	1149	C	N3-C4-N4	-5.73	113.99	118.00
49	C1	369	U	C2-N1-C1'	5.72	124.57	117.70
49	C1	190	G	N9-C4-C5	5.72	107.69	105.40
49	C1	1658	G	C5-C6-O6	5.72	132.03	128.60
49	C1	2203	C	C2-N1-C1'	5.72	125.09	118.80
49	C1	1114	C	N3-C2-O2	-5.71	117.91	121.90
49	C1	371	U	N3-C2-O2	-5.70	118.21	122.20
49	C1	1150	C	C2-N1-C1'	5.70	125.08	118.80
49	C1	776	C	C2-N1-C1'	5.70	125.07	118.80
49	C1	1000	A	O4'-C1'-N9	5.70	112.76	108.20
49	C1	2071	G	O4'-C1'-N9	-5.70	103.64	108.20
50	C2	38	G	O4'-C1'-N9	-5.70	103.64	108.20
20	CD	102	LEU	CA-CB-CG	5.69	128.40	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	C1	2195	U	N1-C2-O2	5.69	126.79	122.80
49	C1	986	C	N1-C2-O2	5.69	122.31	118.90
49	C1	228	G	C5-C6-O6	-5.69	125.19	128.60
49	C1	2173	G	C5-N7-C8	-5.68	101.46	104.30
49	C1	1136	G	N1-C6-O6	-5.68	116.49	119.90
49	C1	1140	A	N1-C6-N6	5.68	122.01	118.60
50	C2	79	G	N9-C4-C5	-5.68	103.13	105.40
32	CR	766	LEU	CA-CB-CG	5.68	128.36	115.30
49	C1	758	U	C6-N1-C1'	-5.68	113.25	121.20
49	C1	2110	C	C2-N1-C1'	5.68	125.04	118.80
49	C1	2209	U	N1-C2-O2	5.68	126.77	122.80
49	C1	2164	C	C6-N1-C2	-5.67	118.03	120.30
49	C1	454	C	C6-N1-C1'	-5.67	113.99	120.80
32	CS	766	LEU	CA-CB-CG	5.67	128.34	115.30
49	C1	582	G	P-O3'-C3'	5.66	126.49	119.70
49	C1	2177	G	O4'-C1'-N9	5.65	112.72	108.20
49	C1	1714	G	N3-C4-C5	-5.64	125.78	128.60
49	C1	2210	U	C5-C4-O4	5.64	129.29	125.90
49	C1	190	G	N1-C6-O6	-5.64	116.52	119.90
50	C2	251	U	C2-N1-C1'	5.64	124.47	117.70
49	C1	2106	U	C5-C6-N1	5.64	125.52	122.70
49	C1	2178	U	C5-C4-O4	-5.64	122.52	125.90
49	C1	134	C	N1-C2-O2	5.64	122.28	118.90
49	C1	1120	C	N3-C2-O2	-5.63	117.96	121.90
49	C1	1155	G	C5-N7-C8	-5.63	101.48	104.30
49	C1	1736	A	N9-C4-C5	-5.63	103.55	105.80
49	C1	160	C	C5-C6-N1	5.63	123.81	121.00
49	C1	1136	G	C5-C6-N1	5.62	114.31	111.50
13	UQ	648	LEU	CA-CB-CG	5.62	128.21	115.30
49	C1	1136	G	C2-N3-C4	5.61	114.71	111.90
49	C1	1667	G	C8-N9-C4	-5.61	104.15	106.40
49	C1	1139	A	C8-N9-C4	-5.61	103.56	105.80
49	C1	1625	G	N3-C2-N2	5.61	123.83	119.90
10	UM	674	LEU	CA-CB-CG	5.61	128.19	115.30
50	C2	148	G	C5-C6-O6	5.61	131.96	128.60
49	C1	294	G	N1-C2-N3	5.60	127.26	123.90
49	C1	2227	C	C6-N1-C1'	-5.60	114.08	120.80
32	CS	84	ARG	CG-CD-NE	5.60	123.56	111.80
49	C1	2216	A	N7-C8-N9	5.60	116.60	113.80
49	C1	1759	U	C2-N1-C1'	5.60	124.42	117.70
50	C2	136	C	C2-N1-C1'	5.60	124.95	118.80
37	Ce	38	ALA	C-N-CA	5.59	135.69	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	C1	2047	G	N3-C4-C5	5.59	131.40	128.60
49	C1	2164	C	N3-C2-O2	-5.59	117.98	121.90
51	UV	334	LEU	CA-CB-CG	5.58	128.14	115.30
32	CR	84	ARG	CG-CD-NE	5.58	123.52	111.80
49	C1	676	C	N3-C2-O2	-5.58	118.00	121.90
49	C1	989	C	C6-N1-C1'	-5.58	114.11	120.80
50	C2	67	C	C2-N1-C1'	5.58	124.93	118.80
49	C1	1026	C	N3-C2-O2	-5.55	118.01	121.90
50	C2	246	G	N3-C4-N9	5.55	129.33	126.00
23	CH	202	LEU	CA-CB-CG	5.55	128.07	115.30
49	C1	742	U	P-O3'-C3'	5.55	126.36	119.70
49	C1	1759	U	N3-C2-O2	-5.55	118.31	122.20
49	C1	18	G	C4-N9-C1'	5.55	133.71	126.50
49	C1	2229	C	C6-N1-C2	-5.55	118.08	120.30
49	C1	134	C	OP1-P-O3'	5.54	117.40	105.20
49	C1	18	G	N3-C4-C5	-5.54	125.83	128.60
49	C1	988	G	C8-N9-C1'	-5.54	119.80	127.00
49	C1	2203	C	N3-C2-O2	-5.54	118.02	121.90
49	C1	769	C	C6-N1-C2	-5.54	118.09	120.30
49	C1	1666	C	C2-N1-C1'	5.54	124.89	118.80
49	C1	203	C	C6-N1-C1'	-5.53	114.16	120.80
50	C2	147	G	C8-N9-C1'	-5.53	119.81	127.00
50	C2	251	U	N3-C2-O2	-5.52	118.34	122.20
49	C1	1149	C	C5-C6-N1	-5.51	118.25	121.00
49	C1	485	G	N3-C4-N9	-5.51	122.70	126.00
49	C1	2176	A	C6-N1-C2	-5.51	115.30	118.60
49	C1	254	G	C8-N9-C4	-5.50	104.20	106.40
24	CI	240	THR	C-N-CA	-5.50	107.94	121.70
49	C1	1633	A	N1-C6-N6	-5.50	115.30	118.60
49	C1	2071	G	N3-C2-N2	5.50	123.75	119.90
50	C2	92	A	C4-N9-C1'	5.49	136.19	126.30
49	C1	1166	U	C5-C6-N1	5.49	125.44	122.70
49	C1	446	C	N1-C2-O2	5.48	122.19	118.90
49	C1	1081	G	N1-C6-O6	-5.47	116.62	119.90
49	C1	2054	A	P-O3'-C3'	5.47	126.27	119.70
49	C1	2352	U	N1-C2-O2	5.47	126.63	122.80
49	C1	2069	G	C4-N9-C1'	5.46	133.60	126.50
49	C1	2195	U	N3-C2-O2	-5.46	118.38	122.20
49	C1	1144	U	N3-C4-O4	5.46	123.22	119.40
49	C1	1736	A	C6-C5-N7	-5.46	128.48	132.30
49	C1	860	C	C6-N1-C1'	5.46	127.35	120.80
49	C1	2180	A	N1-C6-N6	5.46	121.87	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	C2	131	U	N1-C2-O2	5.45	126.62	122.80
49	C1	135	A	N7-C8-N9	5.45	116.53	113.80
49	C1	204	U	C2-N1-C1'	-5.45	111.16	117.70
49	C1	2084	C	C6-N1-C2	-5.45	118.12	120.30
49	C1	692	U	C2-N1-C1'	5.45	124.23	117.70
49	C1	1757	C	C6-N1-C2	-5.44	118.12	120.30
49	C1	206	C	O4'-C1'-N1	5.43	112.55	108.20
49	C1	2180	A	C4-N9-C1'	5.43	136.08	126.30
6	UG	355	LEU	CA-CB-CG	5.43	127.78	115.30
50	C2	92	A	N3-C4-C5	-5.43	123.00	126.80
28	CM	321	TYR	CB-CG-CD2	-5.42	117.75	121.00
49	C1	2090	G	N3-C4-N9	-5.42	122.75	126.00
49	C1	1547	C	C6-N1-C2	-5.41	118.14	120.30
50	C2	147	G	C4-N9-C1'	5.41	133.53	126.50
29	CO	148	LEU	CA-CB-CG	5.40	127.73	115.30
50	C2	92	A	N3-C4-N9	5.40	131.72	127.40
49	C1	505	C	C6-N1-C2	-5.40	118.14	120.30
49	C1	1761	C	C5-C6-N1	5.40	123.70	121.00
49	C1	462	G	N1-C6-O6	-5.40	116.66	119.90
13	UQ	442	LEU	CA-CB-CG	5.39	127.71	115.30
49	C1	2	G	N3-C4-N9	5.39	129.24	126.00
49	C1	618	C	C6-N1-C1'	-5.39	114.33	120.80
49	C1	1148	G	C2-N3-C4	-5.39	109.20	111.90
49	C1	1165	U	C6-N1-C1'	-5.39	113.65	121.20
49	C1	1486	G	N3-C4-N9	5.39	129.24	126.00
49	C1	2230	U	N1-C2-O2	5.39	126.57	122.80
13	UQ	777	LEU	CA-CB-CG	5.39	127.69	115.30
16	UX	52	LEU	CA-CB-CG	5.39	127.69	115.30
49	C1	863	G	N3-C4-N9	-5.38	122.77	126.00
49	C1	354	G	C4-C5-N7	5.37	112.95	110.80
18	CA	290	LEU	CA-CB-CG	5.37	127.64	115.30
49	C1	2106	U	C6-N1-C1'	-5.37	113.69	121.20
49	C1	2156	A	P-O3'-C3'	5.36	126.14	119.70
49	C1	3	G	C5-C6-O6	5.36	131.82	128.60
49	C1	1760	G	C6-C5-N7	-5.36	127.18	130.40
50	C2	74	C	N1-C2-O2	5.36	122.12	118.90
49	C1	148	C	C6-N1-C1'	5.35	127.22	120.80
51	UV	414	LEU	CA-CB-CG	5.35	127.61	115.30
49	C1	2177	G	C6-C5-N7	-5.35	127.19	130.40
49	C1	205	C	P-O3'-C3'	5.35	126.12	119.70
4	UD	397	LEU	CA-CB-CG	5.34	127.59	115.30
49	C1	68	U	N3-C2-O2	-5.34	118.46	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	C1	1026	C	N1-C2-O2	5.34	122.11	118.90
50	C2	63	G	N3-C4-C5	-5.33	125.93	128.60
50	C2	244	G	C5-C6-O6	5.33	131.80	128.60
49	C1	68	U	C5-C6-N1	5.33	125.36	122.70
49	C1	485	G	C5-C6-O6	5.32	131.79	128.60
49	C1	988	G	N3-C4-N9	5.32	129.19	126.00
49	C1	2203	C	C6-N1-C2	-5.32	118.17	120.30
49	C1	281	U	OP1-P-O3'	5.32	116.90	105.20
50	C2	82	U	C2-N1-C1'	5.32	124.08	117.70
49	C1	658	A	N1-C2-N3	5.31	131.96	129.30
49	C1	988	G	C4-N9-C1'	5.31	133.41	126.50
50	C2	28	U	C5-C6-N1	-5.31	120.04	122.70
49	C1	402	U	C2-N1-C1'	5.31	124.07	117.70
49	C1	1485	A	P-O3'-C3'	5.30	126.06	119.70
49	C1	986	C	C6-N1-C2	-5.30	118.18	120.30
49	C1	1071	G	C6-C5-N7	-5.30	127.22	130.40
49	C1	2171	G	N1-C6-O6	-5.30	116.72	119.90
49	C1	860	C	N3-C2-O2	-5.29	118.19	121.90
49	C1	912	U	N3-C2-O2	-5.29	118.50	122.20
49	C1	1183	A	N7-C8-N9	5.29	116.44	113.80
49	C1	346	C	C6-N1-C2	-5.29	118.18	120.30
49	C1	491	G	N3-C4-N9	5.29	129.17	126.00
49	C1	942	U	O4'-C1'-N1	5.29	112.43	108.20
49	C1	684	U	P-O3'-C3'	5.28	126.04	119.70
49	C1	404	C	C6-N1-C1'	-5.28	114.47	120.80
49	C1	2182	C	O5'-P-OP2	-5.28	100.95	105.70
49	C1	231	U	N1-C2-O2	5.27	126.49	122.80
50	C2	131	U	C5-C6-N1	5.27	125.33	122.70
49	C1	18	G	N3-C4-N9	5.27	129.16	126.00
50	C2	90	C	C2-N1-C1'	-5.27	113.00	118.80
50	C2	79	G	C5-C6-N1	5.27	114.13	111.50
49	C1	910	G	N1-C6-O6	-5.26	116.74	119.90
49	C1	1140	A	C2-N3-C4	-5.26	107.97	110.60
49	C1	865	G	N1-C2-N2	-5.26	111.47	116.20
49	C1	2172	C	N1-C2-O2	5.26	122.05	118.90
49	C1	129	G	C2-N3-C4	-5.25	109.27	111.90
49	C1	218	G	N3-C4-C5	-5.25	125.97	128.60
49	C1	408	C	N3-C2-O2	-5.25	118.22	121.90
49	C1	2071	G	N1-C6-O6	-5.25	116.75	119.90
49	C1	359	C	N3-C2-O2	-5.25	118.22	121.90
49	C1	1124	G	O4'-C1'-N9	5.25	112.40	108.20
50	C2	203	C	C6-N1-C2	-5.25	118.20	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	C1	228	G	C8-N9-C4	-5.24	104.30	106.40
49	C1	1708	A	N7-C8-N9	5.24	116.42	113.80
49	C1	129	G	N3-C4-C5	5.24	131.22	128.60
49	C1	2111	U	N3-C2-O2	-5.24	118.53	122.20
49	C1	262	G	N3-C4-N9	5.24	129.14	126.00
49	C1	743	U	O5'-P-OP1	-5.24	100.99	105.70
32	CS	295	MET	CA-CB-CG	5.23	122.19	113.30
49	C1	80	C	C6-N1-C1'	5.23	127.08	120.80
49	C1	770	C	C2-N1-C1'	5.23	124.55	118.80
32	CR	784	LYS	CA-CB-CG	5.23	124.90	113.40
50	C2	82	U	N3-C2-O2	-5.23	118.54	122.20
9	UL	601	LEU	CA-CB-CG	5.23	127.32	115.30
49	C1	2180	A	N9-C4-C5	-5.23	103.71	105.80
50	C2	73	C	N3-C2-O2	-5.22	118.24	121.90
49	C1	56	C	C6-N1-C1'	-5.22	114.53	120.80
49	C1	1458	U	N1-C2-O2	5.22	126.45	122.80
49	C1	1745	C	N1-C2-O2	5.22	122.03	118.90
32	CR	295	MET	CA-CB-CG	5.22	122.17	113.30
49	C1	1760	G	N9-C4-C5	-5.22	103.31	105.40
49	C1	2116	C	C6-N1-C2	-5.21	118.21	120.30
50	C2	161	G	C4-N9-C1'	5.21	133.28	126.50
56	UE	214	LEU	CB-CG-CD1	-5.21	102.14	111.00
49	C1	1102	A	O4'-C1'-N9	5.21	112.37	108.20
32	CS	784	LYS	CA-CB-CG	5.21	124.86	113.40
49	C1	246	G	N3-C4-N9	5.21	129.12	126.00
49	C1	909	G	N3-C4-N9	5.21	129.12	126.00
49	C1	1050	U	N3-C2-O2	-5.21	118.56	122.20
56	UI	214	LEU	CB-CG-CD1	-5.21	102.15	111.00
49	C1	995	C	C6-N1-C1'	-5.20	114.56	120.80
49	C1	2173	G	C4-N9-C1'	5.20	133.26	126.50
49	C1	2238	A	N7-C8-N9	5.20	116.40	113.80
49	C1	1125	A	C4-N9-C1'	5.19	135.65	126.30
49	C1	2181	U	O5'-P-OP1	-5.19	101.03	105.70
49	C1	3	G	N9-C4-C5	5.19	107.48	105.40
49	C1	1175	A	C5-C6-N6	-5.19	119.55	123.70
49	C1	593	G	P-O3'-C3'	5.19	125.93	119.70
2	UB	818	ASP	CB-CG-OD2	5.18	122.97	118.30
49	C1	1646	U	O4'-C1'-N1	5.18	112.35	108.20
49	C1	726	U	N3-C2-O2	-5.18	118.57	122.20
49	C1	345	U	N1-C2-O2	5.18	126.43	122.80
49	C1	1448	A	C5-C6-N1	5.18	120.29	117.70
49	C1	2119	G	C4-N9-C1'	5.18	133.24	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	C1	111	U	N3-C2-O2	-5.18	118.58	122.20
49	C1	294	G	C2-N3-C4	-5.18	109.31	111.90
50	C2	61	G	O4'-C1'-N9	5.17	112.34	108.20
49	C1	889	C	C5-C6-N1	5.17	123.58	121.00
9	UL	376	LEU	C-N-CA	-5.16	108.79	121.70
49	C1	112	C	C2-N1-C1'	5.16	124.48	118.80
50	C2	18	G	N1-C6-O6	-5.16	116.80	119.90
49	C1	218	G	N9-C4-C5	-5.16	103.33	105.40
50	C2	147	G	N9-C4-C5	-5.16	103.34	105.40
49	C1	2069	G	N1-C6-O6	-5.16	116.81	119.90
49	C1	2178	U	C4-C5-C6	-5.15	116.61	119.70
49	C1	1101	U	N3-C2-O2	-5.15	118.59	122.20
49	C1	402	U	N3-C2-O2	-5.15	118.60	122.20
49	C1	146	C	N1-C2-O2	5.14	121.98	118.90
49	C1	29	C	C5-C6-N1	5.14	123.57	121.00
49	C1	246	G	N3-C4-C5	-5.13	126.03	128.60
51	UV	661	LEU	CA-CB-CG	5.13	127.11	115.30
49	C1	2216	A	C8-N9-C4	-5.13	103.75	105.80
49	C1	1089	A	N1-C6-N6	-5.13	115.52	118.60
49	C1	2179	C	N3-C4-N4	-5.13	114.41	118.00
49	C1	446	C	N3-C2-O2	-5.13	118.31	121.90
49	C1	614	U	C2-N1-C1'	5.13	123.85	117.70
49	C1	485	G	N9-C4-C5	5.12	107.45	105.40
49	C1	496	U	N1-C2-O2	5.12	126.39	122.80
49	C1	768	C	C5-C6-N1	5.12	123.56	121.00
49	C1	1052	A	C4-C5-N7	5.12	113.26	110.70
26	CK	89	LEU	CA-CB-CG	5.12	127.07	115.30
49	C1	448	C	N3-C2-O2	-5.12	118.32	121.90
49	C1	228	G	C6-C5-N7	-5.11	127.33	130.40
49	C1	1085	U	P-O3'-C3'	5.11	125.83	119.70
49	C1	1626	G	C6-N1-C2	-5.11	122.03	125.10
32	CS	559	MET	CG-SD-CE	5.11	108.37	100.20
50	C2	246	G	C6-C5-N7	-5.11	127.34	130.40
49	C1	343	C	N1-C2-O2	5.11	121.96	118.90
49	C1	1081	G	N1-C2-N3	5.11	126.96	123.90
49	C1	1148	G	N3-C4-C5	5.10	131.15	128.60
49	C1	915	G	N9-C4-C5	5.10	107.44	105.40
50	C2	131	U	N3-C2-O2	-5.10	118.63	122.20
49	C1	1667	G	C6-C5-N7	-5.10	127.34	130.40
32	CR	559	MET	CG-SD-CE	5.10	108.36	100.20
49	C1	137	C	N3-C2-O2	-5.10	118.33	121.90
10	UM	524	ILE	C-N-CD	5.09	139.09	128.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	C1	2078	C	N3-C2-O2	-5.09	118.34	121.90
49	C1	750	C	C2-N1-C1'	5.09	124.40	118.80
49	C1	434	A	N1-C6-N6	-5.09	115.55	118.60
49	C1	145	C	N1-C2-O2	5.08	121.95	118.90
49	C1	56	C	O5'-P-OP1	5.08	116.79	110.70
49	C1	225	C	C6-N1-C2	-5.07	118.27	120.30
54	UT	1938	LEU	CA-CB-CG	5.07	126.95	115.30
24	CI	833	LEU	CB-CG-CD2	-5.06	102.39	111.00
50	C2	23	A	P-O3'-C3'	5.06	125.77	119.70
32	CR	84	ARG	CD-NE-CZ	5.05	130.68	123.60
49	C1	2180	A	C8-N9-C1'	-5.05	118.61	127.70
49	C1	200	A	C8-N9-C4	5.05	107.82	105.80
49	C1	363	G	C6-C5-N7	-5.05	127.37	130.40
49	C1	1735	A	C2-N3-C4	5.04	113.12	110.60
49	C1	2202	C	C6-N1-C1'	-5.04	114.75	120.80
49	C1	1052	A	N1-C6-N6	5.04	121.62	118.60
49	C1	220	A	C4-N9-C1'	5.04	135.37	126.30
7	UJ	682	LEU	CA-CB-CG	5.03	126.87	115.30
49	C1	1158	G	N3-C4-C5	5.03	131.12	128.60
49	C1	148	C	C5-C4-N4	5.03	123.72	120.20
50	C2	65	C	C6-N1-C2	-5.03	118.29	120.30
50	C2	244	G	N1-C6-O6	-5.02	116.89	119.90
49	C1	1547	C	C2-N3-C4	5.02	122.41	119.90
49	C1	369	U	N3-C2-O2	-5.02	118.69	122.20
49	C1	228	G	N7-C8-N9	5.01	115.61	113.10
49	C1	888	U	N3-C2-O2	-5.01	118.69	122.20
49	C1	2047	G	C6-C5-N7	5.01	133.41	130.40
49	C1	2083	C	N1-C2-O2	5.01	121.91	118.90
49	C1	684	U	N1-C2-O2	5.01	126.31	122.80
32	CS	84	ARG	CD-NE-CZ	5.01	130.61	123.60
49	C1	462	G	C5-C6-O6	5.01	131.60	128.60
61	CZ	552	LEU	CA-CB-CG	5.01	126.81	115.30
49	C1	154	C	C2-N1-C1'	5.00	124.31	118.80
49	C1	1658	G	N9-C4-C5	5.00	107.40	105.40
49	C1	2106	U	OP2-P-O3'	5.00	116.21	105.20
49	C1	2358	U	N1-C2-O2	5.00	126.30	122.80

