



## Full wwPDB EM Validation Report ⓘ

Dec 17, 2022 – 11:34 pm GMT

PDB ID : 6ZQA  
EMDB ID : EMD-11357  
Title : Cryo-EM structure of the 90S pre-ribosome from *Saccharomyces cerevisiae*, state A (Poly-Ala)  
Authors : Cheng, J.; Lau, B.; Venuta, G.L.; Berninghausen, O.; Hurt, E.; Beckmann, R.  
Deposited on : 2020-07-09  
Resolution : 4.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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) : 2.31.3

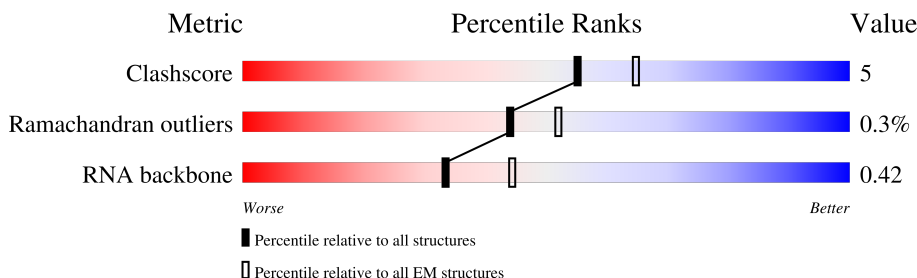
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.40 Å.

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





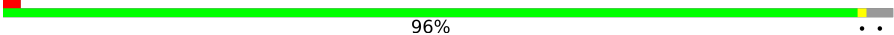



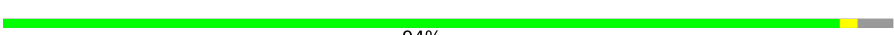




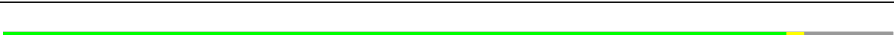









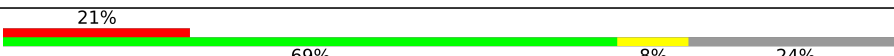
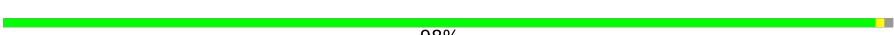
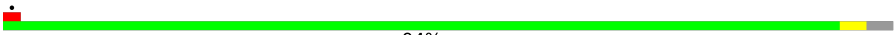

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
RNA backbone	4643	859

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	UA	923	
2	UB	810	
3	UC	610	
4	UD	776	
5	UE	643	
6	UF	440	
7	UG	554	
8	UH	713	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	UI	575	
10	UJ	1769	
11	UK	250	
12	UL	943	
13	UM	817	
14	UN	899	
15	UO	513	
16	UP	214	
17	UQ	896	
18	UR	594	
19	US	552	
20	UU	939	
21	UV	1237	
22	UX	189	
23	UZ	274	
24	CA	327	
24	CB	327	
25	CD	504	
26	CE	511	
27	CF	126	
27	CG	126	
28	CH	573	
29	CI	183	
30	CJ	290	
31	CK	593	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
32	CL	1183	
33	CM	367	
34	CN	297	
35	JF	252	
35	JG	252	
36	JH	483	
37	JJ	274	
38	JM	217	
39	JN	346	
40	JO	316	
41	JP	489	
42	JQ	206	
43	DA	255	
44	DF	225	
45	DH	190	
46	DJ	197	
47	DN	151	
48	DO	137	
49	DQ	143	
50	DS	146	
51	DW	130	
52	DX	145	
53	Db	82	
54	Dc	67	
55	D2	700	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
56	D3	1379	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>7%18%28%9%43%</div></div>
57	D4	175	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>40%46%13%</div></div>

## 2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 125991 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Periodic tryptophan protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	UA	834	Total	C	N	O	0	0
			4121	2453	834	834		

- Molecule 2 is a protein called Nucleolar complex protein 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	UB	504	Total	C	N	O	0	0
			2512	1504	504	504		

- Molecule 3 is a protein called Something about silencing protein 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	UC	128	Total	C	N	O	0	0
			628	372	128	128		

- Molecule 4 is a protein called U3 small nucleolar RNA-associated protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	UD	675	Total	C	N	O	0	0
			3339	1989	675	675		

- Molecule 5 is a protein called U3 small nucleolar RNA-associated protein 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	UE	475	Total	C	N	O	0	0
			2353	1403	475	475		

- Molecule 6 is a protein called U3 small nucleolar RNA-associated protein 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	UF	293	Total	C	N	O	0	0
			1456	870	293	293		

- Molecule 7 is a protein called U3 small nucleolar RNA-associated protein 7.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	UG	533	Total	C	N	O	0	0
			2629	1563	533	533		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	UH	442	Total	C	N	O	0	0
			2190	1306	442	442		

- Molecule 9 is a protein called U3 small nucleolar RNA-associated protein 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	UI	104	Total	C	N	O	0	0
			517	309	104	104		

- Molecule 10 is a protein called U3 small nucleolar RNA-associated protein 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	UJ	726	Total	C	N	O	0	0
			3621	2169	726	726		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	UK	242	Total	C	N	O	0	0
			1203	719	242	242		

- Molecule 12 is a protein called U3 small nucleolar RNA-associated protein 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	UL	842	Total	C	N	O	0	0
			4163	2479	842	842		

- Molecule 13 is a protein called U3 small nucleolar RNA-associated protein 13.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	UM	762	Total	C	N	O	0	0
			3763	2239	762	762		

- Molecule 14 is a protein called U3 small nucleolar RNA-associated protein 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	UN	147	Total	C	N	O	0	0
			733	439	147	147		

- Molecule 15 is a protein called U3 small nucleolar RNA-associated protein 15.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	UO	493	Total	C	N	O	0	0
			2441	1455	493	493		

- Molecule 16 is a protein called Bud site selection protein 21.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	UP	60	Total	C	N	O	0	0
			298	178	60	60		

- Molecule 17 is a protein called NET1-associated nuclear protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	UQ	832	Total	C	N	O	0	0
			4122	2458	832	832		

- Molecule 18 is a protein called U3 small nucleolar RNA-associated protein 18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	UR	482	Total	C	N	O	0	0
			2377	1413	482	482		

- Molecule 19 is a protein called Nucleolar complex protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	US	473	Total	C	N	O	0	0
			2357	1411	473	473		

- Molecule 20 is a protein called U3 small nucleolar RNA-associated protein 21.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	UU	848	Total	C	N	O	0	0
			4181	2485	848	848		

- Molecule 21 is a protein called U3 small nucleolar RNA-associated protein 22.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	UV	1098	Total	C	N	O	0	0
			5442	3246	1098	1098		

- Molecule 22 is a protein called rRNA-processing protein FCF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	UX	174	Total	C	N	O	0	0
			862	514	174	174		

- Molecule 23 is a protein called Ribosome biogenesis protein UTP30.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	UZ	247	Total	C	N	O	0	0
			1224	730	247	247		

- Molecule 24 is a protein called rRNA 2'-O-methyltransferase fibrillarin.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	CA	242	Total	C	N	O	0	0
			1190	706	242	242		
24	CB	228	Total	C	N	O	0	0
			1122	666	228	228		

- Molecule 25 is a protein called Nucleolar protein 56.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	CD	380	Total	C	N	O	0	0
			1880	1120	380	380		

- Molecule 26 is a protein called Nucleolar protein 58.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	CE	435	Total	C	N	O	0	0
			2155	1285	435	435		

- Molecule 27 is a protein called 13 kDa ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	CF	123	Total	C	N	O	0	0
			611	365	123	123		
27	CG	123	Total	C	N	O	0	0
			611	365	123	123		

- Molecule 28 is a protein called Ribosomal RNA-processing protein 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	CH	438	Total	C	N	O	0	0
			2158	1282	438	438		

- Molecule 29 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	CI	182	Total	C	N	O	0	0
			905	541	182	182		

- Molecule 30 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	CJ	282	Total	C	N	O	0	0
			1397	833	282	282		

- Molecule 31 is a protein called U3 small nucleolar RNA-associated protein MPP10.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	CK	207	Total	C	N	O	0	0
			1031	617	207	207		

- Molecule 32 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	CL	781	Total	C	N	O	0	0
			3859	2298	781	780		

- Molecule 33 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	CM	360	Total	C	N	O	0	0
			1767	1047	360	360		

- Molecule 34 is a protein called Ribosomal RNA-processing protein 7.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	CN	232	Total	C	N	O	0	0
			1154	690	232	232		

- Molecule 35 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	JF	216	Total	C	N	O	0	0
			1071	639	216	216		
35	JG	230	Total	C	N	O	0	0
			1141	681	230	230		

- Molecule 36 is a protein called Essential nuclear protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	JH	261	Total	C	N	O	0	0
			1295	773	261	261		

- Molecule 37 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	JJ	182	Total	C	N	O	0	0
			898	534	182	182		

- Molecule 38 is a protein called rRNA-processing protein FCF2.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	JM	135	Total	C	N	O	0	0
			671	401	135	135		

- Molecule 39 is a protein called Protein FAF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	JN	186	Total	C	N	O	0	0
			918	546	186	186		

- Molecule 40 is a protein called KRR1 small subunit processome component.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	JO	188	Total	C	N	O	0	0
			933	557	188	188		

- Molecule 41 is a protein called Protein SOF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	JP	461	Total	C	N	O	0	0
			2283	1361	461	461		

- Molecule 42 is a protein called Regulator of rDNA transcription protein 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	JQ	63	Total	C	N	O	0	0
			312	186	63	63		

- Molecule 43 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	DA	240	Total	C	N	O	0	0
			1187	707	240	240		

- Molecule 44 is a protein called Rps5p.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	DF	213	Total	C	N	O	0	0
			1055	629	213	213		

- Molecule 45 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	DH	184	Total	C	N	O	0	0
			913	545	184	184		

- Molecule 46 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	DJ	185	Total	C	N	O	0	0
			915	545	185	185		

- Molecule 47 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	DN	150	Total	C	N	O	0	0
			742	442	150	150		

- Molecule 48 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	DO	120	Total	C	N	O	0	0
			587	347	120	120		

- Molecule 49 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	DQ	125	Total	C	N	O	0	0
			616	366	125	125		

- Molecule 50 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	DS	105	Total	C	N	O	0	0
			521	311	105	105		

- Molecule 51 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	DW	129	Total	C	N	O	0	0
			634	376	129	129		

- Molecule 52 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	DX	103	Total	C	N	O	0	0
			503	297	103	103		

- Molecule 53 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	Db	81	Total	C	N	O	0	0
			400	238	81	81		

- Molecule 54 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	Dc	63	Total	C	N	O	0	0
			310	184	63	63		

- Molecule 55 is a RNA chain called 5ETS RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	D2	523	Total	C	N	O	P	0	0
			11160	4987	1981	3669	523		

- Molecule 56 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	D3	787	Total	C	N	O	P	0	0
			16806	7509	3018	5492	787		

- Molecule 57 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	D4	175	Total	C	N	O	P	0	0
			3712	1661	648	1228	175		

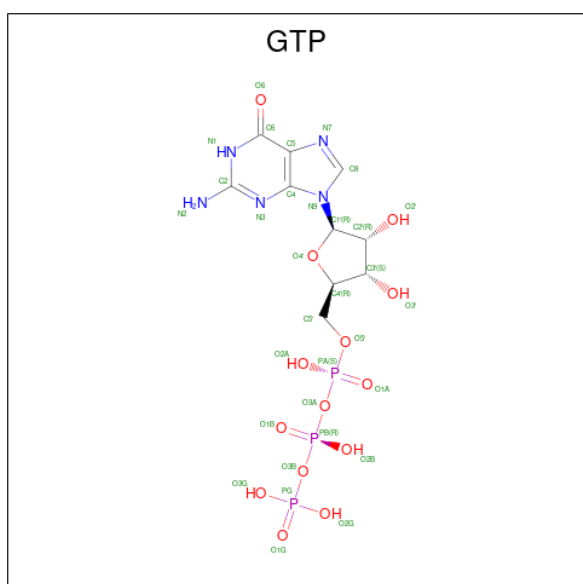
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
58	UX	1	Total	Zn	0
			1	1	
58	Db	1	Total	Zn	0
			1	1	

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
59	UX	1	Total	Mg	0
			1	1	
59	CL	1	Total	Mg	0
			1	1	

- Molecule 60 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).

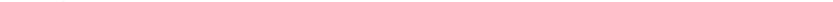


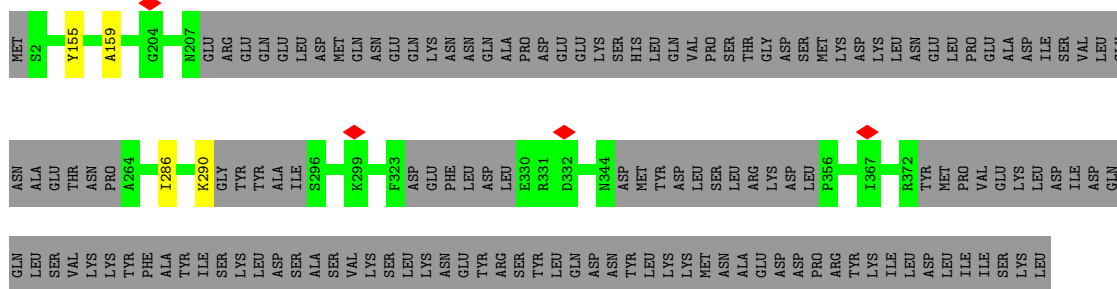
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
60	CL	1	32	10	5	14	3	0

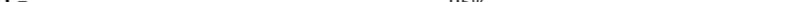


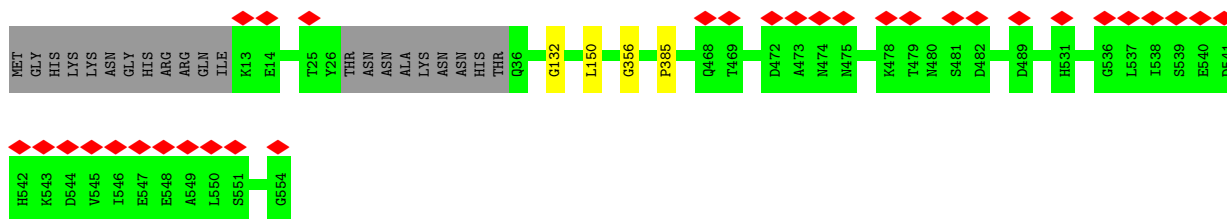


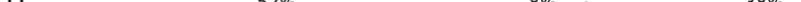
ARG	ASP	THR	MET
LEU	ILE	SER	ASP
GLU	HIS	LEU	S3
THR	SER	GLN	R36
GLU	SER	GLN	ALA
GLN	GLU	GLU	THR
SER	PRO	GLN	ALA
ASP	VAL	ALA	SER
GLY	VAL	LYS	SER
GLU	GLU	PRO	GLY
GLU	GLU	PRO	VAL
GLU	ASP	GLN	ASP
ALA	GLU	ALA	THR
GLY	ASP	ASN	VAL
TYR	ASP	GLU	W46
ASP	VAL	LEU	M67
GLU	GLU	LEU	LEU
VAL	TYR	THR	ALA
GLU	ASN	GLU	SER
GLU	GLU	THR	SER
GLU	GLU	PHE	SER
LEU	LEU	GLY	D72
ASP	ASP	ASP	Q162
ALA	ALA	LYS	A166
GLY	GLY	LEU	I173
LEU	LEU	SER	V191
ILE	ILE	THR	A206
ASP	ASP	VAL	T248
GLY	GLY	ALA	S262
TYR	TYR	ARG	SER
GLY	GLY	LYS	SER
SER	SER	THR	THR
GLU	GLU	ASN	LYS
GLU	GLU	LEU	LYS
GLU	GLU	LYS	ARG
GLU	GLU	GLY	G269
GLY	GLY	SER	S283
ASP	ASP	ASN	G359
SER	SER	LEU	V372
GLU	GLU	THR	ASP
GLN	GLN	THR	ALA
LYS	LYS	ALA	ALA
THR	THR	THR	ILE
T434	L472	L587	LYS
ASP	SER	SER	SER
GLN	THR	ASN	TRP
LYS	HIS	LYS	ARG
THR	THR	TYR	GLU
SER	SER	GLU	ARG
GLN	GLN	ALA	GLU
ASP	ASP	GLY	

