Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 01:11 am GMT

PDB ID	:	6FT6
EMDB ID	:	EMD-4302
Title	:	Structure of the Nop53 pre-60S particle bound to the exosome nuclear cofactors
Authors	:	Schuller, J.M.; Falk, S.; Conti, E.
Deposited on	:	2018-02-20
Resolution	:	3.90 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:

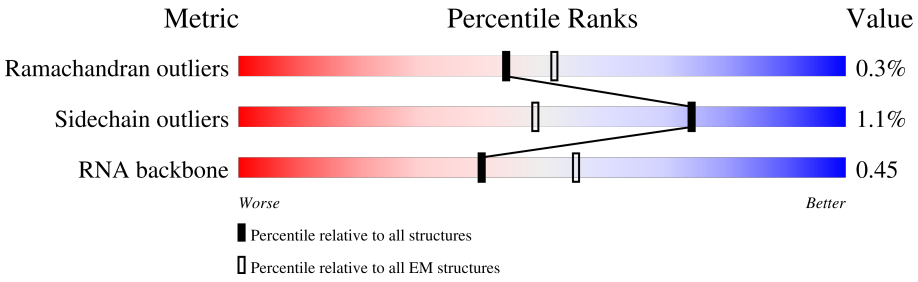
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.90 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.



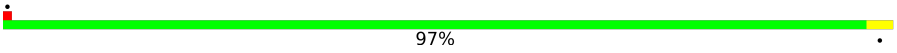
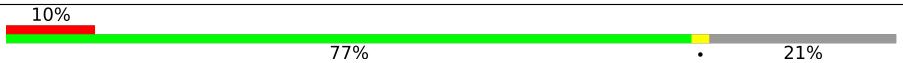
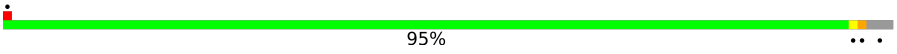
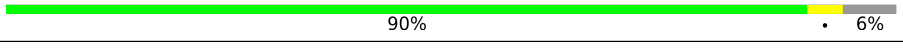
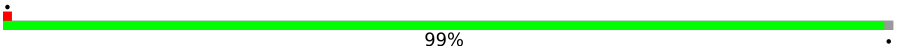
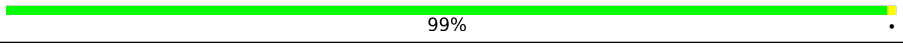
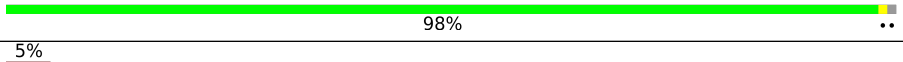
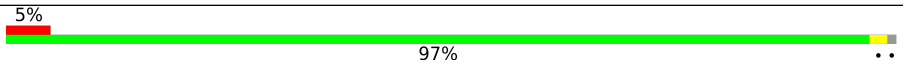
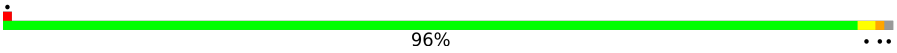
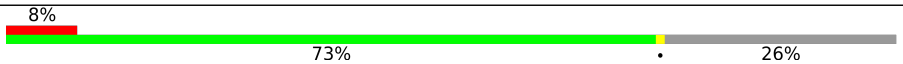
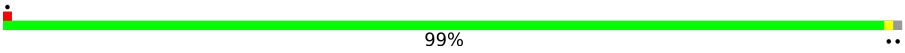
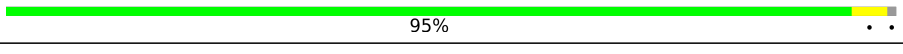
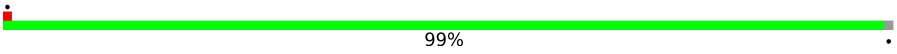
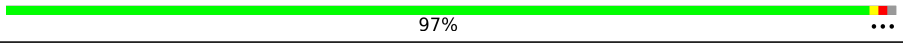
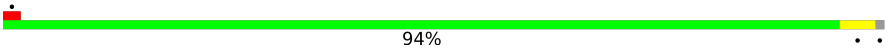
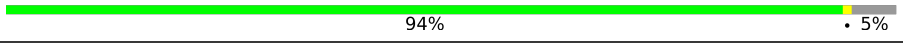
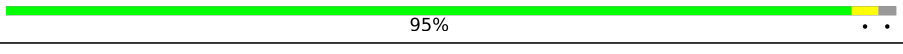
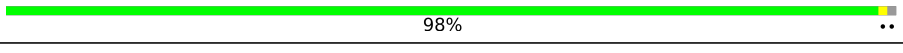
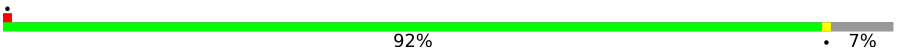
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	2	162	70% 27%
2	A	254	83% 16%
3	B	387	97%
4	C	362	98%
5	D	297	5% 91% 7%
6	E	176	88% 11%
7	F	244	90% 9%
8	G	256	89% 9%

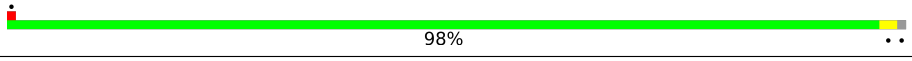
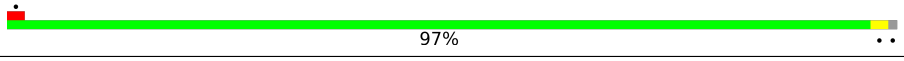
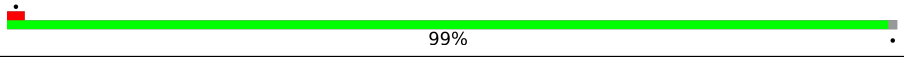
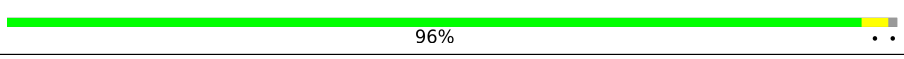
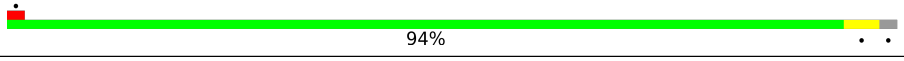
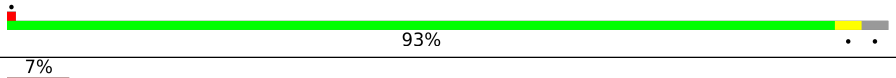
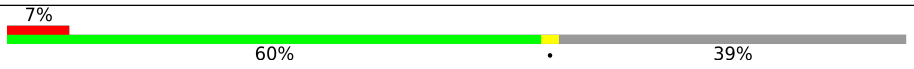
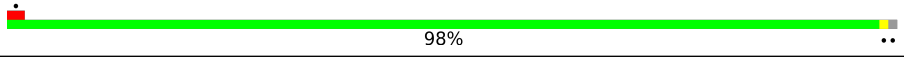
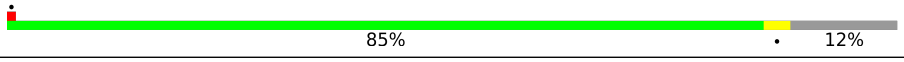
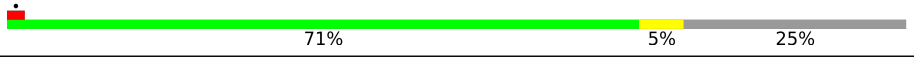
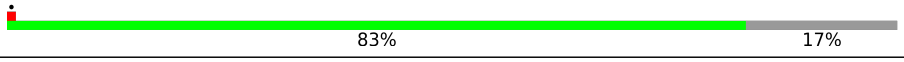
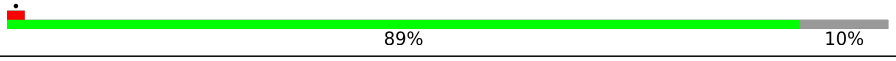
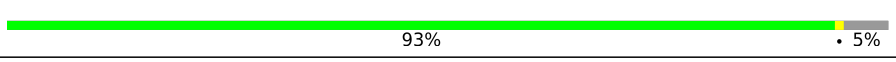
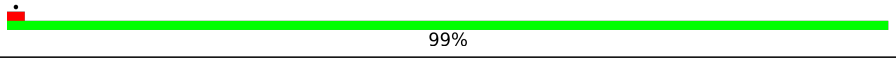
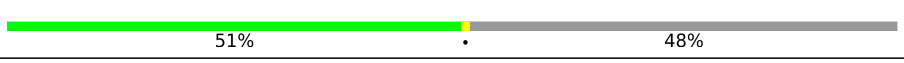
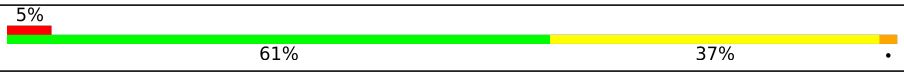
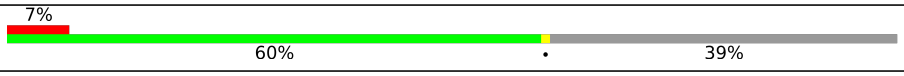
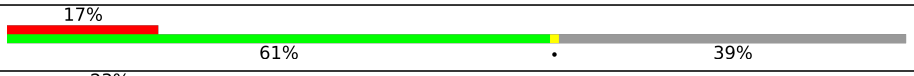
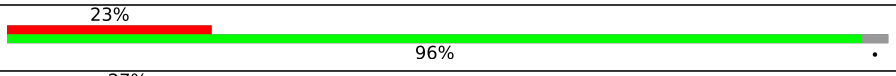
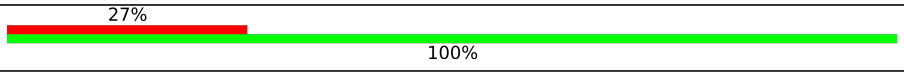
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	H	191	
10	I	166	
11	J	174	
12	L	199	
13	M	138	
14	N	204	
15	O	199	
16	P	184	
17	Q	186	
18	R	189	
19	S	172	
20	T	160	
21	U	121	
22	V	137	
23	W	236	
24	X	142	
25	Y	127	
26	Z	136	
27	a	149	
28	b	647	
29	c	105	
30	d	113	
31	e	130	
32	f	107	
33	g	121	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	h	120	
35	i	100	
36	j	88	
37	k	78	
38	l	51	
39	m	486	
40	n	605	
41	p	92	
42	r	261	
43	s	520	
44	u	199	
45	v	344	
46	w	203	
47	x	515	
48	y	245	
49	z	106	
50	1	3396	
51	3	121	
52	4	593	
53	5	120	
54	KK	733	
55	LL	184	
56	MM	1011	
57	NN	11	

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 157395 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 RNA chain called 7S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	162	3441	1540	606	1133	162	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	157	A	-	expression tag	GB 1279395616
2	158	A	-	expression tag	GB 1279395616
2	159	A	-	expression tag	GB 1279395616
2	160	A	-	expression tag	GB 1279395616
2	161	U	-	expression tag	GB 1279395616
2	162	U	-	expression tag	GB 1279395616

- Molecule 2 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	213	1634	1023	326	284	1	0	0

- Molecule 3 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	386	3081	1956	584	533	8	0	0

- Molecule 4 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	361	2749	1730	522	494	3	0	0

- Molecule 5 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	276	Total	C	N	O	S	0	0
			2211	1397	391	421	2		

- Molecule 6 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 7 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 8 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	233	Total	C	N	O	S	0	0
			1817	1159	326	329	3		

- Molecule 9 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 10 is a protein called Bud site selection protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	131	Total	C	N	O	S	0	0
			1059	662	195	198	4		

- Molecule 11 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 12 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	187	Total	C	N	O	0	0
			1499	934	307	258		

- Molecule 13 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	137	Total	C	N	O	S	0	0
			1059	678	200	179	2		

- Molecule 14 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 15 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 16 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	P	183	Total	C	N	O	0	0
			1442	896	287	259		

- Molecule 17 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	134	Total	C	N	O	S	0	0
			1035	659	196	179	1		

- Molecule 18 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	156	Total	C	N	O	0	0
			1258	781	265	212		

- Molecule 19 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	171	Total	C	N	O	S	0	0
			1437	925	266	243	3		

- Molecule 20 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	119	Total	C	N	O	S	0	0
			943	595	180	165	3		

- Molecule 21 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	106	Total	C	N	O	0	0
			844	545	138	161		

- Molecule 22 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 23 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	234	Total	C	N	O	S	0	0
			1885	1194	323	362	6		

- Molecule 24 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	122	Total	C	N	O	S	0	0
			977	629	172	174	2		

- Molecule 25 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Y	126	Total	C	N	O	0	0
			993	625	192	176		

- Molecule 26 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	Z	135	Total	C	N	O	0	0
			1092	710	202	180		

- Molecule 27 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	93	Total	C	N	O	S	0	0
			735	479	130	125	1		

- Molecule 28 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	642	Total	C	N	O	S	0	0
			5185	3251	938	970	26		

- Molecule 29 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 30 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	107	Total	C	N	O	S	0	0
			873	553	165	154	1		

- Molecule 31 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 32 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 33 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	112	Total	C	N	O	S	0	0
			881	546	179	152	4		

- Molecule 34 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 35 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 36 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	j	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 37 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	k	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 38 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	l	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 39 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	m	469	Total	C	N	O	S	0	0
			3774	2381	685	699	9		

- Molecule 40 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	n	371	Total	C	N	O	S	0	0
			3030	1963	523	534	10		

- Molecule 41 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 42 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	r	230	Total	C	N	O	S	0	0
			1860	1177	352	324	7		

- Molecule 43 is a protein called Nuclear GTP-binding protein NUG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	s	69	Total	C	N	O	S	0	0
			573	359	113	98	3		

- Molecule 44 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	u	150	Total	C	N	O	S	0	0
			1265	793	253	210	9		

- Molecule 45 is a protein called Ribosome biogenesis protein RPF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	v	287	Total	C	N	O	S	0	0
			2318	1482	408	412	16		

- Molecule 46 is a protein called Regulator of ribosome biosynthesis.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	w	182	Total	C	N	O	S	0	0
			1448	911	261	271	5		

- Molecule 47 is a protein called Ribosome assembly protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	x	488	Total	C	N	O	S	0	0
			3807	2398	677	711	21		

- Molecule 48 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	y	244	Total	C	N	O	S	0	0
			1849	1146	319	377	7		

- Molecule 49 is a protein called UPF0642 protein YBL028C.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	z	55	Total	C	N	O	0	0
			444	273	88	83		

- Molecule 50 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	1	3058	Total	C	N	O	P	0	0
			65427	29223	11807	21339	3058		

- Molecule 51 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 52 is a protein called Probable metalloprotease ARX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	516	Total	C	N	O	S	0	0
			3999	2530	688	766	15		

- Molecule 53 is a protein called rRNA-processing protein CGR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	5	73	Total	C	N	O	S	0	0
			645	395	133	114	3		

- Molecule 54 is a protein called Exosome complex exonuclease RRP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	KK	86	Total	C	N	O	S	0	0
			661	411	112	134	4		

- Molecule 55 is a protein called Exosome complex protein LRP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	LL	113	Total	C	N	O	S	0	0
			894	565	151	174	4		

- Molecule 56 is a protein called ATP-dependent RNA helicase DOB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	MM	977	Total	C	N	O	S	0	0
			7619	4866	1293	1418	42		

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
MM	1	MET	-	initiating methionine	UNP P47047
MM	2	ASP	-	expression tag	UNP P47047
MM	3	SER	-	expression tag	UNP P47047
MM	4	THR	-	expression tag	UNP P47047
MM	5	ASP	-	expression tag	UNP P47047
MM	6	LEU	-	expression tag	UNP P47047
MM	7	PHE	-	expression tag	UNP P47047
MM	8	ASP	-	expression tag	UNP P47047
MM	9	VAL	-	expression tag	UNP P47047
MM	10	PHE	-	expression tag	UNP P47047
MM	11	GLU	-	expression tag	UNP P47047
MM	12	GLU	-	expression tag	UNP P47047
MM	13	THR	-	expression tag	UNP P47047
MM	14	PRO	-	expression tag	UNP P47047
MM	15	VAL	-	expression tag	UNP P47047
MM	16	GLU	-	expression tag	UNP P47047
MM	17	LEU	-	expression tag	UNP P47047

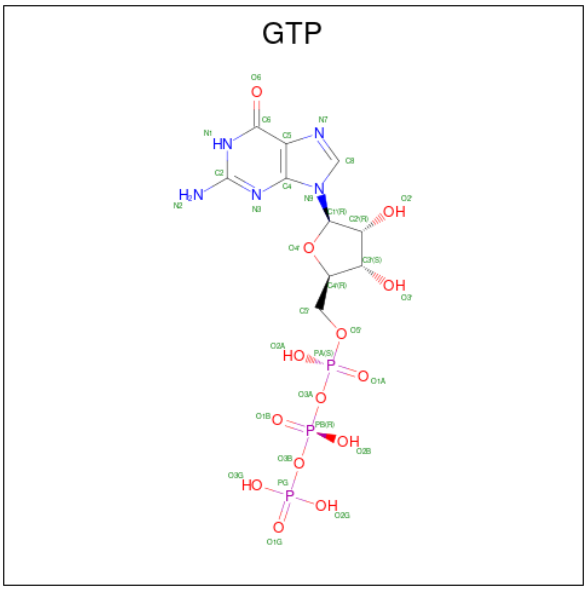
- Molecule 57 is a protein called MPP6.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	NN	11	Total	C	N	O	0	0
			55	33	11	11		

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
58	I	1	Total Zn 1 1	0
58	j	1	Total Zn 1 1	0
58	p	1	Total Zn 1 1	0
58	u	1	Total Zn 1 1	0

- Molecule 59 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms	AltConf
59	b	1	Total C N O P 32 10 5 14 3	0
59	m	1	Total C N O P 32 10 5 14 3	0

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

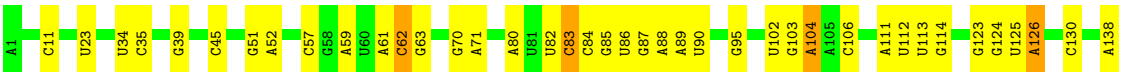
Mol	Chain	Residues	Atoms	AltConf
60	b	1	Total Mg 1 1	0
60	m	1	Total Mg 1 1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 7S ribosomal RNA

Chain 2:

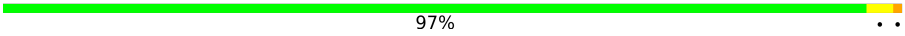


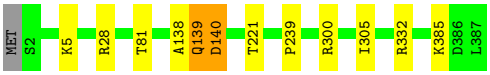
• Molecule 2: 60S ribosomal protein L2-A

Chain A:

• Molecule 3: 60S ribosomal protein L3

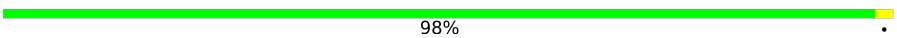
Chain B:





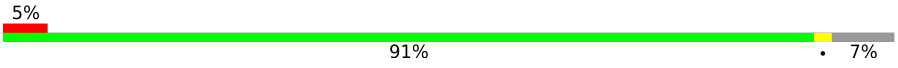
• Molecule 4: 60S ribosomal protein L4-A

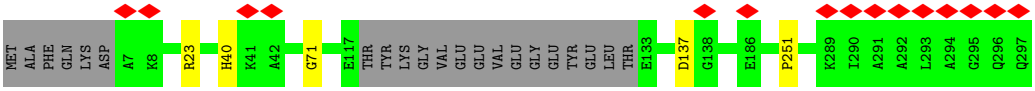
Chain C:



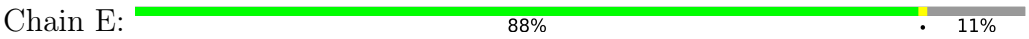
• Molecule 5: 60S ribosomal protein L5

Chain D:

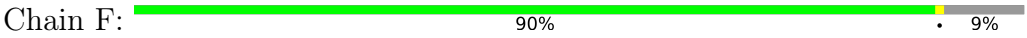


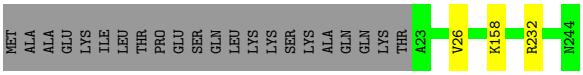


• Molecule 6: 60S ribosomal protein L6-A

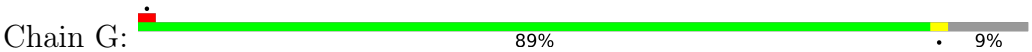


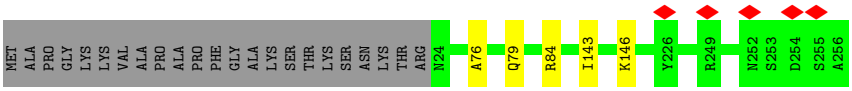
• Molecule 7: 60S ribosomal protein L7-A





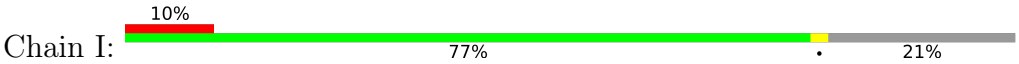
• Molecule 8: 60S ribosomal protein L8-A

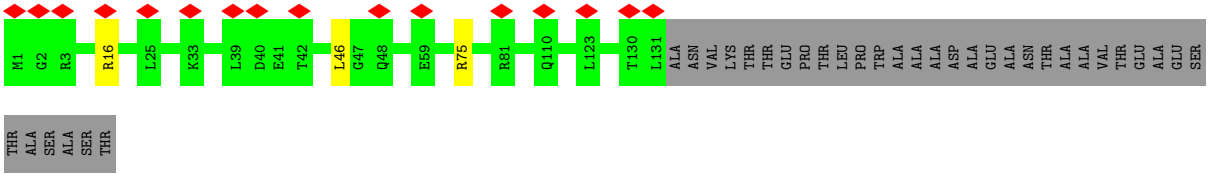




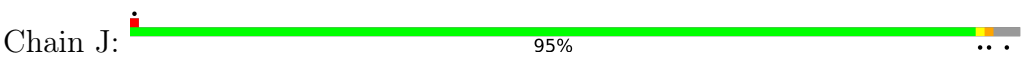
• Molecule 9: 60S ribosomal protein L9-A

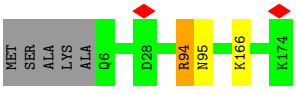
• Molecule 10: Bud site selection protein 20





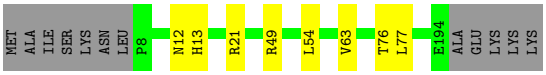
• Molecule 11: 60S ribosomal protein L11-A





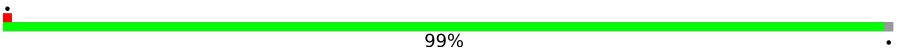
• Molecule 12: 60S ribosomal protein L13-A

Chain L:



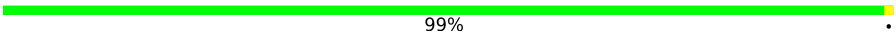
• Molecule 13: 60S ribosomal protein L14-A

Chain M:



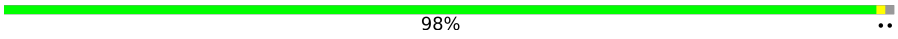
• Molecule 14: 60S ribosomal protein L15-A

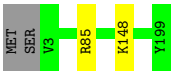
Chain N:



• Molecule 15: 60S ribosomal protein L16-A

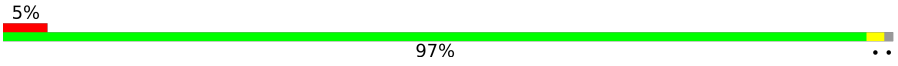
Chain O:

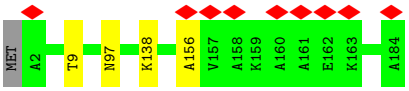




• Molecule 16: 60S ribosomal protein L17-A

Chain P:



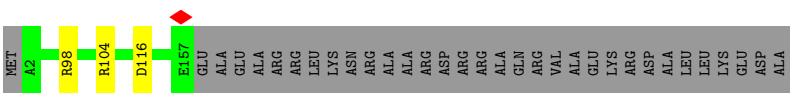


• Molecule 17: 60S ribosomal protein L18-A

Chain Q:

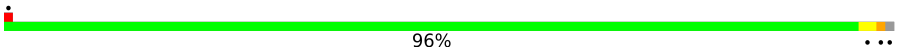
• Molecule 18: 60S ribosomal protein L19-A

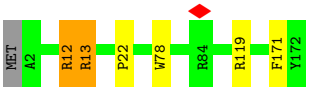
Chain R:



• Molecule 19: 60S ribosomal protein L20-A

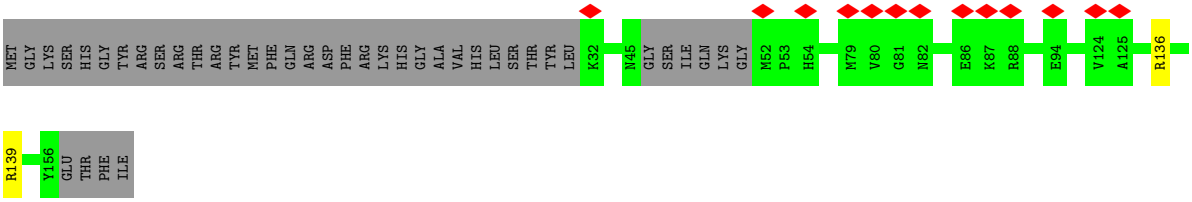
Chain S:





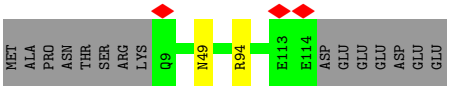
• Molecule 20: 60S ribosomal protein L21-A

Chain T:



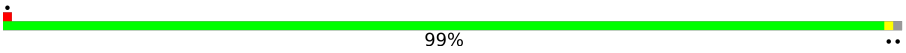
• Molecule 21: 60S ribosomal protein L22-A

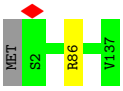
Chain U:



• Molecule 22: 60S ribosomal protein L23-A

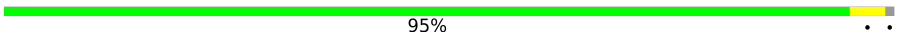
Chain V:





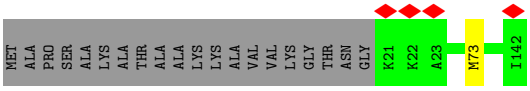
• Molecule 23: Ribosome assembly factor MRT4

Chain W:



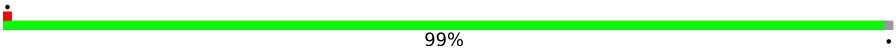
• Molecule 24: 60S ribosomal protein L25

Chain X:



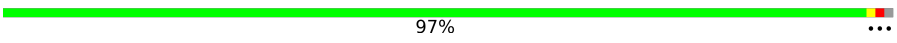
• Molecule 25: 60S ribosomal protein L26-A

Chain Y:



• Molecule 26: 60S ribosomal protein L27-A

Chain Z:

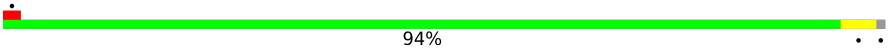


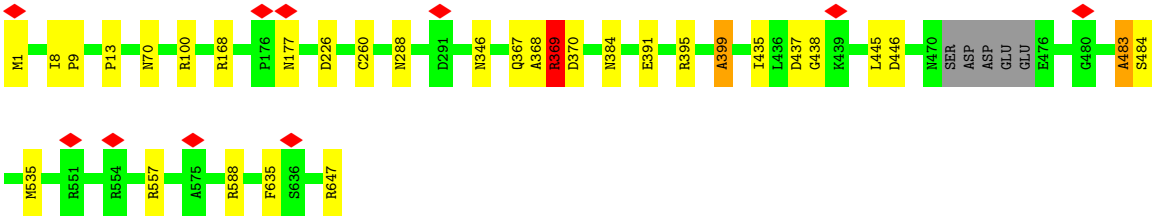
• Molecule 27: 60S ribosomal protein L28

Chain a:

• Molecule 28: Nucleolar GTP-binding protein 1

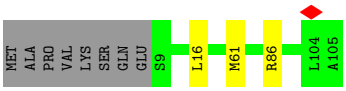
Chain b:





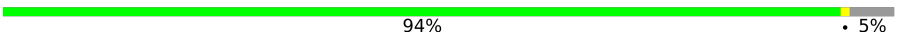
• Molecule 29: 60S ribosomal protein L30

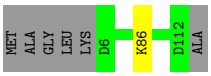
Chain c:



• Molecule 30: 60S ribosomal protein L31-A

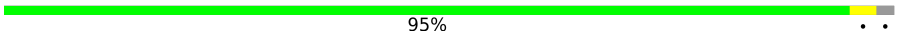
Chain d:





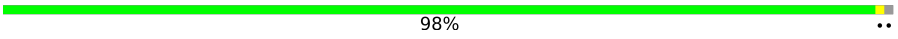
• Molecule 31: 60S ribosomal protein L32

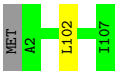
Chain e:



• Molecule 32: 60S ribosomal protein L33-A

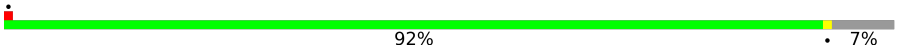
Chain f:

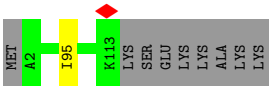




• Molecule 33: 60S ribosomal protein L34-A

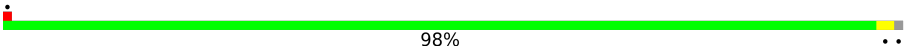
Chain g:

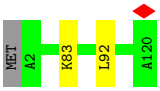




• Molecule 34: 60S ribosomal protein L35-A

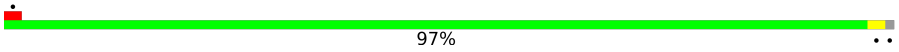
Chain h:

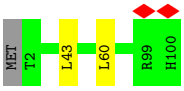




• Molecule 35: 60S ribosomal protein L36-A

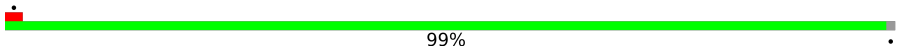
Chain i:

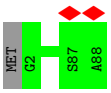




• Molecule 36: 60S ribosomal protein L37-A

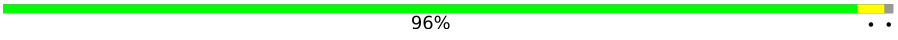
Chain j:

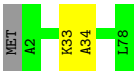




• Molecule 37: 60S ribosomal protein L38

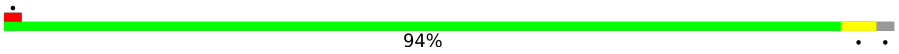
Chain k:

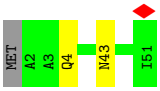




• Molecule 38: 60S ribosomal protein L39

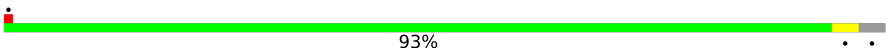
Chain l:

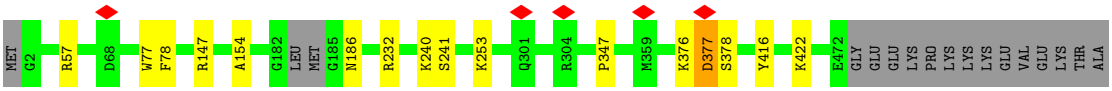




• Molecule 39: Nucleolar GTP-binding protein 2

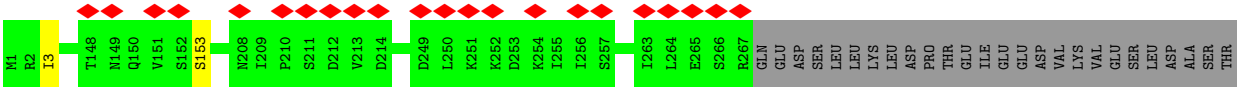
Chain m:

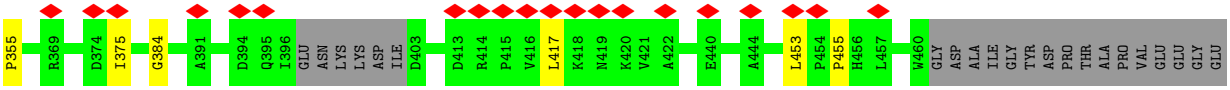




• Molecule 40: Pescadillo homolog

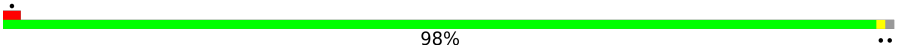
Chain n:

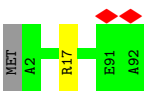




• Molecule 41: 60S ribosomal protein L43-A

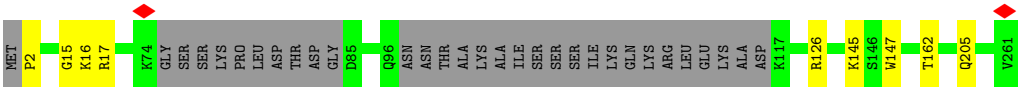
Chain p:





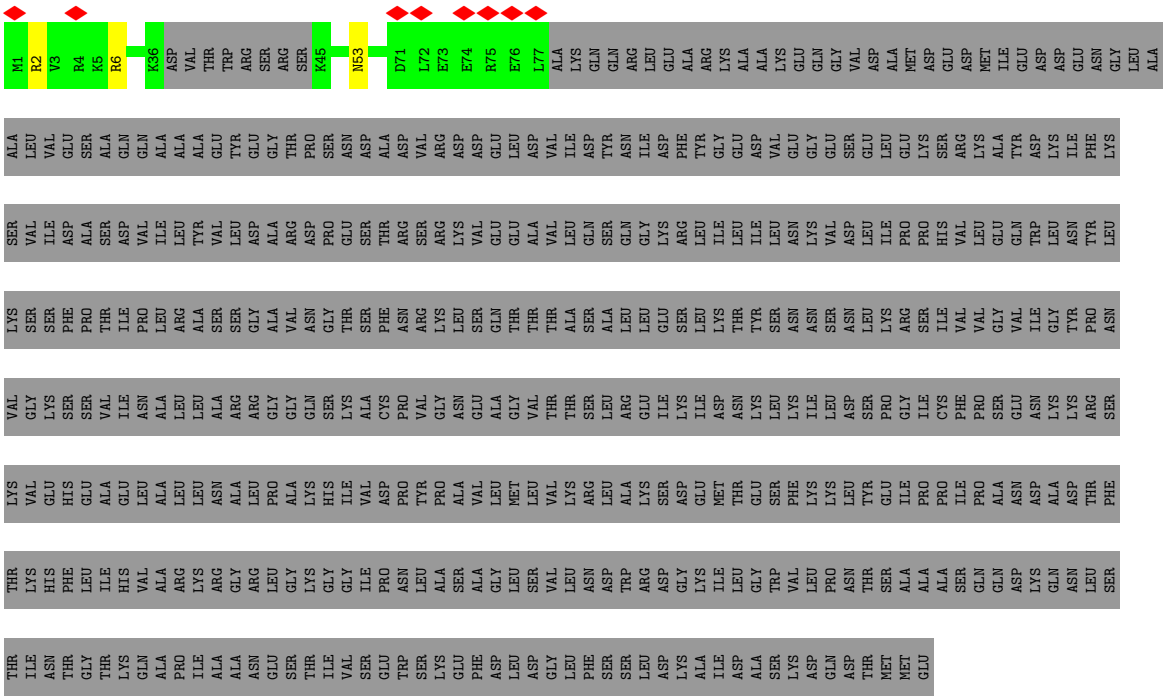
• Molecule 42: Ribosome biogenesis protein NSA2

Chain r:



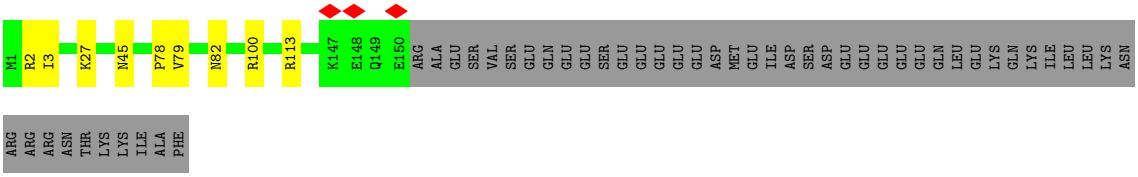
• Molecule 43: Nuclear GTP-binding protein NUG1

Chain s:



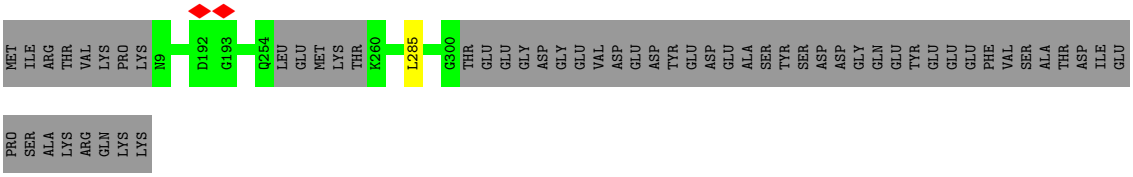
• Molecule 44: Ribosome biogenesis protein RLP24

Chain u:



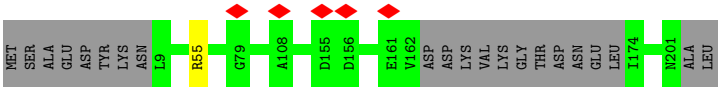
• Molecule 45: Ribosome biogenesis protein RPF2

Chain v:



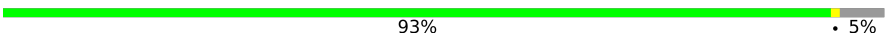
• Molecule 46: Regulator of ribosome biosynthesis

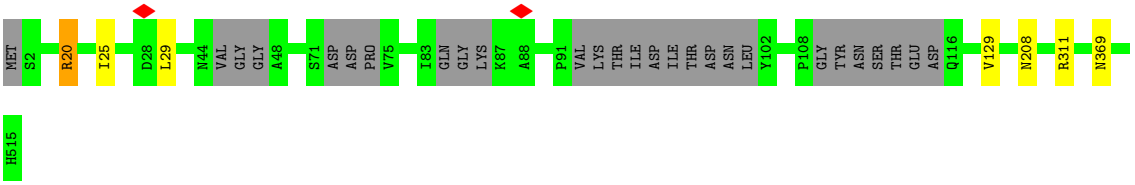
Chain w:



• Molecule 47: Ribosome assembly protein 4

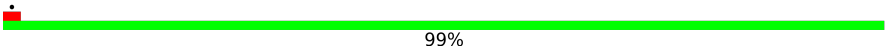
Chain x:

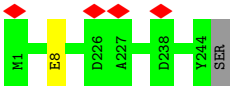




• Molecule 48: Eukaryotic translation initiation factor 6

Chain y:



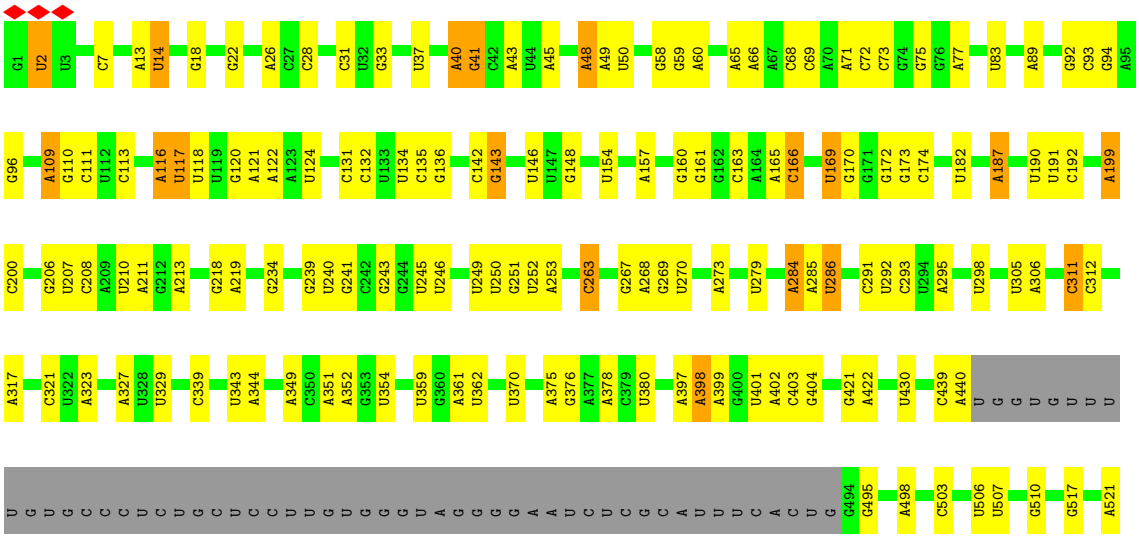


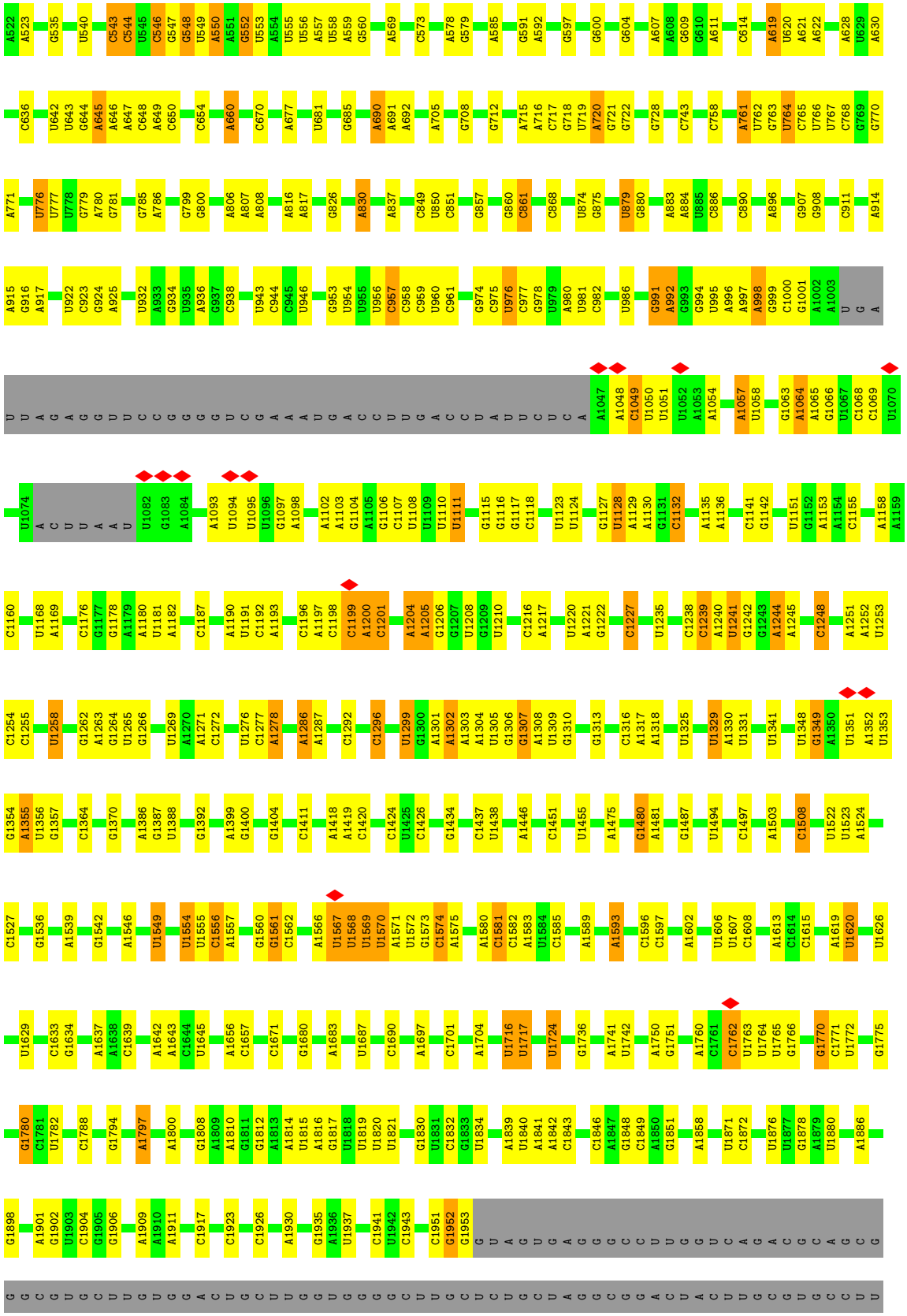
• Molecule 49: UPF0642 protein YBL028C

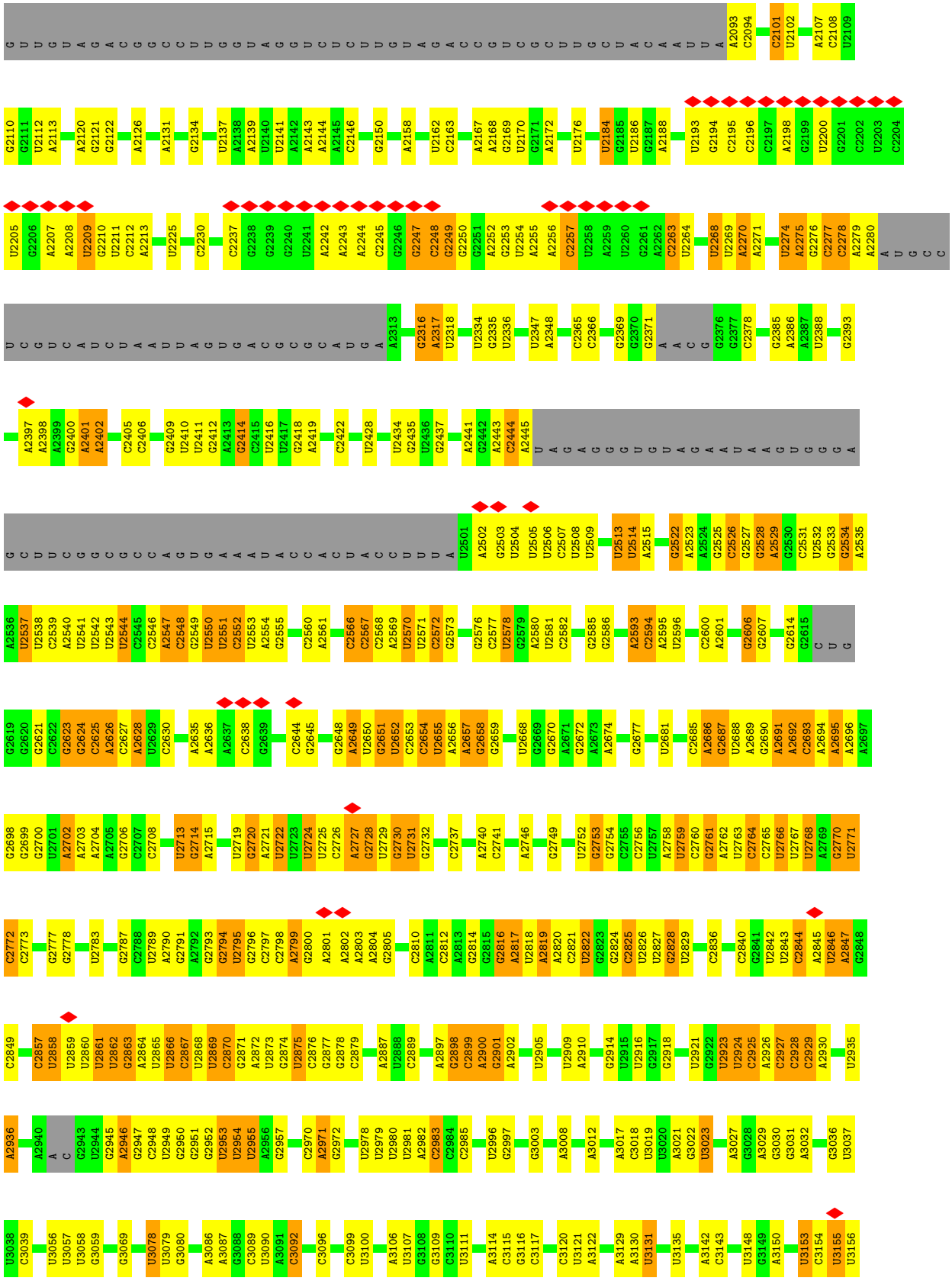
Chain z:

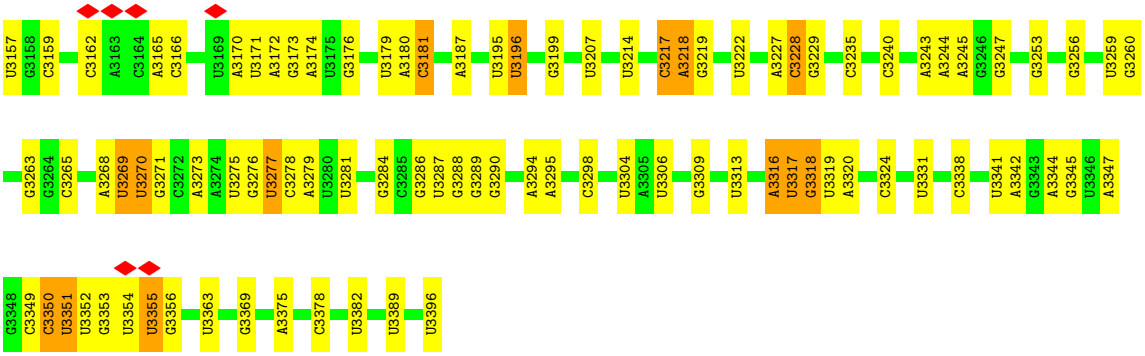
• Molecule 50: 25S ribosomal RNA

Chain 1:



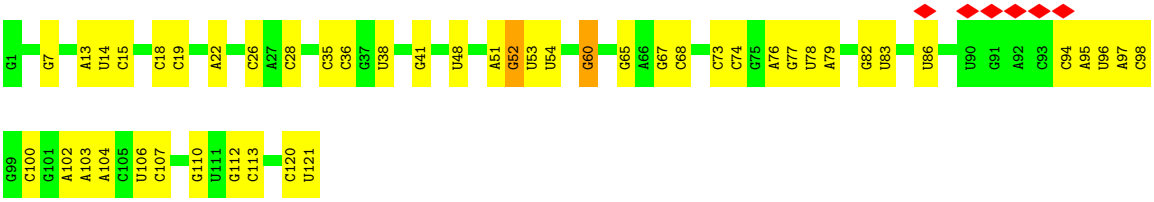






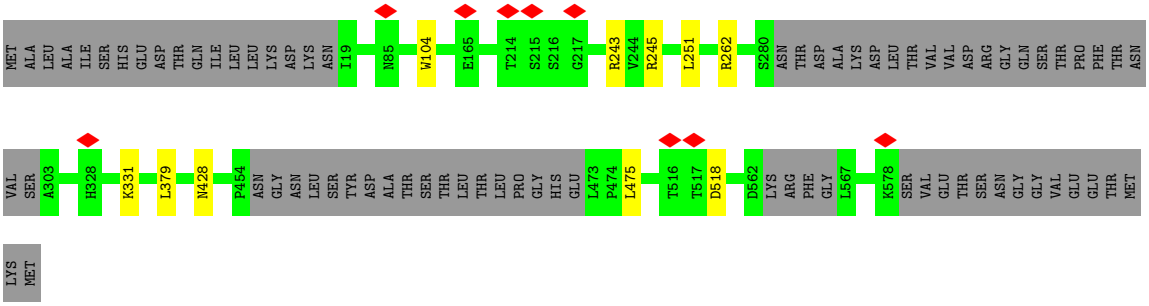
• Molecule 51: 5S ribosomal RNA

Chain 3:



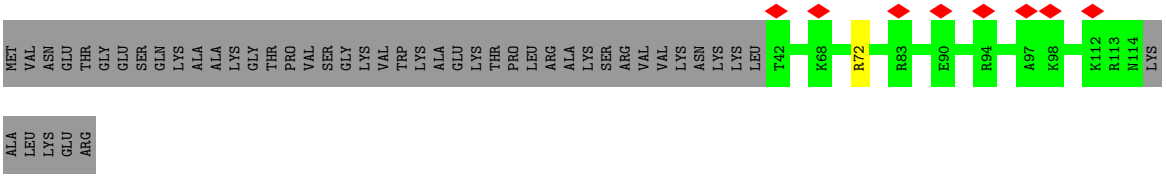
• Molecule 52: Probable metalloprotease ARX1

Chain 4:



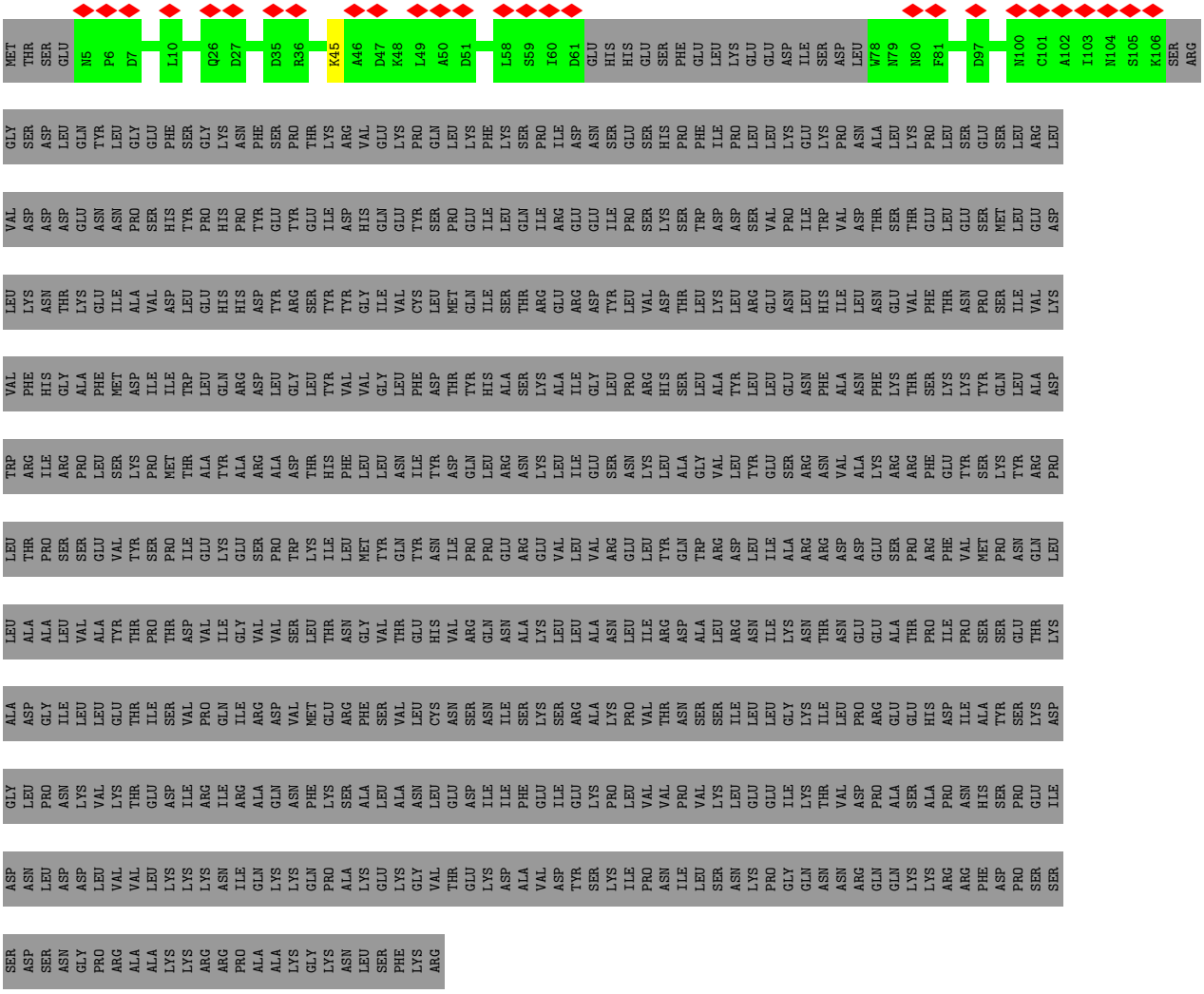
• Molecule 53: rRNA-processing protein CGR1

Chain 5:



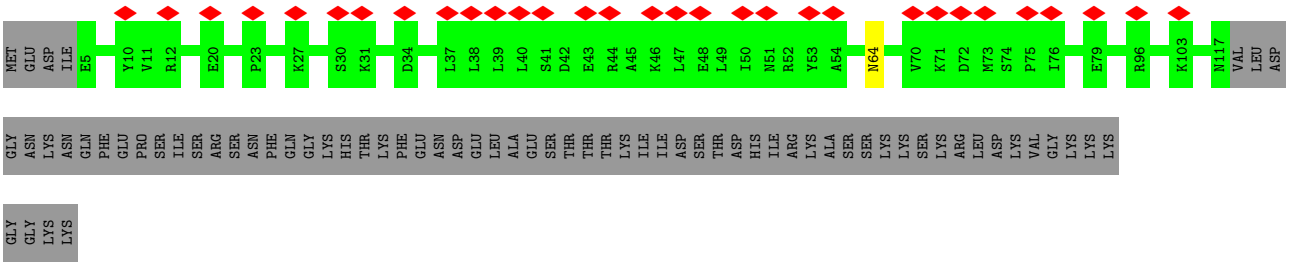
• Molecule 54: Exosome complex exonuclease RRP6

Chain KK:



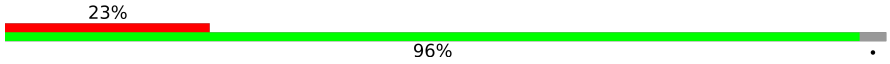
• Molecule 55: Exosome complex protein LRP1

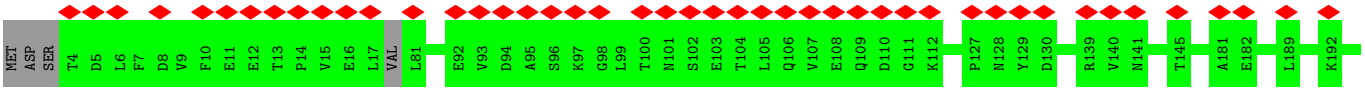
Chain LL:

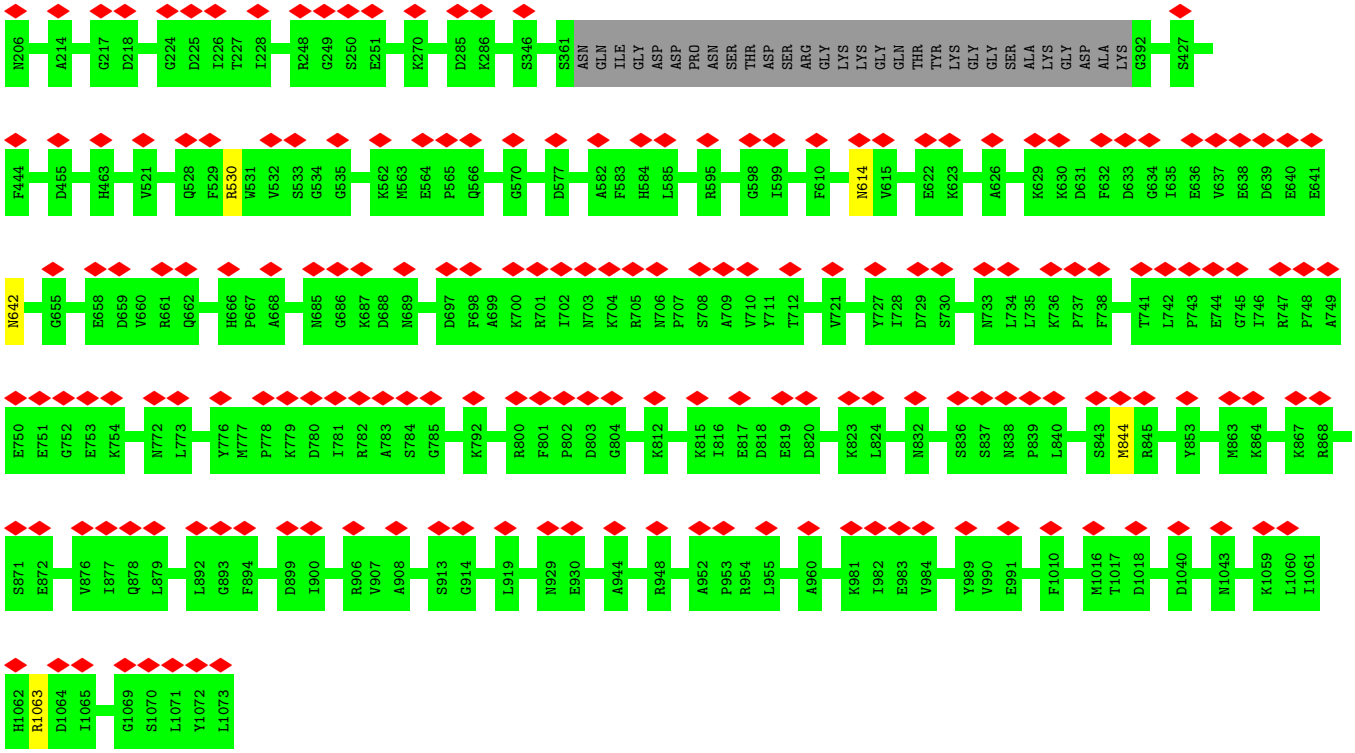


• Molecule 56: ATP-dependent RNA helicase DOB1

Chain MM:

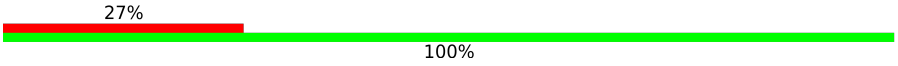


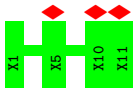




- Molecule 57: MPP6

Chain NN:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22439	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 ($e^-/Å^2$)	38.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.072	Depositor
Minimum map value	-0.024	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	594.0, 594.0, 594.0	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG, 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	2	1.47	6/3846 (0.2%)	1.21	11/5988 (0.2%)
2	A	0.65	0/1666	0.65	0/2241
3	B	0.70	0/3152	0.72	1/4239 (0.0%)
4	C	0.62	0/2801	0.69	1/3792 (0.0%)
5	D	0.51	0/2257	0.63	0/3043
6	E	0.56	0/1260	0.60	0/1694
7	F	0.64	0/1821	0.66	0/2451
8	G	0.61	0/1849	0.67	1/2495 (0.0%)
9	H	0.60	0/1539	0.69	1/2073 (0.0%)
10	I	0.41	0/1075	0.57	1/1443 (0.1%)
11	J	0.41	0/1374	0.68	0/1842
12	L	0.63	1/1524 (0.1%)	0.71	0/2046
13	M	0.59	0/1074	0.63	0/1446
14	N	0.73	0/1757	0.71	1/2354 (0.0%)
15	O	0.69	0/1585	0.64	0/2128
16	P	0.63	0/1465	0.64	0/1968
17	Q	0.60	0/1050	0.69	2/1419 (0.1%)
18	R	0.61	0/1275	0.67	1/1702 (0.1%)
19	S	0.65	1/1473 (0.1%)	0.68	1/1980 (0.1%)
20	T	0.43	0/957	0.63	0/1285
21	U	0.56	0/861	0.64	0/1167
22	V	0.69	0/1018	0.71	0/1369
23	W	0.55	0/1918	0.69	0/2586
24	X	0.63	0/992	0.66	0/1336
25	Y	0.60	0/1004	0.68	0/1341
26	Z	0.60	0/1118	0.67	1/1497 (0.1%)
27	a	0.61	0/751	0.68	0/1013
28	b	0.55	1/5270 (0.0%)	0.68	0/7080
29	c	0.62	0/751	0.65	0/1008
30	d	0.63	0/887	0.63	0/1191
31	e	0.59	1/1041 (0.1%)	0.64	0/1394
32	f	0.76	1/868 (0.1%)	0.64	0/1168

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	g	0.65	0/891	0.65	0/1191
34	h	0.63	0/978	0.71	0/1301
35	i	0.55	0/778	0.68	1/1034 (0.1%)
36	j	0.71	0/696	0.69	0/923
37	k	0.55	0/618	0.66	0/826
38	l	0.68	0/443	0.68	0/588
39	m	0.60	0/3848	0.73	1/5181 (0.0%)
40	n	0.52	0/3101	0.69	2/4187 (0.0%)
41	p	0.64	0/701	0.68	0/934
42	r	0.62	0/1892	0.75	1/2528 (0.0%)
43	s	0.57	1/577 (0.2%)	0.60	0/752
44	u	0.51	0/1287	0.59	0/1711
45	v	0.49	0/2361	0.63	1/3153 (0.0%)
46	w	0.46	0/1471	0.64	0/1980
47	x	0.56	1/3897 (0.0%)	0.65	0/5282
48	y	0.57	0/1872	0.66	0/2548
49	z	0.52	0/445	0.57	0/585
50	1	1.39	72/73234 (0.1%)	1.34	769/114167 (0.7%)
51	3	0.89	1/2883 (0.0%)	1.31	44/4491 (1.0%)
52	4	0.50	0/4069	0.66	1/5520 (0.0%)
53	5	0.43	0/649	0.59	0/848
54	KK	0.29	0/667	0.45	0/899
55	LL	0.32	0/903	0.51	0/1210
56	MM	0.36	0/7765	0.55	0/10511
All	All	1.04	86/167305 (0.1%)	1.06	842/242129 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	1
3	B	0	3
4	C	0	3
5	D	0	4
7	F	0	2
8	G	0	2
9	H	0	1
10	I	0	1
11	J	0	1
12	L	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
16	P	0	2
19	S	0	3
23	W	0	2
26	Z	0	3
27	a	0	1
28	b	0	15
30	d	0	1
34	h	0	1
37	k	0	2
38	l	0	1
39	m	0	8
40	n	0	3
42	r	0	4
43	s	0	1
44	u	0	3
47	x	0	4
48	y	0	1
52	4	0	2
56	MM	0	1
All	All	0	78

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	1	2702	A	N9-C4	-8.81	1.32	1.37
32	f	102	LEU	C-N	-8.72	1.14	1.34
50	1	1200	A	N9-C4	-8.66	1.32	1.37
50	1	116	A	N9-C4	-7.88	1.33	1.37
43	s	53	ASN	C-N	-7.41	1.17	1.34
12	L	13	HIS	CA-CB	-6.83	1.39	1.53
50	1	199	A	N9-C4	-6.83	1.33	1.37
50	1	883	A	N9-C4	-6.63	1.33	1.37
50	1	327	A	N9-C4	-6.38	1.34	1.37
50	1	1546	A	N9-C4	-6.31	1.34	1.37
1	2	126	A	N9-C4	-6.26	1.34	1.37
50	1	2348	A	N9-C4	-6.23	1.34	1.37
50	1	2249	G	N9-C4	-6.21	1.32	1.38
50	1	1169	A	N9-C4	-6.20	1.34	1.37
50	1	716	A	N9-C4	-6.17	1.34	1.37
50	1	1418	A	N9-C4	-6.16	1.34	1.37
50	1	1697	A	N9-C4	-6.11	1.34	1.37
50	1	1286	A	N9-C4	-6.05	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	1	830	A	N9-C4	-6.04	1.34	1.37
50	1	187	A	N9-C4	-6.02	1.34	1.37
50	1	1480	G	N9-C4	-6.01	1.33	1.38
50	1	1656	A	N9-C4	-6.00	1.34	1.37
50	1	109	A	N9-C4	-5.91	1.34	1.37
19	S	78	TRP	CB-CG	-5.86	1.39	1.50
50	1	2139	A	N9-C4	-5.85	1.34	1.37
50	1	690	A	N9-C4	-5.67	1.34	1.37
50	1	1524	A	N9-C4	-5.66	1.34	1.37
1	2	149	A	N9-C4	-5.64	1.34	1.37
31	e	51	SER	C-N	-5.64	1.21	1.34
50	1	2414	G	N9-C8	-5.63	1.33	1.37
50	1	3106	A	N9-C4	-5.62	1.34	1.37
1	2	104	A	N9-C4	-5.60	1.34	1.37
50	1	2692	A	N9-C4	-5.59	1.34	1.37
50	1	2799	A	N9-C4	-5.58	1.34	1.37
50	1	361	A	N9-C4	-5.58	1.34	1.37
50	1	2936	A	N9-C4	-5.57	1.34	1.37
50	1	2143	A	N9-C4	-5.57	1.34	1.37
50	1	2167	A	N9-C4	-5.57	1.34	1.37
50	1	2686	A	N9-C4	-5.56	1.34	1.37
50	1	1797	A	N9-C4	-5.54	1.34	1.37
1	2	71	A	N9-C4	-5.53	1.34	1.37
28	b	391	GLU	C-N	-5.52	1.21	1.34
50	1	3008	A	N9-C4	-5.50	1.34	1.37
50	1	352	A	N9-C4	-5.50	1.34	1.37
50	1	925	A	N9-C4	-5.49	1.34	1.37
50	1	273	A	N9-C4	-5.48	1.34	1.37
1	2	61	A	N9-C4	-5.46	1.34	1.37
50	1	1602	A	N9-C4	-5.44	1.34	1.37
50	1	1911	A	N9-C4	-5.43	1.34	1.37
50	1	2929	C	N1-C6	-5.43	1.33	1.37
50	1	816	A	N9-C4	-5.40	1.34	1.37
50	1	2172	A	N9-C4	-5.39	1.34	1.37
50	1	2971	A	N9-C4	-5.35	1.34	1.37
51	3	104	A	C5-C6	-5.35	1.36	1.41
1	2	89	A	N9-C4	-5.35	1.34	1.37
50	1	1302	A	N7-C5	-5.34	1.36	1.39
50	1	992	A	N9-C4	-5.32	1.34	1.37
50	1	660	A	N9-C4	-5.32	1.34	1.37
50	1	2168	A	N9-C4	-5.32	1.34	1.37
50	1	2623	G	N9-C4	-5.28	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	1	2275	A	N9-C4	-5.25	1.34	1.37
50	1	585	A	N9-C4	-5.24	1.34	1.37
50	1	1704	A	N9-C4	-5.22	1.34	1.37
50	1	1593	A	N9-C4	-5.22	1.34	1.37
50	1	1244	A	N9-C4	-5.20	1.34	1.37
50	1	33	G	N9-C4	-5.20	1.33	1.38
50	1	1278	A	N9-C4	-5.19	1.34	1.37
50	1	48	A	N9-C4	-5.15	1.34	1.37
50	1	1158	A	N9-C4	-5.15	1.34	1.37
50	1	268	A	N9-C4	-5.15	1.34	1.37
50	1	317	A	N9-C4	-5.15	1.34	1.37
50	1	2601	A	N9-C4	-5.14	1.34	1.37
50	1	1318	A	N9-C4	-5.13	1.34	1.37
50	1	1800	A	N9-C4	-5.12	1.34	1.37
50	1	2910	A	N9-C4	-5.12	1.34	1.37
50	1	630	A	N9-C4	-5.12	1.34	1.37
50	1	3318	G	N3-C4	-5.12	1.31	1.35
50	1	2657	A	N9-C4	-5.11	1.34	1.37
47	x	129	VAL	C-N	-5.09	1.22	1.34
50	1	2902	A	N9-C4	-5.07	1.34	1.37
50	1	199	A	C5-C4	-5.07	1.35	1.38
50	1	915	A	N7-C5	-5.06	1.36	1.39
50	1	2900	A	N9-C4	-5.04	1.34	1.37
50	1	2580	A	N9-C4	-5.02	1.34	1.37
50	1	2844	C	C5-C6	-5.02	1.30	1.34
50	1	398	A	N9-C4	-5.01	1.34	1.37