There are no chirality outliers.

All (74) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	CB	293	GLU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
21	CE	33	GLN	Peptide
21	CF	14	ASP	Peptide
21	CF	60	GLN	Peptide
23	CH	170	ARG	Peptide
24	CI	132	VAL	Peptide
24	CI	141	ASP	Peptide
24	CI	211	ASN	Peptide
24	CI	303	PRO	Peptide
24	CI	855	THR	Peptide
24	CI	885	CYS	Peptide
25	CJ	101	VAL	Peptide
25	CJ	144	ARG	Peptide
26	CK	173	ARG	Peptide
28	CM	322	HIS	Peptide
29	CO	84	ILE	Peptide
29	CO	88	ARG	Peptide
32	CR	901	LEU	Peptide
32	CS	901	LEU	Peptide
52	CV	88	LYS	Peptide
52	CV	91	HIS	Peptide
60	CY	374	ARG	Peptide
37	Ce	38	ALA	Peptide
41	Ci	137	ASP	Peptide
42	Cj	126	PRO	Peptide
42	Cj	39	PHE	Peptide
42	Cj	40	ALA	Peptide
58	Cl	79	TYR	Peptide
45	Cn	68	ILE	Peptide
46	Co	365	ASN	Peptide
63	Cz	1628	THR	Peptide
1	UA	273	GLY	Peptide
1	UA	320	GLY	Peptide
1	UA	386	THR	Peptide
1	UA	424	GLU	Peptide
1	UA	443	GLY	Peptide
1	UA	506	PRO	Peptide
1	UA	618	LEU	Peptide
1	UA	622	GLN	Peptide
1	UA	641	ASP	Peptide
1	UA	667	ARG	Peptide
5	UF	120	VAL	Peptide
6	UG	227	TYR	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
6	UG	264	LEU	Peptide
55	UH	753	THR	Peptide
8	UK	12	ALA	Peptide
8	UK	83	PHE	Peptide
9	UL	150	GLY	Peptide
9	UL	17	VAL	Peptide
10	UM	204	ASP	Peptide
10	UM	328	LEU	Peptide
10	UM	383	LEU	Peptide
10	UM	589	VAL	Peptide
11	UN	901	LEU	Peptide
12	UO	282	ALA	Peptide
13	UQ	707	PRO	Peptide
13	UQ	849	ALA	Peptide
54	UT	1516	LEU	Peptide
54	UT	1566	GLU	Peptide
54	UT	408	PRO	Peptide
54	UT	486	GLU	Peptide
54	UT	781	TRP	Peptide
15	UU	397	ASP	Peptide
15	UU	402	GLU	Peptide
15	UU	758	HIS	Peptide
15	UU	759	THR	Peptide
51	UV	1013	ASP	Peptide
51	UV	1058	TYR	Peptide
51	UV	1104	LEU	Peptide
51	UV	57	PHE	Peptide
16	UX	-5	LYS	Peptide
16	UX	126	LYS	Peptide
17	UZ	103	ASP	Peptide
17	UZ	273	GLN	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 PDB entries followed by that with respect to all EM

entries.