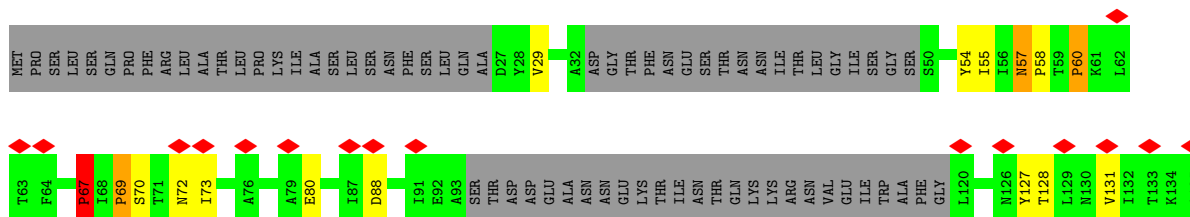
Chain UF:  66% 33%

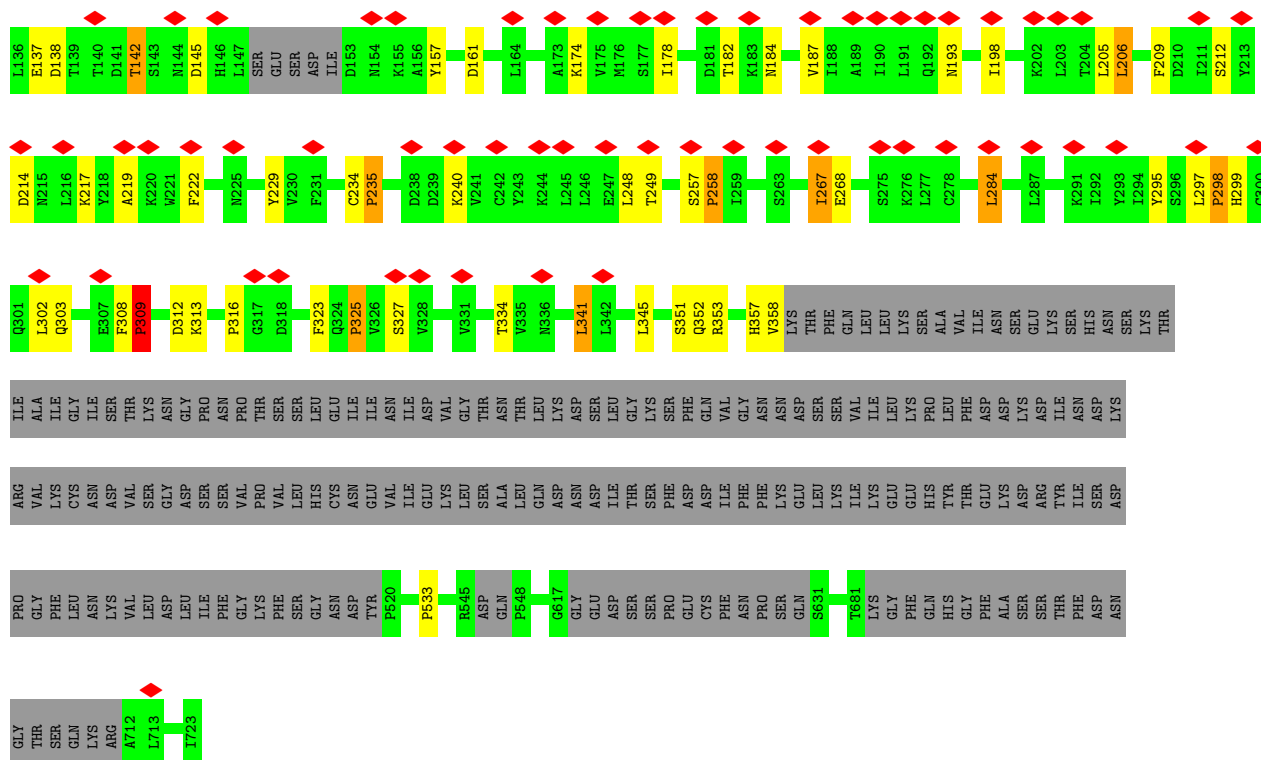


Chain UG:  6% 95% ..



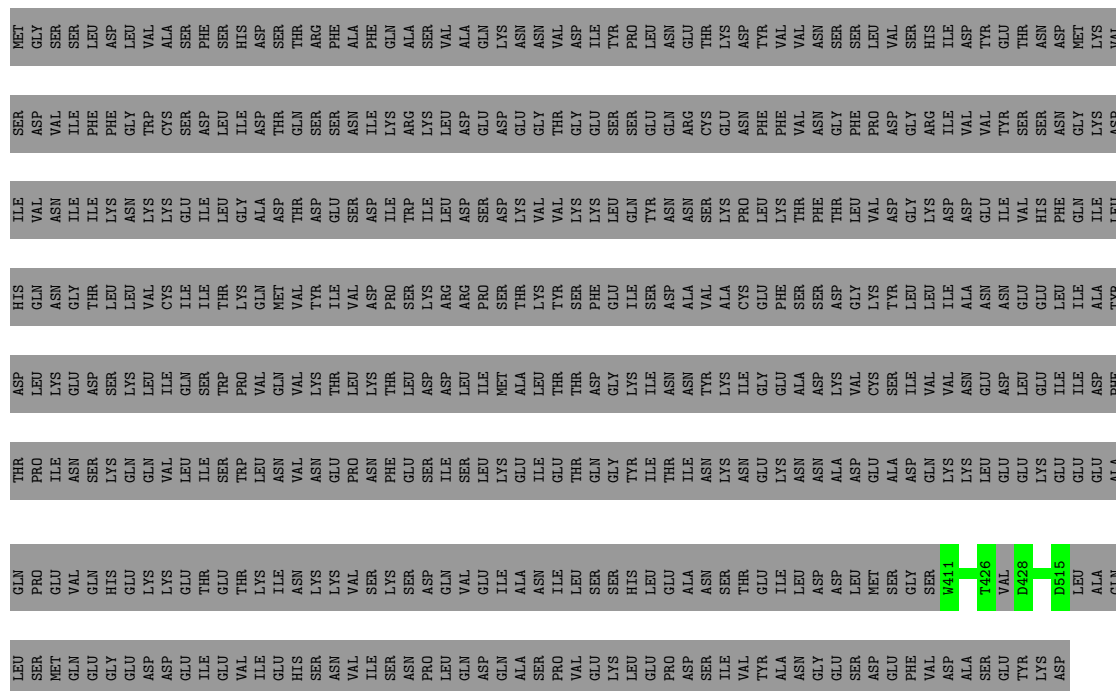
Chain UH: 





• Molecule 9: U3 small nucleolar RNA-associated protein 9

Chain UI: 18% 82%



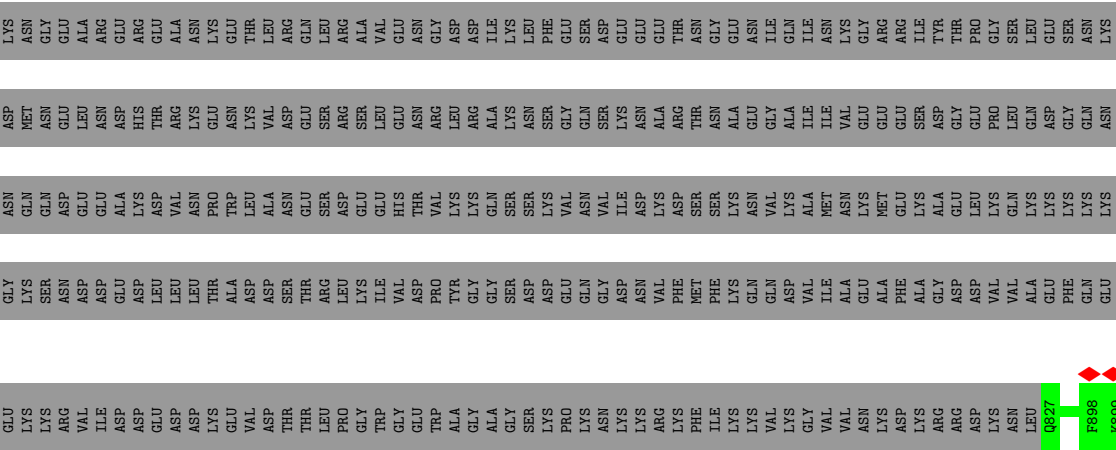
• Molecule 10: U3 small nucleolar RNA-associated protein 10

Chain UJ: 12% 40% 59%

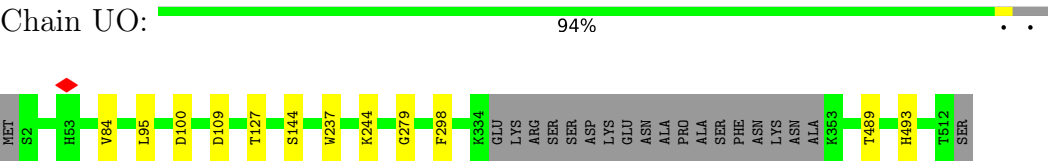




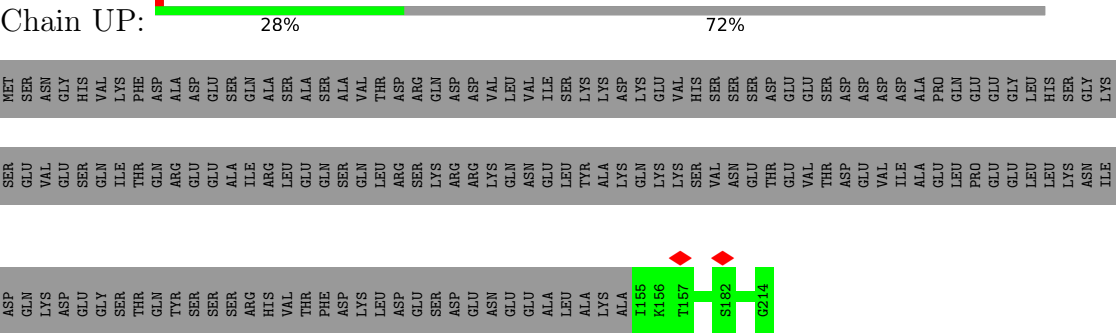
[illegible]



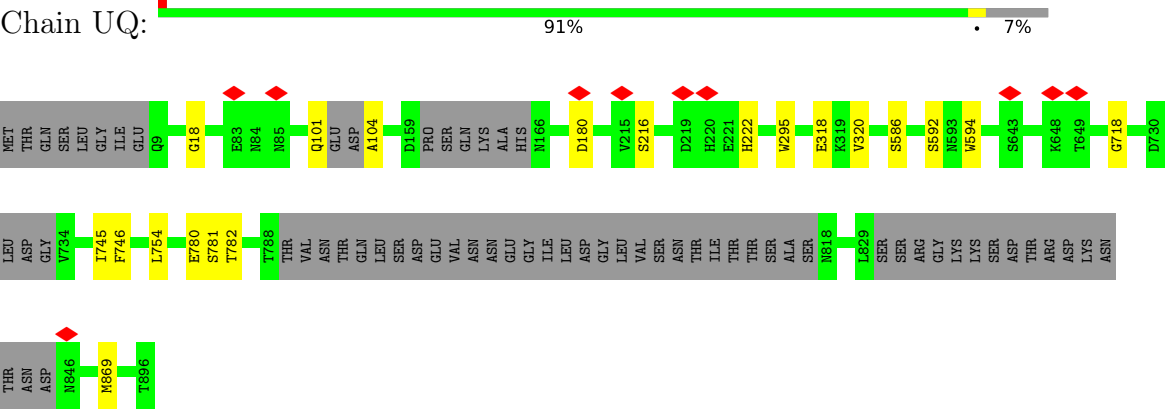
• Molecule 15: U3 small nucleolar RNA-associated protein 15



• Molecule 16: Bud site selection protein 21

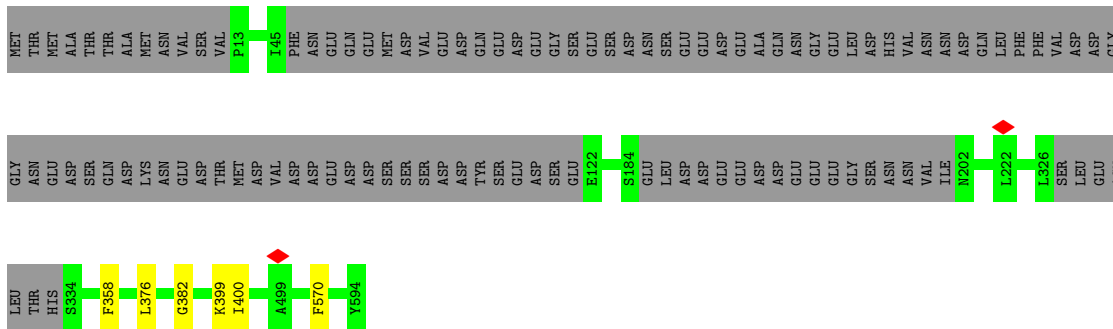


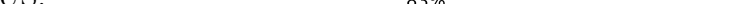
• Molecule 17: NET1-associated nuclear protein 1

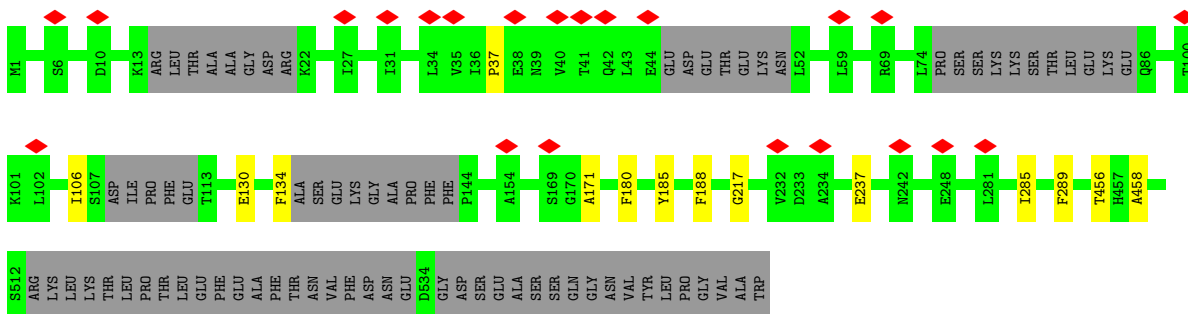


• Molecule 18: U3 small nucleolar RNA-associated protein 18

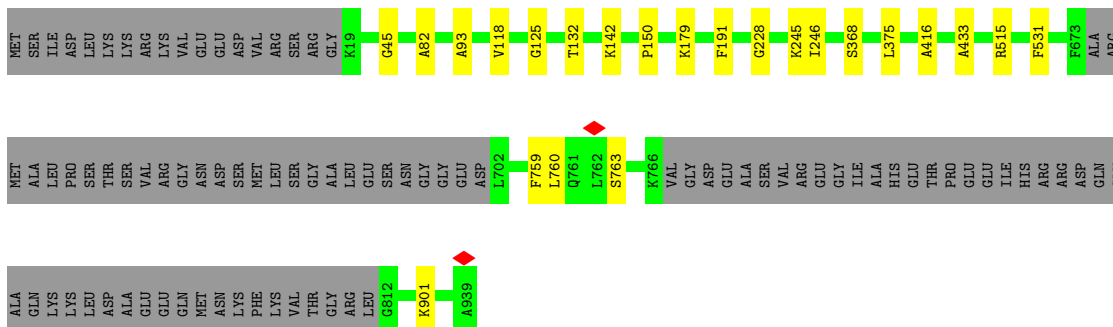
Response	Percentage
Yes, I have used a mobile app to book a flight	80%
No, I have not used a mobile app to book a flight	19%