All (842) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	1	2861	U	C2-N1-C1'	13.39	133.76	117.70
50	1	2528	G	O4'-C1'-N9	12.55	118.24	108.20
50	1	2695	A	O5'-P-OP1	-11.59	95.27	105.70
50	1	2759	U	N3-C2-O2	-11.34	114.26	122.20
50	1	2901	G	O5'-P-OP2	-11.31	95.52	105.70
50	1	2867	C	N1-C2-O2	11.29	125.67	118.90
50	1	2724	U	N3-C2-O2	-11.25	114.33	122.20
50	1	2923	U	N1-C2-O2	11.03	130.52	122.80
50	1	2724	U	N1-C2-O2	11.00	130.50	122.80
50	1	2923	U	C2-N1-C1'	10.96	130.86	117.70
50	1	2506	U	N1-C2-O2	10.74	130.32	122.80
50	1	2724	U	C2-N1-C1'	10.62	130.45	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	1	3217	C	N1-C2-O2	10.46	125.18	118.90
51	3	104	A	C5-C6-N6	-10.32	115.45	123.70
50	1	2506	U	C2-N1-C1'	10.19	129.92	117.70
50	1	2722	U	N3-C2-O2	-10.18	115.08	122.20
50	1	1239	C	N1-C2-O2	10.17	125.00	118.90
50	1	2731	U	C2-N1-C1'	10.15	129.88	117.70
50	1	977	C	N1-C2-O2	10.15	124.99	118.90
50	1	2861	U	C6-N1-C1'	-10.06	107.11	121.20
50	1	2825	C	N1-C2-O2	10.03	124.92	118.90
50	1	2861	U	N1-C2-O2	10.00	129.80	122.80
50	1	2867	C	C5-C6-N1	9.98	125.99	121.00
50	1	2728	G	O4'-C1'-N9	9.75	116.00	108.20
50	1	2759	U	N1-C2-O2	9.72	129.60	122.80
50	1	2713	U	N3-C2-O2	-9.72	115.40	122.20
50	1	2867	C	C6-N1-C2	-9.72	116.41	120.30
50	1	2507	C	N1-C2-O2	9.65	124.69	118.90
50	1	2713	U	N1-C2-O2	9.57	129.50	122.80
50	1	2731	U	N1-C2-O2	9.48	129.44	122.80
50	1	2923	U	N3-C2-O2	-9.42	115.61	122.20
50	1	2594	C	N1-C2-O2	9.26	124.45	118.90
50	1	2867	C	C2-N1-C1'	9.24	128.97	118.80
50	1	292	U	C2-N1-C1'	9.24	128.79	117.70
50	1	2825	C	C2-N1-C1'	9.19	128.91	118.80
50	1	544	C	C6-N1-C2	-9.16	116.64	120.30
51	3	104	A	N1-C6-N6	9.01	124.01	118.60
50	1	2506	U	N3-C2-O2	-8.99	115.91	122.20
50	1	2927	C	N1-C2-O2	8.90	124.24	118.90
50	1	1239	C	N3-C2-O2	-8.89	115.68	121.90
50	1	2836	C	C2-N1-C1'	8.89	128.58	118.80
50	1	3023	U	N1-C2-O2	8.87	129.01	122.80
50	1	995	U	C2-N1-C1'	8.84	128.30	117.70
50	1	2268	U	N3-C2-O2	-8.83	116.02	122.20
50	1	3023	U	N3-C2-O2	-8.76	116.07	122.20
45	v	285	LEU	CA-CB-CG	8.72	135.36	115.30
50	1	2825	C	N3-C2-O2	-8.71	115.80	121.90
50	1	2929	C	C2-N1-C1'	8.64	128.31	118.80
50	1	2955	U	N3-C2-O2	-8.63	116.16	122.20
50	1	3217	C	N3-C2-O2	-8.58	115.90	121.90
50	1	1239	C	C2-N1-C1'	8.55	128.21	118.80
50	1	1299	U	N3-C2-O2	-8.54	116.22	122.20
50	1	1581	C	C6-N1-C2	8.52	123.71	120.30
50	1	2764	C	N1-C2-O2	8.49	123.99	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	1	995	U	N3-C2-O2	-8.48	116.27	122.20
50	1	2955	U	C2-N1-C1'	8.48	127.87	117.70
50	1	1570	U	N3-C2-O2	-8.44	116.29	122.20
50	1	2626	A	O5'-P-OP1	-8.40	98.14	105.70
50	1	764	U	N1-C2-O2	8.39	128.67	122.80
51	3	104	A	C4-C5-N7	8.33	114.87	110.70
50	1	2844	C	N3-C4-C5	8.33	125.23	121.90
50	1	2406	C	N1-C2-O2	8.32	123.89	118.90
50	1	1951	C	N1-C2-O2	8.30	123.88	118.90
50	1	3181	C	C2-N1-C1'	8.28	127.91	118.80
50	1	546	C	C6-N1-C2	-8.28	116.99	120.30
50	1	2955	U	N1-C2-O2	8.27	128.59	122.80
50	1	995	U	N1-C2-O2	8.27	128.59	122.80
50	1	977	C	C2-N1-C1'	8.25	127.88	118.80
50	1	2278	C	N1-C2-O2	8.25	123.85	118.90
50	1	2630	C	C6-N1-C2	-8.24	117.00	120.30
50	1	2836	C	N1-C2-O2	8.22	123.83	118.90
50	1	2861	U	N3-C2-O2	-8.21	116.45	122.20
50	1	2867	C	N3-C2-O2	-8.15	116.19	121.90
50	1	2714	G	C4-N9-C1'	8.14	137.09	126.50
50	1	954	U	C2-N1-C1'	8.14	127.46	117.70
50	1	2849	C	N3-C2-O2	-8.08	116.24	121.90
50	1	2927	C	N3-C2-O2	-8.08	116.25	121.90
50	1	3217	C	C2-N1-C1'	8.06	127.67	118.80
50	1	1187	C	N1-C2-O2	8.05	123.73	118.90
50	1	1819	U	N3-C2-O2	-8.00	116.60	122.20
50	1	1819	U	N1-C2-O2	7.98	128.38	122.80
50	1	2770	G	C5-C6-O6	-7.97	123.82	128.60
50	1	2278	C	N3-C2-O2	-7.96	116.33	121.90
50	1	2655	U	OP2-P-O3'	7.96	122.72	105.20
50	1	2728	G	P-O3'-C3'	7.95	129.24	119.70
50	1	3214	U	C2-N1-C1'	7.95	127.24	117.70
50	1	3019	U	N3-C2-O2	-7.91	116.67	122.20
50	1	2724	U	C6-N1-C1'	-7.85	110.21	121.20
50	1	2771	U	O5'-P-OP2	-7.85	98.64	105.70
50	1	991	G	O5'-P-OP1	7.84	120.11	110.70
50	1	1296	C	N3-C2-O2	-7.84	116.41	121.90
50	1	1411	C	N1-C2-O2	7.84	123.61	118.90
50	1	2731	U	N3-C2-O2	-7.82	116.72	122.20
50	1	2923	U	C6-N1-C1'	-7.80	110.28	121.20
50	1	1255	C	C2-N1-C1'	7.80	127.38	118.80
50	1	1633	C	N1-C2-O2	7.78	123.57	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	3	98	C	C2-N1-C1'	7.74	127.31	118.80
50	1	3019	U	C2-N1-C1'	7.73	126.97	117.70
50	1	1349	G	N3-C4-C5	-7.72	124.74	128.60
50	1	2594	C	N3-C2-O2	-7.71	116.50	121.90
50	1	1187	C	C2-N1-C1'	7.71	127.28	118.80
50	1	263	C	N1-C2-O2	7.69	123.52	118.90
50	1	776	U	N3-C2-O2	-7.68	116.82	122.20
50	1	2249	G	N3-C4-C5	7.68	132.44	128.60
50	1	1204	A	C8-N9-C4	-7.67	102.73	105.80
50	1	2722	U	N1-C2-O2	7.67	128.17	122.80
50	1	2535	A	C5-C6-N6	-7.66	117.58	123.70
50	1	2929	C	C6-N1-C1'	-7.64	111.62	120.80
50	1	1349	G	N3-C4-N9	7.58	130.55	126.00
50	1	1227	C	N1-C2-O2	7.58	123.44	118.90
50	1	776	U	N1-C2-O2	7.57	128.10	122.80
50	1	2652	U	O5'-P-OP1	-7.54	98.91	105.70
50	1	2869	U	N1-C2-O2	7.54	128.08	122.80
51	3	104	A	C5-N7-C8	-7.53	100.14	103.90
50	1	124	U	N3-C2-O2	-7.51	116.94	122.20
50	1	954	U	C5-C6-N1	7.51	126.46	122.70
50	1	1349	G	C4-N9-C1'	7.51	136.26	126.50
50	1	851	C	N1-C2-O2	7.50	123.40	118.90
50	1	2899	C	N1-C2-O2	7.50	123.40	118.90
50	1	2257	C	C2-N1-C1'	7.50	127.05	118.80
50	1	1199	C	N1-C2-O2	7.49	123.40	118.90
50	1	1187	C	N3-C2-O2	-7.48	116.66	121.90
50	1	284	A	P-O3'-C3'	7.47	128.67	119.70
50	1	2761	G	OP1-P-O3'	7.47	121.62	105.20
50	1	2825	C	C6-N1-C1'	-7.46	111.85	120.80
50	1	543	C	N1-C2-O2	7.45	123.37	118.90
50	1	292	U	C6-N1-C1'	-7.44	110.78	121.20
51	3	106	U	N1-C2-O2	7.43	128.00	122.80
50	1	1199	C	C2-N1-C1'	7.41	126.95	118.80
50	1	14	U	O5'-P-OP2	-7.41	99.03	105.70
50	1	776	U	C2-N1-C1'	7.38	126.56	117.70
50	1	2249	G	N3-C4-N9	-7.38	121.57	126.00
50	1	3265	C	N1-C2-O2	7.38	123.33	118.90
50	1	1508	C	N1-C2-O2	7.38	123.33	118.90
50	1	915	A	C2-N3-C4	7.37	114.28	110.60
50	1	2954	U	P-O3'-C3'	7.36	128.53	119.70
50	1	2428	U	C2-N1-C1'	7.36	126.53	117.70
50	1	113	C	N3-C2-O2	-7.36	116.75	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	1	1570	U	N1-C2-O2	7.35	127.94	122.80
50	1	2702	A	N3-C4-C5	7.34	131.94	126.80
51	3	18	C	N1-C2-O2	7.34	123.30	118.90
50	1	2866	U	P-O3'-C3'	7.32	128.48	119.70
50	1	2768	U	C5-C6-N1	7.32	126.36	122.70
50	1	2731	U	C6-N1-C1'	-7.29	111.00	121.20
50	1	263	C	N3-C2-O2	-7.28	116.81	121.90
50	1	3298	C	N1-C2-O2	7.25	123.25	118.90
50	1	116	A	C8-N9-C4	7.25	108.70	105.80
50	1	954	U	N1-C2-O2	7.25	127.87	122.80
50	1	113	C	N1-C2-O2	7.25	123.25	118.90
1	2	130	C	N1-C2-O2	7.23	123.24	118.90
50	1	3057	U	N3-C2-O2	-7.23	117.14	122.20
50	1	1132	C	N1-C2-O2	7.22	123.23	118.90
50	1	1141	C	N1-C2-O2	7.21	123.22	118.90
50	1	2257	C	N1-C2-O2	7.20	123.22	118.90
50	1	2849	C	N1-C2-O2	7.20	123.22	118.90
50	1	1132	C	N3-C2-O2	-7.19	116.86	121.90
50	1	3039	C	N1-C2-O2	7.19	123.22	118.90
50	1	2844	C	C6-N1-C2	7.18	123.17	120.30
50	1	2730	G	C4-N9-C1'	7.17	135.82	126.50
50	1	764	U	C2-N1-C1'	7.17	126.30	117.70
50	1	1581	C	P-O3'-C3'	7.16	128.30	119.70
50	1	549	U	N1-C2-O2	7.15	127.81	122.80
50	1	1299	U	C2-N1-C1'	7.15	126.28	117.70
50	1	1556	C	N1-C2-O2	7.14	123.19	118.90
50	1	1307	G	P-O3'-C3'	7.14	128.26	119.70
50	1	2693	C	N1-C2-O2	7.13	123.18	118.90
50	1	2658	G	P-O3'-C3'	7.12	128.24	119.70
50	1	2819	A	OP2-P-O3'	7.12	120.85	105.20
50	1	544	C	C5-C6-N1	7.10	124.55	121.00
51	3	104	A	N9-C4-C5	-7.09	102.97	105.80
50	1	1951	C	N3-C2-O2	-7.07	116.95	121.90
50	1	1570	U	C2-N1-C1'	7.07	126.18	117.70
50	1	2249	G	C4-N9-C1'	-7.06	117.32	126.50
39	m	377	ASP	N-CA-C	7.06	130.05	111.00
50	1	2714	G	C8-N9-C1'	-7.06	117.83	127.00
50	1	2722	U	C2-N1-C1'	7.05	126.16	117.70
50	1	1248	C	N1-C2-O2	7.04	123.12	118.90
50	1	1568	U	P-O3'-C3'	7.04	128.15	119.70
50	1	2760	C	C2-N1-C1'	7.01	126.51	118.80
50	1	977	C	N3-C2-O2	-7.00	117.00	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	1	2771	U	N1-C2-O2	6.99	127.69	122.80
50	1	2927	C	C2-N1-C1'	6.99	126.48	118.80
50	1	3023	U	C2-N1-C1'	6.97	126.06	117.70
50	1	2547	A	N1-C6-N6	-6.97	114.42	118.60
50	1	2687	G	C8-N9-C4	6.97	109.19	106.40
50	1	2899	C	C2-N1-C1'	6.96	126.45	118.80
50	1	1508	C	N3-C2-O2	-6.95	117.03	121.90
50	1	552	G	N7-C8-N9	6.95	116.58	113.10
50	1	2506	U	C6-N1-C1'	-6.95	111.47	121.20
50	1	2625	C	OP1-P-O3'	6.95	120.49	105.20
50	1	1057	A	OP1-P-O3'	6.95	120.48	105.20
50	1	1570	U	P-O3'-C3'	6.94	128.03	119.70
50	1	1549	U	N1-C2-O2	6.91	127.64	122.80
50	1	2771	U	C2-N1-C1'	6.90	125.98	117.70
50	1	995	U	C6-N1-C1'	-6.90	111.54	121.20
50	1	1239	C	C6-N1-C2	-6.90	117.54	120.30
50	1	2846	U	C2-N1-C1'	6.88	125.96	117.70
50	1	1227	C	N3-C2-O2	-6.88	117.09	121.90
50	1	2537	U	P-O3'-C3'	6.88	127.95	119.70
50	1	3181	C	N1-C2-O2	6.87	123.02	118.90
50	1	124	U	N1-C2-O2	6.86	127.60	122.80
50	1	1634	G	N1-C6-O6	-6.86	115.79	119.90
50	1	292	U	N1-C2-O2	6.85	127.59	122.80
50	1	2535	A	N1-C6-N6	6.84	122.70	118.60
50	1	2759	U	C2-N1-C1'	6.83	125.89	117.70
50	1	3019	U	N1-C2-O2	6.83	127.58	122.80
50	1	2770	G	N1-C6-O6	6.79	123.98	119.90
50	1	977	C	C6-N1-C1'	-6.78	112.66	120.80
50	1	2506	U	C5-C6-N1	6.78	126.09	122.70
50	1	648	C	N1-C2-O2	6.75	122.95	118.90
50	1	2836	C	C6-N1-C1'	-6.75	112.70	120.80
51	3	18	C	N3-C2-O2	-6.75	117.18	121.90
50	1	1049	C	N1-C2-O2	6.75	122.95	118.90
50	1	1716	U	P-O3'-C3'	6.74	127.79	119.70
50	1	758	C	N1-C2-O2	6.73	122.94	118.90
50	1	1567	U	OP2-P-O3'	6.72	119.99	105.20
50	1	1216	C	N1-C2-O2	6.70	122.92	118.90
50	1	292	U	N3-C2-O2	-6.68	117.53	122.20
50	1	764	U	N3-C2-O2	-6.67	117.53	122.20
50	1	2840	C	N1-C2-O2	6.67	122.90	118.90
50	1	1200	A	N3-C4-C5	6.67	131.47	126.80
50	1	2875	U	P-O3'-C3'	6.66	127.69	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	1	3228	C	P-O3'-C3'	6.66	127.70	119.70
50	1	2766	U	O4'-C1'-N1	6.66	113.53	108.20
50	1	1108	U	C2-N1-C1'	6.66	125.69	117.70
50	1	743	C	N1-C2-O2	6.65	122.89	118.90
50	1	2526	C	N3-C2-O2	-6.65	117.25	121.90
50	1	1574	C	P-O3'-C3'	6.64	127.66	119.70
50	1	3324	C	N1-C2-O2	6.63	122.88	118.90
50	1	2730	G	N3-C4-C5	-6.63	125.28	128.60
50	1	1876	U	N3-C2-O2	-6.61	117.58	122.20
50	1	3316	A	P-O3'-C3'	6.61	127.63	119.70
50	1	1064	A	P-O3'-C3'	6.60	127.61	119.70
50	1	2846	U	N1-C2-O2	6.59	127.41	122.80
50	1	2847	A	C8-N9-C4	6.59	108.44	105.80
50	1	2693	C	O4'-C1'-N1	6.58	113.47	108.20
50	1	3039	C	N3-C2-O2	-6.58	117.29	121.90
50	1	3181	C	C6-N1-C1'	-6.57	112.91	120.80
50	1	2657	A	C8-N9-C4	6.57	108.43	105.80
50	1	41	G	C4-N9-C1'	6.56	135.03	126.50
50	1	1108	U	C6-N1-C1'	-6.56	112.02	121.20
50	1	1876	U	N1-C2-O2	6.56	127.39	122.80
50	1	1438	U	N3-C2-O2	-6.55	117.62	122.20
50	1	2766	U	C2-N1-C1'	-6.55	109.84	117.70
50	1	1187	C	C6-N1-C1'	-6.54	112.95	120.80
50	1	2836	C	N3-C2-O2	-6.54	117.32	121.90
50	1	1388	U	N3-C2-O2	-6.52	117.63	122.20
50	1	2582	C	N1-C2-O2	6.52	122.81	118.90
50	1	2730	G	N3-C4-N9	6.51	129.91	126.00
19	S	13	ARG	C-N-CA	6.51	137.98	121.70
51	3	26	C	N3-C2-O2	-6.51	117.34	121.90
50	1	2428	U	C6-N1-C1'	-6.51	112.09	121.20
50	1	1299	U	N1-C2-O2	6.50	127.35	122.80
51	3	36	C	N1-C2-O2	6.50	122.80	118.90
50	1	3116	G	N3-C4-N9	6.50	129.90	126.00
50	1	2257	C	N3-C2-O2	-6.50	117.35	121.90
50	1	922	U	N3-C2-O2	-6.49	117.66	122.20
50	1	2857	C	P-O3'-C3'	6.49	127.49	119.70
50	1	800	G	N3-C4-N9	6.47	129.88	126.00
50	1	1556	C	N3-C2-O2	-6.47	117.37	121.90
50	1	2770	G	C4-C5-N7	6.47	113.39	110.80
50	1	2869	U	N3-C2-O2	-6.47	117.67	122.20
50	1	166	C	N1-C2-O2	6.47	122.78	118.90
50	1	2529	A	C8-N9-C4	-6.46	103.22	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	1	3306	U	N3-C2-O2	-6.46	117.68	122.20
51	3	26	C	N1-C2-O2	6.44	122.77	118.90
50	1	2870	C	N3-C2-O2	-6.44	117.39	121.90
50	1	851	C	N3-C2-O2	-6.44	117.39	121.90
50	1	2249	G	O4'-C1'-N9	6.44	113.35	108.20
50	1	3214	U	N1-C2-O2	6.44	127.31	122.80
50	1	1292	C	N1-C2-O2	6.41	122.75	118.90
50	1	861	C	N1-C2-O2	6.41	122.75	118.90
50	1	208	C	N3-C2-O2	-6.40	117.42	121.90
51	3	36	C	N3-C2-O2	-6.40	117.42	121.90
50	1	2972	G	C4-C5-N7	6.40	113.36	110.80
50	1	2713	U	C5-C6-N1	6.39	125.90	122.70
50	1	321	C	N1-C2-O2	6.39	122.73	118.90
50	1	2277	C	OP1-P-O3'	6.39	119.25	105.20
50	1	2507	C	N3-C2-O2	-6.39	117.43	121.90
50	1	7	C	N1-C2-O2	6.39	122.73	118.90
26	Z	102	GLU	C-N-CA	6.38	137.66	121.70
50	1	2687	G	N3-C4-C5	6.38	131.79	128.60
50	1	3214	U	N3-C2-O2	-6.38	117.73	122.20
50	1	2651	G	P-O3'-C3'	6.38	127.35	119.70
50	1	2760	C	N1-C2-O2	6.38	122.72	118.90
50	1	2274	U	C2-N1-C1'	6.37	125.34	117.70
1	2	130	C	N3-C2-O2	-6.36	117.45	121.90
50	1	1420	C	N3-C2-O2	-6.36	117.45	121.90
50	1	2770	G	N9-C4-C5	-6.36	102.86	105.40
14	N	153	ASP	CB-CG-OD1	6.35	124.02	118.30
50	1	3111	U	N1-C2-O2	6.35	127.25	122.80
50	1	1549	U	N3-C2-O2	-6.34	117.76	122.20
50	1	2406	C	N3-C2-O2	-6.34	117.46	121.90
50	1	293	C	N3-C2-O2	-6.33	117.47	121.90
50	1	1411	C	N3-C2-O2	-6.33	117.47	121.90
50	1	2552	C	N1-C2-O2	6.32	122.69	118.90
50	1	2900	A	OP1-P-O3'	6.32	119.10	105.20
50	1	1567	U	P-O3'-C3'	6.32	127.28	119.70
50	1	2727	A	C8-N9-C4	-6.32	103.27	105.80
50	1	2546	C	N3-C2-O2	-6.31	117.48	121.90
50	1	1923	C	N3-C2-O2	-6.30	117.49	121.90
50	1	1923	C	N1-C2-O2	6.29	122.67	118.90
51	3	100	C	N1-C2-O2	6.29	122.67	118.90
50	1	1168	U	N3-C2-O2	-6.28	117.80	122.20
50	1	2730	G	C8-N9-C1'	-6.28	118.83	127.00
50	1	1349	G	C2-N3-C4	6.28	115.04	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	1	800	G	C4-N9-C1'	6.28	134.66	126.50
50	1	3265	C	N3-C2-O2	-6.28	117.51	121.90
50	1	1832	C	N3-C2-O2	-6.27	117.51	121.90
50	1	2863	G	C8-N9-C4	-6.26	103.89	106.40
50	1	3298	C	N3-C2-O2	-6.26	117.52	121.90
50	1	975	C	N1-C2-O2	6.25	122.65	118.90
18	R	116	ASP	CB-CG-OD1	6.25	123.93	118.30
50	1	922	U	N1-C2-O2	6.25	127.18	122.80
50	1	7	C	N3-C2-O2	-6.25	117.52	121.90
50	1	1349	G	C8-N9-C1'	-6.25	118.88	127.00
50	1	2761	G	P-O3'-C3'	6.24	127.19	119.70
50	1	2274	U	N1-C2-O2	6.24	127.16	122.80
50	1	2849	C	C6-N1-C2	-6.24	117.81	120.30
50	1	40	A	C2-N3-C4	6.23	113.72	110.60
50	1	2702	A	C2-N3-C4	-6.23	107.48	110.60
50	1	2953	U	N1-C2-O2	6.22	127.16	122.80
51	3	28	C	N1-C2-O2	6.22	122.63	118.90
50	1	143	G	N3-C4-N9	6.21	129.73	126.00
50	1	1057	A	P-O3'-C3'	6.21	127.16	119.70
50	1	2630	C	C5-C6-N1	6.20	124.10	121.00
50	1	1296	C	N1-C2-O2	6.20	122.62	118.90
50	1	2983	C	C2-N1-C1'	6.20	125.62	118.80
50	1	1608	C	N3-C2-O2	-6.19	117.56	121.90
50	1	2870	C	N1-C2-O2	6.19	122.61	118.90
50	1	2985	C	N3-C2-O2	-6.19	117.57	121.90
51	3	19	C	N1-C2-O2	6.19	122.61	118.90
50	1	430	U	N3-C2-O2	-6.18	117.87	122.20
51	3	106	U	N3-C2-O2	-6.18	117.87	122.20
50	1	1238	C	N3-C2-O2	-6.18	117.57	121.90
50	1	3269	U	N3-C2-O2	-6.18	117.87	122.20
50	1	1717	U	N1-C2-O2	6.18	127.12	122.80
50	1	1671	C	N1-C2-O2	6.18	122.61	118.90
50	1	2624	G	OP1-P-O3'	6.17	118.79	105.20
50	1	2702	A	N3-C4-N9	-6.17	122.46	127.40
51	3	100	C	N3-C2-O2	-6.17	117.58	121.90
50	1	1832	C	N1-C2-O2	6.16	122.59	118.90
50	1	1128	U	P-O3'-C3'	6.15	127.08	119.70
50	1	1201	C	C2-N1-C1'	6.15	125.57	118.80
50	1	1068	C	C5-C6-N1	6.15	124.08	121.00
50	1	2594	C	C2-N1-C1'	6.14	125.56	118.80
50	1	3235	C	N1-C2-O2	6.14	122.58	118.90
50	1	1168	U	N1-C2-O2	6.13	127.09	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	1	2753	G	C8-N9-C4	-6.12	103.95	106.40
50	1	40	A	P-O3'-C3'	6.12	127.04	119.70
50	1	2263	C	N3-C2-O2	-6.12	117.62	121.90
50	1	3331	U	N1-C2-O2	6.12	127.08	122.80
50	1	1608	C	N1-C2-O2	6.11	122.57	118.90
50	1	1204	A	N7-C8-N9	6.11	116.86	113.80
50	1	3196	U	N1-C2-O2	6.11	127.08	122.80
50	1	720	A	P-O3'-C3'	6.11	127.03	119.70
50	1	2254	U	C5-C6-N1	6.11	125.75	122.70
50	1	1141	C	N3-C2-O2	-6.10	117.63	121.90
50	1	311	C	N1-C2-O2	6.08	122.55	118.90
50	1	2249	G	C8-N9-C4	6.08	108.83	106.40
50	1	2771	U	N3-C2-O2	-6.08	117.94	122.20
50	1	2401	A	O5'-P-OP2	-6.08	100.23	105.70
50	1	1255	C	C6-N1-C1'	-6.07	113.52	120.80
50	1	143	G	C8-N9-C1'	-6.07	119.11	127.00
50	1	2714	G	N3-C4-N9	6.06	129.64	126.00
50	1	3331	U	N3-C2-O2	-6.05	117.97	122.20
50	1	954	U	N3-C2-O2	-6.04	117.97	122.20
50	1	720	A	OP2-P-O3'	6.04	118.48	105.20
1	2	153	U	C5-C6-N1	6.03	125.72	122.70
50	1	1069	C	C6-N1-C2	-6.03	117.89	120.30
1	2	103	G	N3-C4-N9	-6.03	122.38	126.00
50	1	685	G	O5'-P-OP1	-6.02	100.28	105.70
50	1	132	C	N1-C2-O2	6.02	122.51	118.90
50	1	991	G	O5'-P-OP2	-6.01	100.29	105.70
50	1	1952	G	N3-C4-N9	6.01	129.61	126.00
50	1	619	A	P-O3'-C3'	6.01	126.91	119.70
50	1	2550	U	N1-C2-O2	6.00	127.00	122.80
50	1	3222	U	N1-C2-O2	6.00	127.00	122.80
50	1	3344	A	C5-N7-C8	-6.00	100.90	103.90
50	1	2	U	N1-C2-O2	6.00	127.00	122.80
50	1	380	U	N1-C2-O2	5.99	126.99	122.80
50	1	208	C	N1-C2-O2	5.99	122.49	118.90
50	1	2101	C	P-O3'-C3'	5.99	126.88	119.70
52	4	251	LEU	CA-CB-CG	5.99	129.07	115.30
1	2	62	C	C6-N1-C2	5.99	122.69	120.30
51	3	26	C	C6-N1-C2	-5.98	117.91	120.30
17	Q	41	ASP	CB-CG-OD1	5.98	123.68	118.30
50	1	2658	G	O4'-C1'-N9	5.97	112.97	108.20
50	1	2901	G	O5'-P-OP1	5.96	117.86	110.70
50	1	166	C	N3-C2-O2	-5.96	117.73	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	1	1952	G	C5-C6-O6	-5.96	125.03	128.60
50	1	2737	C	N3-C2-O2	-5.96	117.73	121.90
50	1	2434	U	N3-C2-O2	-5.96	118.03	122.20
50	1	2274	U	N3-C2-O2	-5.95	118.03	122.20
50	1	2578	U	N3-C2-O2	-5.95	118.04	122.20
50	1	743	C	N3-C2-O2	-5.94	117.74	121.90
50	1	1049	C	C2-N3-C4	5.94	122.87	119.90
50	1	2746	A	N1-C6-N6	5.94	122.16	118.60
50	1	3196	U	N3-C2-O2	-5.94	118.04	122.20
50	1	31	C	N3-C2-O2	-5.93	117.75	121.90
50	1	3354	U	C2-N1-C1'	5.93	124.82	117.70
50	1	2514	U	O5'-P-OP1	-5.92	100.37	105.70
50	1	1701	C	N1-C2-O2	5.92	122.45	118.90
50	1	2899	C	N3-C2-O2	-5.92	117.76	121.90
51	3	98	C	N1-C2-O2	5.91	122.44	118.90
50	1	2209	U	P-O3'-C3'	5.91	126.78	119.70
51	3	82	G	N7-C8-N9	5.91	116.05	113.10
50	1	2624	G	P-O3'-C3'	5.90	126.78	119.70
50	1	886	C	N1-C2-O2	5.90	122.44	118.90
50	1	2257	C	C6-N1-C2	-5.90	117.94	120.30
50	1	2567	C	N1-C2-O2	5.90	122.44	118.90
50	1	2268	U	N1-C2-O2	5.90	126.93	122.80
50	1	2578	U	N1-C2-O2	5.90	126.93	122.80
50	1	3350	C	C5-C6-N1	5.90	123.95	121.00
50	1	3324	C	N3-C2-O2	-5.89	117.78	121.90
50	1	648	C	C2-N1-C1'	5.89	125.28	118.80
50	1	1216	C	N3-C2-O2	-5.89	117.78	121.90
50	1	2840	C	N3-C2-O2	-5.89	117.78	121.90
50	1	1438	U	N1-C2-O2	5.88	126.92	122.80
50	1	2972	G	C6-C5-N7	-5.88	126.87	130.40