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	
1	UA	835/904 (92%)	733 (88%)	102 (12%)	0	100	100
2	UB	502/907 (55%)	472 (94%)	30 (6%)	0	100	100
3	UC	72/648 (11%)	58 (81%)	14 (19%)	0	100	100
4	UD	754/884 (85%)	708 (94%)	46 (6%)	0	100	100
5	UF	325/414 (78%)	303 (93%)	21 (6%)	1 (0%)	41	76
6	UG	475/558 (85%)	433 (91%)	39 (8%)	3 (1%)	25	65
7	UJ	1062/1802 (59%)	1000 (94%)	62 (6%)	0	100	100
8	UK	211/270 (78%)	196 (93%)	15 (7%)	0	100	100
9	UL	767/962 (80%)	704 (92%)	63 (8%)	0	100	100
10	UM	645/912 (71%)	595 (92%)	49 (8%)	1 (0%)	47	81
11	UN	171/938 (18%)	161 (94%)	9 (5%)	1 (1%)	25	65
12	UO	498/557 (89%)	459 (92%)	39 (8%)	0	100	100
13	UQ	775/960 (81%)	703 (91%)	71 (9%)	1 (0%)	51	85
14	UR	437/618 (71%)	400 (92%)	37 (8%)	0	100	100
15	UU	890/1049 (85%)	797 (90%)	93 (10%)	0	100	100
16	UX	188/193 (97%)	172 (92%)	16 (8%)	0	100	100
17	UZ	229/391 (59%)	206 (90%)	23 (10%)	0	100	100
18	CA	238/313 (76%)	218 (92%)	20 (8%)	0	100	100
18	CB	235/313 (75%)	216 (92%)	19 (8%)	0	100	100
19	CC	383/523 (73%)	361 (94%)	22 (6%)	0	100	100
20	CD	416/582 (72%)	384 (92%)	32 (8%)	0	100	100
21	CE	119/127 (94%)	112 (94%)	7 (6%)	0	100	100
21	CF	118/127 (93%)	109 (92%)	9 (8%)	0	100	100
22	CG	402/630 (64%)	366 (91%)	36 (9%)	0	100	100
23	CH	383/411 (93%)	344 (90%)	38 (10%)	1 (0%)	41	76
24	CI	812/1163 (70%)	732 (90%)	80 (10%)	0	100	100
25	CJ	177/183 (97%)	154 (87%)	23 (13%)	0	100	100
26	CK	295/297 (99%)	255 (86%)	40 (14%)	0	100	100
27	CL	225/785 (29%)	205 (91%)	20 (9%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	CM	443/446 (99%)	402 (91%)	41 (9%)	0	100	100
29	CN	222/252 (88%)	202 (91%)	20 (9%)	0	100	100
29	CO	211/252 (84%)	196 (93%)	13 (6%)	2 (1%)	17	56
30	CP	185/322 (58%)	181 (98%)	4 (2%)	0	100	100
31	CQ	171/259 (66%)	165 (96%)	6 (4%)	0	100	100
32	CR	746/1073 (70%)	692 (93%)	54 (7%)	0	100	100
32	CS	746/1073 (70%)	692 (93%)	54 (7%)	0	100	100
33	CT	127/203 (63%)	111 (87%)	16 (13%)	0	100	100
34	Cb	230/264 (87%)	211 (92%)	19 (8%)	0	100	100
35	Cc	188/212 (89%)	166 (88%)	22 (12%)	0	100	100
36	Cd	224/239 (94%)	208 (93%)	16 (7%)	0	100	100
37	Ce	155/203 (76%)	145 (94%)	10 (6%)	0	100	100
38	Cf	170/202 (84%)	162 (95%)	8 (5%)	0	100	100
39	Cg	157/190 (83%)	149 (95%)	8 (5%)	0	100	100
40	Ch	47/151 (31%)	47 (100%)	0	0	100	100
41	Ci	113/150 (75%)	100 (88%)	13 (12%)	0	100	100
42	Cj	124/143 (87%)	109 (88%)	15 (12%)	0	100	100
43	Ck	136/161 (84%)	131 (96%)	5 (4%)	0	100	100
44	Cm	122/130 (94%)	116 (95%)	6 (5%)	0	100	100
45	Cn	92/145 (63%)	83 (90%)	9 (10%)	0	100	100
46	Co	90/136 (66%)	82 (91%)	8 (9%)	0	100	100
47	Cp	59/68 (87%)	55 (93%)	4 (7%)	0	100	100
48	CU	106/311 (34%)	99 (93%)	7 (7%)	0	100	100
51	UV	1057/1171 (90%)	948 (90%)	108 (10%)	1 (0%)	51	85
52	CV	144/322 (45%)	129 (90%)	14 (10%)	1 (1%)	22	62
53	CW	380/668 (57%)	349 (92%)	31 (8%)	0	100	100
54	UT	1982/2612 (76%)	1878 (95%)	100 (5%)	4 (0%)	47	81
55	UH	349/930 (38%)	335 (96%)	14 (4%)	0	100	100
56	UE	121/410 (30%)	111 (92%)	9 (7%)	1 (1%)	19	60
56	UI	121/410 (30%)	111 (92%)	9 (7%)	1 (1%)	19	60
57	US	443/549 (81%)	420 (95%)	23 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	Cl	78/156 (50%)	74 (95%)	4 (5%)	0	100	100
59	CX	265/480 (55%)	251 (95%)	14 (5%)	0	100	100
60	CY	118/381 (31%)	109 (92%)	9 (8%)	0	100	100
61	CZ	40/609 (7%)	32 (80%)	8 (20%)	0	100	100
62	UP	52/364 (14%)	45 (86%)	7 (14%)	0	100	100
63	Cz	273/1796 (15%)	261 (96%)	12 (4%)	0	100	100
All	All	22926/35864 (64%)	21113 (92%)	1795 (8%)	18 (0%)	54	85

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	UG	176	LEU
29	CO	85	SER
51	UV	1059	ASP
54	UT	487	ILE
5	UF	121	LYS
29	CO	84	ILE
54	UT	457	TRP
6	UG	56	PRO
13	UQ	708	SER
54	UT	1567	PHE
6	UG	322	ASN
54	UT	408	PRO
11	UN	902	ARG
52	CV	92	SER
56	UE	208	PRO
10	UM	329	PRO
56	UI	208	PRO
23	CH	258	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 PDB entries followed by that with respect to all EM entries.

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	
1	UA	651/775 (84%)	647 (99%)	4 (1%)	86	92
2	UB	425/788 (54%)	423 (100%)	2 (0%)	88	93
3	UC	61/536 (11%)	61 (100%)	0	100	100
4	UD	653/738 (88%)	650 (100%)	3 (0%)	88	93
5	UF	248/341 (73%)	246 (99%)	2 (1%)	81	89
6	UG	373/474 (79%)	371 (100%)	2 (0%)	88	93
7	UJ	898/1526 (59%)	890 (99%)	8 (1%)	78	88
8	UK	159/227 (70%)	156 (98%)	3 (2%)	57	75
9	UL	667/821 (81%)	665 (100%)	2 (0%)	92	95
10	UM	569/770 (74%)	567 (100%)	2 (0%)	91	94
11	UN	146/765 (19%)	146 (100%)	0	100	100
12	UO	404/456 (89%)	401 (99%)	3 (1%)	84	90
13	UQ	650/817 (80%)	650 (100%)	0	100	100
14	UR	360/524 (69%)	359 (100%)	1 (0%)	92	95
15	UU	672/863 (78%)	668 (99%)	4 (1%)	86	92
16	UX	150/167 (90%)	147 (98%)	3 (2%)	55	73
17	UZ	186/329 (56%)	184 (99%)	2 (1%)	73	85
18	CA	175/228 (77%)	172 (98%)	3 (2%)	60	78
18	CB	195/228 (86%)	195 (100%)	0	100	100
19	CC	287/435 (66%)	286 (100%)	1 (0%)	92	95
20	CD	319/489 (65%)	318 (100%)	1 (0%)	92	95
21	CE	91/108 (84%)	91 (100%)	0	100	100
21	CF	88/108 (82%)	88 (100%)	0	100	100
22	CG	331/525 (63%)	329 (99%)	2 (1%)	86	92
23	CH	303/320 (95%)	298 (98%)	5 (2%)	60	78
24	CI	661/1009 (66%)	653 (99%)	8 (1%)	71	84
25	CJ	147/169 (87%)	147 (100%)	0	100	100
26	CK	245/266 (92%)	241 (98%)	4 (2%)	62	79
27	CL	181/642 (28%)	181 (100%)	0	100	100
28	CM	364/383 (95%)	361 (99%)	3 (1%)	81	89
29	CN	202/223 (91%)	202 (100%)	0	100	100
29	CO	193/223 (86%)	190 (98%)	3 (2%)	62	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	CP	164/287 (57%)	163 (99%)	1 (1%)	86	92
31	CQ	145/215 (67%)	145 (100%)	0	100	100
32	CR	654/916 (71%)	512 (78%)	142 (22%)	1	6
32	CS	654/916 (71%)	512 (78%)	142 (22%)	1	6
33	CT	108/167 (65%)	108 (100%)	0	100	100
34	Cb	199/221 (90%)	198 (100%)	1 (0%)	88	93
35	Cc	149/178 (84%)	145 (97%)	4 (3%)	44	66
36	Cd	192/204 (94%)	191 (100%)	1 (0%)	88	93
37	Ce	137/177 (77%)	135 (98%)	2 (2%)	65	80
38	Cf	139/164 (85%)	138 (99%)	1 (1%)	84	90
39	Cg	122/162 (75%)	122 (100%)	0	100	100
40	Ch	41/130 (32%)	40 (98%)	1 (2%)	49	69
41	Ci	74/117 (63%)	73 (99%)	1 (1%)	67	81
42	Cj	92/115 (80%)	91 (99%)	1 (1%)	73	85
43	Ck	126/143 (88%)	125 (99%)	1 (1%)	81	89
44	Cm	103/113 (91%)	102 (99%)	1 (1%)	76	86
45	Cn	70/116 (60%)	69 (99%)	1 (1%)	67	81
46	Co	79/115 (69%)	78 (99%)	1 (1%)	69	82
47	Cp	46/61 (75%)	46 (100%)	0	100	100
48	CU	92/260 (35%)	91 (99%)	1 (1%)	73	85
51	UV	908/989 (92%)	895 (99%)	13 (1%)	67	81
52	CV	129/276 (47%)	127 (98%)	2 (2%)	62	79
53	CW	309/587 (53%)	307 (99%)	2 (1%)	86	92
54	UT	1724/2276 (76%)	1715 (100%)	9 (0%)	88	93
55	UH	301/788 (38%)	298 (99%)	3 (1%)	76	86
56	UE	105/346 (30%)	76 (72%)	29 (28%)	0	3
56	UI	105/346 (30%)	76 (72%)	29 (28%)	0	3
57	US	404/493 (82%)	403 (100%)	1 (0%)	93	96
58	Cl	71/135 (53%)	69 (97%)	2 (3%)	43	65
59	CX	225/411 (55%)	223 (99%)	2 (1%)	78	88
60	CY	100/322 (31%)	100 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
61	CZ	36/519 (7%)	34 (94%)	2 (6%)	21	48
62	UP	44/314 (14%)	44 (100%)	0	100	100
63	Cz	235/1533 (15%)	233 (99%)	2 (1%)	78	88
All	All	19136/30385 (63%)	18667 (98%)	469 (2%)	50	68