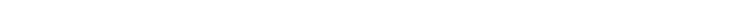


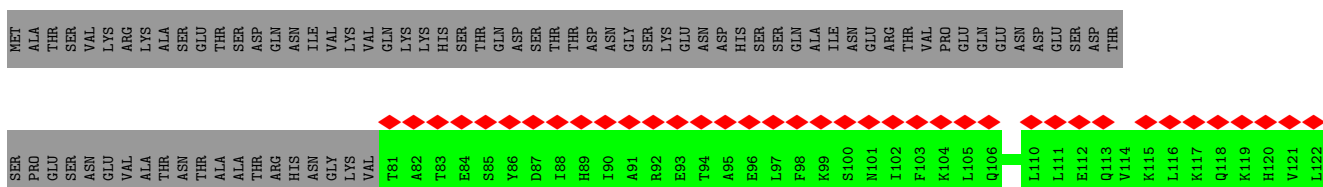
- Chain US:  83% 14%



- Chain UU:  88% 10%

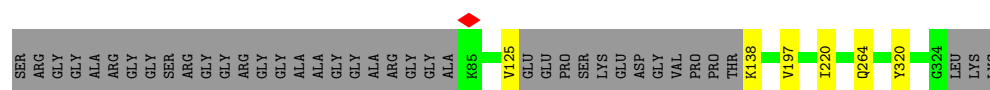


- Chain UV:  84% 87% 11%



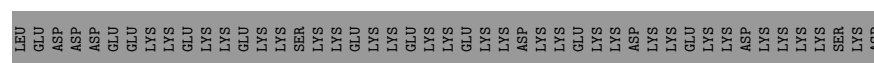
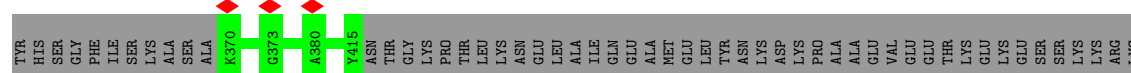
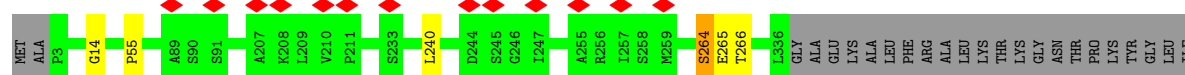
K123	V124	E125	K126	F127	L128	H129	K130	L131	I132	D133	I134	L135	Q136	E137	I138	P139	D140	W141	E142	E143	K144	S145	L146	A147	E148	V149	D150	S151	F152	F153	K154	N155	K156	I157	V158	S159	V160	P161	F162	V163	D164	P165	K166	P167	I168	P169	Q170	N171	T172	N173	Y174	K175	F176	N177	Y178	K179	K180	P181	D182	
I183	S184	L185	I186	G187	S188	F189	A190	G194	I195	Y196	Q197	P198	N199	G200	S201	D204	T205	L206	L207	T208	M209	P210	K211	E212	L213	F214	E215	K216	K217	D218	F219	L220	N221	F222	R223	C224	L225	H226	K227	R228	S229	V230	Y231	L232	A233	Y234	L235	T236	H237	H238	P239	Y300	K301	V302	F303	E304	P305			
D246	K247	L248	D249	S250	F251	L252	Q253	Q254	E255	Y256	S257	Y258	F259	D260	N261	D262	P263	L264	L265	P266	L267	L268	R269	I270	S271	C272	S273	K274	PRO	THR	GLY	ASP	SER	LEU	SER	D282	Y283	N284	F285	Y286	K287	T288	R289	F290	S291	L292	N293	L294	L295	I296	G297	F298	P299	V300	A362	T363	V364	L365		
K306	K307	L308	L309	P310	N311	N312	N313	C314	I315	R316	S377	I317	ALA	GLN	GLU	LYS	GLU	GLN	SER	L326	P327	A328	T329	P330	L331	Y332	N333	F334	S335	V336	L337	S338	S339	S340	T341	H342	E343	N344	Y345	L346	K347	Y348	L349	Y350	K351	T352	K353	K354	Q355	T356	E357	S358	F359	V360	E361	A362	T363	V364	L365	
G366	R367	L368	W369	L370	Q371	Q372	R373	G374	F375	S376	I377	N378	M379	S380	H381	S382	G383	S384	L385	G386	G387	F388	G389	T390	F391	E392	F393	T394	I395	L396	M397	A398	A399	L400	L401	N402	G403	G404	G405	M406	M407	S408	M409	K410	I411	L412	L413	Q355	H414	G415	F416	S417	S418	Y419	Q420	L421	F422	K423	G424	V425
I426	K427	Y428	L429	A430	M432	D433	L434	C435	H436	D437	G438	H439	N500	N501	V502	V503	Q504	D505	Q506	PRO	GLU	ASN	SER	SER	SER	P453	A454	S455	K456	Y457	I458	D459	E460	G461	F462	Q463	T464	P465	T466	L467	F468	D469	T472	K473	V474	M475	I476	L477	L478	K479	M480	T481	V482	S483	S484	Y485	Q486			
I487	L488	K489	E490	Y491	A492	G493	E494	T495	L496	R497	M498	L499	N500	N501	V502	V503	Q504	D505	Q506	PRO	GLU	ASN	SER	SER	SER	P453	A454	S455	K456	Y457	I458	D459	E460	G461	F462	Q463	T464	P465	T466	L467	F468	D469	T472	K473	V474	M475	I476	L477	L478	K479	M480	T481	V482	S483	S484	Y485	Q486			
I487	L488	K489	E490	Y491	A492	G493	E494	T495	L496	R497	M498	L499	N500	N501	V502	V503	Q504	D505	Q506	PRO	GLU	ASN	SER	SER	SER	P453	A454	S455	K456	Y457	I458	D459	E460	G461	F462	Q463	T464	P465	T466	L467	F468	D469	T472	K473	V474	M475	I476	L477	L478	K479	M480	T481	V482	S483	S484	Y485	Q486			
I487	L488	K489	E490	Y491	A492	G493	E494	T495	L496	R497	M498	L499	N500	N501	V502	V503	Q504	D505	Q506	PRO	GLU	ASN	SER	SER	SER	P453	A454	S455	K456	Y457	I458	D459	E460	G461	F462	Q463	T464	P465	T466	L467	F468	D469	T472	K473	V474	M475	I476	L477	L478	K479	M480	T481	V482	S483	S484	Y485	Q486			
I487	L488	K489	E490	Y491	A492	G493	E494	T495	L496	R497	M498	L499	N500	N501	V502	V503	Q504	D505	Q506	PRO	GLU	ASN	SER	SER	SER	P453	A454	S455	K456	Y457	I458	D459	E460	G461	F462	Q463	T464	P465	T466	L467	F468	D469	T472	K473	V474	M475	I476	L477	L478	K479	M480	T481	V482	S483	S484	Y485	Q486			
I487	L488	K489	E490	Y491	A492	G493	E494	T495	L496	R497	M498	L499	N500	N501	V502	V503	Q504	D505	Q506	PRO	GLU	ASN	SER	SER	SER	P453	A454	S455	K456	Y457	I458	D459	E460	G461	F462	Q463	T464	P465	T466	L467	F468	D469	T472	K473	V474	M475	I476	L477	L478	K479	M480	T481	V482	S483	S484	Y485	Q486			
I487	L488	K489	E490	Y491	A492	G493	E494	T495	L496	R497	M498	L499	N500	N501	V502	V503	Q504	D505	Q506	PRO	GLU	ASN	SER	SER	SER	P453	A454	S455	K456	Y457	I458	D459	E460	G461	F462	Q463	T464	P465	T466	L467	F468	D469	T472	K473	V474	M475	I476	L477	L478	K479	M480	T481	V482	S483	S484	Y485	Q486			
I487	L488	K489	E490	Y491	A492	G493	E494	T495	L496	R497	M498	L499	N500	N501	V502	V503	Q504	D505	Q506	PRO	GLU	ASN	SER	SER	SER	P453	A454	S455	K456	Y457	I458	D459	E460	G461	F462	Q463	T464	P465	T466	L467	F468	D469	T472	K473	V474	M475	I476	L477	L478	K479	M480	T481	V482	S483	S484	Y485	Q486			
I487	L488	K489	E490	Y491	A492	G493	E494	T495	L496	R497	M498	L499	N500	N501	V502	V503	Q504	D505	Q506	PRO	GLU	ASN	SER	SER	SER	P453	A454	S455	K456	Y457	I458	D459	E460	G461	F462	Q463	T464	P465	T466	L467	F468	D469	T472	K473	V474	M475	I476	L477	L478	K479	M480	T481	V482	S483	S484	Y485	Q486			
I487	L488	K489	E490	Y491	A492	G493	E494	T495	L496	R497	M498	L499	N500	N501	V502	V503	Q504	D505	Q506	PRO	GLU	ASN	SER	SER	SER	P453	A454	S455	K456	Y457	I458	D459	E460	G461	F462	Q463	T464	P465	T466	L467	F468	D469	T472	K473	V474	M475	I476	L477	L478	K479	M480	T481	V482	S483	S484	Y485	Q486			
I487	L488	K489	E490	Y491	A492	G493	E494	T495	L496	R497	M498	L499	N500	N501	V502	V503	Q504	D505	Q506	PRO	GLU	ASN	SER	SER	SER	P453	A454	S455	K456	Y457	I458	D459	E460	G461	F462	Q463	T464	P465	T466	L467	F468	D469	T472	K473	V474	M475	I476	L477	L478	K479	M480	T481	V482	S483	S484	Y485	Q486			
I487	L488	K489	E490	Y491	A492	G493	E494	T495	L496	R497	M498	L499	N500	N501	V502	V503	Q504	D505	Q506	PRO	GLU	ASN	SER	SER	SER	P453	A454	S455	K456	Y457	I458	D459	E460	G461	F462	Q463	T464	P465	T466	L467	F468	D469	T472	K473	V474	M475	I476	L477	L478	K479	M480	T481	V482	S483	S484	Y485	Q486			
I487	L488	K489	E490	Y491	A492	G493	E494	T495	L496	R497	M498	L499	N500	N501	V502	V503	Q504	D505	Q506	PRO	GLU	ASN	SER	SER	SER	P453	A454	S455	K456	Y457	I458	D459	E460	G461	F462	Q463	T464	P465	T466	L467	F468	D469	T472	K473	V474	M475	I476	L477	L478	K479	M480	T481	V482	S483	S484	Y485	Q486			
I487	L488	K489	E490	Y491	A492	G493	E494	T495	L496	R497	M498	L499	N500	N501	V502	V503	Q504	D505	Q506	PRO	GLU	ASN	SER	SER	SER	P453	A454	S455	K456	Y457	I458	D459	E460	G461	F462	Q463	T464	P465	T466	L467	F468	D469	T472	K473	V474	M475	I476	L477	L478	K479	M480	T481	V482	S483	S484	Y485	Q486			
I487	L488	K489	E490	Y491	A492	G493	E494	T495	L496	R497	M498	L499	N500	N501	V502	V503	Q504	D505	Q506	PRO	GLU	ASN	SER	SER	SER	P453	A454	S455	K456	Y457	I458	D459	E460	G461	F462	Q463	T464	P465	T466	L467	F468	D469	T472	K473	V474	M475	I476	L477	L478	K479	M480	T481	V482	S483	S484	Y485	Q486			
I487	L488	K489	E490	Y491	A492	G493	E494	T495	L496	R497	M498	L499	N500	N501	V502	V503	Q504	D505	Q506	PRO	GLU	ASN	SER	SER	SER	P453	A454	S455	K456	Y457	I458	D459	E460	G461	F462	Q463	T464	P465	T466	L467	F468	D469	T472	K473	V474	M475	I476	L477	L478	K479	M480	T481	V482	S483	S484	Y485	Q486			
I487	L488	K489	E490	Y491	A492	G493	E494	T495	L496	R497	M498	L499	N500	N501	V502	V503	Q504	D505	Q506	PRO	GLU	ASN	SER	SER	SER	P453	A454	S455	K456	Y457	I458	D459	E460	G461	F462	Q463	T464	P465	T466	L467	F468	D469	T472	K473	V474	M475	I476	L477	L478	K479	M480	T481	V482	S483	S484	Y485	Q486			
I487	L488	K489	E490	Y491	A492	G493	E494	T495	L496	R497	M498	L499	N500	N501	V502	V503	Q504	D505	Q506	PRO	GLU	ASN	SER	SER	SER	P453	A454	S455	K456	Y457	I458	D459	E460	G461	F462	Q463	T464	P465	T466	L467	F468	D469	T472	K473	V474	M475	I476	L477	L478	K479	M480	T481	V482	S483	S484	Y485	Q486			
I487	L488	K489	E490	Y491	A492	G493	E494	T495	L496	R497	M498	L499	N500	N501	V502	V503	Q504	D505	Q506	PRO	GLU	ASN	SER	SER	SER	P453	A454	S455	K456	Y457	I458	D459	E460	G461	F462	Q463	T464	P465	T466	L467	F468	D469	T472	K473	V474	M475	I476	L477	L478	K479	M480	T481	V482	S483	S484	Y485	Q486			
I487	L488	K489	E490	Y491	A492	G493	E494	T495	L496	R497	M498	L499	N500	N501	V502	V503	Q504	D505	Q506	PRO	GLU	ASN	SER	SER	SER	P453	A454	S455	K456	Y457	I458	D459	E460	G461	F462	Q463	T464	P465	T466	L467	F468	D469	T472	K473	V474	M475	I476	L477	L478	K479	M480	T481	V482	S483	S484	Y485	Q486			
I487	L488	K489	E490	Y491	A492	G493	E494	T495	L496	R497	M498	L499	N500	N501	V502	V503	Q504	D505	Q506	PRO	GLU	ASN	SER	SER	SER	P453	A454	S455	K456	Y457	I458	D459	E460	G461	F462	Q463	T464	P465	T466	L467	F468	D469	T472	K473	V474	M475	I476	L477	L478	K479	M480	T481	V482	S483	S484	Y485	Q486			
I487	L488	K489	E490	Y491	A492	G493	E494	T495	L496	R497	M49																																																	





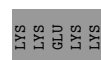
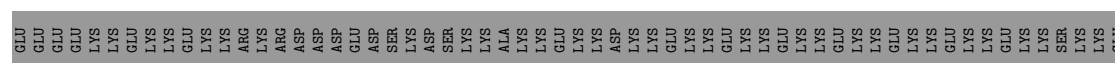
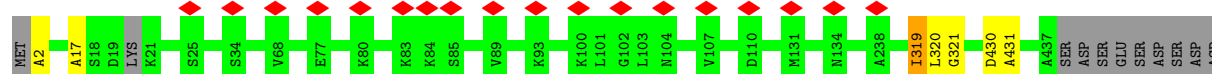
• Molecule 25: Nucleolar protein 56

Chain CD: 74% 25%



• Molecule 26: Nucleolar protein 58

Chain CE: 84% 15%



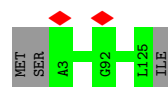
• Molecule 27: 13 kDa ribonucleoprotein-associated protein

Chain CF: 96%



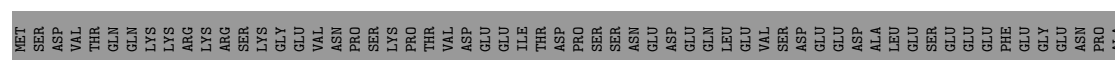
• Molecule 27: 13 kDa ribonucleoprotein-associated protein

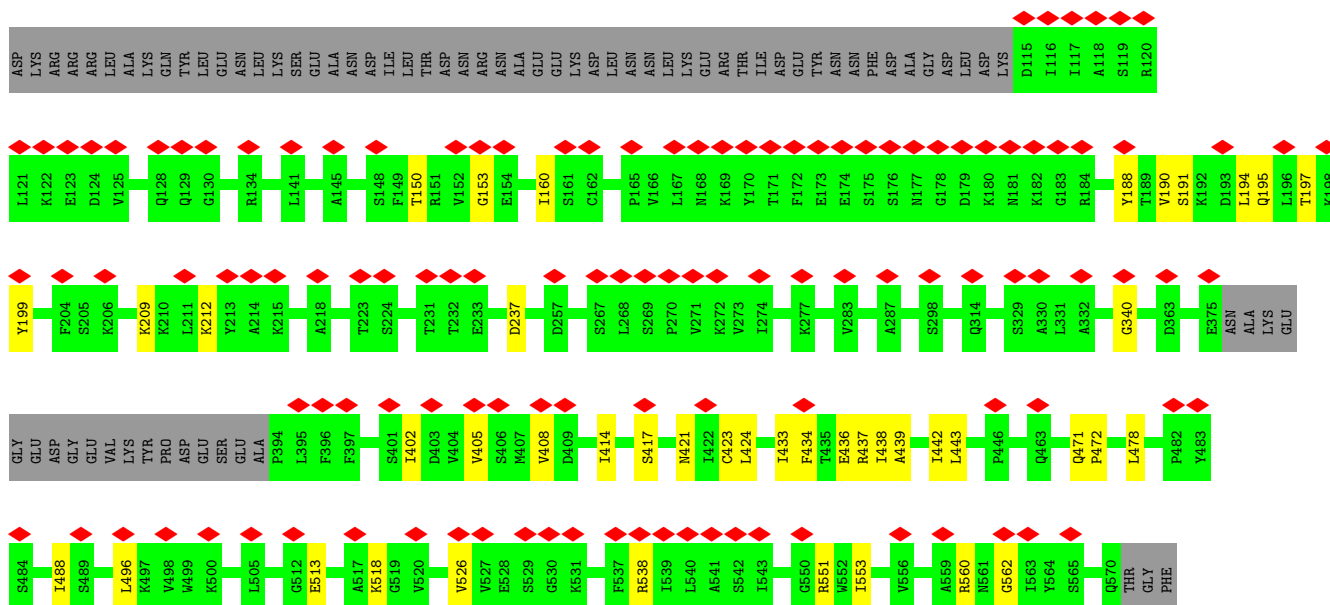
Chain CG: 98%



• Molecule 28: Ribosomal RNA-processing protein 9

Chain CH: 21% 69% 8% 24%





- Molecule 29: U3 small nucleolar ribonucleoprotein protein IMP3



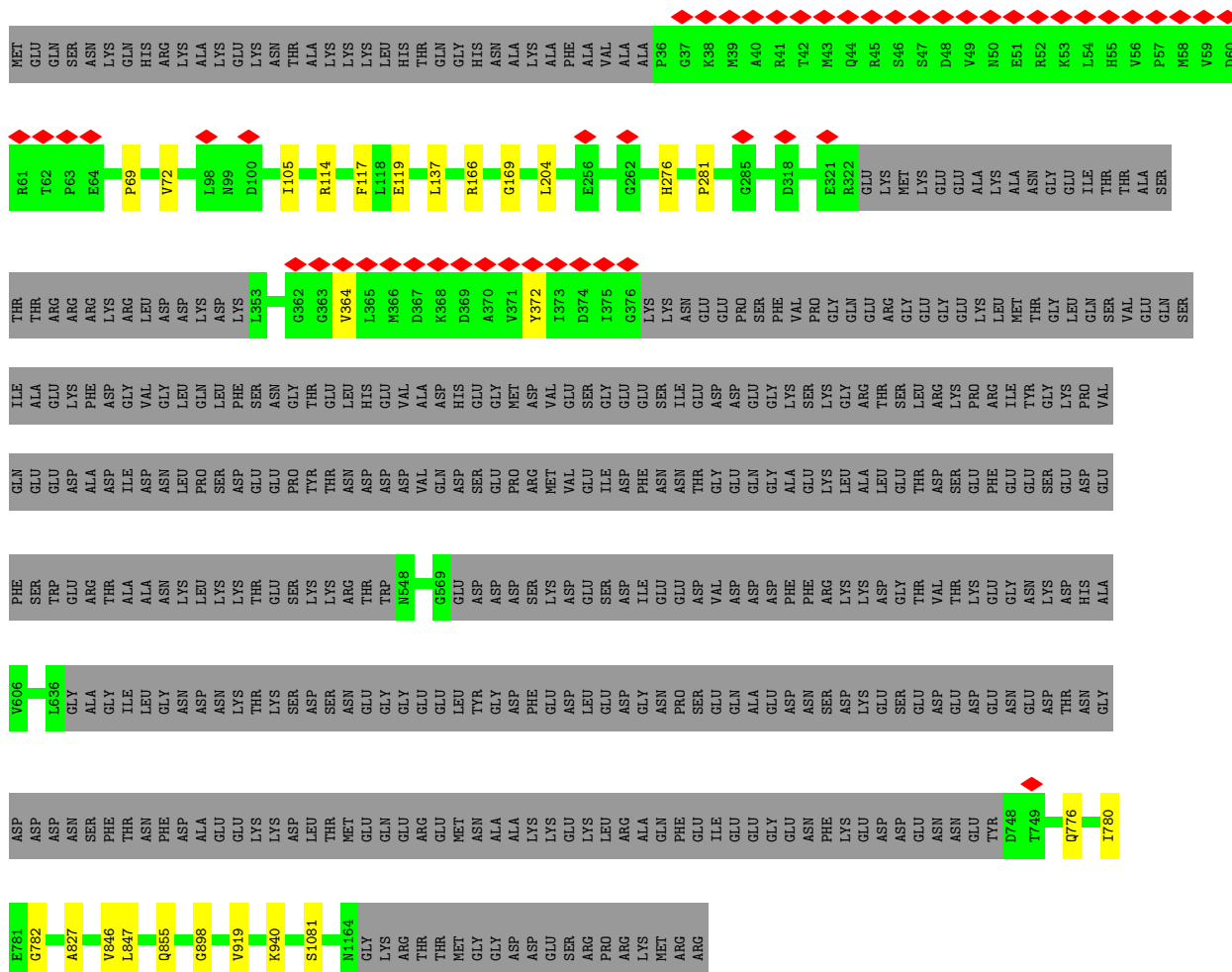
- Molecule 30: U3 small nucleolar ribonucleoprotein protein IMP4