50	1	1200	A	N3-C4-N9	-5.88	122.70	127.40
50	1	1238	C	N1-C2-O2	5.88	122.43	118.90
50	1	2927	C	C6-N1-C2	-5.88	117.95	120.30
50	1	2137	U	C2-N1-C1'	5.88	124.75	117.70
50	1	3278	C	C2-N1-C1'	5.88	125.27	118.80
50	1	312	C	N1-C2-O2	5.87	122.42	118.90
50	1	1248	C	N3-C2-O2	-5.87	117.79	121.90
50	1	2628	A	N1-C6-N6	-5.87	115.08	118.60
50	1	380	U	N3-C2-O2	-5.86	118.10	122.20
50	1	2572	C	N1-C2-O2	5.86	122.42	118.90
50	1	116	A	N3-C4-C5	5.86	130.90	126.80
50	1	1364	C	N1-C2-O2	5.86	122.42	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	1	207	U	N1-C2-O2	5.86	126.90	122.80
50	1	2764	C	C2-N1-C1'	5.86	125.24	118.80
50	1	3116	G	C4-N9-C1'	5.86	134.11	126.50
50	1	1819	U	C2-N1-C1'	5.85	124.72	117.70
50	1	3078	U	P-O3'-C3'	5.85	126.72	119.70
50	1	1241	U	P-O3'-C3'	5.84	126.71	119.70
50	1	1671	C	N3-C2-O2	-5.84	117.81	121.90
50	1	2955	U	C6-N1-C1'	-5.83	113.03	121.20
50	1	2861	U	C5-C6-N1	5.83	125.61	122.70
50	1	2727	A	N7-C8-N9	5.83	116.71	113.80
50	1	3116	G	C8-N9-C1'	-5.82	119.43	127.00
50	1	1620	U	N1-C2-O2	5.82	126.87	122.80
50	1	2731	U	C5-C6-N1	5.82	125.61	122.70
50	1	207	U	N3-C2-O2	-5.81	118.13	122.20
50	1	2691	A	O4'-C1'-N9	-5.81	103.55	108.20
50	1	3217	C	C6-N1-C1'	-5.81	113.83	120.80
50	1	131	C	C6-N1-C2	-5.80	117.98	120.30
50	1	3057	U	N1-C2-O2	5.80	126.86	122.80
50	1	861	C	N3-C2-O2	-5.80	117.84	121.90
50	1	2316	G	C4-N9-C1'	5.79	134.03	126.50
50	1	2186	U	N1-C2-O2	5.79	126.85	122.80
50	1	915	A	N3-C4-C5	-5.79	122.75	126.80
50	1	1633	C	N3-C2-O2	-5.78	117.85	121.90
50	1	3111	U	N3-C2-O2	-5.78	118.15	122.20
50	1	117	U	N1-C2-O2	5.78	126.85	122.80
50	1	915	A	N3-C4-N9	5.78	132.03	127.40
50	1	1199	C	N3-C2-O2	-5.78	117.85	121.90
50	1	2953	U	N3-C2-O2	-5.78	118.15	122.20
50	1	860	G	C4-C5-N7	5.78	113.11	110.80
50	1	998	A	N9-C4-C5	-5.78	103.49	105.80
50	1	1355	A	P-O3'-C3'	5.78	126.64	119.70
50	1	174	C	N1-C2-O2	5.77	122.36	118.90
50	1	68	C	N3-C2-O2	-5.76	117.86	121.90
50	1	800	G	C8-N9-C1'	-5.76	119.51	127.00
50	1	1420	C	N1-C2-O2	5.76	122.36	118.90
50	1	1569	U	N1-C2-O2	5.76	126.83	122.80
50	1	1788	C	N3-C2-O2	-5.76	117.87	121.90
50	1	3092	C	C6-N1-C2	5.76	122.60	120.30
50	1	321	C	N3-C2-O2	-5.75	117.88	121.90
50	1	2899	C	C6-N1-C1'	-5.75	113.90	120.80
50	1	976	U	C5-C6-N1	5.75	125.57	122.70
50	1	2714	G	C6-C5-N7	-5.75	126.95	130.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	1	143	G	C4-N9-C1'	5.74	133.97	126.50
50	1	2862	U	C2-N1-C1'	5.74	124.58	117.70
50	1	1239	C	C5-C6-N1	5.73	123.86	121.00
50	1	1302	A	P-O3'-C3'	5.73	126.58	119.70
50	1	1124	U	C2-N1-C1'	5.73	124.57	117.70
50	1	1626	U	N1-C2-O2	5.72	126.81	122.80
50	1	2211	U	N1-C2-O2	5.72	126.81	122.80
50	1	2416	U	N3-C2-O2	-5.72	118.19	122.20
50	1	2702	A	C8-N9-C4	5.72	108.09	105.80
51	3	113	C	N1-C2-O2	5.72	122.33	118.90
50	1	1124	U	N3-C2-O2	-5.72	118.20	122.20
50	1	117	U	C2-N1-C1'	5.71	124.56	117.70
50	1	2787	G	C4-N9-C1'	5.71	133.93	126.50
51	3	100	C	C6-N1-C2	-5.71	118.02	120.30
50	1	3344	A	C4-C5-N7	5.71	113.56	110.70
50	1	1480	G	N3-C4-C5	5.71	131.45	128.60
50	1	69	C	N3-C2-O2	-5.70	117.91	121.90
51	3	52	G	P-O3'-C3'	5.70	126.54	119.70
50	1	1878	G	C4-N9-C1'	5.70	133.91	126.50
50	1	375	A	OP1-P-O3'	5.70	117.73	105.20
50	1	2317	A	P-O3'-C3'	5.70	126.53	119.70
50	1	1771	C	N1-C2-O2	5.69	122.32	118.90
51	3	104	A	C5-C6-N1	5.69	120.55	117.70
51	3	60	G	N3-C4-N9	5.69	129.42	126.00
50	1	3278	C	N1-C2-O2	5.69	122.31	118.90
50	1	1108	U	C5-C4-O4	-5.69	122.49	125.90
50	1	3235	C	N3-C2-O2	-5.69	117.92	121.90
50	1	2817	A	P-O3'-C3'	5.69	126.52	119.70
50	1	982	C	N1-C2-O2	5.68	122.31	118.90
50	1	1872	C	N1-C2-O2	5.68	122.31	118.90
50	1	2787	G	C8-N9-C1'	-5.68	119.62	127.00
51	3	98	C	N3-C2-O2	-5.68	117.92	121.90
50	1	975	C	N3-C2-O2	-5.68	117.93	121.90
50	1	2566	C	N1-C2-O2	5.68	122.31	118.90
50	1	922	U	C2-N1-C1'	5.67	124.51	117.70
50	1	2546	C	N1-C2-O2	5.67	122.30	118.90
9	H	188	THR	C-N-CA	5.67	135.86	121.70
50	1	41	G	C8-N9-C1'	-5.66	119.64	127.00
50	1	2797	C	N1-C2-O2	5.66	122.30	118.90
50	1	2636	A	C2-N3-C4	5.65	113.43	110.60
50	1	2772	C	N1-C2-O2	5.65	122.29	118.90
50	1	1788	C	N1-C2-O2	5.65	122.29	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	3	83	U	C5-C6-N1	5.64	125.52	122.70
50	1	1952	G	C4-C5-N7	5.64	113.06	110.80
50	1	1296	C	C6-N1-C2	-5.64	118.05	120.30
50	1	2627	C	C2-N1-C1'	5.63	125.00	118.80
50	1	2526	C	N1-C2-O2	5.63	122.28	118.90
51	3	104	A	C6-C5-N7	-5.63	128.36	132.30
50	1	1239	C	C6-N1-C1'	-5.63	114.05	120.80
10	I	46	LEU	CA-CB-CG	5.62	128.23	115.30
50	1	957	C	N1-C2-O2	5.62	122.27	118.90
50	1	2600	C	N1-C2-O2	5.62	122.27	118.90
50	1	2847	A	O4'-C1'-N9	5.62	112.69	108.20
50	1	3306	U	C2-N1-C1'	5.62	124.44	117.70
50	1	2728	G	N9-C1'-C2'	5.62	121.30	114.00
50	1	2625	C	P-O3'-C3'	5.61	126.43	119.70
50	1	2713	U	C6-N1-C2	-5.61	117.63	121.00
50	1	1952	G	C6-C5-N7	-5.61	127.03	130.40
50	1	2505	U	C5-C6-N1	5.61	125.50	122.70
50	1	1724	U	O4'-C1'-N1	5.61	112.69	108.20
50	1	3214	U	C6-N1-C1'	-5.60	113.36	121.20
50	1	1141	C	C2-N1-C1'	5.60	124.96	118.80
50	1	2567	C	N3-C2-O2	-5.59	117.98	121.90
50	1	2900	A	P-O3'-C3'	5.58	126.40	119.70
50	1	2366	C	N1-C2-O2	5.58	122.25	118.90
50	1	2928	C	C6-N1-C2	-5.58	118.07	120.30
50	1	2925	C	N1-C2-O2	5.58	122.25	118.90
50	1	2972	G	C5-N7-C8	-5.58	101.51	104.30
51	3	98	C	C6-N1-C1'	-5.57	114.11	120.80
50	1	879	U	N1-C2-O2	5.57	126.70	122.80
50	1	2816	G	C4-C5-N7	5.57	113.03	110.80
50	1	3195	U	C2-N1-C1'	5.57	124.38	117.70
50	1	2693	C	N3-C2-O2	-5.57	118.00	121.90
50	1	3350	C	N1-C2-O2	5.57	122.24	118.90
50	1	998	A	C8-N9-C4	5.56	108.03	105.80
50	1	2444	C	C2-N1-C1'	5.56	124.92	118.80
50	1	1917	C	N1-C2-O2	5.56	122.24	118.90
50	1	2846	U	N3-C2-O2	-5.56	118.31	122.20
50	1	1269	U	C2-N1-C1'	5.56	124.37	117.70
50	1	1794	G	N3-C4-C5	5.56	131.38	128.60
50	1	1878	G	C8-N9-C1'	-5.56	119.78	127.00
50	1	1904	C	N1-C2-O2	5.56	122.23	118.90
50	1	1329	U	N1-C2-O2	5.56	126.69	122.80
50	1	553	U	N3-C2-O2	-5.55	118.31	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	1	3135	U	N1-C2-O2	5.55	126.69	122.80
50	1	2444	C	O4'-C1'-N1	5.55	112.64	108.20
50	1	2593	A	P-O3'-C3'	5.55	126.36	119.70
50	1	2623	G	N3-C4-N9	-5.55	122.67	126.00
50	1	1794	G	C4-N9-C1'	-5.54	119.30	126.50
50	1	2422	C	N1-C2-O2	5.54	122.22	118.90
50	1	2093	A	C2-N3-C4	5.54	113.37	110.60
50	1	2570	U	C5-C4-O4	-5.53	122.58	125.90
50	1	1222	G	C8-N9-C4	5.53	108.61	106.40
50	1	2858	U	N3-C2-O2	-5.53	118.33	122.20
50	1	3306	U	N1-C2-O2	5.53	126.67	122.80
50	1	169	U	OP1-P-O3'	5.52	117.34	105.20
50	1	2534	G	N9-C4-C5	-5.51	103.19	105.40
50	1	2535	A	C4-C5-N7	5.51	113.45	110.70
50	1	2702	A	C4-C5-C6	-5.51	114.25	117.00
50	1	2946	A	P-O3'-C3'	5.51	126.31	119.70
50	1	976	U	C2-N1-C1'	5.51	124.31	117.70
51	3	106	U	C2-N1-C1'	5.50	124.31	117.70
50	1	2928	C	N3-C2-O2	-5.50	118.05	121.90
50	1	2985	C	N1-C2-O2	5.50	122.20	118.90
50	1	2687	G	C4-N9-C1'	-5.50	119.35	126.50
50	1	2819	A	P-O3'-C3'	5.50	126.30	119.70
51	3	28	C	N3-C2-O2	-5.50	118.05	121.90
1	2	57	C	N1-C2-O2	5.49	122.19	118.90
50	1	1364	C	N3-C2-O2	-5.49	118.06	121.90
50	1	2509	U	N1-C2-O2	5.49	126.64	122.80
50	1	2248	C	C2-N1-C1'	5.49	124.84	118.80
50	1	2770	G	O4'-C1'-N9	-5.49	103.81	108.20
4	C	182	LEU	CA-CB-CG	5.49	127.92	115.30
50	1	2441	A	C2-N3-C4	5.48	113.34	110.60
51	3	107	C	N1-C2-O2	5.48	122.19	118.90
50	1	1701	C	N3-C2-O2	-5.48	118.06	121.90
50	1	286	U	N3-C2-O2	-5.48	118.37	122.20
50	1	1111	U	N3-C2-O2	-5.47	118.37	122.20
50	1	1943	C	N3-C2-O2	-5.47	118.07	121.90
50	1	3349	C	C6-N1-C2	-5.47	118.11	120.30
50	1	2581	U	C2-N1-C1'	5.47	124.26	117.70
50	1	1568	U	OP1-P-OP2	-5.46	111.40	119.60
50	1	2146	C	N3-C2-O2	-5.46	118.08	121.90
50	1	1309	U	OP1-P-O3'	5.46	117.22	105.20
50	1	2794	G	N9-C4-C5	-5.46	103.22	105.40
50	1	3153	U	C2-N1-C1'	5.45	124.24	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	1	2550	U	C2-N1-C1'	5.45	124.24	117.70
50	1	3355	U	N3-C2-O2	-5.45	118.39	122.20
50	1	28	C	N3-C2-O2	-5.45	118.09	121.90
50	1	2849	C	C2-N1-C1'	5.45	124.79	118.80
50	1	293	C	N1-C2-O2	5.44	122.16	118.90
50	1	2529	A	N7-C8-N9	5.44	116.52	113.80
50	1	3019	U	C6-N1-C1'	-5.44	113.59	121.20
50	1	3166	C	C6-N1-C2	-5.44	118.12	120.30
50	1	2651	G	OP1-P-O3'	5.44	117.16	105.20
50	1	3355	U	N1-C2-O2	5.43	126.60	122.80
50	1	352	A	C8-N9-C4	5.43	107.97	105.80
50	1	3240	C	N3-C2-O2	-5.43	118.10	121.90
1	2	45	C	N1-C2-O2	5.43	122.16	118.90
50	1	1597	C	N3-C4-C5	5.42	124.07	121.90
50	1	2760	C	C6-N1-C1'	-5.42	114.29	120.80
42	r	2	PRO	C-N-CA	5.42	135.26	121.70
50	1	2548	C	N1-C2-O2	5.42	122.15	118.90
50	1	312	C	N3-C2-O2	-5.42	118.11	121.90
50	1	807	A	N1-C6-N6	5.42	121.85	118.60
50	1	860	G	C8-N9-C1'	-5.42	119.96	127.00
50	1	758	C	N3-C2-O2	-5.41	118.11	121.90
50	1	2317	A	OP2-P-O3'	5.41	117.11	105.20
50	1	670	C	N1-C2-O2	5.41	122.15	118.90
50	1	1278	A	C5-N7-C8	-5.41	101.20	103.90
50	1	1762	C	C6-N1-C2	-5.41	118.14	120.30
50	1	3218	A	P-O3'-C3'	5.41	126.19	119.70
50	1	2263	C	P-O3'-C3'	5.40	126.18	119.70
50	1	2249	G	N7-C8-N9	-5.40	110.40	113.10
50	1	2	U	N3-C2-O2	-5.39	118.42	122.20
50	1	1255	C	O4'-C1'-N1	5.39	112.51	108.20
50	1	1292	C	N3-C2-O2	-5.39	118.13	121.90
50	1	3338	C	N1-C2-O2	5.39	122.13	118.90
50	1	1222	G	N9-C4-C5	-5.39	103.25	105.40
50	1	41	G	C6-C5-N7	-5.38	127.17	130.40
50	1	2898	G	C4-C5-N7	5.38	112.95	110.80
50	1	2921	U	N3-C2-O2	-5.38	118.43	122.20
50	1	2863	G	N3-C2-N2	-5.38	116.14	119.90
50	1	2534	G	N3-C4-N9	5.38	129.23	126.00
50	1	2544	U	N1-C2-O2	5.38	126.56	122.80
50	1	1205	A	P-O3'-C3'	5.37	126.14	119.70
50	1	2901	G	OP1-P-OP2	-5.37	111.55	119.60
50	1	267	G	N3-C4-N9	5.36	129.22	126.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	1	267	G	C4-C5-N7	5.36	112.94	110.80
50	1	1388	U	N1-C2-O2	5.36	126.55	122.80
50	1	2817	A	OP1-P-O3'	5.36	116.99	105.20
1	2	103	G	N3-C4-C5	5.36	131.28	128.60
50	1	279	U	N1-C2-O2	5.36	126.55	122.80
50	1	2112	U	N3-C2-O2	-5.36	118.45	122.20
50	1	2652	U	P-O3'-C3'	5.36	126.13	119.70
50	1	2137	U	C6-N1-C1'	-5.36	113.70	121.20
50	1	2247	G	C4-N9-C1'	5.36	133.46	126.50
50	1	506	U	N3-C2-O2	-5.35	118.45	122.20
50	1	552	G	C8-N9-C4	-5.35	104.26	106.40
50	1	2550	U	N3-C2-O2	-5.35	118.45	122.20
50	1	860	G	C6-C5-N7	-5.35	127.19	130.40
50	1	1902	G	C6-C5-N7	-5.35	127.19	130.40
50	1	2552	C	C2-N1-C1'	5.35	124.68	118.80
50	1	3131	U	N3-C2-O2	-5.35	118.46	122.20
50	1	548	G	N1-C6-O6	5.35	123.11	119.90
50	1	868	C	N3-C2-O2	-5.34	118.16	121.90
50	1	1108	U	N1-C2-O2	5.34	126.54	122.80
50	1	1554	U	P-O3'-C3'	5.34	126.11	119.70
50	1	2741	C	N1-C2-O2	5.34	122.11	118.90
40	n	417	LEU	CA-CB-CG	5.34	127.59	115.30
50	1	546	C	C5-C6-N1	5.34	123.67	121.00
50	1	3269	U	P-O3'-C3'	5.34	126.11	119.70
50	1	2983	C	C6-N1-C1'	-5.34	114.40	120.80
51	3	35	C	N1-C2-O2	5.33	122.10	118.90
50	1	2828	G	C4-C5-N7	5.33	112.93	110.80
50	1	2953	U	C2-N1-C1'	5.33	124.09	117.70
50	1	2184	U	N3-C2-O2	-5.33	118.47	122.20
50	1	961	C	C2-N1-C1'	5.32	124.65	118.80
50	1	2277	C	P-O3'-C3'	5.32	126.08	119.70
51	3	96	U	C2-N3-C4	5.32	130.19	127.00
50	1	1424	C	C2-N1-C1'	5.32	124.65	118.80
50	1	2703	A	C2-N3-C4	5.32	113.26	110.60
50	1	3338	C	N3-C2-O2	-5.32	118.18	121.90
50	1	1780	G	N3-C4-N9	5.31	129.19	126.00
8	G	143	ILE	CG1-CB-CG2	-5.31	99.71	111.40
50	1	1208	U	N1-C2-O2	5.31	126.52	122.80
50	1	3284	G	N3-C2-N2	-5.31	116.18	119.90
50	1	2795	U	OP1-P-O3'	5.30	116.86	105.20
51	3	100	C	C2-N1-C1'	5.30	124.63	118.80
50	1	860	G	C4-N9-C1'	5.30	133.39	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	1	2655	U	P-O3'-C3'	5.30	126.06	119.70
50	1	3277	U	N3-C2-O2	-5.30	118.49	122.20
50	1	764	U	C6-N1-C1'	-5.29	113.79	121.20
50	1	2551	U	N1-C2-O2	5.29	126.51	122.80
50	1	549	U	C5-C6-N1	5.29	125.34	122.70
50	1	915	A	C4-N9-C1'	5.29	135.81	126.30
50	1	800	G	C6-C5-N7	-5.28	127.23	130.40
50	1	2434	U	N1-C2-O2	5.28	126.50	122.80
50	1	1341	U	N3-C2-O2	-5.28	118.50	122.20
50	1	2606	G	N3-C4-N9	5.28	129.17	126.00
50	1	2783	U	N3-C2-O2	-5.28	118.50	122.20
50	1	1210	U	N1-C2-O2	5.28	126.49	122.80
50	1	1292	C	C2-N1-C1'	5.28	124.61	118.80
50	1	2630	C	N3-C2-O2	-5.28	118.21	121.90
50	1	1132	C	C6-N1-C2	-5.27	118.19	120.30
51	3	104	A	N7-C8-N9	5.27	116.43	113.80
50	1	2577	C	N3-C2-O2	-5.26	118.22	121.90
50	1	2812	C	N3-C2-O2	-5.26	118.22	121.90
50	1	2509	U	N3-C2-O2	-5.25	118.52	122.20
17	Q	122	ILE	CG1-CB-CG2	-5.25	99.86	111.40
50	1	2948	C	N3-C2-O2	-5.25	118.23	121.90
50	1	1585	C	N3-C2-O2	-5.24	118.23	121.90
50	1	3351	U	P-O3'-C3'	5.24	125.99	119.70
51	3	95	A	N9-C4-C5	-5.24	103.70	105.80
50	1	2553	U	C2-N1-C1'	5.24	123.99	117.70
50	1	1329	U	C2-N1-C1'	5.24	123.98	117.70
50	1	1569	U	N3-C2-O2	-5.24	118.53	122.20
50	1	2654	C	C6-N1-C2	-5.24	118.20	120.30
50	1	1451	C	N1-C2-O2	5.24	122.04	118.90
50	1	2760	C	N3-C2-O2	-5.24	118.24	121.90
50	1	2270	A	O5'-P-OP1	-5.23	100.99	105.70
50	1	2444	C	N1-C2-O2	5.23	122.04	118.90
50	1	1426	C	N1-C2-O2	5.23	122.04	118.90
50	1	2722	U	C6-N1-C2	-5.22	117.87	121.00
50	1	1762	C	N1-C2-O2	5.22	122.03	118.90
50	1	41	G	O4'-C1'-N9	5.22	112.38	108.20
50	1	1608	C	C2-N1-C1'	5.22	124.54	118.80
50	1	3195	U	N1-C2-O2	5.22	126.45	122.80
50	1	2816	G	N9-C4-C5	-5.22	103.31	105.40
50	1	2923	U	C5-C6-N1	5.22	125.31	122.70
50	1	1200	A	C8-N9-C4	5.22	107.89	105.80
50	1	1561	G	O4'-C1'-N9	5.22	112.37	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	1	2270	A	C2-N3-C4	5.22	113.21	110.60
51	3	14	U	N1-C2-O2	5.21	126.45	122.80
50	1	2843	U	N1-C2-O2	5.21	126.45	122.80
50	1	1597	C	N3-C2-O2	-5.21	118.25	121.90
50	1	2772	C	C2-N1-C1'	5.20	124.52	118.80
50	1	2150	G	C8-N9-C4	5.20	108.48	106.40
50	1	2764	C	C2-N3-C4	5.20	122.50	119.90
50	1	1637	A	C8-N9-C4	5.19	107.88	105.80
50	1	2867	C	C6-N1-C1'	-5.19	114.57	120.80
50	1	2211	U	N3-C2-O2	-5.19	118.57	122.20
50	1	1199	C	C6-N1-C1'	-5.19	114.57	120.80
50	1	3116	G	N3-C4-C5	-5.19	126.01	128.60
50	1	3096	C	N3-C2-O2	-5.19	118.27	121.90
50	1	199	A	O4'-C1'-N9	5.18	112.35	108.20
50	1	1276	U	N1-C2-O2	5.18	126.43	122.80
50	1	2316	G	C8-N9-C1'	-5.18	120.26	127.00
50	1	770	G	O4'-C1'-N9	5.18	112.34	108.20
50	1	960	U	C2-N1-C1'	5.18	123.92	117.70
50	1	1634	G	C5-C6-N1	5.18	114.09	111.50
50	1	2898	G	C2-N3-C4	-5.18	109.31	111.90
51	3	68	C	N3-C2-O2	-5.18	118.28	121.90
50	1	2263	C	N1-C2-O2	5.17	122.00	118.90
50	1	41	G	N1-C2-N3	5.17	127.00	123.90
50	1	2794	G	C5-C6-O6	-5.17	125.50	128.60
50	1	3316	A	OP2-P-O3'	5.16	116.56	105.20
50	1	40	A	OP1-P-O3'	5.16	116.56	105.20
50	1	169	U	P-O3'-C3'	5.15	125.88	119.70
50	1	2924	U	N1-C2-O2	5.15	126.41	122.80
50	1	552	G	C6-C5-N7	-5.15	127.31	130.40
50	1	645	A	P-O3'-C3'	5.15	125.88	119.70
50	1	1615	C	N3-C2-O2	-5.15	118.30	121.90
3	B	140	ASP	CA-C-N	5.15	126.49	116.20
50	1	2247	G	N3-C4-N9	5.15	129.09	126.00
50	1	2441	A	N3-C4-N9	5.14	131.52	127.40
50	1	2703	A	N3-C4-N9	5.14	131.52	127.40
50	1	2508	U	N1-C2-O2	5.14	126.40	122.80
50	1	2513	U	P-O3'-C3'	5.14	125.86	119.70
50	1	3275	U	OP1-P-O3'	5.14	116.50	105.20
50	1	1255	C	N1-C2-O2	5.13	121.98	118.90
50	1	2829	U	C2-N1-C1'	5.13	123.86	117.70
51	3	106	U	C5-C6-N1	5.13	125.27	122.70
50	1	1770	G	C4-N9-C1'	5.13	133.17	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	1	2535	A	C5-N7-C8	-5.13	101.34	103.90
40	n	453	LEU	CA-CB-CG	5.12	127.08	115.30
50	1	2720	G	C4-N9-C1'	5.12	133.16	126.50
50	1	548	G	C5-C6-O6	-5.12	125.53	128.60
50	1	868	C	N1-C2-O2	5.12	121.97	118.90
50	1	1258	U	N1-C2-O2	5.12	126.39	122.80
50	1	3290	G	C6-N1-C2	5.12	128.17	125.10
50	1	2623	G	N3-C4-C5	5.12	131.16	128.60
50	1	614	C	N3-C2-O2	-5.12	118.32	121.90
50	1	1142	G	C2-N3-C4	-5.11	109.34	111.90
50	1	3317	U	N3-C2-O2	-5.11	118.62	122.20
51	3	35	C	N3-C2-O2	-5.11	118.32	121.90
50	1	1355	A	OP2-P-O3'	5.11	116.44	105.20
50	1	2703	A	C4-N9-C1'	5.10	135.49	126.30
50	1	883	A	C8-N9-C4	5.10	107.84	105.80
50	1	2247	G	N3-C4-C5	-5.10	126.05	128.60
50	1	3222	U	N3-C2-O2	-5.10	118.63	122.20
50	1	1302	A	N7-C8-N9	5.10	116.35	113.80
50	1	2950	G	C4-C5-N7	5.09	112.84	110.80
50	1	3159	C	N3-C2-O2	-5.09	118.33	121.90
50	1	550	A	N9-C4-C5	-5.09	103.76	105.80
50	1	1771	C	N3-C2-O2	-5.09	118.33	121.90
50	1	2649	A	C2-N3-C4	5.09	113.15	110.60
50	1	2652	U	OP1-P-O3'	5.09	116.41	105.20
50	1	549	U	C2-N3-C4	5.09	130.06	127.00
50	1	2928	C	N1-C2-O2	5.09	121.95	118.90
50	1	3270	U	C5-C6-N1	-5.09	120.16	122.70
50	1	761	A	P-O3'-C3'	5.08	125.80	119.70
50	1	2753	G	P-O3'-C3'	5.08	125.80	119.70
50	1	553	U	N1-C2-O2	5.08	126.36	122.80
50	1	3196	U	C2-N1-C1'	5.08	123.80	117.70
50	1	270	U	N3-C2-O2	-5.08	118.64	122.20
50	1	2230	C	C5-C6-N1	5.08	123.54	121.00
50	1	40	A	N3-C4-N9	5.07	131.45	127.40
50	1	3018	C	N3-C2-O2	-5.07	118.35	121.90
51	3	28	C	C6-N1-C2	-5.07	118.27	120.30
50	1	2553	U	N3-C2-O2	-5.06	118.66	122.20
50	1	2402	A	N9-C1'-C2'	5.06	120.58	114.00
1	2	11	C	N3-C2-O2	-5.06	118.36	121.90
50	1	1904	C	N3-C2-O2	-5.05	118.36	121.90
50	1	2822	U	C2-N1-C1'	5.05	123.77	117.70
50	1	2921	U	N1-C2-O2	5.05	126.34	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	1	1128	U	OP1-P-O3'	5.05	116.32	105.20
50	1	354	U	N3-C2-O2	-5.05	118.66	122.20
50	1	430	U	N1-C2-O2	5.05	126.34	122.80
50	1	1200	A	C2-N3-C4	-5.05	108.08	110.60
50	1	163	C	N1-C2-O2	5.05	121.93	118.90
50	1	552	G	C5-N7-C8	-5.05	101.78	104.30
50	1	3078	U	OP2-P-O3'	5.04	116.29	105.20
50	1	1843	C	N1-C2-O2	5.04	121.92	118.90
35	i	43	LEU	CA-CB-CG	5.04	126.89	115.30
50	1	573	C	N3-C2-O2	-5.04	118.37	121.90
50	1	3120	C	N1-C2-O2	5.04	121.92	118.90
51	3	38	U	N3-C2-O2	-5.04	118.68	122.20
1	2	102	U	N3-C2-O2	-5.03	118.68	122.20
50	1	1522	U	C5-C6-N1	-5.03	120.18	122.70
50	1	2414	G	N7-C8-N9	5.03	115.62	113.10
50	1	2582	C	N3-C2-O2	-5.03	118.38	121.90
50	1	1690	C	N3-C2-O2	-5.03	118.38	121.90
50	1	2764	C	N3-C2-O2	-5.03	118.38	121.90
50	1	2	U	C2-N1-C1'	5.03	123.73	117.70
50	1	1132	C	C2-N1-C1'	5.02	124.32	118.80
50	1	2909	U	N3-C2-O2	-5.02	118.68	122.20
50	1	2400	G	N1-C2-N2	-5.02	111.68	116.20
50	1	2685	C	N1-C2-O2	5.02	121.91	118.90
50	1	718	G	N3-C4-C5	5.02	131.11	128.60
50	1	654	C	N1-C2-O2	5.01	121.91	118.90
1	2	83	C	C6-N1-C2	5.01	122.30	120.30
50	1	2708	C	N1-C2-O2	5.01	121.91	118.90
50	1	3162	C	N1-C2-O2	5.01	121.91	118.90
50	1	3155	U	N3-C2-O2	-5.01	118.69	122.20
50	1	654	C	N3-C2-O2	-5.00	118.40	121.90
50	1	2905	U	N3-C2-O2	-5.00	118.70	122.20
50	1	2522	G	N3-C4-N9	5.00	129.00	126.00