All (469) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	UA	33	VAL
1	UA	150	HIS
1	UA	471	VAL
1	UA	493	ARG
2	UB	87	ARG
2	UB	786	ARG
4	UD	228	ASP
4	UD	264	LYS
4	UD	346	ASP
5	UF	113	TYR
5	UF	121	LYS
6	UG	41	ARG
6	UG	121	VAL
7	UJ	25	LEU
7	UJ	393	LYS
7	UJ	405	LYS
7	UJ	840	LYS
7	UJ	1509	LYS
7	UJ	1517	LYS
7	UJ	1656	LYS
7	UJ	1720	LYS
8	UK	58	ARG
8	UK	65	PHE
8	UK	160	LYS
9	UL	71	THR
9	UL	93	ARG
10	UM	755	ARG
10	UM	889	ARG
12	UO	253	ASN
12	UO	258	LEU
12	UO	264	LYS
14	UR	437	ARG
15	UU	394	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	UU	503	SER
15	UU	618	THR
15	UU	1000	ARG
16	UX	-1	LYS
16	UX	31	LYS
16	UX	58	VAL
17	UZ	140	TYR
17	UZ	170	THR
18	CA	211	ARG
18	CA	218	MET
18	CA	292	LEU
19	CC	51	ARG
20	CD	68	LYS
22	CG	345	VAL
22	CG	352	ARG
23	CH	73	THR
23	CH	208	LEU
23	CH	273	THR
23	CH	304	VAL
23	CH	354	ARG
24	CI	91	ARG
24	CI	113	ARG
24	CI	222	LEU
24	CI	840	ARG
24	CI	841	ARG
24	CI	854	ARG
24	CI	863	THR
24	CI	1073	GLU
26	CK	92	THR
26	CK	108	ARG
26	CK	246	ARG
26	CK	280	VAL
28	CM	39	GLU
28	CM	208	VAL
28	CM	408	LYS
29	CO	135	LYS
29	CO	209	MET
29	CO	241	PHE
30	CP	49	ARG
32	CR	3	VAL
32	CR	8	ASP
32	CR	10	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	CR	14	LEU
32	CR	19	LEU
32	CR	25	SER
32	CR	32	ASP
32	CR	41	LEU
32	CR	45	MET
32	CR	49	ASP
32	CR	50	VAL
32	CR	54	LYS
32	CR	55	SER
32	CR	62	LYS
32	CR	65	LEU
32	CR	69	SER
32	CR	75	GLU
32	CR	77	LYS
32	CR	78	ILE
32	CR	79	LYS
32	CR	80	LYS
32	CR	83	LYS
32	CR	84	ARG
32	CR	87	ARG
32	CR	88	GLU
32	CR	95	PHE
32	CR	107	CYS
32	CR	112	THR
32	CR	116	LEU
32	CR	119	THR
32	CR	129	GLU
32	CR	131	ILE
32	CR	132	THR
32	CR	140	ILE
32	CR	141	GLU
32	CR	142	THR
32	CR	148	LEU
32	CR	149	VAL
32	CR	159	LEU
32	CR	162	LEU
32	CR	167	MET
32	CR	168	ASP
32	CR	195	SER
32	CR	198	SER
32	CR	209	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	CR	249	ILE
32	CR	252	LEU
32	CR	253	ILE
32	CR	266	LEU
32	CR	270	ASP
32	CR	277	LEU
32	CR	280	THR
32	CR	282	THR
32	CR	284	THR
32	CR	289	ARG
32	CR	292	SER
32	CR	295	MET
32	CR	297	VAL
32	CR	299	ILE
32	CR	313	THR
32	CR	314	SER
32	CR	316	SER
32	CR	372	ILE
32	CR	387	VAL
32	CR	402	LEU
32	CR	408	VAL
32	CR	412	SER
32	CR	424	LEU
32	CR	426	LEU
32	CR	429	ILE
32	CR	432	LEU
32	CR	470	LYS
32	CR	471	GLU
32	CR	475	SER
32	CR	480	TYR
32	CR	488	LYS
32	CR	492	THR
32	CR	494	LEU
32	CR	502	ARG
32	CR	510	CYS
32	CR	512	ASP
32	CR	528	SER
32	CR	532	VAL
32	CR	534	GLU
32	CR	535	LYS
32	CR	536	PHE
32	CR	537	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	CR	539	GLN
32	CR	540	MET
32	CR	545	VAL
32	CR	547	SER
32	CR	552	SER
32	CR	555	ASP
32	CR	557	GLN
32	CR	560	SER
32	CR	567	LEU
32	CR	571	THR
32	CR	576	GLU
32	CR	581	GLU
32	CR	586	ILE
32	CR	589	SER
32	CR	590	LEU
32	CR	612	ASP
32	CR	617	LEU
32	CR	619	SER
32	CR	625	ASP
32	CR	631	SER
32	CR	638	ILE
32	CR	640	THR
32	CR	643	ASP
32	CR	645	MET
32	CR	647	MET
32	CR	651	SER
32	CR	657	LEU
32	CR	708	LEU
32	CR	710	SER
32	CR	713	SER
32	CR	719	LYS
32	CR	733	LEU
32	CR	739	ARG
32	CR	745	VAL
32	CR	750	THR
32	CR	773	SER
32	CR	784	LYS
32	CR	789	LEU
32	CR	796	GLU
32	CR	800	ILE
32	CR	853	VAL
32	CR	854	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	CR	855	LEU
32	CR	860	THR
32	CR	867	THR
32	CR	870	LEU
32	CR	879	LEU
32	CR	884	LEU
32	CR	887	LEU
32	CR	892	LYS
32	CR	894	ILE
32	CR	897	LEU
32	CR	901	LEU
32	CR	902	ASN
32	CR	909	LEU
32	CS	3	VAL
32	CS	8	ASP
32	CS	10	ARG
32	CS	14	LEU
32	CS	19	LEU
32	CS	25	SER
32	CS	32	ASP
32	CS	41	LEU
32	CS	45	MET
32	CS	49	ASP
32	CS	50	VAL
32	CS	54	LYS
32	CS	55	SER
32	CS	62	LYS
32	CS	65	LEU
32	CS	69	SER
32	CS	75	GLU
32	CS	77	LYS
32	CS	78	ILE
32	CS	79	LYS
32	CS	80	LYS
32	CS	83	LYS
32	CS	84	ARG
32	CS	87	ARG
32	CS	88	GLU
32	CS	95	PHE
32	CS	107	CYS
32	CS	112	THR
32	CS	116	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	CS	119	THR
32	CS	129	GLU
32	CS	131	ILE
32	CS	132	THR
32	CS	140	ILE
32	CS	141	GLU
32	CS	142	THR
32	CS	148	LEU
32	CS	149	VAL
32	CS	159	LEU
32	CS	162	LEU
32	CS	167	MET
32	CS	168	ASP
32	CS	195	SER
32	CS	198	SER
32	CS	209	LEU
32	CS	249	ILE
32	CS	252	LEU
32	CS	253	ILE
32	CS	266	LEU
32	CS	270	ASP
32	CS	277	LEU
32	CS	280	THR
32	CS	282	THR
32	CS	284	THR
32	CS	289	ARG
32	CS	292	SER
32	CS	295	MET
32	CS	297	VAL
32	CS	299	ILE
32	CS	313	THR
32	CS	314	SER
32	CS	316	SER
32	CS	372	ILE
32	CS	387	VAL
32	CS	402	LEU
32	CS	408	VAL
32	CS	412	SER
32	CS	424	LEU
32	CS	426	LEU
32	CS	429	ILE
32	CS	432	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	CS	470	LYS
32	CS	471	GLU
32	CS	475	SER
32	CS	480	TYR
32	CS	488	LYS
32	CS	492	THR
32	CS	494	LEU
32	CS	502	ARG
32	CS	510	CYS
32	CS	512	ASP
32	CS	528	SER
32	CS	532	VAL
32	CS	534	GLU
32	CS	535	LYS
32	CS	536	PHE
32	CS	537	LEU
32	CS	539	GLN
32	CS	540	MET
32	CS	545	VAL
32	CS	547	SER
32	CS	552	SER
32	CS	555	ASP
32	CS	557	GLN
32	CS	560	SER
32	CS	567	LEU
32	CS	571	THR
32	CS	576	GLU
32	CS	581	GLU
32	CS	586	ILE
32	CS	589	SER
32	CS	590	LEU
32	CS	612	ASP
32	CS	617	LEU
32	CS	619	SER
32	CS	625	ASP
32	CS	631	SER
32	CS	638	ILE
32	CS	640	THR
32	CS	643	ASP
32	CS	645	MET
32	CS	647	MET
32	CS	651	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	CS	657	LEU
32	CS	708	LEU
32	CS	710	SER
32	CS	713	SER
32	CS	719	LYS
32	CS	733	LEU
32	CS	739	ARG
32	CS	745	VAL
32	CS	750	THR
32	CS	773	SER
32	CS	784	LYS
32	CS	789	LEU
32	CS	796	GLU
32	CS	800	ILE
32	CS	853	VAL
32	CS	854	VAL
32	CS	855	LEU
32	CS	860	THR
32	CS	867	THR
32	CS	870	LEU
32	CS	879	LEU
32	CS	884	LEU
32	CS	887	LEU
32	CS	892	LYS
32	CS	894	ILE
32	CS	897	LEU
32	CS	901	LEU
32	CS	902	ASN
32	CS	909	LEU
34	Cb	133	ARG
35	Cc	41	ARG
35	Cc	66	VAL
35	Cc	130	ARG
35	Cc	144	ARG
36	Cd	111	LEU
37	Ce	90	LYS
37	Ce	184	ARG
38	Cf	18	ARG
40	Ch	100	LYS
41	Ci	105	LYS
42	Cj	111	GLN
43	Ck	72	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	Cm	32	LYS
45	Cn	78	LYS
46	Co	368	LYS
48	CU	129	ARG
51	UV	36	ARG
51	UV	91	LYS
51	UV	248	ARG
51	UV	577	ARG
51	UV	612	ARG
51	UV	668	VAL
51	UV	676	ARG
51	UV	733	LYS
51	UV	784	LYS
51	UV	941	THR
51	UV	982	ARG
51	UV	989	LYS
51	UV	1099	LYS
52	CV	156	LYS
52	CV	167	LYS
53	CW	85	ARG
53	CW	337	THR
54	UT	8	ARG
54	UT	139	LYS
54	UT	324	ARG
54	UT	1006	ARG
54	UT	1472	THR
54	UT	1564	LYS
54	UT	1635	LYS
54	UT	1857	LEU
54	UT	1940	ARG
55	UH	624	MET
55	UH	748	LYS
55	UH	902	LYS
56	UE	157	LEU
56	UE	163	THR
56	UE	170	GLU
56	UE	180	ILE
56	UE	187	ARG
56	UE	191	SER
56	UE	196	LEU
56	UE	199	LYS
56	UE	206	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	UE	210	ARG
56	UE	214	LEU
56	UE	218	ILE
56	UE	219	GLN
56	UE	222	LEU
56	UE	231	THR
56	UE	234	ASP
56	UE	241	GLU
56	UE	254	SER
56	UE	255	SER
56	UE	259	LEU
56	UE	262	LYS
56	UE	263	LEU
56	UE	264	ASP
56	UE	265	MET
56	UE	266	LEU
56	UE	267	ASP
56	UE	270	LEU
56	UE	271	LYS
56	UE	278	MET
57	US	425	LYS
58	CI	25	LYS
58	CI	80	LYS
59	CX	204	LYS
59	CX	247	CYS
61	CZ	554	ASN
61	CZ	575	THR
56	UI	157	LEU
56	UI	163	THR
56	UI	170	GLU
56	UI	180	ILE
56	UI	187	ARG
56	UI	191	SER
56	UI	196	LEU
56	UI	199	LYS
56	UI	206	ARG
56	UI	210	ARG
56	UI	214	LEU
56	UI	218	ILE
56	UI	219	GLN
56	UI	222	LEU
56	UI	231	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	UI	234	ASP
56	UI	241	GLU
56	UI	254	SER
56	UI	255	SER
56	UI	259	LEU
56	UI	262	LYS
56	UI	263	LEU
56	UI	264	ASP
56	UI	265	MET
56	UI	266	LEU
56	UI	267	ASP
56	UI	270	LEU
56	UI	271	LYS
56	UI	278	MET
63	Cz	1664	LEU
63	Cz	1701	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (279) such sidechains are listed below:

Mol	Chain	Res	Type
1	UA	19	ASN
1	UA	45	ASN
1	UA	131	ASN
1	UA	207	GLN
1	UA	328	GLN
1	UA	344	ASN
1	UA	353	GLN
1	UA	508	GLN
1	UA	576	ASN
1	UA	846	ASN
2	UB	5	GLN
2	UB	525	ASN
2	UB	683	HIS
4	UD	176	GLN
4	UD	195	GLN
4	UD	277	GLN
4	UD	324	HIS
4	UD	416	ASN
4	UD	473	ASN
4	UD	532	GLN
4	UD	536	HIS
4	UD	673	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	UD	697	GLN
4	UD	755	GLN
4	UD	828	HIS
5	UF	154	ASN
6	UG	95	ASN
6	UG	216	HIS
6	UG	243	GLN
6	UG	278	GLN
6	UG	331	ASN
6	UG	378	GLN
6	UG	427	ASN
7	UJ	15	ASN
7	UJ	51	GLN
7	UJ	158	GLN
7	UJ	250	GLN
7	UJ	448	ASN
7	UJ	515	ASN
7	UJ	731	ASN
7	UJ	785	ASN
7	UJ	842	ASN
7	UJ	1645	ASN
7	UJ	1723	ASN
7	UJ	1745	GLN
8	UK	9	GLN
9	UL	21	ASN
9	UL	151	HIS
9	UL	154	GLN
9	UL	207	HIS
9	UL	215	GLN
9	UL	296	HIS
9	UL	453	ASN
9	UL	506	HIS
9	UL	630	ASN
9	UL	688	GLN
9	UL	832	ASN
10	UM	231	HIS
10	UM	236	GLN
10	UM	338	GLN
10	UM	628	ASN
10	UM	644	ASN
10	UM	706	ASN
10	UM	741	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	UM	743	GLN
10	UM	747	ASN
10	UM	772	ASN
11	UN	332	HIS
11	UN	333	ASN
11	UN	362	GLN
11	UN	916	GLN
12	UO	393	ASN
13	UQ	209	ASN
13	UQ	262	HIS
13	UQ	473	GLN
13	UQ	477	HIS
13	UQ	783	ASN
13	UQ	924	GLN
14	UR	177	GLN
14	UR	185	GLN
14	UR	440	GLN
14	UR	493	ASN
14	UR	498	ASN
15	UU	62	GLN
15	UU	89	GLN
15	UU	143	GLN
15	UU	197	ASN
15	UU	314	ASN
15	UU	577	GLN
15	UU	634	ASN
15	UU	727	GLN
15	UU	740	HIS
15	UU	963	ASN
15	UU	1023	GLN
16	UX	63	ASN
17	UZ	79	GLN
17	UZ	90	ASN
17	UZ	110	ASN
17	UZ	143	GLN
18	CB	195	ASN
18	CB	232	GLN
18	CB	235	GLN
18	CB	277	GLN
18	CB	289	GLN
20	CD	106	ASN
20	CD	147	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	CD	219	ASN
20	CD	404	ASN
20	CD	422	ASN
21	CE	112	ASN
22	CG	243	GLN
22	CG	274	ASN
22	CG	330	GLN
22	CG	430	HIS
23	CH	90	ASN
23	CH	127	HIS
23	CH	233	ASN
23	CH	244	ASN
23	CH	316	GLN
23	CH	323	GLN
24	CI	55	HIS
24	CI	165	ASN
24	CI	823	HIS
24	CI	888	GLN
24	CI	930	ASN
24	CI	1030	ASN
25	CJ	8	HIS
25	CJ	30	HIS
25	CJ	39	GLN
25	CJ	59	HIS
25	CJ	135	HIS
25	CJ	169	ASN
26	CK	5	GLN
26	CK	8	GLN
26	CK	48	ASN
26	CK	121	ASN
26	CK	132	GLN
26	CK	159	HIS
26	CK	168	HIS
26	CK	169	ASN
26	CK	242	HIS
27	CL	525	HIS
28	CM	65	HIS
28	CM	77	ASN
28	CM	120	ASN
28	CM	151	GLN
28	CM	206	ASN
28	CM	262	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	CM	282	HIS
28	CM	376	ASN
29	CN	81	ASN
29	CN	111	GLN
29	CO	94	GLN
29	CO	105	ASN
30	CP	110	GLN
30	CP	190	ASN
31	CQ	203	ASN
31	CQ	247	ASN
32	CR	102	ASN
32	CR	126	GLN
32	CR	279	ASN
32	CR	485	ASN
32	CR	655	GLN
32	CR	749	GLN
32	CR	810	ASN
32	CS	102	ASN
32	CS	126	GLN
32	CS	279	ASN
32	CS	485	ASN
32	CS	557	GLN
32	CS	655	GLN
32	CS	749	GLN
32	CS	810	ASN
34	Cb	57	ASN
34	Cb	67	GLN
34	Cb	197	HIS
35	Cc	31	ASN
35	Cc	82	ASN
35	Cc	87	HIS
35	Cc	109	HIS
35	Cc	115	ASN
35	Cc	211	ASN
36	Cd	129	HIS
36	Cd	163	GLN
36	Cd	179	GLN
36	Cd	189	HIS
36	Cd	200	GLN
37	Ce	36	ASN
38	Cf	94	ASN
39	Cg	121	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	Cg	140	ASN
42	Cj	77	GLN
42	Cj	107	GLN
43	Ck	22	ASN
43	Ck	111	ASN
43	Ck	115	HIS
43	Ck	132	GLN
43	Ck	143	ASN
44	Cm	42	GLN
44	Cm	64	GLN
44	Cm	113	HIS
45	Cn	48	HIS
45	Cn	79	ASN
46	Co	353	GLN
46	Co	360	HIS
48	CU	211	GLN
51	UV	106	GLN
51	UV	107	ASN
51	UV	260	GLN
51	UV	355	GLN
51	UV	368	ASN
51	UV	378	GLN
51	UV	494	ASN
51	UV	526	GLN
51	UV	542	ASN
51	UV	615	GLN
51	UV	809	HIS
51	UV	813	HIS
51	UV	841	HIS
51	UV	974	GLN
51	UV	1092	ASN
52	CV	198	HIS
53	CW	80	HIS
53	CW	177	GLN
53	CW	243	GLN
53	CW	361	ASN
54	UT	24	ASN
54	UT	25	HIS
54	UT	87	ASN
54	UT	311	HIS
54	UT	365	ASN
54	UT	377	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	UT	389	HIS
54	UT	495	GLN
54	UT	768	ASN
54	UT	780	GLN
54	UT	803	ASN
54	UT	909	GLN
54	UT	971	ASN
54	UT	1026	GLN
54	UT	1272	HIS
54	UT	1314	ASN
54	UT	1315	GLN
54	UT	1345	GLN
54	UT	1416	ASN
54	UT	1437	ASN
54	UT	1454	ASN
54	UT	1599	GLN
54	UT	1602	ASN
54	UT	1795	HIS
54	UT	1874	GLN
54	UT	1909	GLN
54	UT	1985	ASN
54	UT	2052	GLN
54	UT	2097	ASN
54	UT	2141	GLN
54	UT	2163	ASN
55	UH	590	ASN
56	UE	186	ASN
56	UE	237	ASN
57	US	152	HIS
57	US	184	HIS
57	US	225	ASN
57	US	253	HIS
57	US	391	ASN
57	US	468	HIS
58	CI	21	ASN
58	CI	74	GLN
59	CX	290	ASN
59	CX	355	GLN
59	CX	364	ASN
59	CX	423	ASN
56	UI	186	ASN
56	UI	237	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
62	UP	325	ASN
62	UP	341	ASN
63	Cz	1556	ASN
63	Cz	1578	ASN
63	Cz	1617	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
49	C1	1461/2323 (62%)	559 (38%)	35 (2%)
50	C2	226/230 (98%)	86 (38%)	6 (2%)
All	All	1687/2553 (66%)	645 (38%)	41 (2%)