- Molecule 31: U3 small nucleolar RNA-associated protein MPP10



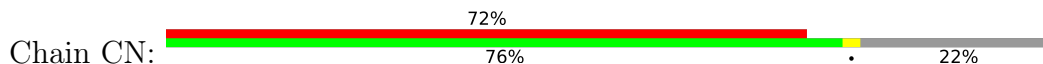
- Molecule 32: Ribosome biogenesis protein BMS1



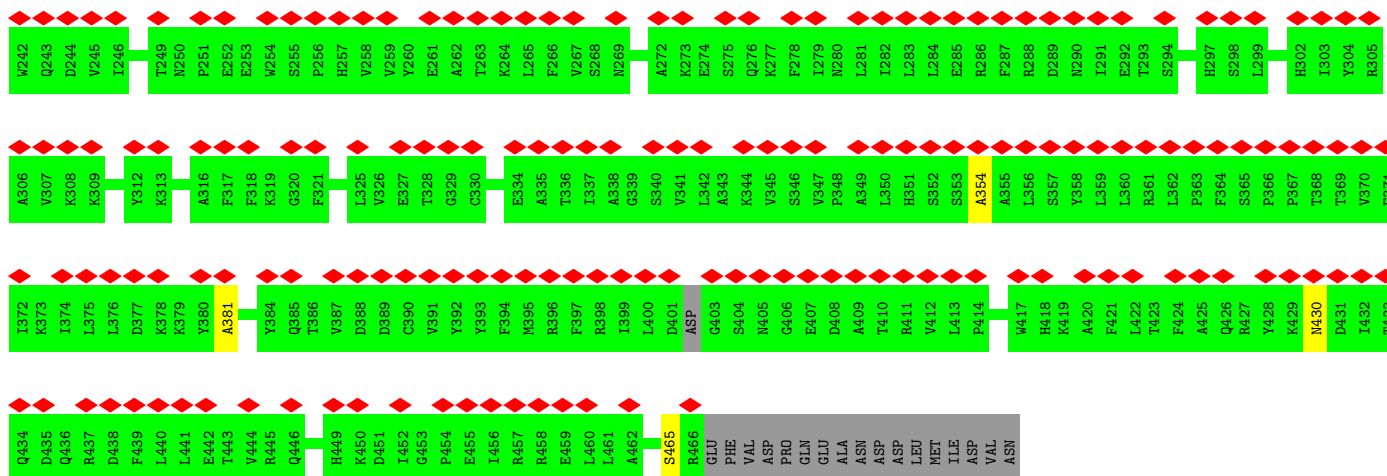
- Molecule 33: RNA 3'-terminal phosphate cyclase-like protein



- Molecule 34: Ribosomal RNA-processing protein 7

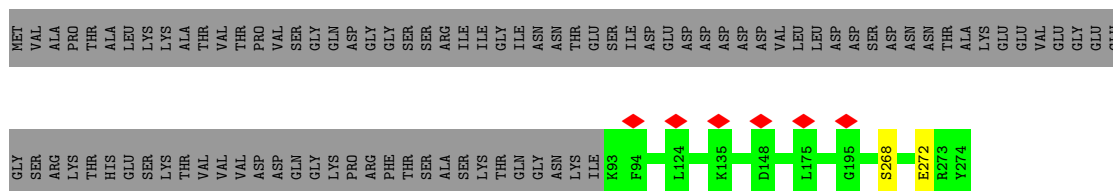






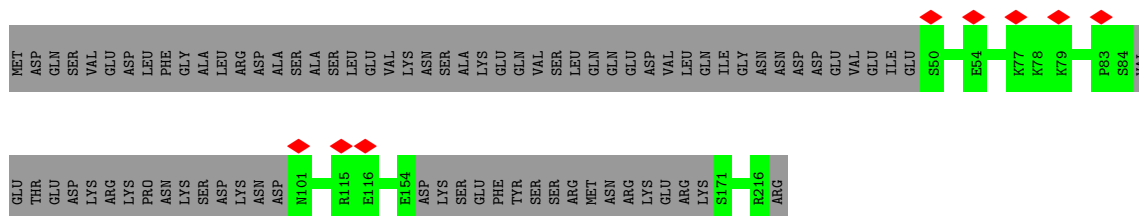
• Molecule 37: Pre-rRNA-processing protein PNO1

Chain JJ: 66% 34%



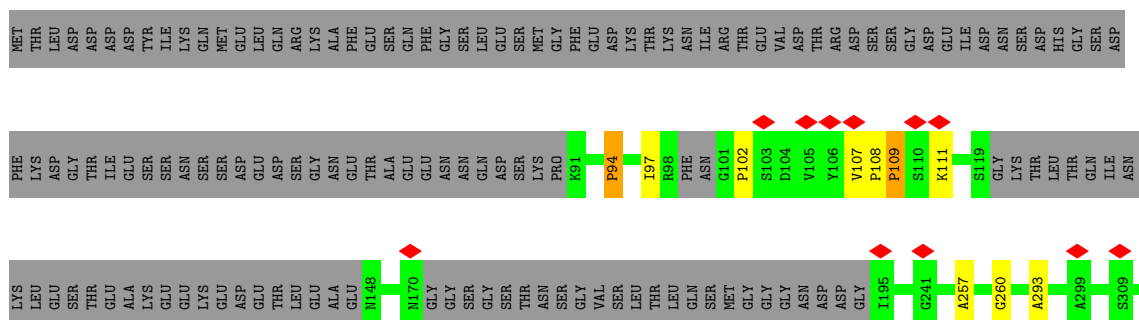
• Molecule 38: rRNA-processing protein FCF2

Chain JM: 62% 38%

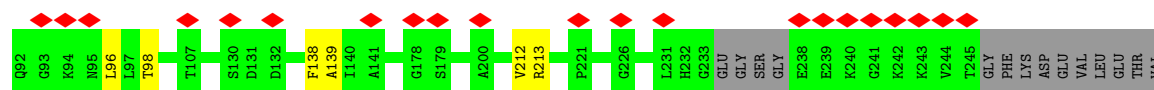


• Molecule 39: Protein FAF1

Chain JN: 51% 46%







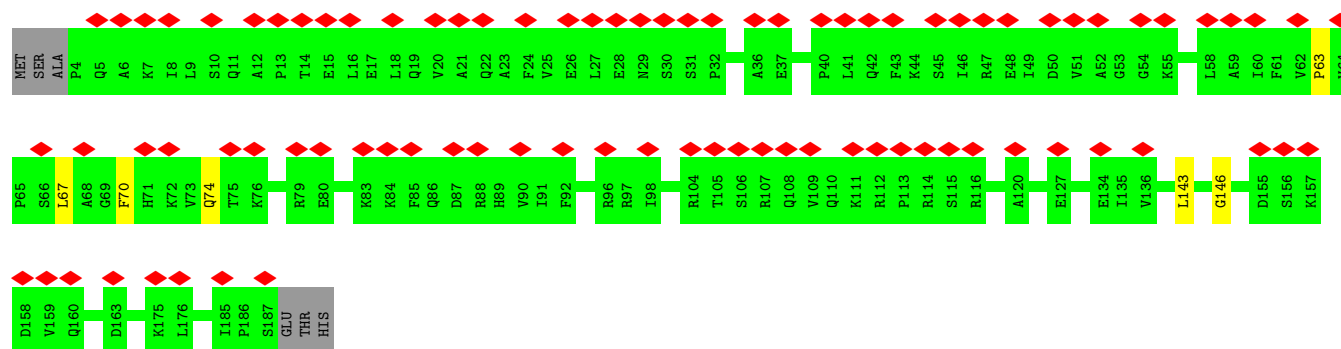
- Molecule 44: Rps5p

Chain DF: 94% 5%



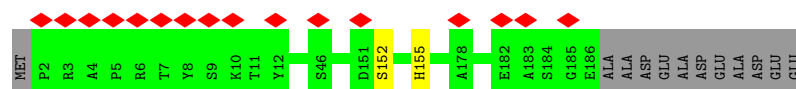
- Molecule 45: 40S ribosomal protein S7-A

Chain DH: 45% 94% . .



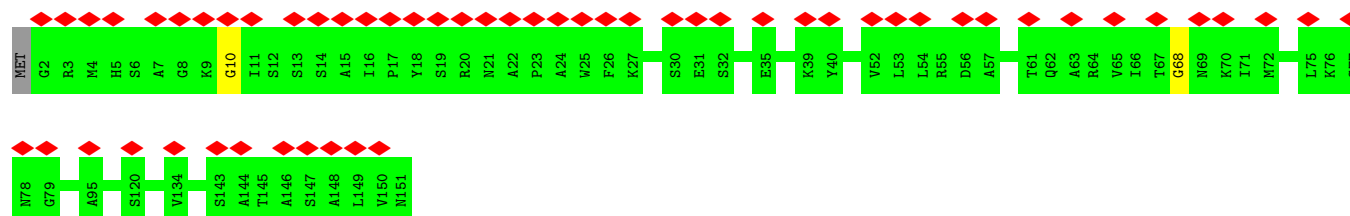
- Molecule 46: 40S ribosomal protein S9-A

Chain DJ: 8% 93% . 6%



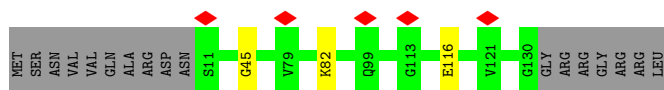
- Molecule 47: 40S ribosomal protein S13

Chain DN: 37% 98% . .

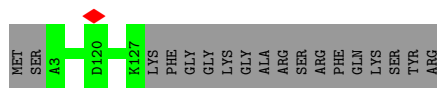


- Molecule 48: 40S ribosomal protein S14-A

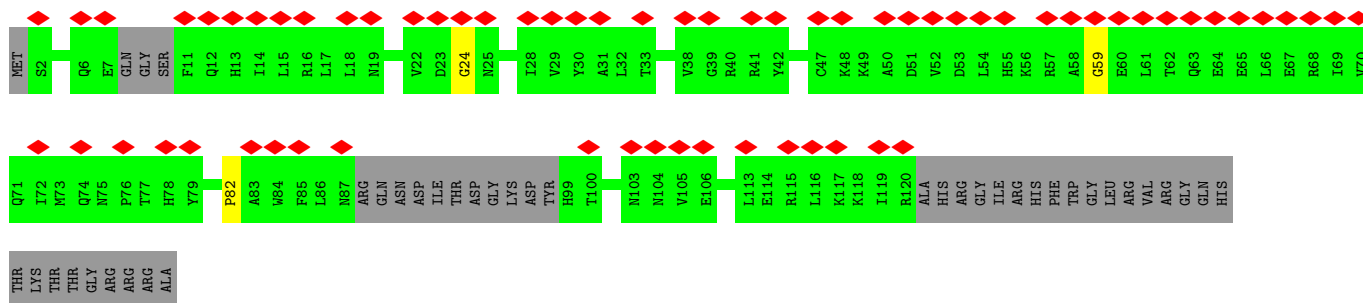
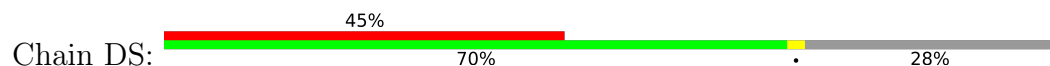
Chain DO: 85% 12%



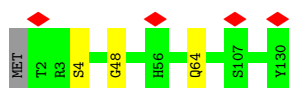
- Molecule 49: 40S ribosomal protein S16-A



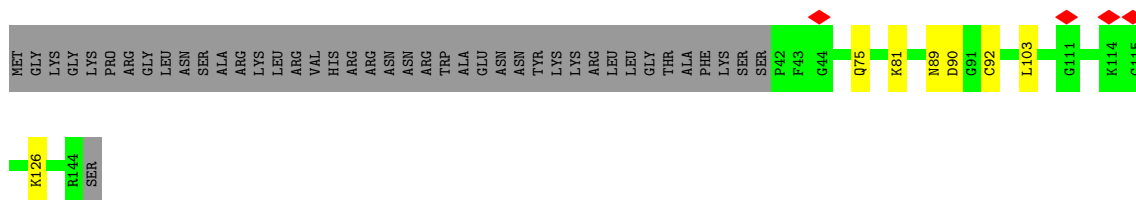
- Molecule 50: 40S ribosomal protein S18-A



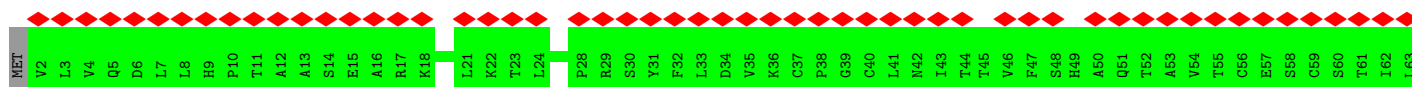
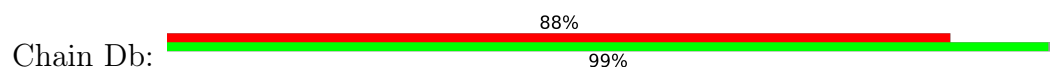
- Molecule 51: 40S ribosomal protein S22-A

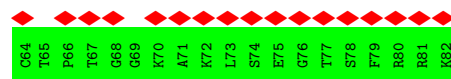


- Molecule 52: 40S ribosomal protein S23-A



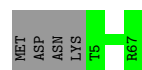
- Molecule 53: 40S ribosomal protein S27-A