There are no chirality outliers.

All (78) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
52	4	104	TRP	Peptide
52	4	379	LEU	Peptide
2	A	143	GLU	Peptide
3	B	138	ALA	Peptide
3	B	139	GLN	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
3	B	221	THR	Peptide
4	C	132	ALA	Peptide
4	C	318	LEU	Peptide
4	C	338	LYS	Peptide
5	D	137	ASP	Peptide
5	D	251	PRO	Peptide
5	D	40	HIS	Peptide
5	D	71	GLY	Peptide
7	F	158	LYS	Peptide
7	F	232	ARG	Peptide
8	G	76	ALA	Peptide
8	G	79	GLN	Peptide
9	H	21	LYS	Peptide
10	I	16	ARG	Peptide
11	J	94	ARG	Peptide
12	L	49	ARG	Peptide
12	L	76	THR	Peptide
56	MM	1063	ARG	Peptide
16	P	156	ALA	Peptide
16	P	9	THR	Peptide
19	S	12	ARG	Peptide
19	S	171	PHE	Peptide
19	S	22	PRO	Peptide
23	W	175	ILE	Peptide
23	W	177	ALA	Peptide
26	Z	101	PHE	Peptide
26	Z	102	GLU	Peptide
26	Z	58	GLY	Peptide
27	a	96	LYS	Peptide
28	b	13	PRO	Peptide
28	b	226	ASP	Peptide
28	b	260	CYS	Peptide
28	b	367	GLN	Peptide
28	b	368	ALA	Peptide
28	b	369	ARG	Mainchain,Peptide
28	b	399	ALA	Peptide
28	b	435	ILE	Peptide
28	b	437	ASP	Peptide
28	b	438	GLY	Peptide
28	b	446	ASP	Peptide
28	b	483	ALA	Peptide
28	b	635	PHE	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
28	b	8	ILE	Peptide
30	d	86	LYS	Peptide
34	h	83	LYS	Peptide
37	k	33	LYS	Peptide
37	k	34	ALA	Peptide
38	l	4	GLN	Peptide
39	m	154	ALA	Peptide
39	m	240	LYS	Peptide
39	m	253	LYS	Peptide
39	m	376	LYS	Peptide
39	m	377	ASP	Peptide
39	m	378	SER	Peptide
39	m	416	TYR	Peptide
39	m	77	TRP	Peptide
40	n	3	ILE	Peptide
40	n	354	SER	Peptide
40	n	375	ILE	Peptide
42	r	145	LYS	Peptide
42	r	15	GLY	Peptide
42	r	16	LYS	Peptide
42	r	205	GLN	Peptide
43	s	2	ARG	Peptide
44	u	2	ARG	Peptide
44	u	78	PRO	Peptide
44	u	79	VAL	Peptide
47	x	20	ARG	Peptide
47	x	208	ASN	Peptide
47	x	25	ILE	Peptide
47	x	29	LEU	Peptide
48	y	8	GLU	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	
2	A	211/254 (83%)	194 (92%)	17 (8%)	0	100	100
3	B	384/387 (99%)	327 (85%)	53 (14%)	4 (1%)	15	52
4	C	359/362 (99%)	317 (88%)	39 (11%)	3 (1%)	19	57
5	D	272/297 (92%)	251 (92%)	21 (8%)	0	100	100
6	E	152/176 (86%)	140 (92%)	12 (8%)	0	100	100
7	F	220/244 (90%)	204 (93%)	16 (7%)	0	100	100
8	G	231/256 (90%)	210 (91%)	21 (9%)	0	100	100
9	H	189/191 (99%)	171 (90%)	18 (10%)	0	100	100
10	I	129/166 (78%)	113 (88%)	16 (12%)	0	100	100
11	J	167/174 (96%)	146 (87%)	20 (12%)	1 (1%)	25	63
12	L	185/199 (93%)	162 (88%)	21 (11%)	2 (1%)	14	51
13	M	135/138 (98%)	125 (93%)	10 (7%)	0	100	100
14	N	201/204 (98%)	182 (90%)	19 (10%)	0	100	100
15	O	195/199 (98%)	188 (96%)	7 (4%)	0	100	100
16	P	181/184 (98%)	169 (93%)	12 (7%)	0	100	100
17	Q	132/186 (71%)	124 (94%)	7 (5%)	1 (1%)	19	57
18	R	154/189 (82%)	150 (97%)	4 (3%)	0	100	100
19	S	169/172 (98%)	154 (91%)	14 (8%)	1 (1%)	25	63
20	T	115/160 (72%)	104 (90%)	11 (10%)	0	100	100
21	U	104/121 (86%)	92 (88%)	12 (12%)	0	100	100
22	V	134/137 (98%)	125 (93%)	9 (7%)	0	100	100
23	W	232/236 (98%)	215 (93%)	15 (6%)	2 (1%)	17	54
24	X	120/142 (84%)	112 (93%)	8 (7%)	0	100	100
25	Y	124/127 (98%)	118 (95%)	6 (5%)	0	100	100
26	Z	133/136 (98%)	114 (86%)	18 (14%)	1 (1%)	19	57
27	a	91/149 (61%)	83 (91%)	8 (9%)	0	100	100
28	b	638/647 (99%)	562 (88%)	70 (11%)	6 (1%)	17	54
29	c	95/105 (90%)	92 (97%)	3 (3%)	0	100	100
30	d	105/113 (93%)	96 (91%)	9 (9%)	0	100	100
31	e	125/130 (96%)	119 (95%)	6 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	f	104/107 (97%)	96 (92%)	8 (8%)	0	100	100
33	g	110/121 (91%)	101 (92%)	9 (8%)	0	100	100
34	h	117/120 (98%)	106 (91%)	10 (8%)	1 (1%)	17	54
35	i	97/100 (97%)	86 (89%)	11 (11%)	0	100	100
36	j	85/88 (97%)	78 (92%)	7 (8%)	0	100	100
37	k	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
38	l	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
39	m	465/486 (96%)	404 (87%)	58 (12%)	3 (1%)	25	63
40	n	365/605 (60%)	310 (85%)	51 (14%)	4 (1%)	14	51
41	p	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
42	r	224/261 (86%)	189 (84%)	32 (14%)	3 (1%)	12	48
43	s	65/520 (12%)	59 (91%)	6 (9%)	0	100	100
44	u	148/199 (74%)	138 (93%)	9 (6%)	1 (1%)	22	60
45	v	283/344 (82%)	262 (93%)	21 (7%)	0	100	100
46	w	178/203 (88%)	152 (85%)	26 (15%)	0	100	100
47	x	476/515 (92%)	432 (91%)	44 (9%)	0	100	100
48	y	242/245 (99%)	225 (93%)	17 (7%)	0	100	100
49	z	53/106 (50%)	50 (94%)	3 (6%)	0	100	100
52	4	508/593 (86%)	454 (89%)	54 (11%)	0	100	100
53	5	71/120 (59%)	69 (97%)	2 (3%)	0	100	100
54	KK	82/733 (11%)	80 (98%)	2 (2%)	0	100	100
55	LL	111/184 (60%)	111 (100%)	0	0	100	100
56	MM	971/1011 (96%)	926 (95%)	45 (5%)	0	100	100
All	All	10649/13063 (82%)	9689 (91%)	927 (9%)	33 (0%)	44	75

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	339	LEU
11	J	95	ASN
28	b	484	SER
39	m	241	SER
42	r	17	ARG
3	B	139	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	140	ASP
4	C	131	VAL
23	W	178	GLY
28	b	370	ASP
39	m	78	PHE
40	n	153	SER
40	n	384	GLY
4	C	130	ALA
12	L	63	VAL
12	L	77	LEU
19	S	13	ARG
28	b	369	ARG
28	b	399	ALA
28	b	483	ALA
34	h	92	LEU
40	n	355	PRO
42	r	147	TRP
42	r	162	THR
3	B	5	LYS
3	B	239	PRO
17	Q	41	ASP
26	Z	102	GLU
28	b	9	PRO
44	u	3	ILE
23	W	126	ARG
39	m	347	PRO
40	n	455	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
2	A	166/196 (85%)	165 (99%)	1 (1%)	86 91
3	B	322/323 (100%)	316 (98%)	6 (2%)	57 75
4	C	288/289 (100%)	287 (100%)	1 (0%)	92 95

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	D	227/245 (93%)	226 (100%)	1 (0%)	91 94
6	E	134/153 (88%)	133 (99%)	1 (1%)	84 90
7	F	186/205 (91%)	185 (100%)	1 (0%)	88 93
8	G	191/208 (92%)	189 (99%)	2 (1%)	76 86
9	H	171/171 (100%)	167 (98%)	4 (2%)	50 71
10	I	117/141 (83%)	116 (99%)	1 (1%)	78 87
11	J	147/150 (98%)	145 (99%)	2 (1%)	67 81
12	L	149/159 (94%)	146 (98%)	3 (2%)	55 74
13	M	108/109 (99%)	108 (100%)	0	100 100
14	N	175/176 (99%)	174 (99%)	1 (1%)	86 91
15	O	160/162 (99%)	158 (99%)	2 (1%)	69 82
16	P	145/146 (99%)	143 (99%)	2 (1%)	67 81
17	Q	110/151 (73%)	109 (99%)	1 (1%)	78 87
18	R	129/154 (84%)	127 (98%)	2 (2%)	62 79
19	S	155/156 (99%)	153 (99%)	2 (1%)	69 82
20	T	102/137 (74%)	100 (98%)	2 (2%)	55 74
21	U	93/107 (87%)	91 (98%)	2 (2%)	52 71
22	V	104/105 (99%)	103 (99%)	1 (1%)	76 86
23	W	211/213 (99%)	206 (98%)	5 (2%)	49 69
24	X	106/118 (90%)	105 (99%)	1 (1%)	78 87
25	Y	109/110 (99%)	109 (100%)	0	100 100
26	Z	115/116 (99%)	115 (100%)	0	100 100
27	a	76/119 (64%)	75 (99%)	1 (1%)	69 82
28	b	568/573 (99%)	553 (97%)	15 (3%)	46 68
29	c	81/88 (92%)	78 (96%)	3 (4%)	34 60
30	d	94/97 (97%)	94 (100%)	0	100 100
31	e	109/111 (98%)	106 (97%)	3 (3%)	43 66
32	f	90/91 (99%)	90 (100%)	0	100 100
33	g	95/103 (92%)	94 (99%)	1 (1%)	73 84
34	h	104/105 (99%)	104 (100%)	0	100 100
35	i	81/82 (99%)	80 (99%)	1 (1%)	71 83

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
36	j	70/71 (99%)	70 (100%)	0	100 100
37	k	68/69 (99%)	68 (100%)	0	100 100
38	l	45/46 (98%)	44 (98%)	1 (2%)	52 71
39	m	413/428 (96%)	408 (99%)	5 (1%)	71 83
40	n	334/548 (61%)	333 (100%)	1 (0%)	92 95
41	p	71/72 (99%)	70 (99%)	1 (1%)	67 81
42	r	203/229 (89%)	202 (100%)	1 (0%)	88 93
43	s	62/445 (14%)	61 (98%)	1 (2%)	62 79
44	u	133/180 (74%)	128 (96%)	5 (4%)	33 59
45	v	258/309 (84%)	258 (100%)	0	100 100
46	w	161/179 (90%)	160 (99%)	1 (1%)	86 91
47	x	428/451 (95%)	425 (99%)	3 (1%)	84 90
48	y	210/211 (100%)	210 (100%)	0	100 100
49	z	48/95 (50%)	47 (98%)	1 (2%)	53 73
52	4	453/520 (87%)	446 (98%)	7 (2%)	65 80
53	5	67/106 (63%)	66 (98%)	1 (2%)	65 80
54	KK	75/671 (11%)	74 (99%)	1 (1%)	69 82
55	LL	99/168 (59%)	98 (99%)	1 (1%)	76 86
56	MM	809/895 (90%)	805 (100%)	4 (0%)	88 93
All	All	9225/11262 (82%)	9123 (99%)	102 (1%)	74 84

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	193	ARG
3	B	28	ARG
3	B	81	THR
3	B	300	ARG
3	B	305	ILE
3	B	332	ARG
3	B	385	LYS
4	C	197	ARG
5	D	23	ARG
6	E	51	ARG
7	F	26	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	G	84	ARG
8	G	146	LYS
9	H	23	ARG
9	H	118	LEU
9	H	124	ARG
9	H	157	ASN
10	I	75	ARG
11	J	94	ARG
11	J	166	LYS
12	L	12	ASN
12	L	21	ARG
12	L	54	LEU
14	N	188	ARG
15	O	85	ARG
15	O	148	LYS
16	P	97	ASN
16	P	138	LYS
17	Q	147	ARG
18	R	98	ARG
18	R	104	ARG
19	S	12	ARG
19	S	119	ARG
20	T	136	ARG
20	T	139	ARG
21	U	49	ASN
21	U	94	ARG
22	V	86	ARG
23	W	22	ASN
23	W	113	LYS
23	W	128	ASN
23	W	231	THR
23	W	232	ASN
24	X	73	MET
27	a	120	ASN
28	b	1	MET
28	b	70	ASN
28	b	100	ARG
28	b	168	ARG
28	b	177	ASN
28	b	288	ASN
28	b	346	ASN
28	b	369	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	b	384	ASN
28	b	395	ARG
28	b	445	LEU
28	b	535	MET
28	b	557	ARG
28	b	588	ARG
28	b	647	ARG
29	c	16	LEU
29	c	61	MET
29	c	86	ARG
31	e	27	ARG
31	e	87	MET
31	e	126	LEU
33	g	95	ILE
35	i	60	LEU
38	l	43	ASN
39	m	57	ARG
39	m	147	ARG
39	m	186	ASN
39	m	232	ARG
39	m	422	LYS
40	n	351	LYS
41	p	17	ARG
42	r	126	ARG
43	s	6	ARG
44	u	27	LYS
44	u	45	ASN
44	u	82	ASN
44	u	100	ARG
44	u	113	ARG
46	w	55	ARG
47	x	20	ARG
47	x	311	ARG
47	x	369	ASN
49	z	19	ARG
52	4	243	ARG
52	4	245	ARG
52	4	262	ARG
52	4	331	LYS
52	4	428	ASN
52	4	475	LEU
52	4	518	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	5	72	ARG
54	KK	45	LYS
55	LL	64	ASN
56	MM	530	ARG
56	MM	614	ASN
56	MM	642	ASN
56	MM	844	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (112) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	79	ASN
3	B	243	HIS
4	C	58	HIS
4	C	110	ASN
4	C	116	ASN
4	C	260	GLN
5	D	90	HIS
5	D	178	ASN
5	D	264	GLN
6	E	167	ASN
7	F	48	ASN
8	G	38	GLN
8	G	41	GLN
8	G	137	ASN
8	G	138	HIS
8	G	221	ASN
10	I	36	ASN
10	I	49	HIS
10	I	73	HIS
11	J	95	ASN
12	L	12	ASN
12	L	25	HIS
12	L	37	ASN
14	N	37	HIS
14	N	57	GLN
14	N	182	ASN
16	P	54	HIS
16	P	55	GLN
16	P	118	GLN
18	R	134	HIS
19	S	74	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	S	89	ASN
19	S	154	HIS
20	T	90	ASN
20	T	95	HIS
20	T	149	GLN
21	U	49	ASN
23	W	22	ASN
23	W	74	GLN
23	W	232	ASN
24	X	65	GLN
26	Z	36	HIS
26	Z	78	ASN
27	a	67	HIS
27	a	120	ASN
28	b	26	GLN
28	b	70	ASN
28	b	78	HIS
28	b	107	GLN
28	b	177	ASN
28	b	217	GLN
28	b	288	ASN
28	b	333	ASN
28	b	346	ASN
28	b	384	ASN
30	d	57	GLN
31	e	104	ASN
32	f	77	ASN
34	h	59	ASN
34	h	113	GLN
35	i	91	ASN
38	l	43	ASN
39	m	90	GLN
39	m	175	GLN
39	m	186	ASN
39	m	227	HIS
40	n	137	ASN
40	n	164	ASN
40	n	230	HIS
40	n	437	ASN
42	r	70	GLN
44	u	17	HIS
44	u	45	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	u	76	ASN
44	u	82	ASN
45	v	29	GLN
45	v	64	ASN
45	v	280	GLN
46	w	57	ASN
46	w	63	ASN
46	w	83	GLN
46	w	180	ASN
47	x	325	HIS
47	x	359	ASN
47	x	369	ASN
47	x	401	HIS
47	x	407	HIS
47	x	449	GLN
48	y	21	ASN
48	y	86	ASN
48	y	162	HIS
49	z	12	ASN
52	4	26	ASN
52	4	273	HIS
52	4	348	HIS
52	4	405	ASN
52	4	428	ASN
52	4	551	GLN
53	5	100	HIS
54	KK	26	GLN
55	LL	64	ASN
55	LL	95	ASN
55	LL	113	ASN
56	MM	87	GLN
56	MM	117	HIS
56	MM	445	ASN
56	MM	446	ASN
56	MM	614	ASN
56	MM	651	GLN
56	MM	703	ASN
56	MM	838	ASN
56	MM	1012	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	161/162 (99%)	36 (22%)	2 (1%)
50	1	3048/3396 (89%)	902 (29%)	80 (2%)
51	3	120/121 (99%)	28 (23%)	1 (0%)
All	All	3329/3679 (90%)	966 (29%)	83 (2%)