All (645) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
49	C1	4	G
49	C1	5	G
49	C1	7	A
49	C1	13	G
49	C1	14	G
49	C1	15	G
49	C1	16	U
49	C1	17	C
49	C1	18	G
49	C1	19	C
49	C1	23	G
49	C1	26	C
49	C1	38	G
49	C1	40	A
49	C1	41	G
49	C1	42	C
49	C1	43	C
49	C1	47	G
49	C1	49	G
49	C1	56	C
49	C1	59	U
49	C1	60	A
49	C1	61	G
49	C1	62	U
49	C1	63	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	C1	66	G
49	C1	68	U
49	C1	71	A
49	C1	72	U
49	C1	73	A
49	C1	74	C
49	C1	75	G
49	C1	77	C
49	C1	84	A
49	C1	88	C
49	C1	89	G
49	C1	90	A
49	C1	93	G
49	C1	96	C
49	C1	104	U
49	C1	105	A
49	C1	121	G
49	C1	126	C
49	C1	127	C
49	C1	128	G
49	C1	134	C
49	C1	135	A
49	C1	136	C
49	C1	139	C
49	C1	143	A
49	C1	152	G
49	C1	154	C
49	C1	155	G
49	C1	158	C
49	C1	159	C
49	C1	160	C
49	C1	161	A
49	C1	162	G
49	C1	166	A
49	C1	169	G
49	C1	180	G
49	C1	182	C
49	C1	183	C
49	C1	188	C
49	C1	192	A
49	C1	193	U
49	C1	198	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	C1	201	G
49	C1	202	A
49	C1	203	C
49	C1	204	U
49	C1	205	C
49	C1	206	C
49	C1	207	U
49	C1	208	A
49	C1	209	A
49	C1	210	G
49	C1	211	G
49	C1	212	C
49	C1	219	G
49	C1	220	A
49	C1	222	U
49	C1	223	A
49	C1	224	C
49	C1	228	G
49	C1	234	G
49	C1	236	C
49	C1	241	G
49	C1	242	U
49	C1	243	U
49	C1	244	G
49	C1	256	U
49	C1	257	G
49	C1	258	C
49	C1	260	U
49	C1	265	G
49	C1	266	C
49	C1	268	G
49	C1	269	G
49	C1	271	C
49	C1	273	G
49	C1	276	C
49	C1	277	U
49	C1	278	A
49	C1	282	C
49	C1	283	A
49	C1	285	A
49	C1	286	G
49	C1	289	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	C1	290	C
49	C1	291	C
49	C1	292	G
49	C1	297	U
49	C1	298	A
49	C1	309	G
49	C1	334	U
49	C1	339	C
49	C1	340	G
49	C1	346	C
49	C1	347	C
49	C1	349	C
49	C1	351	U
49	C1	352	G
49	C1	353	G
49	C1	362	G
49	C1	368	G
49	C1	378	C
49	C1	382	U
49	C1	383	G
49	C1	384	C
49	C1	386	G
49	C1	397	U
49	C1	402	U
49	C1	403	G
49	C1	406	G
49	C1	408	C
49	C1	409	A
49	C1	410	G
49	C1	411	C
49	C1	416	U
49	C1	417	G
49	C1	419	G
49	C1	425	C
49	C1	427	G
49	C1	433	G
49	C1	435	A
49	C1	436	A
49	C1	438	C
49	C1	440	G
49	C1	441	A
49	C1	442	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	C1	443	G
49	C1	453	G
49	C1	454	C
49	C1	458	A
49	C1	459	C
49	C1	467	C
49	C1	468	C
49	C1	469	G
49	C1	471	C
49	C1	473	G
49	C1	474	A
49	C1	475	C
49	C1	483	U
49	C1	484	G
49	C1	491	G
49	C1	492	C
49	C1	494	G
49	C1	499	G
49	C1	500	C
49	C1	501	U
49	C1	502	A
49	C1	504	C
49	C1	581	C
49	C1	582	G
49	C1	583	A
49	C1	584	U
49	C1	585	A
49	C1	586	G
49	C1	587	U
49	C1	591	C
49	C1	594	G
49	C1	602	U
49	C1	604	C
49	C1	609	A
49	C1	610	G
49	C1	612	C
49	C1	613	A
49	C1	614	U
49	C1	618	C
49	C1	621	G
49	C1	627	A
49	C1	628	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	C1	636	C
49	C1	646	C
49	C1	650	G
49	C1	652	A
49	C1	653	U
49	C1	655	A
49	C1	656	G
49	C1	659	A
49	C1	660	U
49	C1	664	A
49	C1	666	A
49	C1	667	G
49	C1	678	A
49	C1	679	A
49	C1	680	U
49	C1	682	G
49	C1	683	C
49	C1	685	C
49	C1	686	A
49	C1	687	U
49	C1	688	U
49	C1	689	A
49	C1	690	A
49	C1	692	U
49	C1	693	C
49	C1	697	U
49	C1	700	C
49	C1	702	U
49	C1	703	U
49	C1	710	A
49	C1	711	U
49	C1	713	G
49	C1	714	U
49	C1	719	U
49	C1	720	A
49	C1	728	G
49	C1	729	A
49	C1	730	U
49	C1	735	G
49	C1	740	A
49	C1	741	A
49	C1	742	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	C1	743	U
49	C1	744	C
49	C1	745	U
49	C1	756	C
49	C1	758	U
49	C1	760	C
49	C1	764	A
49	C1	765	A
49	C1	767	U
49	C1	768	C
49	C1	769	C
49	C1	770	C
49	C1	771	G
49	C1	772	A
49	C1	774	U
49	C1	775	U
49	C1	776	C
49	C1	777	G
49	C1	778	G
49	C1	780	A
49	C1	782	G
49	C1	785	U
49	C1	786	G
49	C1	797	A
49	C1	816	C
49	C1	828	G
49	C1	832	U
49	C1	833	U
49	C1	834	C
49	C1	841	A
49	C1	845	C
49	C1	849	A
49	C1	850	A
49	C1	851	U
49	C1	856	C
49	C1	858	G
49	C1	860	C
49	C1	861	U
49	C1	862	U
49	C1	863	G
49	C1	864	C
49	C1	865	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	C1	871	G
49	C1	880	U
49	C1	886	U
49	C1	888	U
49	C1	889	C
49	C1	892	C
49	C1	893	C
49	C1	897	U
49	C1	898	C
49	C1	900	A
49	C1	903	U
49	C1	905	C
49	C1	906	G
49	C1	907	A
49	C1	910	G
49	C1	913	G
49	C1	915	G
49	C1	916	U
49	C1	921	G
49	C1	925	G
49	C1	927	C
49	C1	930	G
49	C1	931	G
49	C1	934	A
49	C1	935	C
49	C1	936	A
49	C1	941	G
49	C1	942	U
49	C1	943	A
49	C1	944	A
49	C1	953	U
49	C1	958	C
49	C1	971	A
49	C1	972	A
49	C1	974	G
49	C1	983	A
49	C1	984	A
49	C1	985	A
49	C1	986	C
49	C1	988	G
49	C1	989	C
49	C1	990	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	C1	995	C
49	C1	1000	A
49	C1	1001	A
49	C1	1002	G
49	C1	1005	A
49	C1	1007	G
49	C1	1015	C
49	C1	1017	C
49	C1	1019	C
49	C1	1020	A
49	C1	1021	A
49	C1	1022	A
49	C1	1023	U
49	C1	1024	U
49	C1	1025	A
49	C1	1027	C
49	C1	1028	C
49	C1	1029	A
49	C1	1030	A
49	C1	1035	G
49	C1	1036	A
49	C1	1037	C
49	C1	1038	A
49	C1	1039	C
49	C1	1043	G
49	C1	1044	A
49	C1	1052	A
49	C1	1053	C
49	C1	1054	A
49	C1	1057	A
49	C1	1059	A
49	C1	1061	A
49	C1	1069	A
49	C1	1076	U
49	C1	1077	U
49	C1	1078	U
49	C1	1079	C
49	C1	1080	G
49	C1	1083	U
49	C1	1085	U
49	C1	1086	U
49	C1	1087	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	C1	1088	U
49	C1	1089	A
49	C1	1093	G
49	C1	1094	G
49	C1	1095	A
49	C1	1097	U
49	C1	1098	G
49	C1	1099	A
49	C1	1103	C
49	C1	1104	A
49	C1	1105	A
49	C1	1111	A
49	C1	1116	U
49	C1	1120	C
49	C1	1123	G
49	C1	1124	G
49	C1	1125	A
49	C1	1126	A
49	C1	1127	C
49	C1	1128	A
49	C1	1129	A
49	C1	1134	A
49	C1	1141	G
49	C1	1145	G
49	C1	1147	U
49	C1	1148	G
49	C1	1149	C
49	C1	1150	C
49	C1	1154	A
49	C1	1156	C
49	C1	1157	C
49	C1	1158	G
49	C1	1159	C
49	C1	1163	A
49	C1	1164	A
49	C1	1166	U
49	C1	1167	C
49	C1	1168	C
49	C1	1169	A
49	C1	1171	C
49	C1	1177	U
49	C1	1178	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	C1	1179	G
49	C1	1181	G
49	C1	1186	U
49	C1	1218	G
49	C1	1219	A
49	C1	1222	C
49	C1	1223	U
49	C1	1444	A
49	C1	1447	A
49	C1	1448	A
49	C1	1449	U
49	C1	1450	A
49	C1	1451	G
49	C1	1452	G
49	C1	1458	U
49	C1	1461	G
49	C1	1471	U
49	C1	1479	U
49	C1	1480	G
49	C1	1481	U
49	C1	1483	A
49	C1	1484	G
49	C1	1486	G
49	C1	1489	G
49	C1	1491	A
49	C1	1497	U
49	C1	1498	G
49	C1	1499	G
49	C1	1507	G
49	C1	1517	A
49	C1	1518	A
49	C1	1519	C
49	C1	1520	U
49	C1	1525	A
49	C1	1527	G
49	C1	1529	A
49	C1	1536	A
49	C1	1544	U
49	C1	1545	U
49	C1	1546	U
49	C1	1547	C
49	C1	1549	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	C1	1551	A
49	C1	1554	C
49	C1	1555	A
49	C1	1624	A
49	C1	1625	G
49	C1	1628	A
49	C1	1636	G
49	C1	1637	C
49	C1	1639	U
49	C1	1642	A
49	C1	1643	U
49	C1	1644	U
49	C1	1645	U
49	C1	1656	C
49	C1	1665	A
49	C1	1666	C
49	C1	1667	G
49	C1	1668	A
49	C1	1669	U
49	C1	1670	A
49	C1	1673	U
49	C1	1675	A
49	C1	1676	A
49	C1	1677	A
49	C1	1678	A
49	C1	1698	G
49	C1	1699	U
49	C1	1700	A
49	C1	1709	A
49	C1	1710	G
49	C1	1711	G
49	C1	1712	C
49	C1	1713	U
49	C1	1716	A
49	C1	1730	G
49	C1	1733	G
49	C1	1734	G
49	C1	1735	A
49	C1	1741	A
49	C1	1742	C
49	C1	1743	C
49	C1	1744	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	C1	1751	G
49	C1	1761	C
49	C1	2054	A
49	C1	2055	C
49	C1	2056	U
49	C1	2057	G
49	C1	2059	C
49	C1	2061	G
49	C1	2068	C
49	C1	2069	G
49	C1	2070	A
49	C1	2071	G
49	C1	2072	U
49	C1	2073	A
49	C1	2074	C
49	C1	2075	U
49	C1	2077	C
49	C1	2078	C
49	C1	2085	G
49	C1	2086	A
49	C1	2087	G
49	C1	2088	A
49	C1	2107	A
49	C1	2109	A
49	C1	2114	G
49	C1	2115	U
49	C1	2118	U
49	C1	2119	G
49	C1	2120	C
49	C1	2121	U
49	C1	2157	G
49	C1	2158	G
49	C1	2166	A
49	C1	2167	G
49	C1	2173	G
49	C1	2175	A
49	C1	2176	A
49	C1	2177	G
49	C1	2178	U
49	C1	2179	C
49	C1	2181	U
49	C1	2183	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	C1	2184	G
49	C1	2185	C
49	C1	2193	G
49	C1	2196	U
49	C1	2197	A
49	C1	2199	G
49	C1	2201	C
49	C1	2210	U
49	C1	2211	U
49	C1	2212	G
49	C1	2213	U
49	C1	2214	A
49	C1	2215	C
49	C1	2216	A
49	C1	2217	C
49	C1	2220	C
49	C1	2222	C
49	C1	2223	C
49	C1	2227	C
49	C1	2329	A
49	C1	2330	G
49	C1	2351	G
49	C1	2352	U
49	C1	2358	U
49	C1	2362	U
49	C1	2363	G
49	C1	2364	A
49	C1	2365	A
49	C1	2366	C
49	C1	2374	G
50	C2	6	C
50	C2	8	A
50	C2	10	A
50	C2	11	C
50	C2	15	A
50	C2	22	C
50	C2	23	A
50	C2	24	U
50	C2	25	U
50	C2	26	U
50	C2	28	U
50	C2	29	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	C2	31	A
50	C2	32	G
50	C2	33	U
50	C2	34	A
50	C2	36	U
50	C2	39	U
50	C2	48	G
50	C2	57	A
50	C2	58	A
50	C2	62	A
50	C2	63	G
50	C2	67	C
50	C2	91	G
50	C2	92	A
50	C2	94	A
50	C2	95	U
50	C2	101	G
50	C2	104	C
50	C2	105	C
50	C2	111	G
50	C2	124	U
50	C2	125	U
50	C2	126	U
50	C2	127	A
50	C2	128	C
50	C2	131	U
50	C2	132	C
50	C2	135	U
50	C2	136	C
50	C2	140	C
50	C2	142	G
50	C2	145	A
50	C2	147	G
50	C2	148	G
50	C2	153	G
50	C2	156	C
50	C2	160	U
50	C2	162	C
50	C2	163	C
50	C2	164	U
50	C2	165	C
50	C2	166	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	C2	167	U
50	C2	168	C
50	C2	170	C
50	C2	174	G
50	C2	177	G
50	C2	178	U
50	C2	179	A
50	C2	181	A
50	C2	182	G
50	C2	187	U
50	C2	189	G
50	C2	190	C
50	C2	192	A
50	C2	193	U
50	C2	194	G
50	C2	198	U
50	C2	199	G
50	C2	200	U
50	C2	201	A
50	C2	244	G
50	C2	246	G
50	C2	247	G
50	C2	249	U
50	C2	250	G
50	C2	255	U
50	C2	256	G
50	C2	259	A
50	C2	260	G
50	C2	261	U
50	C2	262	C
50	C2	265	A
50	C2	266	C