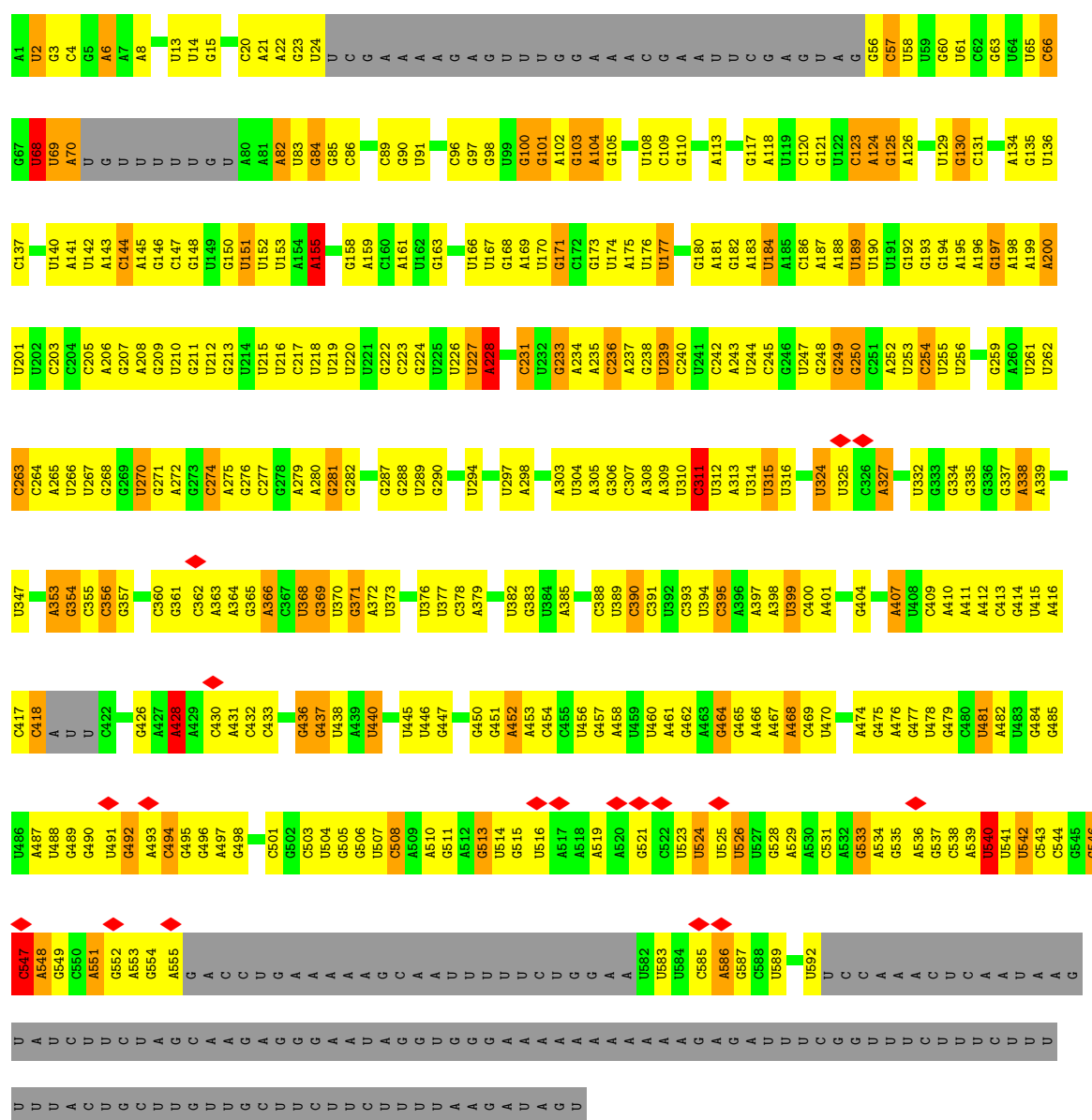
- Molecule 54: 40S ribosomal protein S28-A

Chain Dc: 94% 6%



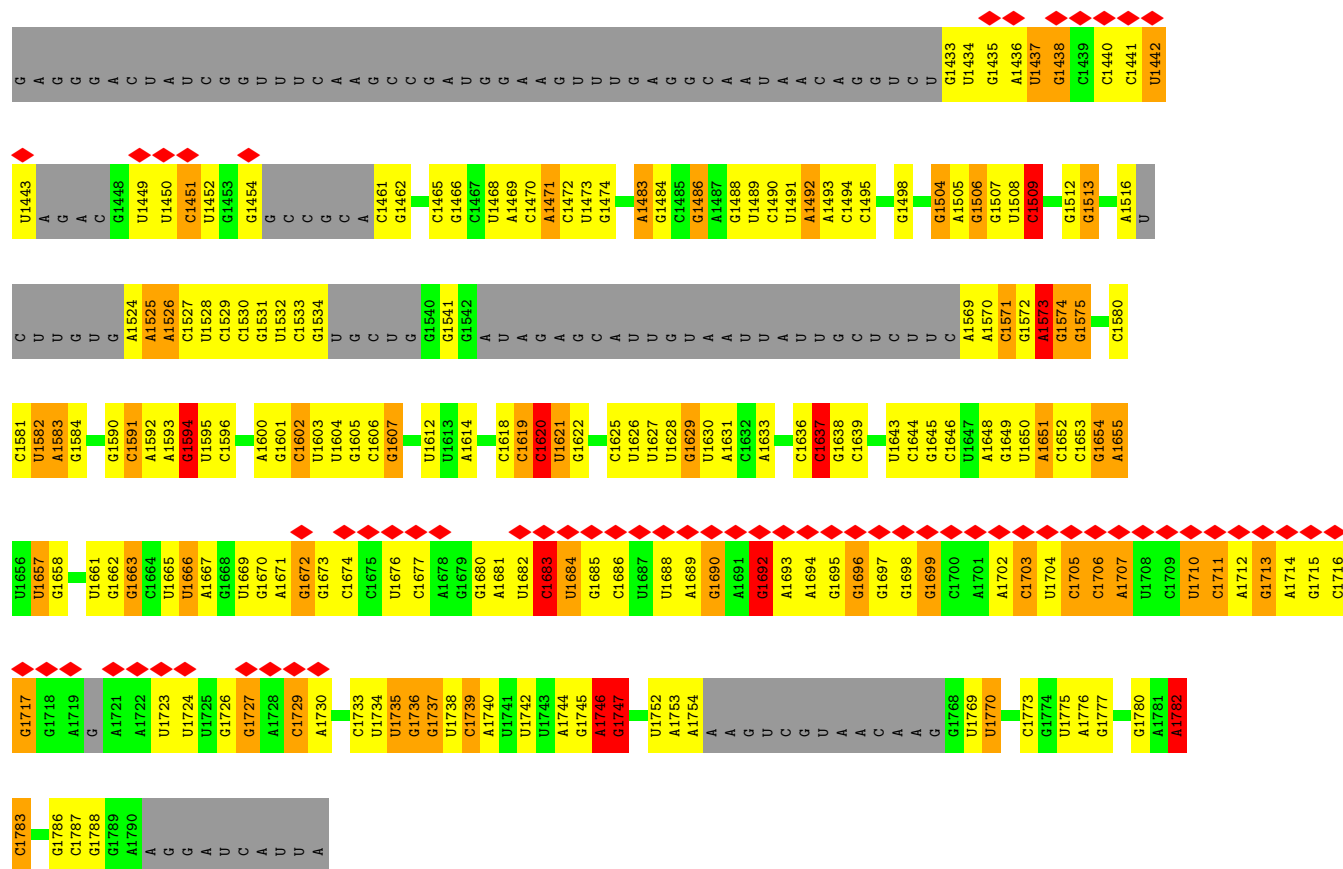
- Molecule 55: 5ETS RNA

Chain D2: 24% 40% 10% 25%

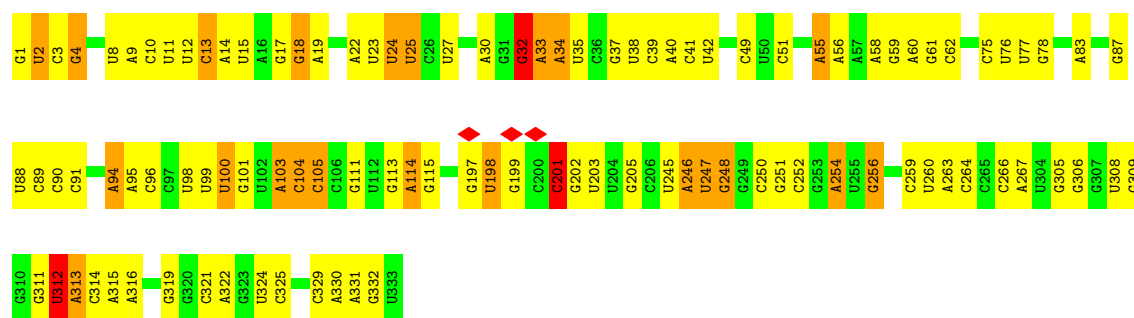


- Molecule 56: 18S rRNA





### • Molecule 57: U3 snoRNA



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11194	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	44, 44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k), GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.062	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size ( $\text{\AA}$ )	508.32, 508.32, 508.32	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.059, 1.059, 1.059	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	UA	0.42	0/4119	0.64	0/5734
2	UB	0.33	0/2506	0.57	4/3494 (0.1%)
3	UC	0.35	0/626	0.56	0/866
4	UD	0.39	0/3333	0.64	0/4635
5	UE	0.40	0/2348	0.64	1/3266 (0.0%)
6	UF	0.36	0/1451	0.50	0/2018
7	UG	0.44	0/2627	0.61	0/3653
8	UH	0.32	0/2182	0.67	10/3030 (0.3%)
9	UI	0.32	0/515	0.50	0/716
10	UJ	0.34	0/3618	0.53	0/5055
11	UK	0.37	0/1201	0.52	0/1674
12	UL	0.34	0/4156	0.61	0/5779
13	UM	0.32	0/3757	0.61	0/5222
14	UN	0.34	0/731	0.57	0/1019
15	UO	0.39	0/2439	0.59	0/3397
16	UP	0.33	0/297	0.53	0/413
17	UQ	0.37	0/4116	0.61	1/5730 (0.0%)
18	UR	0.45	1/2373 (0.0%)	0.61	0/3296
19	US	0.34	0/2350	0.55	1/3274 (0.0%)
20	UU	0.41	0/4178	0.61	0/5809
21	UV	0.25	0/5436	0.51	0/7572
22	UX	0.38	0/860	0.56	0/1196
23	UZ	0.34	0/1223	0.56	0/1704
24	CA	0.42	0/1188	0.59	0/1648
24	CB	0.37	0/1120	0.64	0/1554
25	CD	0.34	0/1878	0.54	0/2614
26	CE	0.34	0/2153	0.55	0/2999
27	CF	0.39	0/610	0.58	0/850
27	CG	0.37	0/610	0.58	0/850
28	CH	0.30	0/2156	0.66	0/2996
29	CI	0.42	0/904	0.60	0/1261
30	CJ	0.40	0/1395	0.61	0/1942

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
31	CK	0.36	0/1029	0.58	0/1435
32	CL	0.37	1/3854 (0.0%)	0.56	1/5361 (0.0%)
33	CM	0.33	0/1766	0.58	0/2451
34	CN	0.25	0/1150	0.50	0/1600
35	JF	0.33	0/1069	0.55	0/1488
35	JG	0.36	0/1139	0.59	0/1586
36	JH	0.29	0/1293	0.54	0/1801
37	JJ	0.31	0/897	0.54	0/1247
38	JM	0.36	0/668	0.54	0/928
39	JN	0.32	0/914	0.65	4/1266 (0.3%)
40	JO	0.32	0/932	0.56	0/1299
41	JP	0.42	1/2281 (0.0%)	0.63	0/3177
42	JQ	0.33	0/310	0.52	0/429
43	DA	0.29	0/1185	0.57	0/1648
44	DF	0.38	0/1054	0.54	0/1468
45	DH	0.29	0/912	0.56	0/1271
46	DJ	0.34	0/914	0.55	0/1272
47	DN	0.28	0/741	0.55	0/1031
48	DO	0.34	0/586	0.57	0/811
49	DQ	0.37	0/615	0.60	0/854
50	DS	0.28	0/518	0.52	0/718
51	DW	0.32	0/633	0.58	0/878
52	DX	0.34	0/502	0.56	0/694
53	Db	0.26	0/399	0.54	0/554
54	Dc	0.40	0/309	0.56	0/428
55	D2	0.89	2/12482 (0.0%)	1.28	112/19446 (0.6%)
56	D3	0.76	3/18789 (0.0%)	1.36	243/29248 (0.8%)
57	D4	0.91	1/4142 (0.0%)	1.28	27/6435 (0.4%)
All	All	0.53	9/129539 (0.0%)	0.87	404/186090 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	UA	0	1
2	UB	0	1
4	UD	0	3
5	UE	0	2
10	UJ	0	2
12	UL	0	5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
13	UM	0	4
14	UN	0	1
17	UQ	0	2
20	UU	0	1
23	UZ	0	1
25	CD	0	1
26	CE	0	1
28	CH	0	3
31	CK	0	1
32	CL	0	1
34	CN	0	1
40	JO	0	1
41	JP	0	3
44	DF	0	1
All	All	0	36

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	D3	1158	C	N3-C4	-8.09	1.28	1.33
56	D3	1164	G	C6-O6	-7.08	1.17	1.24
41	JP	313	PHE	C-N	-5.88	1.20	1.34
57	D4	83	A	N9-C4	-5.55	1.34	1.37
55	D2	388	C	C2-O2	-5.50	1.19	1.24
56	D3	553	G	C2-N3	-5.49	1.28	1.32
32	CL	1081	SER	CA-CB	-5.47	1.44	1.52
55	D2	298	A	N9-C4	-5.12	1.34	1.37
18	UR	570	PHE	C-N	-5.12	1.22	1.34