All (966) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	23	U
1	2	34	U
1	2	35	C
1	2	39	G
1	2	51	G
1	2	52	A
1	2	59	A
1	2	62	C
1	2	63	G
1	2	70	G
1	2	80	A
1	2	82	U
1	2	83	C
1	2	84	C
1	2	85	G
1	2	86	U
1	2	87	G
1	2	88	A
1	2	90	U
1	2	95	G
1	2	104	A
1	2	106	C
1	2	111	A
1	2	112	U
1	2	113	U
1	2	114	G
1	2	124	G
1	2	125	U
1	2	126	A
1	2	138	A
1	2	148	G
1	2	151	C
1	2	152	G
1	2	154	C
1	2	156	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2	157	A
50	1	2	U
50	1	13	A
50	1	14	U
50	1	18	G
50	1	22	G
50	1	26	A
50	1	37	U
50	1	40	A
50	1	41	G
50	1	43	A
50	1	45	A
50	1	48	A
50	1	49	A
50	1	50	U
50	1	58	G
50	1	59	G
50	1	60	A
50	1	65	A
50	1	66	A
50	1	71	A
50	1	72	C
50	1	73	C
50	1	75	G
50	1	77	A
50	1	83	U
50	1	89	A
50	1	92	G
50	1	93	C
50	1	94	G
50	1	96	G
50	1	109	A
50	1	110	G
50	1	111	C
50	1	116	A
50	1	117	U
50	1	118	U
50	1	120	G
50	1	121	A
50	1	122	A
50	1	134	U
50	1	135	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1	136	G
50	1	142	C
50	1	143	G
50	1	146	U
50	1	148	G
50	1	154	U
50	1	157	A
50	1	161	G
50	1	165	A
50	1	166	C
50	1	169	U
50	1	170	G
50	1	172	G
50	1	173	G
50	1	182	U
50	1	187	A
50	1	190	U
50	1	191	U
50	1	192	C
50	1	199	A
50	1	200	C
50	1	206	G
50	1	210	U
50	1	211	A
50	1	213	A
50	1	218	G
50	1	219	A
50	1	234	G
50	1	240	U
50	1	241	G
50	1	243	G
50	1	245	U
50	1	246	U
50	1	249	U
50	1	250	U
50	1	251	G
50	1	252	U
50	1	253	A
50	1	263	C
50	1	269	G
50	1	284	A
50	1	285	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1	286	U
50	1	291	C
50	1	295	A
50	1	298	U
50	1	305	U
50	1	306	A
50	1	311	C
50	1	323	A
50	1	329	U
50	1	339	C
50	1	343	U
50	1	344	A
50	1	349	A
50	1	351	A
50	1	359	U
50	1	362	U
50	1	370	U
50	1	376	G
50	1	378	A
50	1	397	A
50	1	398	A
50	1	399	A
50	1	401	U
50	1	402	A
50	1	403	C
50	1	404	G
50	1	421	G
50	1	422	A
50	1	439	C
50	1	440	A
50	1	495	G
50	1	498	A
50	1	503	C
50	1	507	U
50	1	510	G
50	1	517	G
50	1	521	A
50	1	523	A
50	1	535	G
50	1	540	U
50	1	543	C
50	1	544	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1	546	C
50	1	547	G
50	1	548	G
50	1	550	A
50	1	552	G
50	1	555	U
50	1	556	U
50	1	557	A
50	1	558	U
50	1	559	A
50	1	560	G
50	1	569	A
50	1	578	A
50	1	579	G
50	1	591	G
50	1	592	A
50	1	597	G
50	1	600	G
50	1	604	G
50	1	607	A
50	1	609	G
50	1	611	A
50	1	620	U
50	1	621	A
50	1	622	A
50	1	628	A
50	1	636	C
50	1	642	U
50	1	643	U
50	1	644	G
50	1	645	A
50	1	646	A
50	1	647	A
50	1	650	C
50	1	660	A
50	1	677	A
50	1	681	U
50	1	690	A
50	1	691	A
50	1	692	A
50	1	705	A
50	1	708	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1	712	G
50	1	715	A
50	1	717	C
50	1	719	U
50	1	720	A
50	1	721	G
50	1	722	G
50	1	728	G
50	1	761	A
50	1	762	U
50	1	763	G
50	1	764	U
50	1	765	C
50	1	766	U
50	1	767	U
50	1	768	C
50	1	771	A
50	1	776	U
50	1	777	U
50	1	779	G
50	1	780	A
50	1	781	G
50	1	785	G
50	1	786	A
50	1	799	G
50	1	806	A
50	1	808	A
50	1	817	A
50	1	826	G
50	1	830	A
50	1	837	A
50	1	849	C
50	1	850	U
50	1	857	G
50	1	861	C
50	1	874	U
50	1	875	G
50	1	879	U
50	1	880	G
50	1	884	A
50	1	890	C
50	1	896	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1	907	G
50	1	908	G
50	1	911	C
50	1	914	A
50	1	916	G
50	1	917	A
50	1	923	C
50	1	924	G
50	1	932	U
50	1	934	G
50	1	936	A
50	1	938	C
50	1	943	U
50	1	944	C
50	1	946	U
50	1	953	G
50	1	956	U
50	1	957	C
50	1	958	C
50	1	959	C
50	1	974	G
50	1	976	U
50	1	978	G
50	1	980	A
50	1	981	U
50	1	986	U
50	1	991	G
50	1	992	A
50	1	994	G
50	1	996	A
50	1	997	A
50	1	998	A
50	1	999	G
50	1	1000	C
50	1	1001	G
50	1	1048	A
50	1	1049	C
50	1	1050	U
50	1	1051	U
50	1	1054	A
50	1	1057	A
50	1	1058	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1	1063	G
50	1	1064	A
50	1	1065	A
50	1	1066	G
50	1	1093	A
50	1	1094	U
50	1	1095	U
50	1	1097	G
50	1	1098	A
50	1	1102	A
50	1	1103	A
50	1	1104	G
50	1	1106	G
50	1	1107	C
50	1	1110	U
50	1	1111	U
50	1	1115	G
50	1	1116	G
50	1	1117	G
50	1	1118	C
50	1	1123	U
50	1	1127	G
50	1	1128	U
50	1	1129	A
50	1	1130	A
50	1	1132	C
50	1	1135	A
50	1	1136	A
50	1	1151	U
50	1	1153	A
50	1	1155	C
50	1	1160	C
50	1	1176	C
50	1	1178	G
50	1	1180	A
50	1	1181	U
50	1	1182	A
50	1	1190	A
50	1	1191	U
50	1	1192	C
50	1	1193	A
50	1	1196	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1	1197	A
50	1	1198	C
50	1	1199	C
50	1	1200	A
50	1	1201	C
50	1	1204	A
50	1	1206	G
50	1	1217	A
50	1	1220	U
50	1	1221	A
50	1	1227	C
50	1	1235	U
50	1	1239	C
50	1	1240	A
50	1	1241	U
50	1	1242	G
50	1	1244	A
50	1	1245	A
50	1	1248	C
50	1	1251	A
50	1	1252	A
50	1	1253	U
50	1	1254	C
50	1	1258	U
50	1	1262	G
50	1	1263	A
50	1	1264	G
50	1	1265	U
50	1	1266	G
50	1	1271	A
50	1	1272	C
50	1	1277	C
50	1	1278	A
50	1	1286	A
50	1	1287	A
50	1	1296	C
50	1	1299	U
50	1	1301	A
50	1	1302	A
50	1	1303	A
50	1	1304	A
50	1	1305	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1	1306	G
50	1	1307	G
50	1	1308	A
50	1	1310	G
50	1	1313	G
50	1	1316	C
50	1	1317	A
50	1	1325	U
50	1	1330	A
50	1	1331	U
50	1	1348	U
50	1	1349	G
50	1	1351	U
50	1	1352	A
50	1	1353	U
50	1	1354	G
50	1	1355	A
50	1	1356	U
50	1	1357	G
50	1	1370	G
50	1	1386	A
50	1	1387	G
50	1	1392	G
50	1	1399	A
50	1	1400	G
50	1	1404	G
50	1	1419	A
50	1	1434	G
50	1	1437	C
50	1	1446	A
50	1	1455	U
50	1	1475	A
50	1	1480	G
50	1	1481	A
50	1	1487	G
50	1	1494	U
50	1	1497	C
50	1	1503	A
50	1	1508	C
50	1	1523	U
50	1	1527	C
50	1	1536	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1	1539	A
50	1	1542	G
50	1	1549	U
50	1	1554	U
50	1	1555	U
50	1	1556	C
50	1	1557	A
50	1	1560	G
50	1	1561	G
50	1	1562	C
50	1	1566	A
50	1	1567	U
50	1	1568	U
50	1	1569	U
50	1	1570	U
50	1	1571	A
50	1	1572	U
50	1	1573	G
50	1	1575	A
50	1	1580	A
50	1	1581	C
50	1	1582	C
50	1	1583	A
50	1	1589	A
50	1	1593	A
50	1	1596	C
50	1	1606	U
50	1	1607	U
50	1	1613	A
50	1	1619	A
50	1	1620	U
50	1	1629	U
50	1	1639	C
50	1	1642	A
50	1	1643	A
50	1	1645	U
50	1	1657	C
50	1	1680	G
50	1	1683	A
50	1	1687	U
50	1	1716	U
50	1	1717	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1	1724	U
50	1	1736	G
50	1	1741	A
50	1	1742	U
50	1	1750	A
50	1	1751	G
50	1	1760	A
50	1	1762	C
50	1	1763	U
50	1	1764	U
50	1	1765	U
50	1	1766	G
50	1	1770	G
50	1	1772	U
50	1	1775	G
50	1	1780	G
50	1	1782	U
50	1	1797	A
50	1	1808	G
50	1	1810	A
50	1	1812	G
50	1	1814	A
50	1	1815	U
50	1	1816	A
50	1	1817	G
50	1	1820	U
50	1	1821	U
50	1	1830	G
50	1	1834	U
50	1	1839	A
50	1	1840	U
50	1	1841	A
50	1	1842	A
50	1	1846	C
50	1	1848	G
50	1	1849	C
50	1	1851	G
50	1	1858	A
50	1	1871	U
50	1	1880	U
50	1	1886	A
50	1	1898	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1	1901	A
50	1	1906	G
50	1	1909	A
50	1	1926	C
50	1	1930	A
50	1	1935	G
50	1	1937	U
50	1	1941	C
50	1	1952	G
50	1	1953	G
50	1	2094	C
50	1	2102	U
50	1	2107	A
50	1	2108	C
50	1	2110	G
50	1	2113	A
50	1	2120	A
50	1	2121	G
50	1	2122	G
50	1	2126	A
50	1	2131	A
50	1	2134	G
50	1	2141	U
50	1	2144	A
50	1	2158	A
50	1	2162	U
50	1	2163	C
50	1	2169	G
50	1	2170	U
50	1	2176	U
50	1	2184	U
50	1	2188	A
50	1	2193	U
50	1	2194	G
50	1	2195	C
50	1	2196	C
50	1	2198	A
50	1	2200	U
50	1	2205	U
50	1	2207	A
50	1	2208	A
50	1	2210	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1	2212	C
50	1	2213	A
50	1	2225	U
50	1	2237	C
50	1	2242	A
50	1	2243	A
50	1	2244	A
50	1	2245	C
50	1	2247	G
50	1	2248	C
50	1	2249	G
50	1	2250	G
50	1	2252	A
50	1	2253	G
50	1	2255	A
50	1	2256	A
50	1	2257	C
50	1	2264	U
50	1	2268	U
50	1	2269	U
50	1	2270	A
50	1	2271	A
50	1	2274	U
50	1	2275	A
50	1	2276	G
50	1	2277	C
50	1	2278	C
50	1	2279	A
50	1	2280	A
50	1	2316	G
50	1	2317	A
50	1	2318	U
50	1	2334	U
50	1	2335	G
50	1	2336	U
50	1	2347	U
50	1	2365	C
50	1	2369	G
50	1	2371	G
50	1	2378	C
50	1	2385	G
50	1	2386	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1	2388	U
50	1	2393	G
50	1	2397	A
50	1	2398	A
50	1	2401	A
50	1	2402	A
50	1	2405	C
50	1	2409	G
50	1	2410	U
50	1	2411	U
50	1	2412	G
50	1	2414	G
50	1	2418	G
50	1	2419	A
50	1	2435	G
50	1	2437	G
50	1	2443	A
50	1	2444	C
50	1	2445	A
50	1	2502	A
50	1	2503	G
50	1	2504	U
50	1	2514	U
50	1	2515	A
50	1	2522	G
50	1	2523	A
50	1	2525	G
50	1	2526	C
50	1	2527	G
50	1	2528	G
50	1	2529	A
50	1	2531	C
50	1	2532	U
50	1	2533	G
50	1	2534	G
50	1	2537	U
50	1	2538	U
50	1	2539	C
50	1	2540	A
50	1	2541	U
50	1	2542	U
50	1	2543	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1	2544	U
50	1	2547	A
50	1	2548	C
50	1	2549	G
50	1	2550	U
50	1	2551	U
50	1	2552	C
50	1	2554	A
50	1	2555	G
50	1	2560	C
50	1	2561	A
50	1	2566	C
50	1	2567	C
50	1	2568	C
50	1	2569	A
50	1	2570	U
50	1	2571	U
50	1	2572	C
50	1	2573	G
50	1	2576	G
50	1	2578	U
50	1	2585	G
50	1	2586	G
50	1	2593	A
50	1	2594	C
50	1	2595	A
50	1	2596	U
50	1	2606	G
50	1	2607	G
50	1	2614	G
50	1	2621	G
50	1	2623	G
50	1	2625	C
50	1	2626	A
50	1	2628	A
50	1	2635	A
50	1	2638	C
50	1	2644	C
50	1	2645	G
50	1	2648	G
50	1	2649	A
50	1	2650	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1	2651	G
50	1	2652	U
50	1	2653	C
50	1	2654	C
50	1	2655	U
50	1	2656	A
50	1	2657	A
50	1	2659	G
50	1	2668	U
50	1	2670	G
50	1	2672	G
50	1	2674	A
50	1	2677	G
50	1	2681	U
50	1	2686	A
50	1	2687	G
50	1	2688	U
50	1	2689	A
50	1	2690	G
50	1	2691	A
50	1	2692	A
50	1	2693	C
50	1	2694	A
50	1	2695	A
50	1	2696	A
50	1	2698	G
50	1	2699	G
50	1	2700	G
50	1	2702	A
50	1	2704	A
50	1	2706	G
50	1	2713	U
50	1	2714	G
50	1	2715	A
50	1	2719	U
50	1	2720	G
50	1	2721	A
50	1	2722	U
50	1	2724	U
50	1	2725	U
50	1	2726	C
50	1	2727	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1	2728	G
50	1	2729	U
50	1	2730	G
50	1	2731	U
50	1	2732	G
50	1	2740	A
50	1	2749	G
50	1	2752	U
50	1	2754	G
50	1	2756	C
50	1	2758	A
50	1	2759	U
50	1	2761	G
50	1	2762	A
50	1	2763	U
50	1	2764	C
50	1	2765	C
50	1	2766	U
50	1	2767	U
50	1	2768	U
50	1	2770	G
50	1	2771	U
50	1	2772	C
50	1	2773	C
50	1	2777	G
50	1	2778	G
50	1	2789	U
50	1	2790	A
50	1	2791	G
50	1	2793	G
50	1	2794	G
50	1	2795	U
50	1	2796	G
50	1	2798	C
50	1	2799	A
50	1	2800	G
50	1	2801	A
50	1	2802	A
50	1	2803	A
50	1	2804	A
50	1	2805	G
50	1	2810	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1	2814	G
50	1	2816	G
50	1	2817	A
50	1	2818	U
50	1	2820	A
50	1	2821	C
50	1	2822	U
50	1	2824	G
50	1	2825	C
50	1	2826	U
50	1	2827	U
50	1	2842	U
50	1	2844	C
50	1	2845	A
50	1	2846	U
50	1	2847	A
50	1	2857	C
50	1	2858	U
50	1	2859	U
50	1	2860	U
50	1	2861	U
50	1	2862	U
50	1	2863	G
50	1	2864	A
50	1	2865	U
50	1	2866	U
50	1	2867	C
50	1	2868	U
50	1	2869	U
50	1	2870	C
50	1	2871	G
50	1	2872	A
50	1	2873	U
50	1	2874	G
50	1	2875	U
50	1	2876	C
50	1	2877	G
50	1	2878	G
50	1	2879	C
50	1	2887	A
50	1	2889	C
50	1	2897	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1	2898	G
50	1	2899	C
50	1	2901	G
50	1	2914	G
50	1	2916	U
50	1	2918	G
50	1	2923	U
50	1	2924	U
50	1	2925	C
50	1	2926	A
50	1	2927	C
50	1	2928	C
50	1	2929	C
50	1	2930	A
50	1	2935	U
50	1	2936	A
50	1	2945	G
50	1	2946	A
50	1	2947	G
50	1	2949	U
50	1	2951	G
50	1	2952	G
50	1	2953	U
50	1	2954	U
50	1	2955	U
50	1	2957	G
50	1	2970	C
50	1	2971	A
50	1	2978	U
50	1	2979	U
50	1	2980	U
50	1	2981	U
50	1	2982	A
50	1	2983	C
50	1	2996	U
50	1	2997	G
50	1	3003	G
50	1	3012	A
50	1	3017	A
50	1	3021	A
50	1	3022	G
50	1	3023	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1	3027	A
50	1	3029	A
50	1	3030	G
50	1	3031	G
50	1	3032	A
50	1	3036	G
50	1	3037	U
50	1	3056	U
50	1	3058	U
50	1	3059	G
50	1	3069	G
50	1	3078	U
50	1	3079	U
50	1	3080	G
50	1	3086	A
50	1	3087	A
50	1	3089	C
50	1	3090	U
50	1	3092	C
50	1	3099	C
50	1	3100	U
50	1	3107	U
50	1	3109	G
50	1	3114	A
50	1	3115	C
50	1	3117	C
50	1	3122	A
50	1	3129	A
50	1	3130	A
50	1	3131	U
50	1	3142	A
50	1	3143	C
50	1	3148	U
50	1	3150	A
50	1	3153	U
50	1	3154	C
50	1	3155	U
50	1	3156	U
50	1	3157	U
50	1	3165	A
50	1	3170	A
50	1	3172	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1	3173	G
50	1	3174	A
50	1	3176	G
50	1	3179	U
50	1	3180	A
50	1	3181	C
50	1	3187	A
50	1	3196	U
50	1	3199	G
50	1	3207	U
50	1	3217	C
50	1	3218	A
50	1	3219	G
50	1	3227	A
50	1	3228	C
50	1	3229	G
50	1	3243	A
50	1	3244	A
50	1	3245	A
50	1	3247	G
50	1	3253	G
50	1	3256	G
50	1	3259	U
50	1	3260	G
50	1	3263	G
50	1	3268	A
50	1	3270	U
50	1	3271	G
50	1	3273	A
50	1	3276	G
50	1	3277	U
50	1	3279	A
50	1	3281	U
50	1	3286	G
50	1	3287	U
50	1	3288	G
50	1	3289	G
50	1	3294	A
50	1	3295	A
50	1	3304	U
50	1	3309	G
50	1	3313	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1	3316	A
50	1	3317	U
50	1	3318	G
50	1	3319	U
50	1	3320	A
50	1	3341	U
50	1	3342	A
50	1	3345	G
50	1	3347	A
50	1	3351	U
50	1	3352	U
50	1	3353	G
50	1	3355	U
50	1	3356	G
50	1	3363	U
50	1	3369	G
50	1	3375	A
50	1	3378	C
50	1	3382	U
50	1	3389	U
50	1	3396	U
51	3	7	G
51	3	13	A
51	3	15	C
51	3	22	A
51	3	41	G
51	3	48	U
51	3	51	A
51	3	52	G
51	3	53	U
51	3	54	U
51	3	60	G
51	3	65	G
51	3	67	G
51	3	73	C
51	3	74	C
51	3	76	A
51	3	77	G
51	3	78	U
51	3	79	A
51	3	86	U
51	3	94	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	3	97	A
51	3	102	A
51	3	103	A
51	3	110	G
51	3	112	G
51	3	120	C
51	3	121	U

All (83) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	88	A
1	2	123	G
50	1	13	A
50	1	40	A
50	1	160	G
50	1	169	U
50	1	239	G
50	1	284	A
50	1	619	A
50	1	645	A
50	1	649	A
50	1	720	A
50	1	761	A
50	1	765	C
50	1	849	C
50	1	916	G
50	1	1057	A
50	1	1064	A
50	1	1097	G
50	1	1102	A
50	1	1103	A
50	1	1128	U
50	1	1192	C
50	1	1205	A
50	1	1241	U
50	1	1302	A
50	1	1307	G
50	1	1329	U
50	1	1355	A
50	1	1554	U
50	1	1567	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1	1568	U
50	1	1570	U
50	1	1574	C
50	1	1581	C
50	1	1716	U
50	1	2101	C
50	1	2209	U
50	1	2263	C
50	1	2269	U
50	1	2317	A
50	1	2418	G
50	1	2513	U
50	1	2525	G
50	1	2537	U
50	1	2547	A
50	1	2593	A
50	1	2624	G
50	1	2625	C
50	1	2651	G
50	1	2652	U
50	1	2654	C
50	1	2655	U
50	1	2658	G
50	1	2728	G
50	1	2731	U
50	1	2753	G
50	1	2761	G
50	1	2770	G
50	1	2795	U
50	1	2801	A
50	1	2817	A
50	1	2819	A
50	1	2828	G
50	1	2857	C
50	1	2865	U
50	1	2866	U
50	1	2875	U
50	1	2900	A
50	1	2946	A
50	1	2954	U
50	1	3030	G
50	1	3078	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1	3121	U
50	1	3171	U
50	1	3218	A
50	1	3228	C
50	1	3269	U
50	1	3276	G
50	1	3316	A
50	1	3350	C
50	1	3351	U
51	3	52	G

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	GTP	b	701	60	26,34,34	1.19	1 (3%)	32,54,54	1.62	6 (18%)
59	GTP	m	501	60	26,34,34	1.51	4 (15%)	32,54,54	1.91	6 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	GTP	b	701	60	-	7/18/38/38	0/3/3/3
59	GTP	m	501	60	-	4/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	m	501	GTP	C5-C6	-4.90	1.37	1.47
59	b	701	GTP	C5-C6	-4.13	1.39	1.47
59	m	501	GTP	C5-C4	-2.37	1.37	1.43
59	m	501	GTP	O4'-C4'	-2.18	1.40	1.45
59	m	501	GTP	C2'-C1'	-2.07	1.50	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	m	501	GTP	PB-O3B-PG	-5.90	112.58	132.83
59	m	501	GTP	PA-O3A-PB	-4.34	117.93	132.83
59	b	701	GTP	PB-O3B-PG	-4.28	118.15	132.83
59	b	701	GTP	C5-C6-N1	3.26	119.71	113.95
59	m	501	GTP	C8-N7-C5	3.15	108.99	102.99
59	b	701	GTP	C8-N7-C5	3.10	108.89	102.99
59	m	501	GTP	C2-N1-C6	-3.09	119.40	125.10
59	m	501	GTP	C3'-C2'-C1'	3.07	105.61	100.98
59	b	701	GTP	C2-N1-C6	-2.92	119.71	125.10
59	b	701	GTP	PA-O3A-PB	-2.90	122.89	132.83
59	m	501	GTP	C5-C6-N1	2.87	119.02	113.95
59	b	701	GTP	O6-C6-C5	-2.15	120.16	124.37

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	b	701	GTP	C5'-O5'-PA-O3A
59	b	701	GTP	C5'-O5'-PA-O1A
59	b	701	GTP	C5'-O5'-PA-O2A
59	m	501	GTP	C5'-O5'-PA-O1A
59	b	701	GTP	C4'-C5'-O5'-PA
59	m	501	GTP	C3'-C4'-C5'-O5'
59	b	701	GTP	PA-O3A-PB-O1B
59	b	701	GTP	O4'-C4'-C5'-O5'
59	b	701	GTP	C3'-C4'-C5'-O5'
59	m	501	GTP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

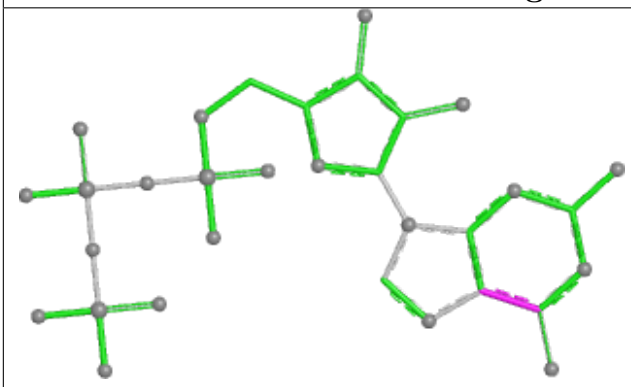
Mol	Chain	Res	Type	Atoms
59	m	501	GTP	C5'-O5'-PA-O3A

There are no ring outliers.

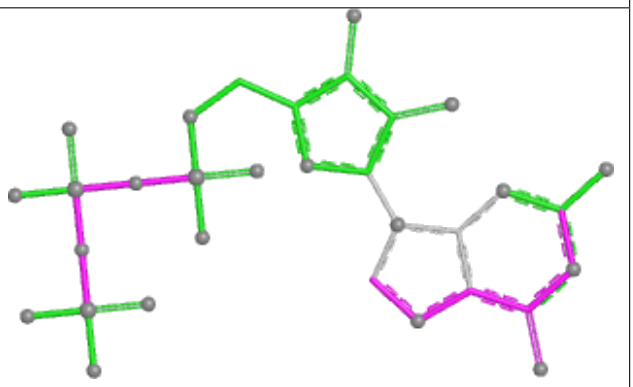
No monomer is involved in short contacts.

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

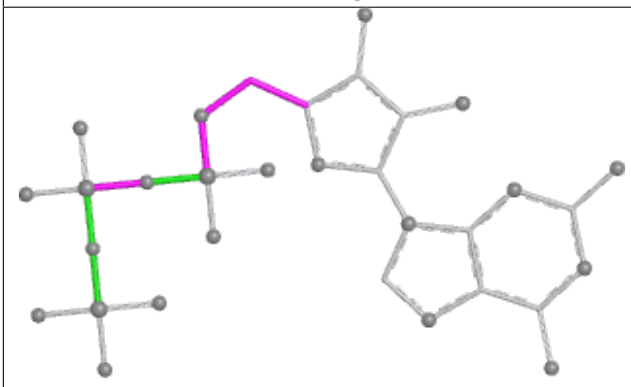
Ligand GTP b 701



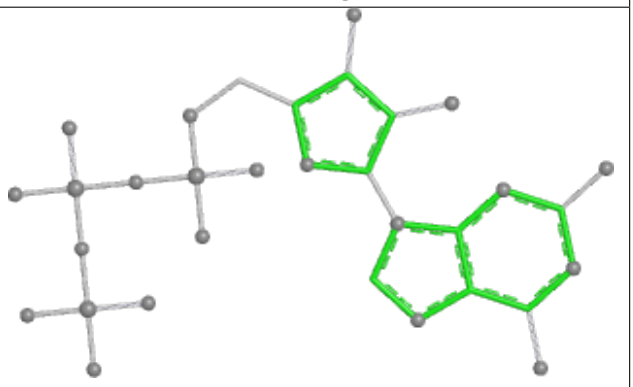
Bond lengths



Bond angles

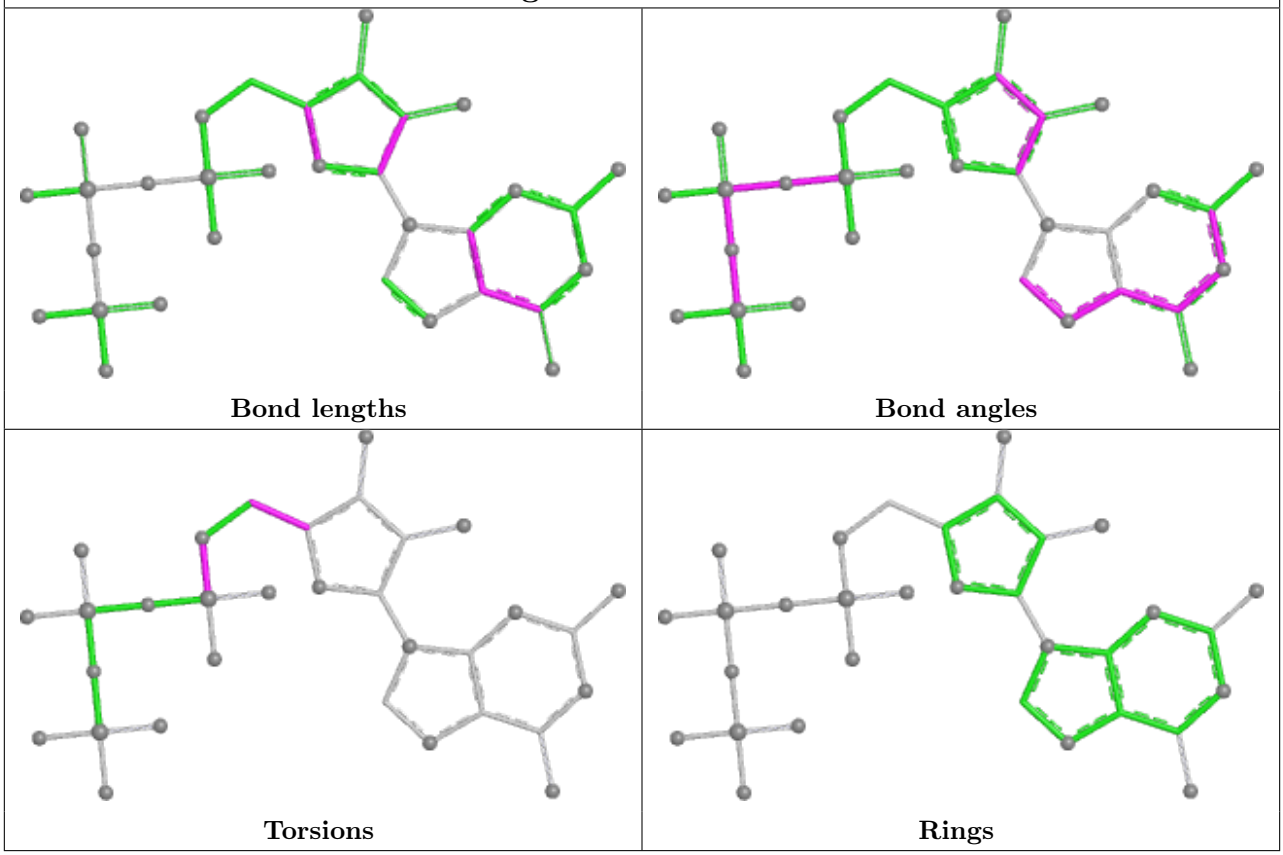


Torsions



Rings

Ligand GTP m 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
43	s	1
32	f	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	s	53:ASN	C	54:PHE	N	1.17
1	f	102:LEU	C	103:TYR	N	1.14

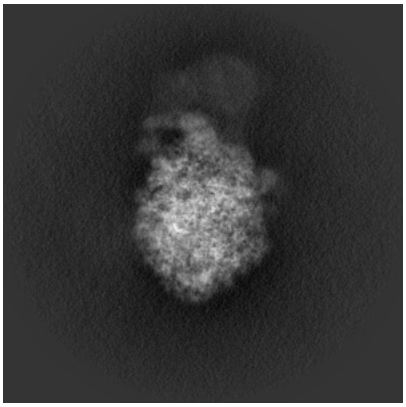
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4302. These allow visual inspection of the internal detail of the map and identification of artifacts.