All (41) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
49	C1	67	G
49	C1	89	G
49	C1	134	C
49	C1	135	A
49	C1	150	C
49	C1	200	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	C1	205	C
49	C1	209	A
49	C1	257	G
49	C1	277	U
49	C1	281	U
49	C1	290	C
49	C1	424	U
49	C1	582	G
49	C1	593	G
49	C1	684	U
49	C1	742	U
49	C1	771	G
49	C1	1001	A
49	C1	1058	A
49	C1	1068	C
49	C1	1077	U
49	C1	1085	U
49	C1	1087	G
49	C1	1163	A
49	C1	1176	A
49	C1	1485	A
49	C1	1712	C
49	C1	1734	G
49	C1	2054	A
49	C1	2070	A
49	C1	2106	U
49	C1	2156	A
49	C1	2166	A
49	C1	2219	C
50	C2	23	A
50	C2	33	U
50	C2	35	G
50	C2	91	G
50	C2	255	U
50	C2	259	A

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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
50	C2	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C2	206:G	O3'	240:C	P	18.94
1	C2	105:C	O3'	110:A	P	15.09
1	C2	119:C	O3'	123:A	P	11.47

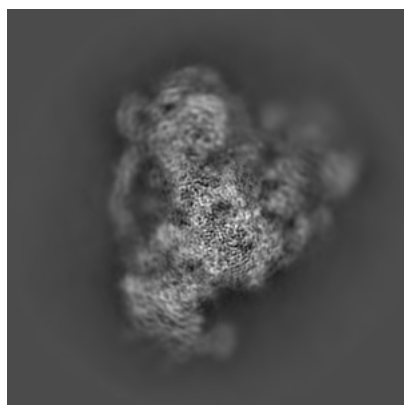
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10056. These allow visual inspection of the internal detail of the map and identification of artifacts.

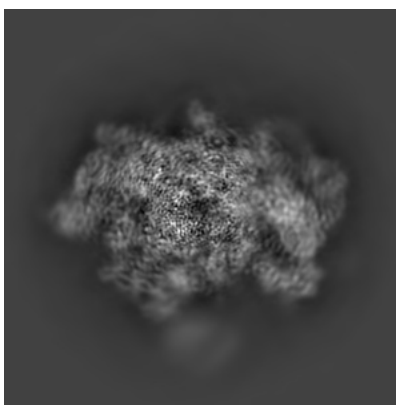
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

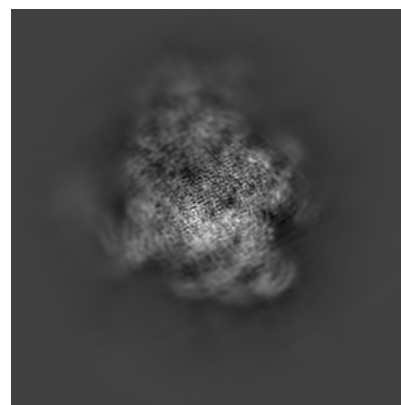
6.1.1 Primary map



X



Y

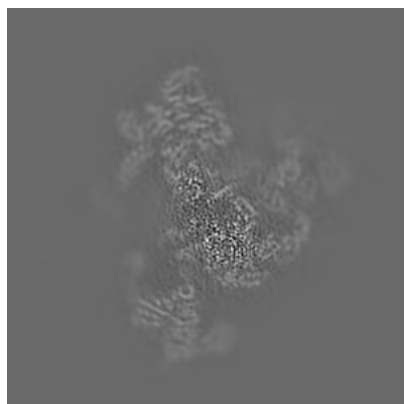


Z

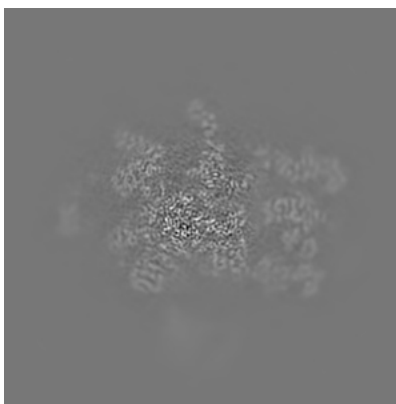
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

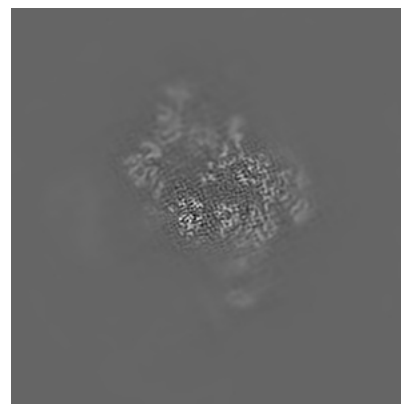
6.2.1 Primary map



X Index: 240



Y Index: 240

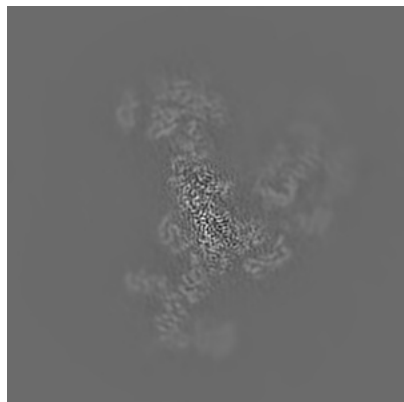


Z Index: 240

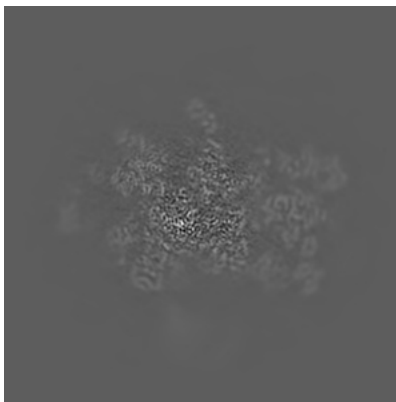
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

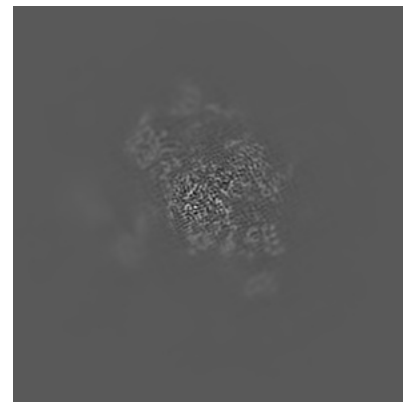
6.3.1 Primary map



X Index: 217



Y Index: 238

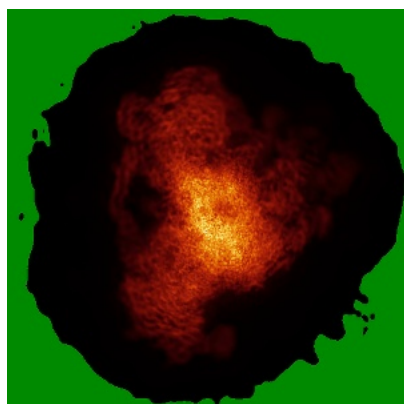


Z Index: 214

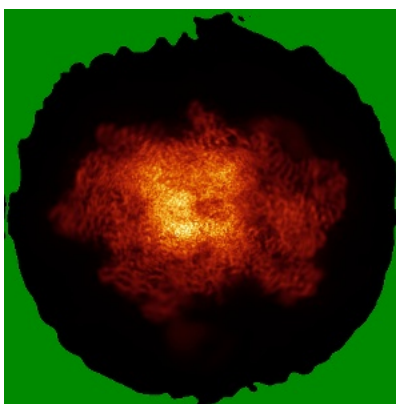
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

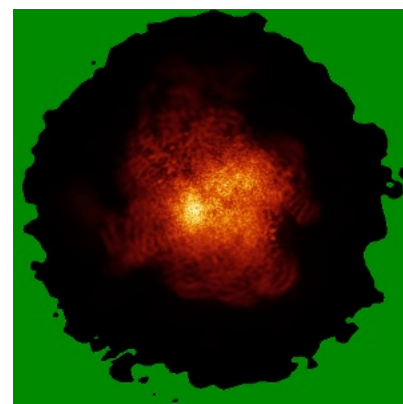
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

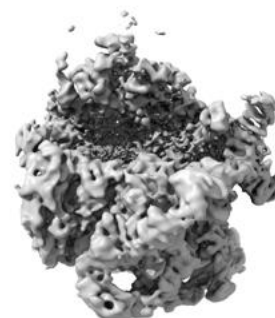
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