All (404) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	D3	1164	G	N1-C6-O6	-29.76	102.04	119.90
56	D3	1158	C	N3-C4-N4	-24.46	100.88	118.00
56	D3	1158	C	C5-C4-N4	19.67	133.97	120.20
56	D3	1164	G	C5-C6-O6	17.37	139.02	128.60
56	D3	1705	C	N3-C2-O2	-12.32	113.28	121.90
55	D2	394	U	C2-N1-C1'	11.55	131.56	117.70
56	D3	1164	G	C5-C6-N1	11.40	117.20	111.50
57	D4	13	C	N1-C2-O2	11.34	125.70	118.90
5	UE	472	LEU	C-N-CA	11.18	149.66	121.70
57	D4	13	C	N3-C2-O2	-10.96	114.23	121.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	D2	356	C	N3-C2-O2	-10.36	114.65	121.90
56	D3	474	A	N1-C6-N6	-10.35	112.39	118.60
56	D3	553	G	N3-C4-N9	-10.28	119.83	126.00
56	D3	1705	C	N1-C2-O2	10.02	124.91	118.90
55	D2	394	U	N1-C2-O2	9.65	129.55	122.80
55	D2	524	U	OP1-P-O3'	-9.61	84.05	105.20
55	D2	151	U	C2-N1-C1'	9.59	129.21	117.70
56	D3	1703	C	N3-C2-O2	-9.49	115.25	121.90
55	D2	524	U	OP2-P-O3'	-9.31	84.72	105.20
55	D2	418	C	N3-C2-O2	-9.29	115.39	121.90
56	D3	1739	C	C6-N1-C2	-9.24	116.60	120.30
56	D3	563	U	N1-C2-O2	9.21	129.24	122.80
55	D2	394	U	N3-C2-O2	-9.13	115.81	122.20
56	D3	553	G	N9-C4-C5	9.12	109.05	105.40
56	D3	1066	C	N3-C2-O2	-8.95	115.64	121.90
56	D3	563	U	C2-N1-C1'	8.93	128.42	117.70
56	D3	1077	C	N3-C2-O2	-8.91	115.67	121.90
56	D3	553	G	C8-N9-C1'	8.86	138.52	127.00
55	D2	356	C	C6-N1-C2	-8.85	116.76	120.30
55	D2	151	U	N1-C2-O2	8.78	128.95	122.80
56	D3	551	G	N3-C4-N9	8.78	131.27	126.00
55	D2	144	C	N1-C2-O2	8.73	124.14	118.90
55	D2	108	U	N1-C2-O2	8.53	128.77	122.80
56	D3	976	G	C4-N9-C1'	8.45	137.49	126.50
55	D2	481	U	N1-C2-O2	8.42	128.70	122.80
56	D3	1128	C	N3-C2-O2	-8.38	116.03	121.90
56	D3	1729	C	N3-C2-O2	-8.36	116.05	121.90
55	D2	263	C	N3-C2-O2	-8.26	116.12	121.90
55	D2	108	U	C2-N1-C1'	8.19	127.53	117.70
56	D3	1653	C	N3-C2-O2	-8.16	116.19	121.90
56	D3	563	U	N3-C2-O2	-8.14	116.50	122.20
56	D3	553	G	C6-C5-N7	8.13	135.28	130.40
56	D3	1066	C	N1-C2-O2	8.10	123.76	118.90
2	UB	400	PRO	N-CA-CB	8.09	113.01	103.30
56	D3	1075	C	C6-N1-C2	-7.96	117.12	120.30
55	D2	123	C	C2-N1-C1'	7.94	127.53	118.80
56	D3	1158	C	N3-C4-C5	7.93	125.07	121.90
55	D2	151	U	N3-C2-O2	-7.92	116.66	122.20
55	D2	355	C	N1-C2-O2	7.92	123.65	118.90
56	D3	1746	A	N1-C6-N6	-7.82	113.91	118.60
56	D3	1495	C	N3-C2-O2	-7.80	116.44	121.90
56	D3	553	G	N3-C2-N2	-7.77	114.46	119.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	D2	394	U	C6-N1-C1'	-7.76	110.33	121.20
55	D2	123	C	N1-C2-O2	7.74	123.54	118.90
55	D2	356	C	N1-C2-O2	7.70	123.52	118.90
56	D3	1163	A	C6-N1-C2	-7.70	113.98	118.60
57	D4	55	A	O4'-C1'-N9	7.67	114.33	108.20
56	D3	1123	C	N1-C2-O2	7.64	123.49	118.90
55	D2	68	U	N3-C2-O2	-7.58	116.89	122.20
56	D3	553	G	C4-N9-C1'	-7.55	116.68	126.50
55	D2	123	C	C6-N1-C2	-7.54	117.28	120.30
56	D3	1449	U	N1-C2-O2	7.50	128.05	122.80
55	D2	481	U	N3-C2-O2	-7.50	116.95	122.20
57	D4	100	U	N3-C2-O2	-7.49	116.96	122.20
55	D2	231	C	C2-N1-C1'	7.48	127.02	118.80
56	D3	976	G	C8-N9-C1'	-7.47	117.29	127.00
56	D3	1727	G	N3-C4-N9	7.47	130.48	126.00
56	D3	1692	G	C2-N3-C4	7.42	115.61	111.90
55	D2	355	C	C2-N1-C1'	7.42	126.96	118.80
56	D3	1210	C	C5-C6-N1	7.42	124.71	121.00
56	D3	551	G	C6-C5-N7	-7.42	125.95	130.40
56	D3	536	C	C2-N1-C1'	7.41	126.95	118.80
56	D3	551	G	C8-N9-C1'	-7.31	117.50	127.00
56	D3	551	G	C4-N9-C1'	7.28	135.97	126.50
56	D3	587	C	N3-C2-O2	-7.28	116.81	121.90
56	D3	1220	C	C5-C6-N1	7.27	124.64	121.00
56	D3	1440	C	C5-C6-N1	7.27	124.64	121.00
56	D3	1705	C	C6-N1-C2	-7.25	117.40	120.30
56	D3	885	G	C4-N9-C1'	7.21	135.87	126.50
56	D3	553	G	N1-C6-O6	-7.20	115.58	119.90
57	D4	100	U	N1-C2-O2	7.17	127.82	122.80
56	D3	1739	C	N3-C2-O2	-7.11	116.92	121.90
57	D4	312	U	C5-C6-N1	7.07	126.23	122.70
56	D3	1747	G	N3-C4-N9	7.02	130.21	126.00
56	D3	1654	G	N9-C4-C5	-7.02	102.59	105.40
56	D3	542	A	N7-C8-N9	7.01	117.30	113.80
56	D3	486	G	O4'-C1'-N9	6.98	113.78	108.20
56	D3	1637	C	N3-C2-O2	-6.98	117.01	121.90
56	D3	14	C	N3-C2-O2	-6.97	117.02	121.90
56	D3	551	G	C4-C5-N7	6.96	113.59	110.80
55	D2	66	C	C5-C6-N1	6.95	124.47	121.00
55	D2	525	U	OP1-P-OP2	6.95	130.02	119.60
55	D2	274	C	N3-C2-O2	-6.94	117.04	121.90
56	D3	551	G	N9-C4-C5	-6.94	102.62	105.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	D2	144	C	C2-N1-C1'	6.92	126.41	118.80
57	D4	312	U	C6-N1-C2	-6.91	116.86	121.00
55	D2	108	U	C6-N1-C1'	-6.88	111.56	121.20
55	D2	231	C	C6-N1-C2	-6.86	117.56	120.30
56	D3	1449	U	N3-C2-O2	-6.85	117.41	122.20
55	D2	481	U	C2-N1-C1'	6.83	125.90	117.70
55	D2	369	G	N3-C4-N9	6.78	130.07	126.00
56	D3	1433	G	C4-N9-C1'	6.78	135.31	126.50
56	D3	1747	G	C6-C5-N7	-6.78	126.33	130.40
55	D2	391	C	C2-N1-C1'	6.77	126.24	118.80
39	JN	108	PRO	N-CA-CB	6.76	111.42	103.30
56	D3	579	A	P-O3'-C3'	6.76	127.81	119.70
55	D2	250	G	C2-N3-C4	-6.74	108.53	111.90
56	D3	1033	C	N1-C2-O2	6.74	122.94	118.90
55	D2	390	C	N3-C2-O2	-6.70	117.21	121.90
56	D3	885	G	C8-N9-C1'	-6.70	118.29	127.00
56	D3	14	C	C6-N1-C2	-6.68	117.63	120.30
56	D3	1056	U	C5-C6-N1	6.68	126.04	122.70
55	D2	123	C	C5-C6-N1	6.66	124.33	121.00
8	UH	235	PRO	N-CA-CB	6.64	111.27	103.30
56	D3	1696	G	C5-C6-O6	6.61	132.57	128.60
55	D2	68	U	N1-C2-O2	6.60	127.42	122.80
56	D3	564	G	C4-C5-N7	6.58	113.43	110.80
56	D3	1164	G	C6-N1-C2	-6.57	121.16	125.10
57	D4	314	C	N3-C2-O2	-6.54	117.32	121.90
56	D3	1527	C	C2-N1-C1'	6.53	125.98	118.80
56	D3	1440	C	C6-N1-C2	-6.50	117.70	120.30
56	D3	1215	C	C6-N1-C2	-6.49	117.70	120.30
55	D2	151	U	C5-C6-N1	6.49	125.95	122.70
56	D3	1033	C	N3-C2-O2	-6.49	117.36	121.90
55	D2	356	C	C2-N1-C1'	6.45	125.90	118.80
57	D4	13	C	C2-N1-C1'	6.45	125.89	118.80
8	UH	325	PRO	N-CA-CB	6.44	111.03	103.30
57	D4	89	C	C6-N1-C2	-6.43	117.73	120.30
39	JN	109	PRO	N-CA-CB	6.42	111.01	103.30
55	D2	508	C	C5-C6-N1	6.41	124.20	121.00
55	D2	144	C	N3-C2-O2	-6.40	117.42	121.90
56	D3	1673	G	C8-N9-C4	-6.40	103.84	106.40
56	D3	563	U	C6-N1-C1'	-6.38	112.26	121.20
56	D3	1674	C	N1-C2-O2	6.38	122.73	118.90
19	US	37	PRO	N-CA-CB	6.37	110.94	103.30
56	D3	912	U	P-O3'-C3'	6.36	127.33	119.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	D3	1128	C	C6-N1-C2	-6.35	117.76	120.30
56	D3	908	U	C5-C6-N1	6.34	125.87	122.70
56	D3	913	G	N3-C4-N9	6.34	129.80	126.00
55	D2	123	C	N3-C2-O2	-6.33	117.47	121.90
56	D3	1077	C	N1-C2-O2	6.33	122.70	118.90
56	D3	1220	C	C2-N1-C1'	6.33	125.76	118.80
56	D3	1746	A	O4'-C1'-N9	6.32	113.26	108.20
56	D3	975	C	C6-N1-C2	-6.31	117.78	120.30
55	D2	547	C	N1-C2-O2	6.31	122.69	118.90
55	D2	216	U	C5-C6-N1	6.30	125.85	122.70
56	D3	1692	G	N3-C4-C5	-6.27	125.47	128.60
56	D3	1729	C	N1-C2-O2	6.26	122.66	118.90
8	UH	67	PRO	N-CA-CB	6.25	110.80	103.30
56	D3	482	U	C2-N1-C1'	6.24	125.19	117.70
56	D3	1079	U	N3-C2-O2	-6.23	117.84	122.20
55	D2	311	C	P-O3'-C3'	6.21	127.15	119.70
55	D2	418	C	C6-N1-C2	-6.21	117.81	120.30
8	UH	309	PRO	N-CA-CB	6.19	110.72	103.30
39	JN	102	PRO	N-CA-CB	6.18	110.72	103.30
56	D3	587	C	N1-C2-O2	6.18	122.61	118.90
56	D3	976	G	N3-C4-N9	6.18	129.71	126.00
55	D2	501	C	C2-N1-C1'	6.17	125.59	118.80
55	D2	393	C	C6-N1-C1'	6.17	128.21	120.80
2	UB	412	PRO	N-CA-CB	6.17	110.70	103.30
56	D3	553	G	C5-C6-O6	6.16	132.29	128.60
56	D3	1060	U	C2-N1-C1'	6.13	125.06	117.70
56	D3	553	G	N1-C2-N2	6.12	121.71	116.20
55	D2	388	C	N3-C2-O2	-6.11	117.62	121.90
56	D3	1433	G	N3-C4-N9	6.10	129.66	126.00
56	D3	1747	G	N7-C8-N9	6.10	116.15	113.10
56	D3	1674	C	C2-N1-C1'	6.08	125.48	118.80
56	D3	1729	C	C6-N1-C2	-6.06	117.87	120.30
39	JN	94	PRO	N-CA-CB	6.06	110.57	103.30
56	D3	1591	C	N1-C2-O2	6.05	122.53	118.90
56	D3	1683	C	C5-C6-N1	6.04	124.02	121.00
56	D3	1653	C	C6-N1-C2	-6.03	117.89	120.30
55	D2	151	U	C6-N1-C1'	-6.03	112.76	121.20
56	D3	1057	U	P-O3'-C3'	6.03	126.93	119.70
57	D4	266	C	N3-C2-O2	-6.02	117.68	121.90
55	D2	369	G	C6-C5-N7	-6.02	126.79	130.40
2	UB	201	PRO	N-CA-CB	6.00	110.50	103.30
56	D3	1692	G	C8-N9-C4	-5.99	104.00	106.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	D3	1037	C	C6-N1-C2	5.98	122.69	120.30
55	D2	394	U	C5-C6-N1	5.96	125.68	122.70
8	UH	258	PRO	N-CA-CB	5.96	110.45	103.30
55	D2	89	C	N1-C2-O2	5.94	122.46	118.90
8	UH	298	PRO	N-CA-CB	5.93	110.42	103.30
56	D3	14	C	N1-C2-N3	5.93	123.36	119.20
56	D3	1513	G	C5-C6-O6	5.93	132.16	128.60
56	D3	469	C	N1-C2-O2	5.93	122.46	118.90
56	D3	1686	C	C2-N1-C1'	5.93	125.33	118.80
55	D2	347	U	N3-C2-O2	-5.93	118.05	122.20
56	D3	1607	G	O5'-P-OP2	-5.93	100.36	105.70
56	D3	1654	G	N3-C2-N2	5.92	124.05	119.90
56	D3	1163	A	N1-C2-N3	5.91	132.26	129.30
55	D2	68	U	C2-N1-C1'	5.91	124.79	117.70
56	D3	1059	U	C2-N1-C1'	5.91	124.79	117.70
56	D3	1056	U	C2-N1-C1'	5.91	124.79	117.70
56	D3	1043	A	N1-C6-N6	-5.90	115.06	118.60
55	D2	91	U	C5-C6-N1	5.89	125.65	122.70
56	D3	1220	C	N1-C2-O2	5.89	122.43	118.90
56	D3	1513	G	C2-N3-C4	-5.88	108.96	111.90
56	D3	1582	U	N3-C2-O2	5.87	126.31	122.20
56	D3	1620	C	N1-C2-O2	5.86	122.42	118.90
56	D3	1207	C	N1-C2-O2	5.85	122.41	118.90
56	D3	1495	C	C6-N1-C2	-5.85	117.96	120.30
56	D3	542	A	C5-N7-C8	-5.84	100.98	103.90
57	D4	89	C	C2-N1-C1'	5.84	125.22	118.80
55	D2	540	U	C2-N1-C1'	5.84	124.70	117.70
56	D3	1696	G	N1-C6-O6	-5.82	116.41	119.90
55	D2	270	U	N3-C2-O2	-5.81	118.13	122.20
56	D3	1727	G	C6-C5-N7	-5.81	126.91	130.40
2	UB	285	PRO	N-CA-CB	5.80	110.26	103.30
55	D2	437	G	C2-N3-C4	-5.80	109.00	111.90
56	D3	1433	G	N3-C4-C5	-5.79	125.70	128.60
56	D3	1747	G	C4-N9-C1'	5.79	134.03	126.50
56	D3	1056	U	N1-C2-O2	5.79	126.85	122.80
56	D3	536	C	N1-C2-O2	5.78	122.37	118.90
56	D3	1449	U	C2-N1-C1'	5.78	124.64	117.70
56	D3	895	G	C5-C6-O6	5.78	132.07	128.60
56	D3	536	C	C6-N1-C1'	-5.76	113.89	120.80
56	D3	1747	G	C4-C5-N7	5.76	113.10	110.80
55	D2	108	U	N3-C2-O2	-5.76	118.17	122.20
56	D3	1620	C	N3-C2-O2	-5.75	117.88	121.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	D3	962	C	N1-C2-O2	5.74	122.34	118.90
55	D2	395	C	N1-C2-O2	5.73	122.34	118.90
56	D3	1451	C	N3-C2-O2	-5.72	117.90	121.90
56	D3	1672	G	N3-C4-N9	5.71	129.43	126.00
56	D3	1433	G	C8-N9-C1'	-5.70	119.58	127.00
8	UH	69	PRO	N-CA-CB	5.70	110.13	103.30
55	D2	355	C	C6-N1-C1'	-5.70	113.97	120.80
56	D3	1746	A	C5-C6-N6	5.69	128.25	123.70
55	D2	436	G	N3-C4-N9	5.68	129.41	126.00
55	D2	66	C	C2-N1-C1'	5.68	125.05	118.80
55	D2	417	C	N1-C2-O2	5.68	122.31	118.90
56	D3	584	C	C6-N1-C1'	5.67	127.61	120.80
57	D4	89	C	N1-C2-O2	5.67	122.30	118.90
55	D2	391	C	N1-C2-O2	5.67	122.30	118.90
56	D3	948	G	C4-N9-C1'	5.66	133.86	126.50
56	D3	933	A	C2-N3-C4	5.66	113.43	110.60
56	D3	960	U	C2-N1-C1'	5.65	124.48	117.70
56	D3	1210	C	C6-N1-C2	-5.65	118.04	120.30
56	D3	1674	C	C5-C6-N1	5.64	123.82	121.00
32	CL	119	GLU	C-N-CA	-5.64	107.60	121.70
57	D4	306	G	C5-C6-O6	5.64	131.98	128.60
56	D3	1746	A	N9-C4-C5	5.63	108.05	105.80
55	D2	184	U	C2-N1-C1'	5.62	124.45	117.70
55	D2	184	U	N1-C2-O2	5.62	126.73	122.80
8	UH	58	PRO	N-CA-CB	5.61	110.03	103.30
55	D2	250	G	C5-C6-O6	5.60	131.96	128.60
55	D2	501	C	N1-C2-O2	5.60	122.26	118.90
56	D3	1209	C	C6-N1-C2	-5.59	118.06	120.30
56	D3	948	G	C8-N9-C1'	-5.59	119.73	127.00
55	D2	390	C	C6-N1-C2	-5.58	118.07	120.30
56	D3	1747	G	N3-C4-C5	-5.58	125.81	128.60
56	D3	1059	U	O4'-C1'-N1	5.58	112.66	108.20
56	D3	1637	C	C6-N1-C2	-5.58	118.07	120.30
56	D3	584	C	C2-N1-C1'	-5.57	112.67	118.80
57	D4	89	C	C5-C6-N1	5.56	123.78	121.00
56	D3	1216	C	N3-C2-O2	-5.56	118.01	121.90
55	D2	250	G	N1-C2-N3	5.56	127.23	123.90
56	D3	1123	C	N3-C2-O2	-5.56	118.01	121.90
56	D3	1673	G	C5-C6-O6	5.55	131.93	128.60
56	D3	553	G	O4'-C1'-N9	5.55	112.64	108.20
56	D3	1075	C	N3-C2-O2	-5.53	118.03	121.90
55	D2	89	C	C2-N1-C1'	5.52	124.88	118.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	D2	338	A	N1-C2-N3	5.52	132.06	129.30
56	D3	1081	A	N7-C8-N9	5.52	116.56	113.80
56	D3	1207	C	N3-C2-O2	-5.52	118.04	121.90
56	D3	534	A	C2-N3-C4	5.52	113.36	110.60
56	D3	1451	C	C6-N1-C2	-5.51	118.09	120.30
56	D3	1637	C	N1-C2-O2	5.50	122.20	118.90
56	D3	1056	U	N3-C2-O2	-5.49	118.36	122.20
55	D2	233	G	C6-C5-N7	-5.48	127.11	130.40
55	D2	492	G	P-O3'-C3'	5.48	126.28	119.70
56	D3	1081	A	C8-N9-C4	-5.48	103.61	105.80
56	D3	1452	U	C2-N1-C1'	5.47	124.27	117.70
57	D4	32	G	C4-N9-C1'	5.46	133.60	126.50
55	D2	369	G	C4-C5-N7	5.46	112.98	110.80
56	D3	542	A	C6-C5-N7	-5.45	128.48	132.30
56	D3	1265	G	N3-C4-N9	5.45	129.27	126.00
56	D3	1209	C	C5-C6-N1	5.44	123.72	121.00
55	D2	57	C	C5-C6-N1	5.43	123.71	121.00
56	D3	1654	G	N3-C4-N9	5.42	129.25	126.00
8	UH	60	PRO	N-CA-CB	5.42	109.80	103.30
55	D2	355	C	N3-C2-O2	-5.41	118.11	121.90
56	D3	976	G	N7-C8-N9	5.41	115.80	113.10
56	D3	1657	U	P-O3'-C3'	5.41	126.19	119.70
57	D4	13	C	C6-N1-C2	-5.40	118.14	120.30
55	D2	508	C	C6-N1-C2	-5.40	118.14	120.30
56	D3	1452	U	C5-C6-N1	5.40	125.40	122.70
56	D3	1654	G	N1-C2-N2	-5.39	111.35	116.20
57	D4	2	U	N3-C2-O2	-5.39	118.43	122.20
56	D3	1591	C	C5-C6-N1	5.38	123.69	121.00
56	D3	1737	G	C6-C5-N7	-5.38	127.17	130.40
56	D3	474	A	C5-C6-N6	5.38	128.00	123.70
56	D3	1571	C	N3-C2-O2	-5.37	118.14	121.90
56	D3	1594	G	P-O3'-C3'	5.37	126.14	119.70
56	D3	1629	G	C5-C6-O6	5.37	131.82	128.60
56	D3	1056	U	C6-N1-C2	-5.37	117.78	121.00
56	D3	1654	G	C4-C5-N7	5.37	112.95	110.80
56	D3	1782	A	N1-C6-N6	-5.37	115.38	118.60
56	D3	1054	U	C2-N1-C1'	5.36	124.13	117.70
55	D2	338	A	C2-N3-C4	-5.36	107.92	110.60
56	D3	962	C	N3-C2-O2	-5.36	118.15	121.90
55	D2	189	U	N1-C2-O2	5.35	126.55	122.80
57	D4	264	C	C6-N1-C2	-5.34	118.16	120.30
56	D3	1620	C	P-O3'-C3'	5.34	126.11	119.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	D3	1452	U	N1-C2-O2	5.34	126.54	122.80
56	D3	1770	U	N3-C2-O2	-5.33	118.47	122.20
55	D2	418	C	N1-C2-O2	5.33	122.10	118.90
55	D2	65	U	N1-C2-O2	5.33	126.53	122.80
56	D3	1058	U	N3-C2-O2	-5.33	118.47	122.20
56	D3	483	A	C6-N1-C2	-5.32	115.41	118.60
56	D3	1727	G	N9-C4-C5	-5.32	103.27	105.40
55	D2	393	C	C2-N1-C1'	-5.32	112.95	118.80
56	D3	564	G	C6-C5-N7	-5.32	127.21	130.40
56	D3	1686	C	C6-N1-C2	-5.31	118.17	120.30
57	D4	18	G	N3-C4-N9	-5.31	122.81	126.00
56	D3	1696	G	N1-C2-N2	-5.31	111.42	116.20
56	D3	960	U	N3-C2-O2	-5.30	118.49	122.20
56	D3	895	G	N1-C6-O6	-5.30	116.72	119.90
56	D3	530	C	C6-N1-C2	-5.30	118.18	120.30
57	D4	27	U	N1-C2-O2	5.29	126.50	122.80
56	D3	1128	C	N1-C2-O2	5.29	122.07	118.90
56	D3	1621	U	N3-C2-O2	-5.28	118.50	122.20
57	D4	105	C	C6-N1-C2	-5.28	118.19	120.30
55	D2	66	C	C6-N1-C2	-5.27	118.19	120.30
55	D2	356	C	C5-C6-N1	5.27	123.64	121.00
56	D3	573	C	N1-C2-O2	5.26	122.06	118.90
56	D3	1652	C	N1-C2-O2	5.24	122.04	118.90
56	D3	962	C	C2-N1-C1'	5.23	124.56	118.80
56	D3	1673	G	N1-C6-O6	-5.23	116.76	119.90
56	D3	1509	C	C6-N1-C2	-5.22	118.21	120.30
56	D3	1654	G	C6-C5-N7	-5.22	127.27	130.40
56	D3	1727	G	C4-N9-C1'	5.22	133.28	126.50
56	D3	1058	U	C2-N1-C1'	5.21	123.95	117.70
55	D2	120	C	C2-N1-C1'	5.21	124.53	118.80
57	D4	306	G	C8-N9-C4	-5.21	104.32	106.40
56	D3	913	G	N3-C4-C5	-5.20	126.00	128.60
56	D3	1058	U	N1-C2-O2	5.19	126.43	122.80
56	D3	885	G	C6-C5-N7	-5.19	127.29	130.40
55	D2	428	A	C8-N9-C4	-5.18	103.73	105.80
55	D2	464	G	C5-C6-O6	5.18	131.71	128.60
55	D2	501	C	C6-N1-C2	-5.18	118.23	120.30
55	D2	144	C	C6-N1-C1'	-5.18	114.58	120.80
56	D3	564	G	C5-N7-C8	-5.17	101.72	104.30
56	D3	1206	U	N3-C2-O2	-5.17	118.58	122.20
8	UH	316	PRO	N-CA-CB	5.17	109.50	103.30
56	D3	469	C	C2-N1-C1'	5.17	124.48	118.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	D3	495	C	C6-N1-C2	-5.17	118.23	120.30
56	D3	1265	G	N3-C4-C5	-5.15	126.02	128.60
55	D2	347	U	N1-C2-O2	5.15	126.41	122.80
55	D2	388	C	C6-N1-C2	-5.15	118.24	120.30
55	D2	249	G	C5-C6-N1	5.14	114.07	111.50
55	D2	86	C	N1-C2-O2	-5.13	115.82	118.90
56	D3	1210	C	C2-N3-C4	5.13	122.47	119.90
57	D4	201	C	C6-N1-C2	-5.13	118.25	120.30
56	D3	1494	C	N3-C2-O2	-5.13	118.31	121.90
55	D2	228	A	N7-C8-N9	5.13	116.36	113.80
56	D3	1209	C	C2-N1-C1'	5.12	124.44	118.80
56	D3	1034	C	C6-N1-C2	-5.12	118.25	120.30
56	D3	573	C	N3-C2-O2	-5.12	118.32	121.90
56	D3	551	G	N3-C2-N2	5.11	123.48	119.90
56	D3	1582	U	C5-C4-O4	-5.11	122.83	125.90
56	D3	1703	C	N1-C2-O2	5.11	121.97	118.90
56	D3	1057	U	OP1-P-O3'	5.10	116.43	105.20
56	D3	542	A	C4-C5-N7	5.10	113.25	110.70
56	D3	1673	G	N9-C4-C5	5.10	107.44	105.40
56	D3	552	G	C2-N3-C4	-5.10	109.35	111.90
55	D2	155	A	C8-N9-C4	-5.10	103.76	105.80
55	D2	355	C	C5-C4-N4	-5.09	116.64	120.20
56	D3	1513	G	N1-C2-N3	5.09	126.96	123.90
56	D3	1140	G	N1-C6-O6	-5.09	116.85	119.90
57	D4	201	C	C2-N1-C1'	5.08	124.39	118.80
56	D3	976	G	C6-C5-N7	-5.08	127.35	130.40
56	D3	1054	U	N1-C2-O2	5.08	126.35	122.80
17	UQ	869	MET	CA-C-N	5.08	128.37	117.20
55	D2	501	C	C5-C6-N1	5.07	123.53	121.00
56	D3	542	A	C4-N9-C1'	5.07	135.42	126.30
56	D3	924	A	C6-C5-N7	-5.07	128.75	132.30
55	D2	369	G	C4-N9-C1'	5.06	133.08	126.50
56	D3	1174	C	N1-C2-O2	5.06	121.94	118.90
56	D3	1534	G	C8-N9-C4	-5.06	104.38	106.40
56	D3	1727	G	C8-N9-C1'	-5.06	120.42	127.00
56	D3	886	U	N3-C2-O2	-5.05	118.66	122.20
55	D2	233	G	C8-N9-C1'	-5.05	120.44	127.00
56	D3	573	C	C6-N1-C2	-5.05	118.28	120.30
56	D3	1573	A	P-O3'-C3'	5.05	125.76	119.70
57	D4	314	C	N1-C2-O2	5.04	121.93	118.90
57	D4	308	U	N3-C2-O2	-5.04	118.67	122.20
56	D3	1262	U	N3-C2-O2	-5.04	118.67	122.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	D3	1174	C	N3-C2-O2	-5.03	118.38	121.90
56	D3	1703	C	C6-N1-C2	-5.03	118.29	120.30
55	D2	231	C	N3-C2-O2	-5.03	118.38	121.90
55	D2	189	U	N3-C2-O2	-5.02	118.68	122.20
56	D3	913	G	C4-N9-C1'	5.02	133.02	126.50
56	D3	0	U	P-O3'-C3'	5.01	125.72	119.70
56	D3	553	G	N3-C4-C5	5.01	131.11	128.60
55	D2	66	C	N1-C2-O2	5.01	121.91	118.90
56	D3	551	G	N3-C4-C5	-5.01	126.09	128.60
56	D3	908	U	N1-C2-O2	5.01	126.31	122.80
55	D2	388	C	N1-C2-N3	5.01	122.71	119.20
56	D3	1696	G	N3-C4-N9	-5.01	123.00	126.00
55	D2	369	G	N9-C4-C5	-5.01	103.40	105.40
55	D2	369	G	C8-N9-C1'	-5.00	120.50	127.00
55	D2	82	A	P-O3'-C3'	5.00	125.70	119.70
55	D2	391	C	C6-N1-C1'	-5.00	114.80	120.80