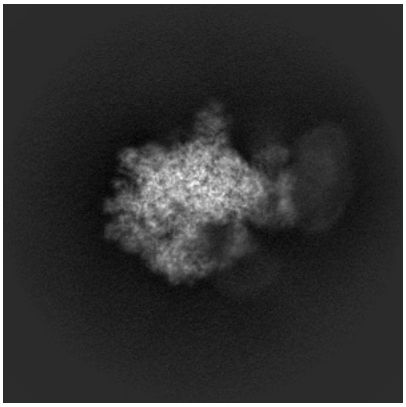
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

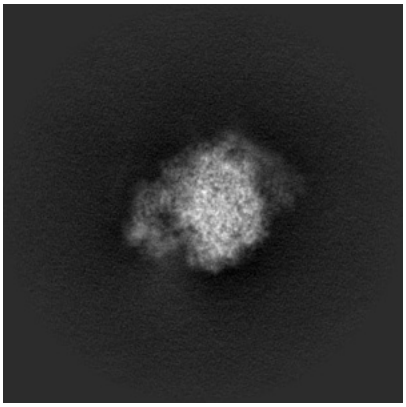
6.1.1 Primary map



X



Y

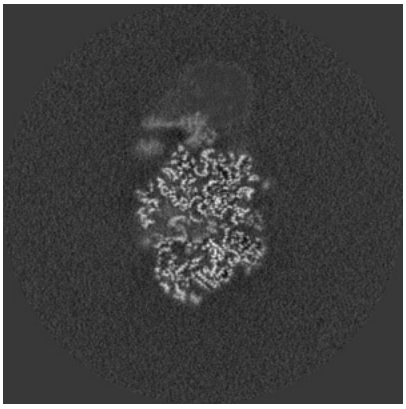


Z

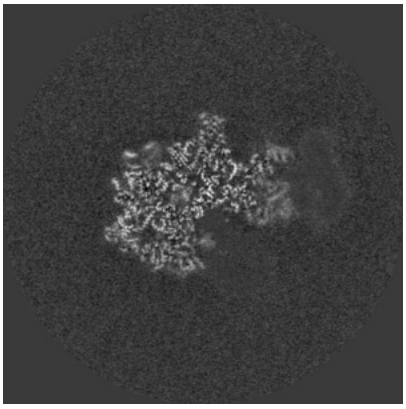
The images above show the map projected in three orthogonal directions.

6.2 Central slices

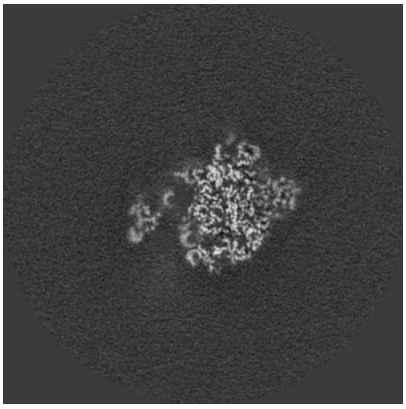
6.2.1 Primary map



X Index: 220



Y Index: 220

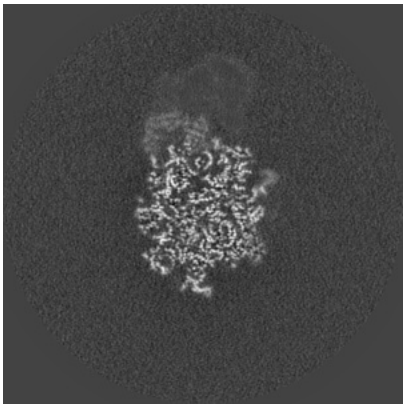


Z Index: 220

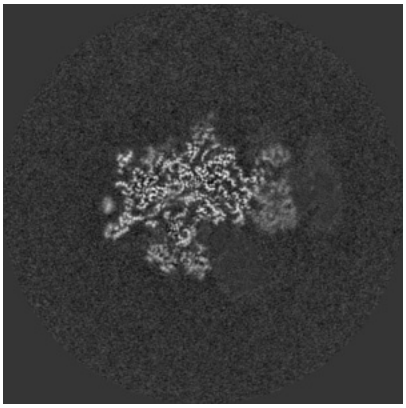
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

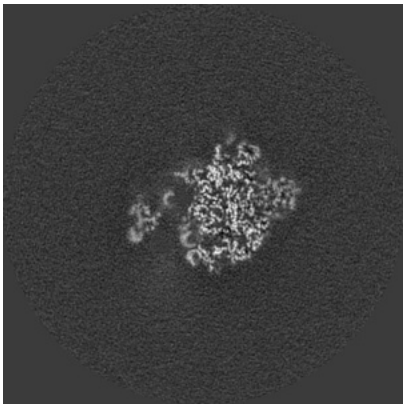
6.3.1 Primary map



X Index: 241



Y Index: 210



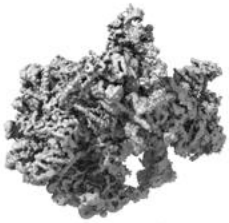
Z Index: 220

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

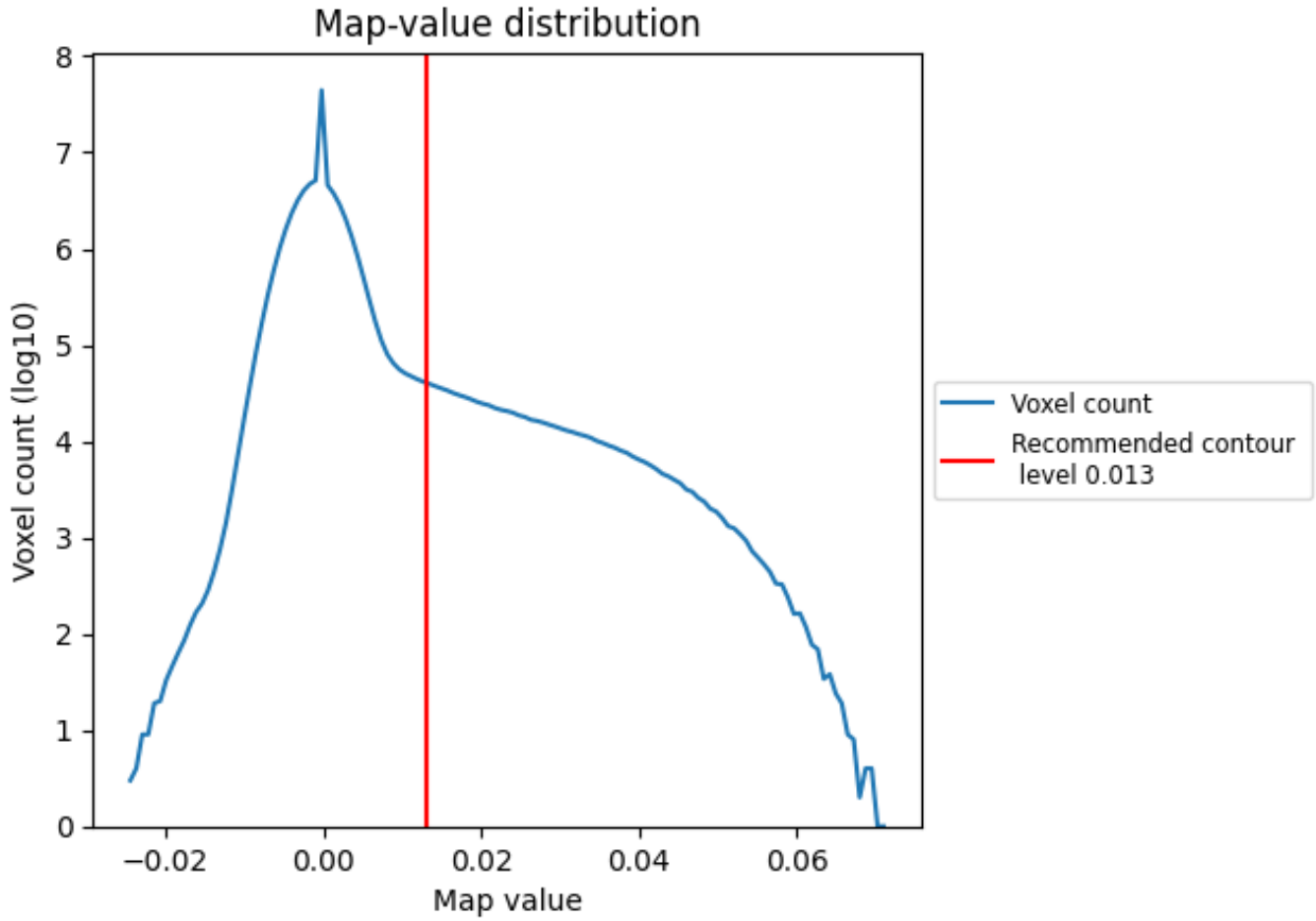
6.5 Mask visualisation (i)

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

7 Map analysis

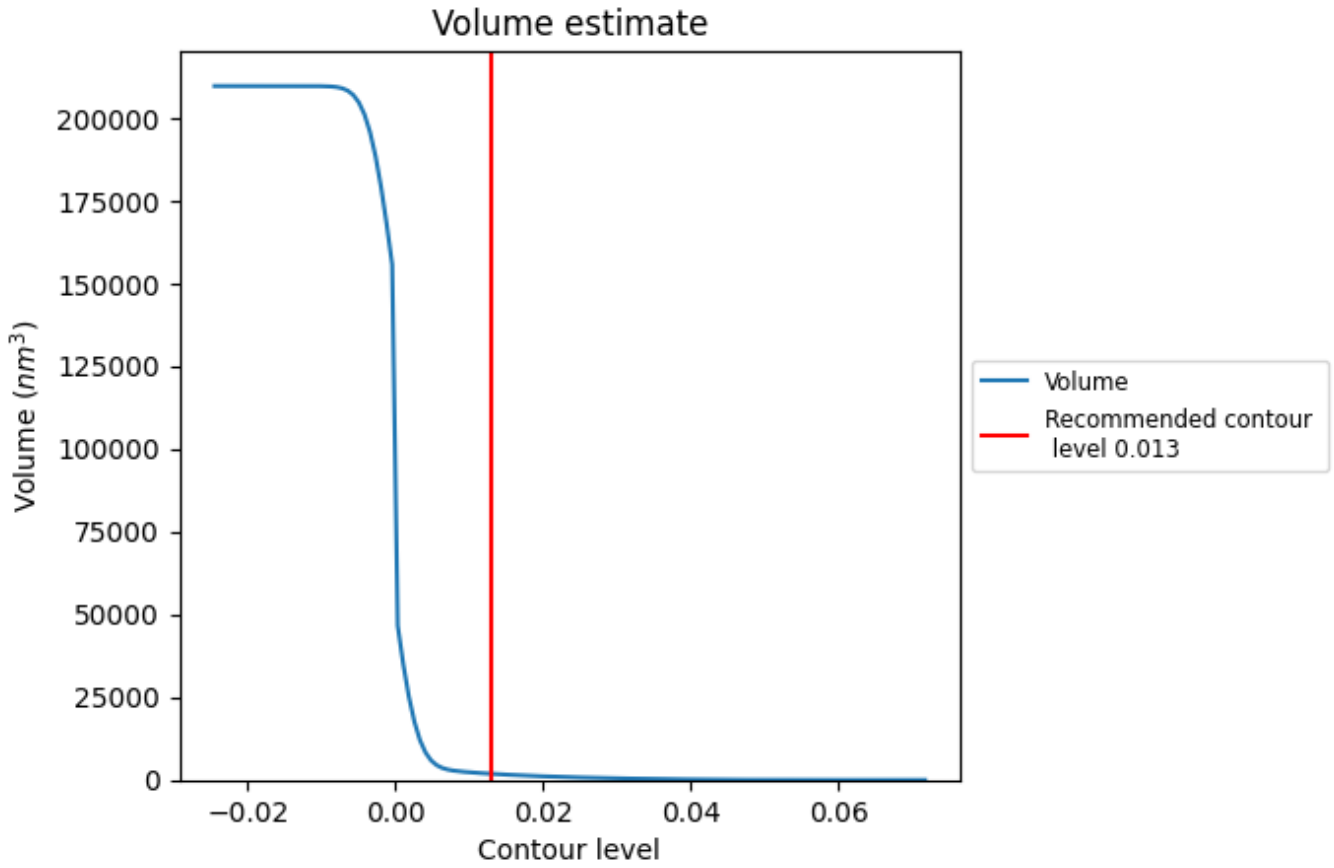
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

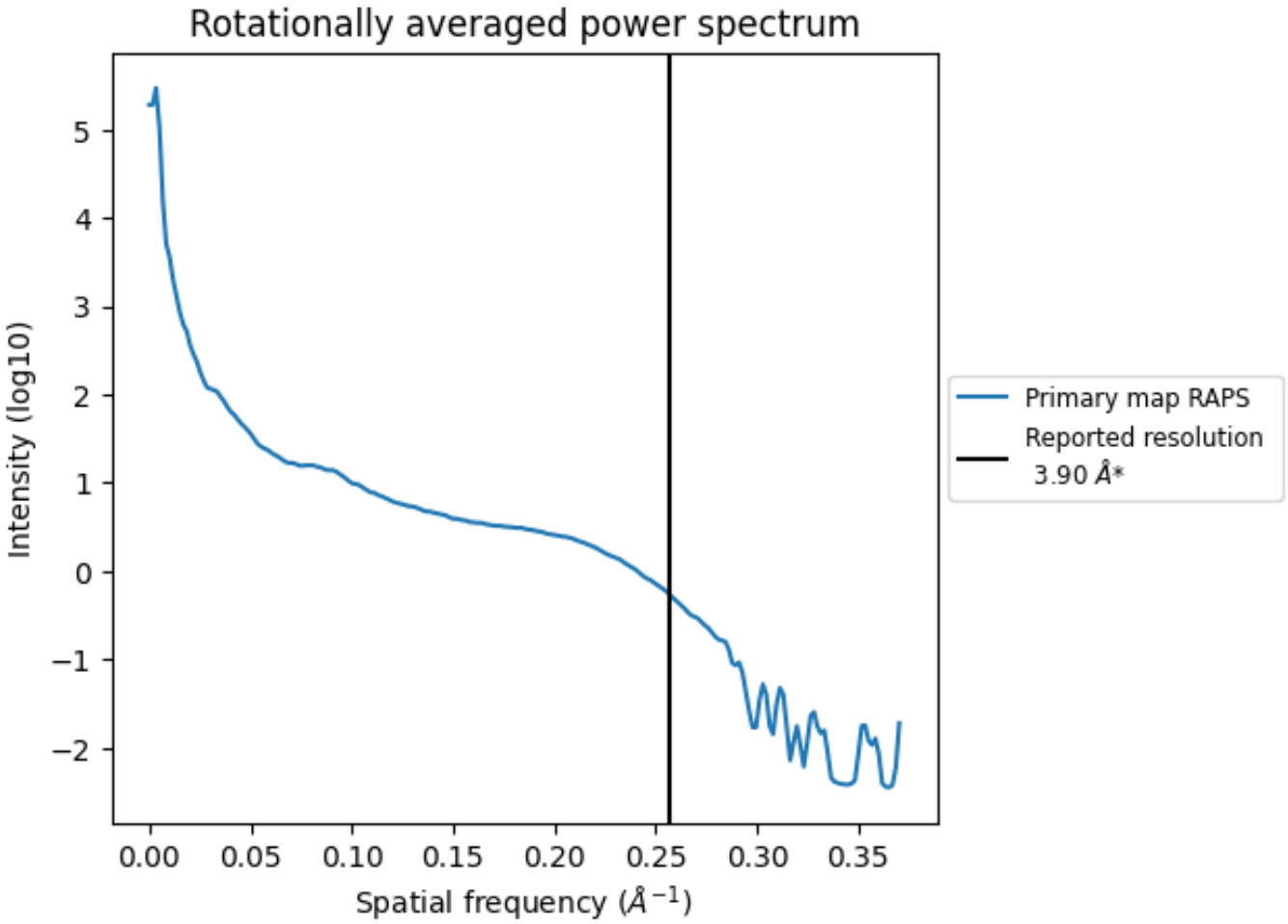
7.2 Volume estimate



The volume at the recommended contour level is 1864 nm^3; this corresponds to an approximate mass of 1683 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 0.256 $Å^{-1}$

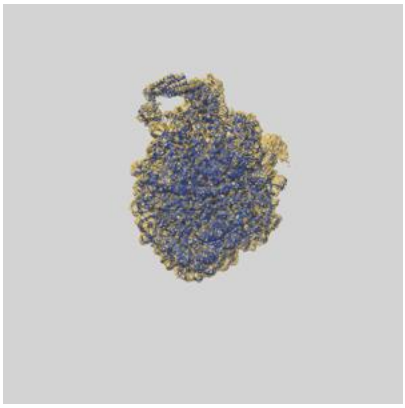
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

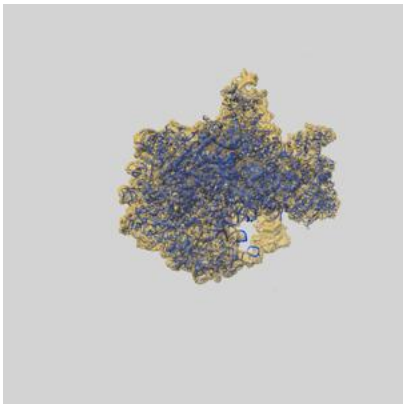
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4302 and PDB model 6FT6. Per-residue inclusion information can be found in section 3 on page 15.

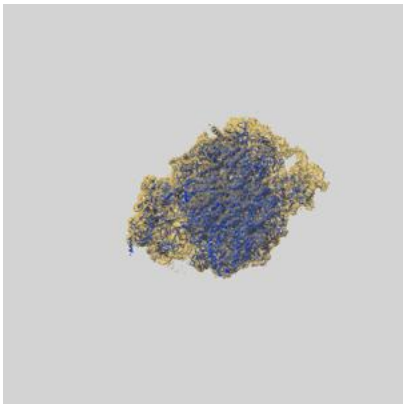
9.1 Map-model overlay



X



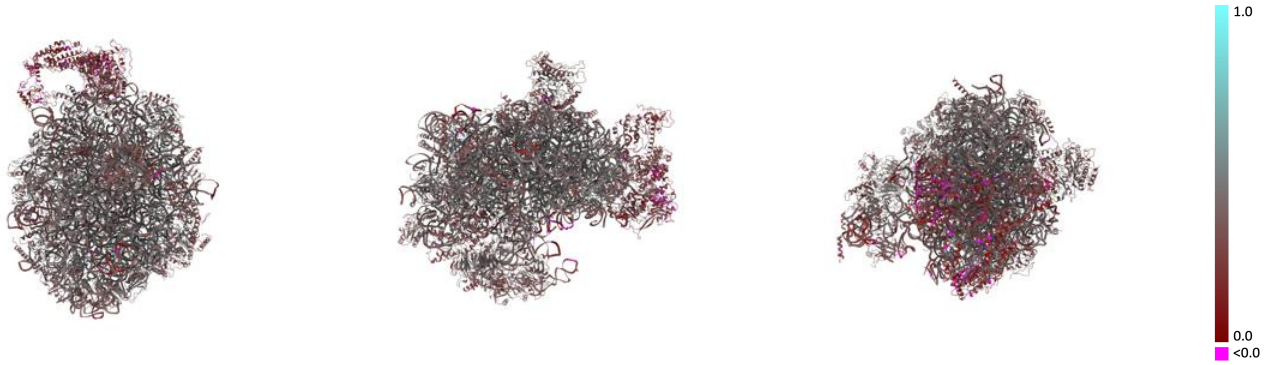
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.013 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.

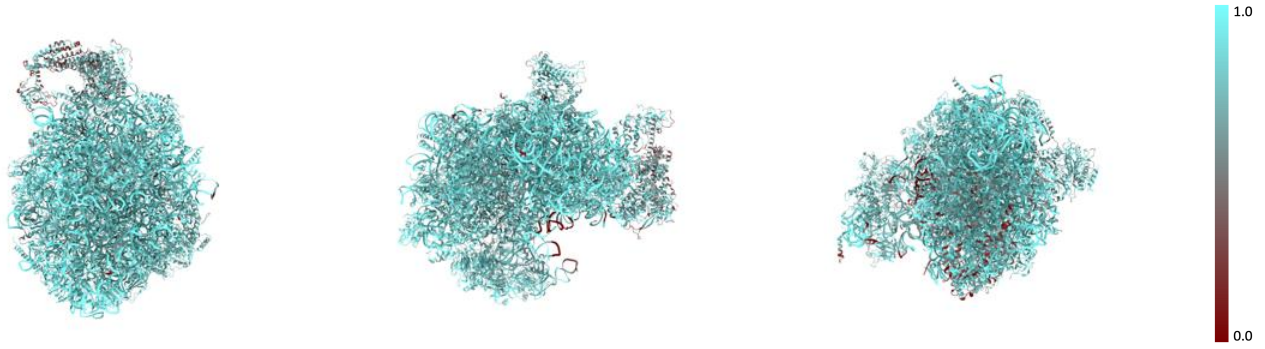
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

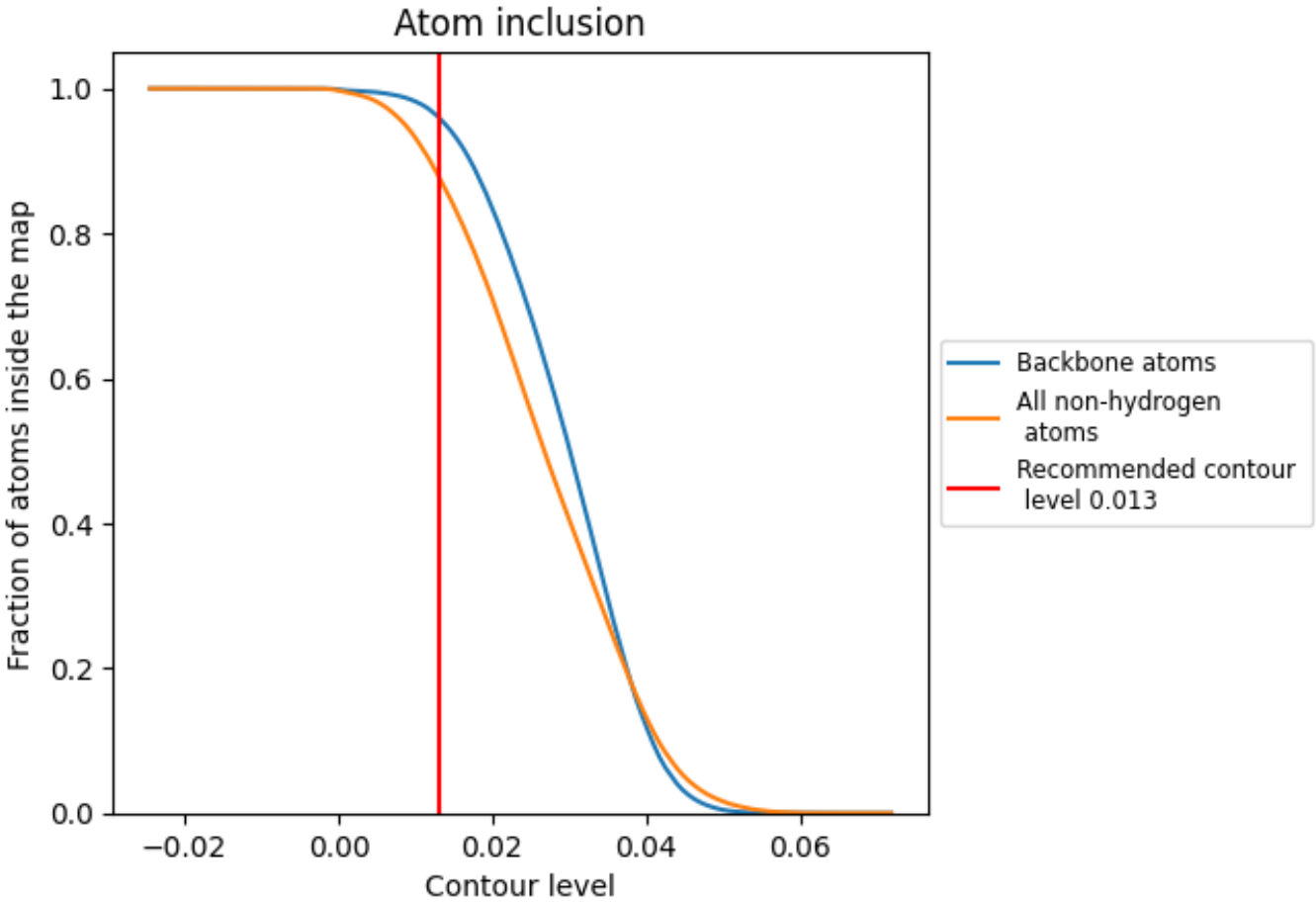
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.013).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 88% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8793	0.3840
1	0.9608	0.4040
2	0.9852	0.4290
3	0.9271	0.3110
4	0.7889	0.3690
5	0.6527	0.2690
A	0.8755	0.4450
B	0.8889	0.4320
C	0.8891	0.4260
D	0.8088	0.3340
E	0.8763	0.4010
F	0.8772	0.4060
G	0.8095	0.3820
H	0.8651	0.4280
I	0.6193	0.3690
J	0.8183	0.2740
KK	0.5328	0.1900
L	0.8787	0.4100
LL	0.5381	0.2130
M	0.8789	0.3930
MM	0.6076	0.2120
N	0.8797	0.4290
NN	0.6545	0.3030
O	0.8910	0.4230
P	0.8517	0.4070
Q	0.8788	0.4130
R	0.8713	0.4120
S	0.8451	0.3950
T	0.7185	0.3480
U	0.8627	0.3780
V	0.8509	0.4410
W	0.8675	0.3620
X	0.8335	0.4200
Y	0.8820	0.4180
Z	0.8842	0.4090

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
a	0.8667	0.4060
b	0.7959	0.3710
c	0.8892	0.3980
d	0.8654	0.4290
e	0.8712	0.4390
f	0.9038	0.4430
g	0.8732	0.4260
h	0.8441	0.3950
i	0.8403	0.3870
j	0.9040	0.4460
k	0.8564	0.3920
l	0.8771	0.4360
m	0.8276	0.3940
n	0.7417	0.2940
p	0.8672	0.4120
r	0.8396	0.4140
s	0.7151	0.3550
u	0.8020	0.3860
v	0.8099	0.3590
w	0.7801	0.3560
x	0.8567	0.3760
y	0.8465	0.3890
z	0.8456	0.3680