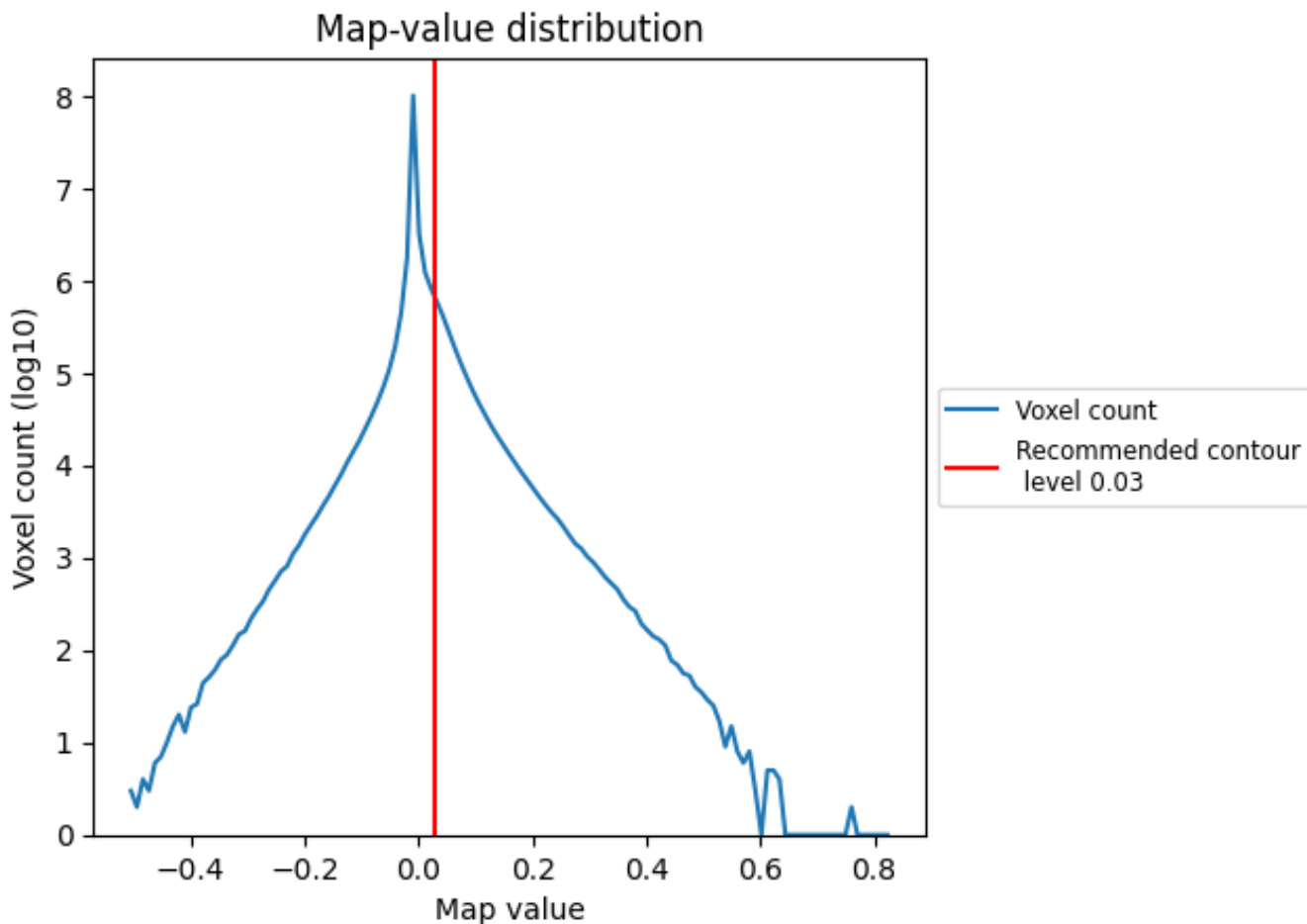
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

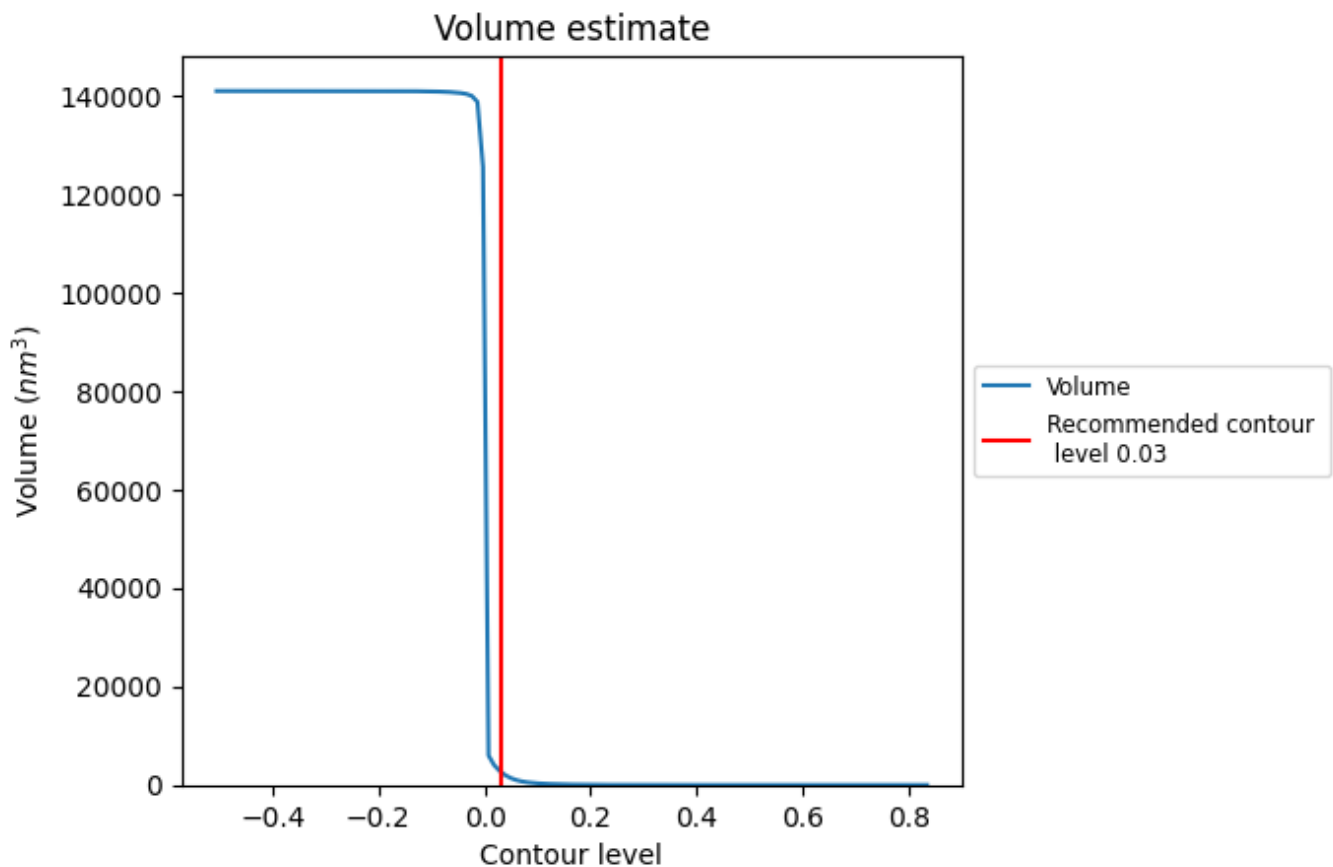
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

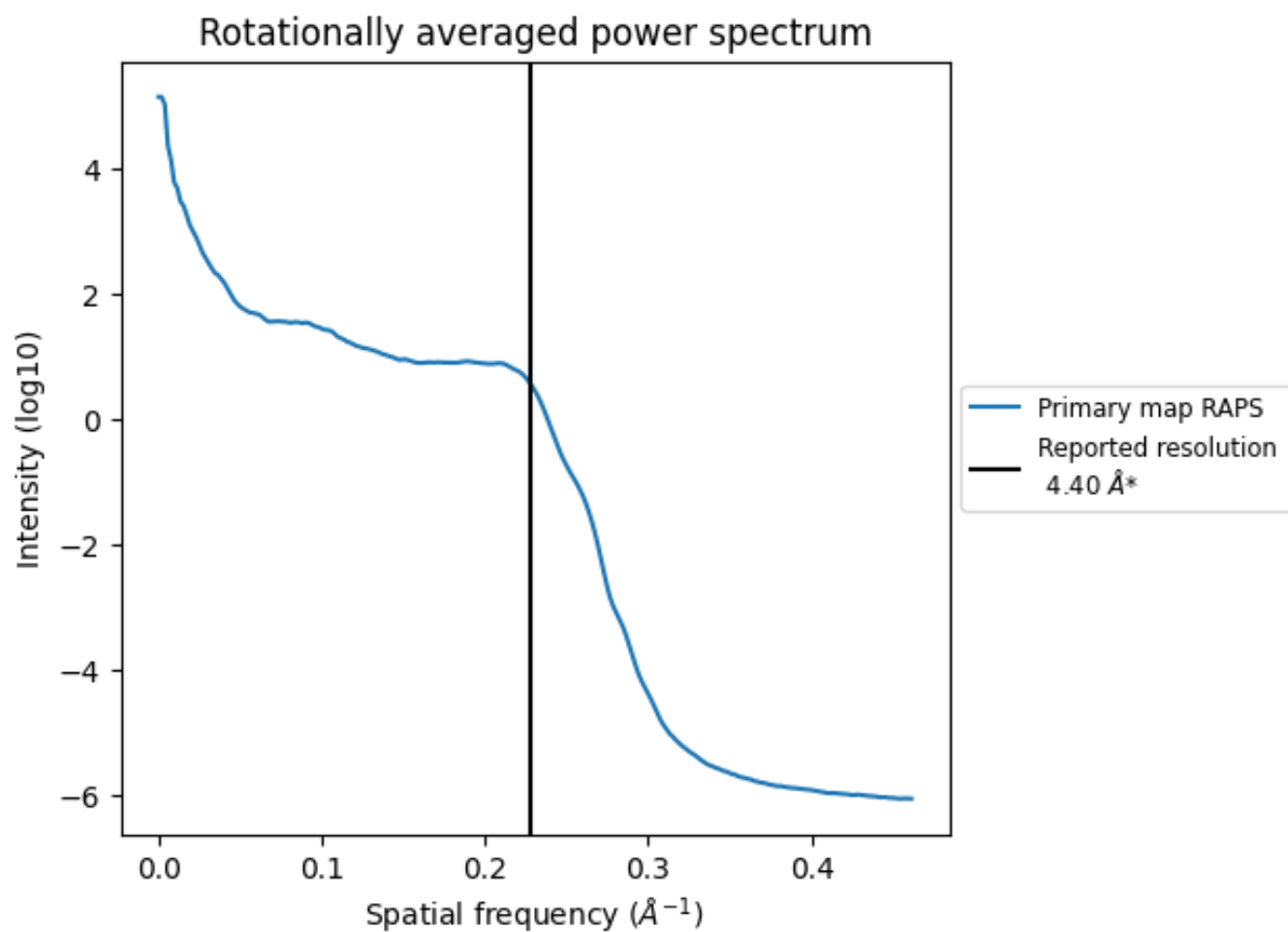
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2721 nm³; this corresponds to an approximate mass of 2458 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