There are no chirality outliers.

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	CD	264	SER	Peptide
26	CE	319	ILE	Peptide
28	CH	237	ASP	Peptide
28	CH	340	GLY	Peptide
28	CH	408	VAL	Peptide
31	CK	453	SER	Peptide
32	CL	276	HIS	Peptide
34	CN	254	LYS	Peptide
44	DF	126	ASP	Peptide
40	JO	191	MET	Peptide
41	JP	283	ASP	Peptide
41	JP	301	PHE	Peptide
41	JP	335	ASN	Peptide
1	UA	289	LEU	Peptide
2	UB	616	LEU	Peptide
4	UD	279	HIS	Peptide
4	UD	309	GLN	Peptide
4	UD	353	GLU	Peptide
5	UE	166	ALA	Peptide
5	UE	248	THR	Peptide
10	UJ	154	ILE	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
10	UJ	602	ASP	Peptide
12	UL	183	ASP	Peptide
12	UL	212	VAL	Peptide
12	UL	243	THR	Peptide
12	UL	451	ASN	Peptide
12	UL	552	ASP	Peptide
13	UM	400	GLY	Peptide
13	UM	421	SER	Peptide
13	UM	426	ILE	Peptide
13	UM	705	SER	Peptide
14	UN	321	HIS	Peptide
17	UQ	180	ASP	Peptide
17	UQ	592	SER	Peptide
20	UU	901	LYS	Peptide
23	UZ	90	ASP	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	UA	4121	0	1858	11	0
2	UB	2512	0	1079	5	0
3	UC	628	0	292	1	0
4	UD	3339	0	1434	15	0
5	UE	2353	0	1028	3	0
6	UF	1456	0	606	2	0
7	UG	2629	0	1182	4	0
8	UH	2190	0	916	23	0
9	UI	517	0	211	0	0
10	UJ	3621	0	1585	8	0
11	UK	1203	0	513	2	0
12	UL	4163	0	1851	31	0
13	UM	3763	0	1688	29	0
14	UN	733	0	308	1	0
15	UO	2441	0	1083	8	0
16	UP	298	0	122	0	0
17	UQ	4122	0	1749	9	0
18	UR	2377	0	1045	4	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	US	2357	0	1007	6	0
20	UU	4181	0	1864	14	0
21	UV	5442	0	2336	8	0
22	UX	862	0	375	2	0
23	UZ	1224	0	510	1	0
24	CA	1190	0	547	2	0
24	CB	1122	0	514	4	0
25	CD	1880	0	871	2	0
26	CE	2155	0	1051	5	0
27	CF	611	0	293	1	0
27	CG	611	0	295	0	0
28	CH	2158	0	965	19	0
29	CI	905	0	380	1	0
30	CJ	1397	0	620	6	0
31	CK	1031	0	456	7	0
32	CL	3859	0	1693	12	0
33	CM	1767	0	795	8	0
34	CN	1154	0	501	3	0
35	JF	1071	0	467	4	0
35	JG	1141	0	500	5	0
36	JH	1295	0	570	3	0
37	JJ	898	0	399	1	0
38	JM	671	0	286	0	0
39	JN	918	0	396	2	0
40	JO	933	0	406	1	0
41	JP	2283	0	999	6	0
42	JQ	312	0	127	0	0
43	DA	1187	0	531	6	0
44	DF	1055	0	496	0	0
45	DH	913	0	400	3	0
46	DJ	915	0	422	1	0
47	DN	742	0	345	1	0
48	DO	587	0	295	2	0
49	DQ	616	0	285	0	0
50	DS	521	0	224	2	0
51	DW	634	0	289	2	0
52	DX	503	0	231	3	0
53	Db	400	0	180	0	0
54	Dc	310	0	134	0	0
55	D2	11160	0	5609	239	0
56	D3	16806	0	8479	350	0
57	D4	3712	0	1882	70	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	Db	1	0	0	0	0
58	UX	1	0	0	0	0
59	CL	1	0	0	0	0
59	UX	1	0	0	0	0
60	CL	32	0	12	0	0
All	All	125991	0	57587	924	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (924) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:D3:1541:G:N2	56:D3:1569:A:C6	1.99	1.31
34:CN:87:LEU:HA	34:CN:125:LEU:O	1.23	1.30
20:UU:228:GLY:HA3	20:UU:246:ILE:O	1.28	1.28
13:UM:30:LYS:HA	13:UM:45:LEU:O	1.22	1.28
7:UG:132:GLY:HA3	7:UG:150:LEU:O	1.26	1.26
18:UR:382:GLY:HA3	18:UR:400:ILE:O	1.35	1.21
56:D3:1541:G:C2	56:D3:1570:A:N6	2.10	1.19
8:UH:341:LEU:HA	8:UH:358:VAL:O	1.02	1.17
8:UH:341:LEU:CA	8:UH:358:VAL:O	1.93	1.17
4:UD:548:GLY:O	4:UD:565:ARG:HA	1.43	1.16
56:D3:1541:G:N2	56:D3:1570:A:C6	2.15	1.14
7:UG:132:GLY:CA	7:UG:150:LEU:O	1.98	1.12
55:D2:101:G:C8	55:D2:103:G:N2	2.17	1.10
56:D3:1677:C:N4	56:D3:1724:U:H3	1.53	1.07
56:D3:1699:G:H21	56:D3:1702:A:N6	1.53	1.06
56:D3:1043:A:H61	56:D3:1075:C:N4	1.53	1.05
56:D3:625:C:H42	56:D3:974:A:N6	1.54	1.05
56:D3:1541:G:C2	56:D3:1569:A:N6	2.26	1.03
56:D3:1654:G:H21	56:D3:1746:A:N6	1.56	1.02
56:D3:1267:G:C6	56:D3:1442:U:N3	2.28	1.01
56:D3:1699:G:N2	56:D3:1702:A:H62	1.58	1.01
56:D3:625:C:N4	56:D3:974:A:H61	1.58	1.01
56:D3:1267:G:O6	56:D3:1442:U:C4	2.14	1.01
56:D3:1158:C:H42	56:D3:1163:A:H61	1.03	1.01
56:D3:1646:C:N4	56:D3:1754:A:H61	1.58	0.99
56:D3:628:G:N2	56:D3:971:A:H62	1.60	0.98
56:D3:1654:G:N2	56:D3:1746:A:N6	2.13	0.96
55:D2:174:U:H3	55:D2:222:G:H1	0.96	0.96

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:D3:1043:A:N6	56:D3:1075:C:H42	1.61	0.96
56:D3:1646:C:H42	56:D3:1754:A:N6	1.61	0.96
56:D3:628:G:H21	56:D3:971:A:N6	1.65	0.95
57:D4:95:A:H61	57:D4:321:C:H42	0.97	0.95
56:D3:625:C:H42	56:D3:974:A:H61	0.96	0.94
57:D4:205:G:N1	57:D4:245:U:C2	2.36	0.94
56:D3:1044:U:H3	56:D3:1074:G:H1	1.04	0.94
56:D3:1654:G:N2	56:D3:1746:A:H62	1.64	0.94
55:D2:254:C:N4	55:D2:440:U:H3	1.65	0.93
56:D3:477:A:N6	56:D3:539:G:H21	1.65	0.93
55:D2:182:G:H1	55:D2:215:U:H3	1.12	0.93
56:D3:1655:A:N6	56:D3:1745:G:H1	1.68	0.92
56:D3:1775:U:H3	56:D3:1786:G:H1	1.13	0.92
56:D3:477:A:H61	56:D3:539:G:H21	1.13	0.91
56:D3:477:A:H61	56:D3:539:G:N2	1.67	0.91
56:D3:867:G:H1	56:D3:961:U:H3	1.14	0.91
56:D3:1655:A:H61	56:D3:1745:G:N2	1.68	0.91
56:D3:895:G:H1	56:D3:917:U:H3	1.16	0.90
15:UO:279:GLY:CA	15:UO:298:PHE:O	2.20	0.90
55:D2:360:C:N4	55:D2:366:A:H61	1.70	0.89
55:D2:254:C:H42	55:D2:440:U:H3	0.91	0.89
56:D3:1267:G:C6	56:D3:1442:U:C4	2.61	0.89
15:UO:279:GLY:HA3	15:UO:298:PHE:O	1.72	0.88
56:D3:976:G:N2	56:D3:978:A:N6	2.21	0.87
33:CM:306:GLU:HA	33:CM:356:GLY:O	1.74	0.87
56:D3:1541:G:N2	56:D3:1570:A:N6	2.18	0.86
56:D3:1689:A:N6	56:D3:1713:G:N2	2.23	0.86
55:D2:546:G:C6	55:D2:592:U:O2	2.28	0.86
56:D3:1541:G:C2	56:D3:1570:A:C6	2.60	0.85
55:D2:467:A:H61	57:D4:49:C:N4	1.73	0.85
56:D3:1541:G:C2	56:D3:1569:A:C6	2.64	0.85
21:UV:143:GLU:HA	21:UV:176:PHE:O	1.76	0.85
55:D2:184:U:H3	55:D2:213:G:H1	1.20	0.85
56:D3:1158:C:N4	56:D3:1163:A:H61	1.74	0.85
56:D3:1582:U:C2	56:D3:1614:A:N7	2.45	0.84
56:D3:1655:A:N6	56:D3:1745:G:H22	1.74	0.84
28:CH:190:VAL:HA	28:CH:195:GLN:O	1.77	0.84
8:UH:57:ASN:O	8:UH:70:SER:HA	1.78	0.83
55:D2:101:G:C5	55:D2:103:G:C2	2.65	0.83
13:UM:542:CYS:O	13:UM:546:LYS:HA	1.77	0.83
56:D3:628:G:H21	56:D3:971:A:H62	0.86	0.82