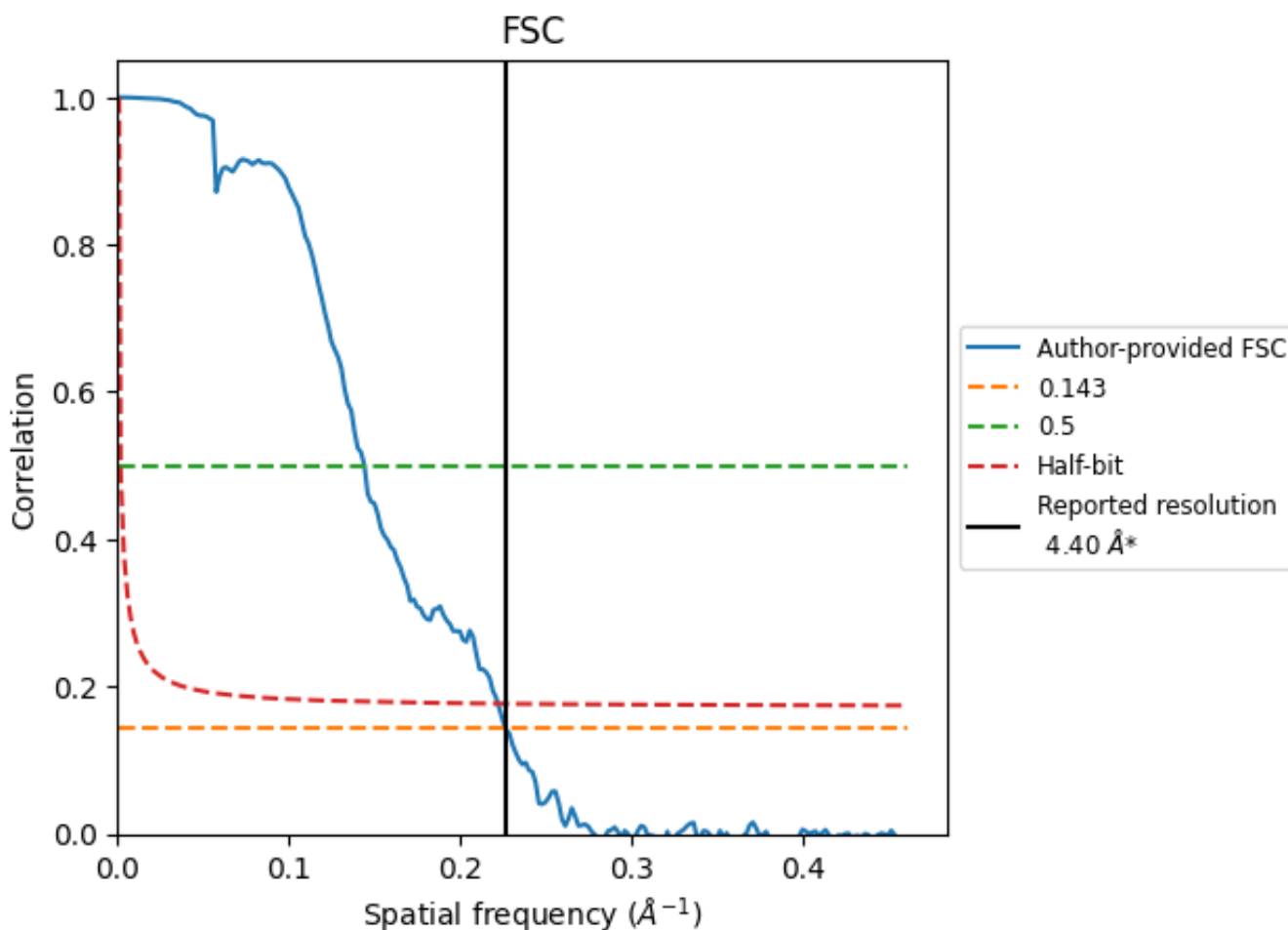


*Reported resolution corresponds to spatial frequency of 0.227\AA^{-1}

8 Fourier-Shell correlation [\(i\)](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

8.2 Resolution estimates [i](#)

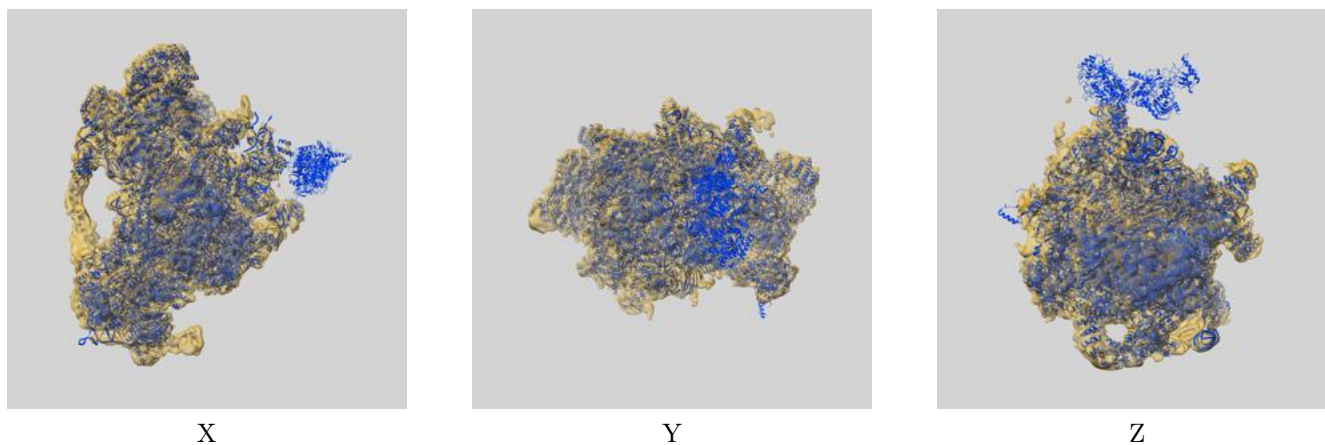
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.42	6.93	4.50
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

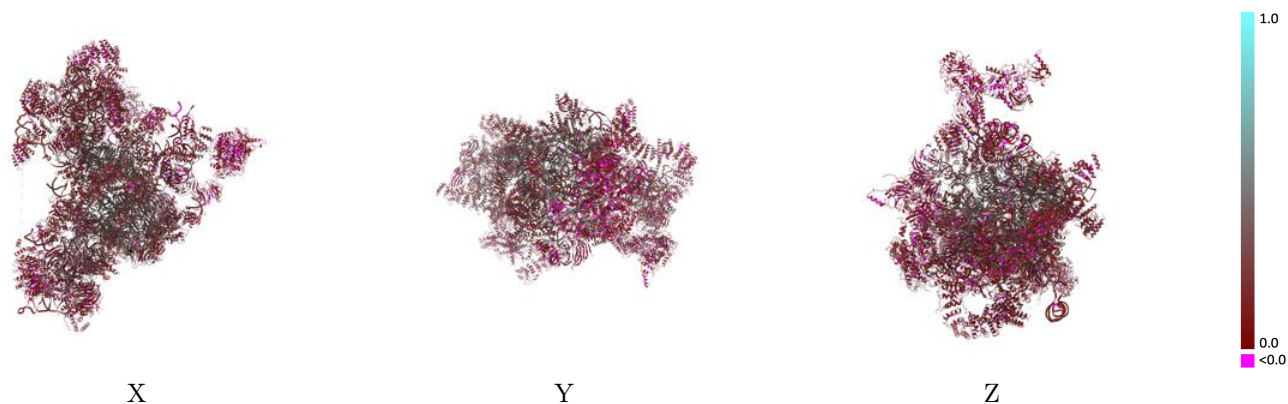
This section contains information regarding the fit between EMDB map EMD-10056 and PDB model 6RXZ. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



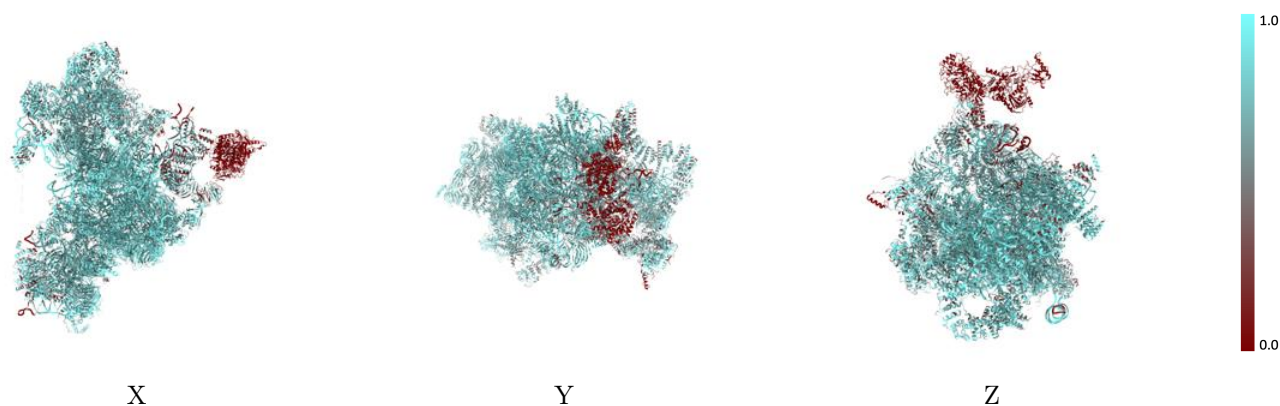
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



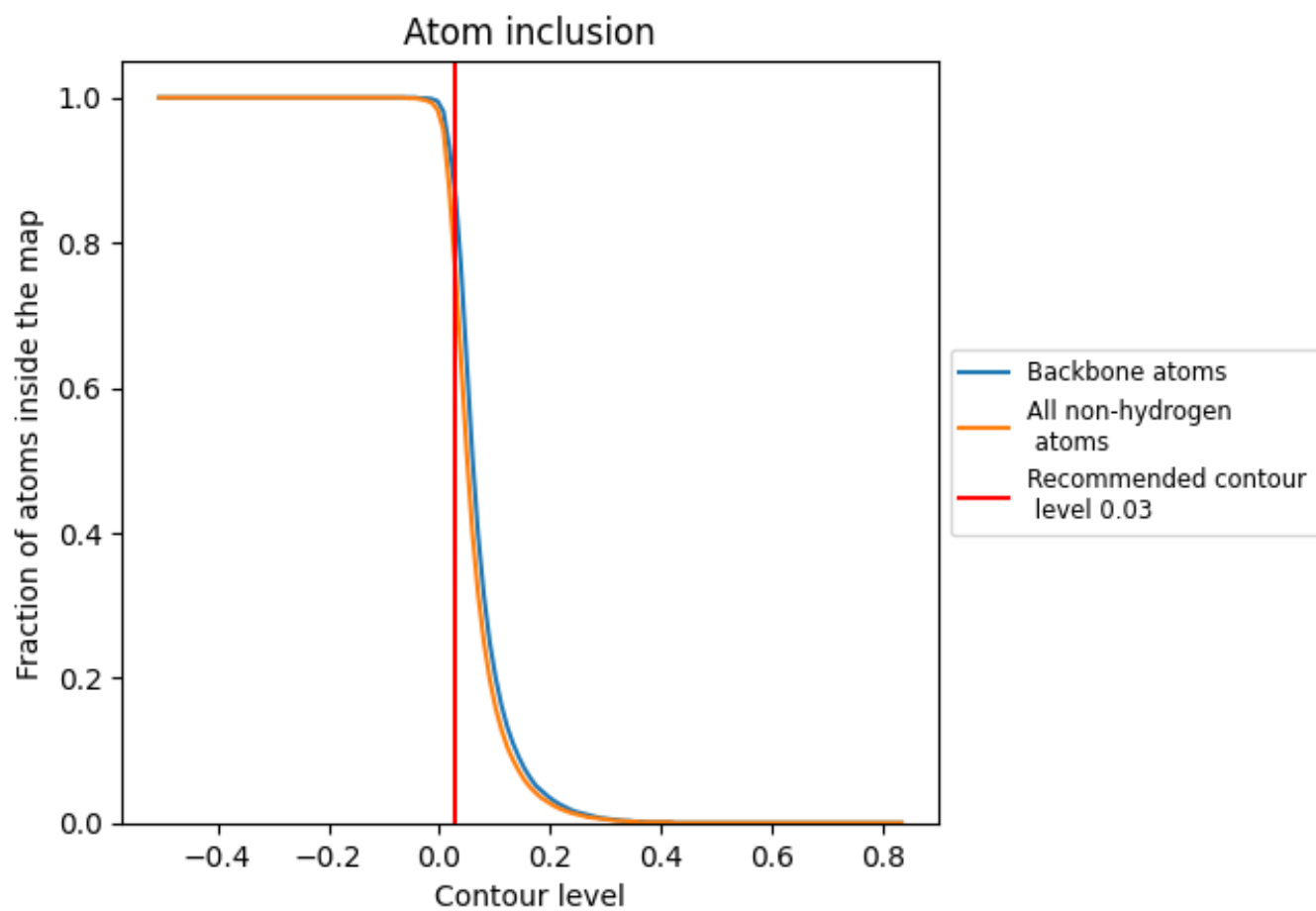
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7520	 0.2270
C1	 0.8700	 0.2580
C2	 0.9050	 0.2760
CA	 0.8720	 0.3590
CB	 0.7420	 0.2130
CC	 0.8130	 0.2470
CD	 0.7940	 0.2420
CE	 0.8610	 0.3370
CF	 0.8180	 0.2680
CG	 0.7830	 0.2070
CH	 0.8130	 0.2770
CI	 0.8790	 0.3550
CJ	 0.9150	 0.4170
CK	 0.8980	 0.4110
CL	 0.8390	 0.3190
CM	 0.8580	 0.3350
CN	 0.7370	 0.2190
CO	 0.6650	 0.1760
CP	 0.5340	 0.1610
CQ	 0.7250	 0.1670
CR	 0.7260	 0.1710
CS	 0.6120	 0.1210
CT	 0.8940	 0.3680
CU	 0.7960	 0.2810
CV	 0.0000	 0.0660
CW	 0.7380	 0.1660
CX	 0.6190	 0.1010
CY	 0.7510	 0.2410
CZ	 0.6960	 0.1540
Cb	 0.7140	 0.1810
Cc	 0.8230	 0.2950
Cd	 0.7370	 0.1700
Ce	 0.5820	 0.1730
Cf	 0.7440	 0.1410
Cg	 0.8540	 0.3460



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Ch	0.5340	0.1030
Ci	0.6460	0.1590
Cj	0.8910	0.4000
Ck	0.6730	0.1430
Cl	0.5030	0.2250
Cm	0.7760	0.2740
Cn	0.9170	0.4400
Co	0.7560	0.2010
Cp	0.8020	0.2540
Cz	0.4380	0.1550
UA	0.8580	0.3350
UB	0.7750	0.2200
UC	0.8880	0.3970
UD	0.7720	0.2150
UE	0.7200	0.1650
UF	0.8260	0.2180
UG	0.8040	0.3170
UH	0.7480	0.1680
UI	0.6510	0.1390
UJ	0.7460	0.2010
UK	0.8760	0.3630
UL	0.7580	0.1780
UM	0.6520	0.1240
UN	0.7670	0.2770
UO	0.7730	0.2240
UP	0.7540	0.2410
UQ	0.7900	0.2070
UR	0.8520	0.3000
US	0.7560	0.1660
UT	0.7440	0.1570
UU	0.8530	0.2850
UV	0.0030	0.0740
UX	0.8960	0.4090
UZ	0.8150	0.2630