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:UM:589:GLN:HA	13:UM:602:TRP:O	1.81	0.81
55:D2:498:G:O6	55:D2:540:U:C4	2.34	0.81
18:UR:382:GLY:O	18:UR:399:LYS:HA	1.81	0.81
56:D3:1541:G:N2	56:D3:1569:A:C5	2.49	0.81
55:D2:121:G:H21	55:D2:124:A:H62	1.28	0.80
56:D3:1646:C:H42	56:D3:1754:A:H61	0.82	0.80
4:UD:548:GLY:O	4:UD:565:ARG:CA	2.26	0.80
56:D3:1677:C:H42	56:D3:1724:U:H3	0.82	0.80
56:D3:1699:G:H21	56:D3:1702:A:H62	0.81	0.79
55:D2:516:U:O2	55:D2:519:A:N7	2.17	0.78
56:D3:1043:A:H61	56:D3:1075:C:H42	0.81	0.78
30:CJ:150:THR:HA	30:CJ:167:LEU:O	1.83	0.77
56:D3:1158:C:H42	56:D3:1163:A:N6	1.81	0.77
55:D2:101:G:H3'	55:D2:103:G:H21	1.49	0.77
13:UM:30:LYS:CA	13:UM:45:LEU:O	2.19	0.76
1:UA:390:VAL:HA	1:UA:406:SER:HA	1.68	0.76
57:D4:95:A:N6	57:D4:321:C:H42	1.81	0.75
26:CE:2:ALA:HB3	26:CE:17:ALA:O	1.87	0.75
55:D2:24:U:H3	55:D2:56:G:H1	1.31	0.75
56:D3:1267:G:N1	56:D3:1442:U:C2	2.55	0.75
55:D2:506:G:N2	55:D2:531:C:O2	2.21	0.74
55:D2:360:C:N4	55:D2:366:A:N6	2.35	0.74
57:D4:114:A:C6	57:D4:254:A:C2	2.76	0.73
4:UD:199:ASP:HA	4:UD:215:ALA:O	1.88	0.73
28:CH:421:ASN:HA	28:CH:436:GLU:O	1.88	0.73
56:D3:1655:A:N6	56:D3:1745:G:N2	2.35	0.73
56:D3:1270:G:N2	56:D3:1441:C:O2	2.22	0.73
55:D2:101:G:N7	55:D2:103:G:N2	2.36	0.73
12:UL:412:GLY:HA3	12:UL:430:CYS:H	1.54	0.72
34:CN:87:LEU:CA	34:CN:125:LEU:O	2.19	0.72
56:D3:1734:U:H2'	56:D3:1735:U:C5'	2.20	0.72
20:UU:125:GLY:HA2	26:CE:430:ASP:HA	1.72	0.72
15:UO:279:GLY:HA2	15:UO:298:PHE:O	1.89	0.71
56:D3:872:G:N2	56:D3:956:C:O2	2.22	0.71
12:UL:364:TYR:O	12:UL:382:THR:O	2.09	0.71
55:D2:238:G:O6	55:D2:275:A:C6	2.43	0.71
56:D3:1663:G:H1	56:D3:1738:U:H3	1.37	0.71
55:D2:121:G:N2	55:D2:124:A:H62	1.88	0.71
56:D3:867:G:N2	56:D3:961:U:O2	2.23	0.71
20:UU:416:ALA:HB3	20:UU:433:ALA:HB3	1.73	0.71
55:D2:121:G:H21	55:D2:124:A:N6	1.89	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:JG:41:MET:O	35:JG:110:LEU:HA	1.91	0.70
56:D3:23:G:C2	56:D3:603:U:O2	2.44	0.70
56:D3:34:G:O6	56:D3:474:A:C5	2.45	0.70
57:D4:114:A:C5	57:D4:254:A:C6	2.79	0.70
56:D3:868:G:H1	56:D3:960:U:H3	1.39	0.69
57:D4:263:A:C6	57:D4:309:G:C2	2.80	0.69
56:D3:473:A:C6	56:D3:474:A:N6	2.60	0.69
56:D3:1689:A:N6	56:D3:1713:G:C2	2.60	0.69
55:D2:554:G:N2	55:D2:583:U:O2	2.25	0.69
56:D3:1164:G:H2'	56:D3:1165:G:H8	1.57	0.69
56:D3:1530:C:H2'	56:D3:1531:G:H8	1.58	0.69
56:D3:1582:U:O2	56:D3:1614:A:C5	2.46	0.69
56:D3:1273:G:O6	56:D3:1437:U:O2	2.11	0.68
19:US:180:PHE:O	19:US:185:TYR:N	2.27	0.68
56:D3:1273:G:O6	56:D3:1437:U:C2	2.47	0.68
12:UL:209:GLY:O	12:UL:219:THR:HA	1.94	0.68
56:D3:625:C:N3	56:D3:974:A:N1	2.42	0.68
24:CB:264:GLN:HA	24:CB:320:TYR:O	1.94	0.68
13:UM:540:SER:O	13:UM:548:LEU:HA	1.93	0.68
55:D2:514:U:H3	55:D2:521:G:H1	1.41	0.68
56:D3:868:G:N2	56:D3:960:U:O2	2.25	0.68
56:D3:1734:U:H2'	56:D3:1735:U:H5'	1.76	0.68
55:D2:101:G:N7	55:D2:103:G:C2	2.62	0.67
55:D2:168:G:H22	55:D2:227:U:H3	1.42	0.67
55:D2:360:C:H42	55:D2:366:A:N6	1.91	0.67
56:D3:1541:G:N2	56:D3:1569:A:N1	2.41	0.67
56:D3:519:C:N4	56:D3:534:A:C8	2.63	0.67
55:D2:554:G:N1	55:D2:583:U:N3	2.43	0.67
56:D3:33:U:O2	56:D3:468:A:C5	2.49	0.66
56:D3:1698:G:C6	56:D3:1704:U:N3	2.64	0.66
55:D2:161:A:N6	55:D2:233:G:C5	2.64	0.66
55:D2:6:A:N6	55:D2:8:A:N3	2.43	0.66
55:D2:103:G:O2'	55:D2:104:A:N7	2.26	0.66
10:UJ:407:PHE:O	10:UJ:410:ILE:O	2.14	0.65
57:D4:312:U:H2'	57:D4:313:A:C8	2.32	0.65
55:D2:467:A:N6	57:D4:49:C:N4	2.44	0.65
56:D3:479:C:O2	56:D3:510:G:N2	2.30	0.65
56:D3:1541:G:N1	56:D3:1569:A:N6	2.44	0.65
41:JP:351:VAL:HA	41:JP:367:SER:HA	1.78	0.65
55:D2:361:G:N2	55:D2:364:A:OP2	2.29	0.65
55:D2:498:G:O6	55:D2:540:U:O4	2.15	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:D3:477:A:N6	56:D3:539:G:N2	2.35	0.64
56:D3:1782:A:OP2	56:D3:1783:C:N4	2.30	0.64
57:D4:113:G:O2'	57:D4:256:G:N2	2.29	0.64
56:D3:23:G:N1	56:D3:603:U:C2	2.65	0.64
10:UJ:550:TYR:O	10:UJ:553:SER:C	2.36	0.64
55:D2:254:C:N3	55:D2:440:U:O4	2.30	0.64
52:DX:89:ASN:O	52:DX:92:CYS:N	2.28	0.64
56:D3:1267:G:C6	56:D3:1442:U:C2	2.85	0.64
35:JG:44:VAL:HA	35:JG:113:TYR:O	1.98	0.64
56:D3:1068:C:H2'	56:D3:1069:A:H8	1.62	0.63
55:D2:125:G:H2'	55:D2:126:A:H8	1.62	0.63
13:UM:304:LEU:O	13:UM:311:LEU:HA	1.97	0.63
55:D2:489:G:N2	55:D2:495:G:O3'	2.31	0.63
56:D3:1663:G:O6	56:D3:1738:U:O4	2.16	0.63
20:UU:118:VAL:HA	20:UU:132:THR:HA	1.81	0.63
57:D4:205:G:N1	57:D4:245:U:N3	2.47	0.63
56:D3:897:C:O2'	56:D3:914:G:N2	2.31	0.63
56:D3:1468:U:H2'	56:D3:1469:A:H8	1.64	0.63
8:UH:312:ASP:HA	8:UH:323:PHE:O	1.98	0.63
20:UU:179:LYS:HA	20:UU:191:PHE:O	1.98	0.63
56:D3:1690:G:N2	56:D3:1711:C:C2	2.65	0.63
41:JP:363:ILE:O	41:JP:374:LEU:HA	1.98	0.63
56:D3:1471:A:OP2	56:D3:1573:A:N6	2.32	0.62
56:D3:1663:G:N1	56:D3:1738:U:N3	2.43	0.62
55:D2:197:G:N2	55:D2:200:A:OP2	2.31	0.62
56:D3:634:G:C2	56:D3:966:A:N6	2.68	0.62
56:D3:1272:U:O2	56:D3:1438:G:O6	2.18	0.62
56:D3:1541:G:N1	56:D3:1570:A:N6	2.47	0.62
12:UL:364:TYR:O	12:UL:382:THR:C	2.37	0.62
12:UL:476:ILE:HA	12:UL:492:SER:HA	1.81	0.62
55:D2:171:G:O6	55:D2:226:U:C4	2.53	0.62
56:D3:1665:U:C2	56:D3:1737:G:N1	2.68	0.62
13:UM:418:ASN:O	13:UM:422:CYS:C	2.38	0.61
33:CM:249:SER:O	33:CM:253:GLY:CA	2.48	0.61
55:D2:353:A:H4'	55:D2:354:G:H5'	1.81	0.61
56:D3:1270:G:C2	56:D3:1441:C:O2	2.52	0.61
21:UV:251:PHE:O	21:UV:272:CYS:HA	2.00	0.61
32:CL:776:GLN:O	32:CL:780:ILE:N	2.30	0.61
5:UE:191:VAL:HA	5:UE:206:ALA:HA	1.81	0.61
56:D3:1164:G:H2'	56:D3:1165:G:C8	2.35	0.61
56:D3:1707:A:H8	56:D3:1707:A:P	2.22	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:UM:418:ASN:O	13:UM:422:CYS:HA	2.01	0.61
33:CM:249:SER:O	33:CM:253:GLY:N	2.33	0.61
56:D3:936:G:OP1	56:D3:1074:G:N2	2.30	0.61
55:D2:20:C:H2'	55:D2:21:A:H8	1.65	0.61
55:D2:123:C:OP2	55:D2:124:A:N6	2.33	0.61
57:D4:8:U:H2'	57:D4:9:A:H8	1.65	0.61
8:UH:212:SER:HA	8:UH:219:ALA:HA	1.83	0.60
55:D2:242:C:H2'	55:D2:243:A:H8	1.65	0.60
56:D3:634:G:N2	56:D3:965:U:OP2	2.34	0.60
1:UA:482:SER:O	1:UA:486:SER:N	2.35	0.60
31:CK:453:SER:O	31:CK:455:HIS:N	2.35	0.60
43:DA:91:VAL:HA	43:DA:96:LEU:HA	1.83	0.60
56:D3:480:G:H2'	56:D3:481:A:H8	1.66	0.60
57:D4:205:G:N2	57:D4:245:U:O2	2.34	0.60
55:D2:436:G:H2'	55:D2:437:G:C8	2.37	0.60
56:D3:32:U:O2	56:D3:595:G:C2	2.55	0.60
57:D4:8:U:H2'	57:D4:9:A:C8	2.37	0.60
57:D4:111:G:O6	57:D4:260:U:O4	2.20	0.60
8:UH:67:PRO:HA	8:UH:80:GLU:O	2.01	0.60
17:UQ:745:ILE:O	17:UQ:754:LEU:N	2.35	0.59
55:D2:184:U:O2	55:D2:213:G:N2	2.32	0.59
8:UH:341:LEU:O	8:UH:357:HIS:HA	2.02	0.59
56:D3:1775:U:H2'	56:D3:1776:A:H8	1.67	0.59
28:CH:518:LYS:O	28:CH:560:ARG:N	2.34	0.59
57:D4:250:C:H2'	57:D4:251:G:C8	2.38	0.59
12:UL:227:LYS:HA	12:UL:246:GLY:O	2.03	0.59
57:D4:3:C:H2'	57:D4:4:G:H8	1.68	0.59
1:UA:581:THR:H	1:UA:596:GLY:HA2	1.68	0.59
56:D3:1715:G:H5'	56:D3:1716:C:OP2	2.03	0.59
13:UM:622:ALA:HB3	13:UM:635:ALA:HB3	1.85	0.59
17:UQ:101:GLN:O	17:UQ:104:ALA:N	2.36	0.59
41:JP:288:TYR:O	41:JP:298:LEU:N	2.36	0.59
55:D2:238:G:H4'	55:D2:239:U:H5'	1.82	0.59
4:UD:595:ASN:N	4:UD:610:VAL:O	2.36	0.59
28:CH:402:ILE:HA	28:CH:417:SER:HA	1.85	0.59
12:UL:940:GLY:HA2	31:CK:465:LEU:HA	1.85	0.59
35:JF:41:MET:O	35:JF:110:LEU:HA	2.02	0.59
56:D3:1707:A:H8	56:D3:1707:A:O5'	1.84	0.59
57:D4:114:A:N6	57:D4:254:A:C2	2.71	0.59
12:UL:88:HIS:O	12:UL:92:ASP:N	2.36	0.58
56:D3:566:C:H2'	56:D3:567:A:H8	1.67	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:UD:534:LEU:HA	4:UD:542:VAL:O	2.02	0.58
56:D3:1202:A:H3'	56:D3:1203:A:H8	1.67	0.58
43:DA:2:ALA:N	48:DO:45:GLY:O	2.36	0.58
13:UM:29:GLY:O	13:UM:45:LEU:O	2.22	0.58
56:D3:629:U:OP2	56:D3:969:C:N4	2.36	0.58
56:D3:1082:C:H2'	56:D3:1083:G:H8	1.68	0.58
1:UA:482:SER:O	1:UA:486:SER:HA	2.04	0.58
56:D3:519:C:N4	56:D3:534:A:N7	2.52	0.58
55:D2:158:G:H2'	55:D2:159:A:H8	1.68	0.58
55:D2:174:U:O4	55:D2:222:G:O6	2.22	0.58
56:D3:1041:G:H2'	56:D3:1042:G:C8	2.38	0.58
57:D4:197:G:N1	57:D4:246:A:OP2	2.37	0.58
28:CH:526:VAL:HA	28:CH:538:ARG:O	2.03	0.58
56:D3:519:C:C4	56:D3:534:A:C5	2.92	0.58
12:UL:48:ASP:HA	12:UL:63:LEU:O	2.02	0.58
13:UM:588:LYS:O	13:UM:604:CYS:N	2.35	0.58
56:D3:1692:G:C6	56:D3:1710:U:C4	2.91	0.58
15:UO:95:LEU:HA	15:UO:109:ASP:HA	1.85	0.57
55:D2:490:G:H1'	55:D2:495:G:H5'	1.86	0.57
55:D2:117:G:H2'	55:D2:118:A:C8	2.39	0.57
57:D4:114:A:C8	57:D4:254:A:N6	2.73	0.57
13:UM:105:SER:HA	13:UM:121:GLY:HA2	1.86	0.57
12:UL:599:ILE:O	12:UL:608:HIS:N	2.38	0.57
28:CH:191:SER:O	28:CH:194:LEU:N	2.37	0.57
30:CJ:43:PRO:O	30:CJ:47:ALA:HB2	2.05	0.57
56:D3:1461:C:H2'	56:D3:1462:G:H8	1.70	0.57
13:UM:550:THR:O	13:UM:557:VAL:HA	2.04	0.57
57:D4:114:A:C6	57:D4:254:A:N1	2.71	0.57
55:D2:210:U:H2'	55:D2:211:G:H8	1.70	0.56
55:D2:490:G:N3	55:D2:494:C:O2'	2.36	0.56
56:D3:1688:U:H2'	56:D3:1689:A:H8	1.68	0.56
13:UM:542:CYS:O	13:UM:546:LYS:CA	2.52	0.56
55:D2:24:U:O4	55:D2:56:G:O6	2.23	0.56
55:D2:334:G:H2'	55:D2:335:G:H8	1.70	0.56
56:D3:467:G:O2'	56:D3:469:C:OP2	2.20	0.56
56:D3:1692:G:O6	56:D3:1710:U:O4	2.23	0.56
56:D3:1716:C:H6	56:D3:1716:C:O5'	1.88	0.56
57:D4:18:G:H2'	57:D4:19:A:H8	1.70	0.56
25:CD:264:SER:O	25:CD:266:THR:N	2.33	0.56
56:D3:1082:C:H2'	56:D3:1083:G:C8	2.39	0.56
56:D3:1204:A:O2'	56:D3:1208:A:N3	2.33	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CL:72:VAL:HA	32:CL:137:LEU:O	2.05	0.56
41:JP:283:ASP:O	41:JP:285:ASN:N	2.37	0.56
56:D3:937:C:H2'	56:D3:938:G:C8	2.41	0.56
11:UK:230:LYS:O	55:D2:236:C:N4	2.27	0.56
55:D2:456:U:H2'	55:D2:457:G:C8	2.41	0.56
56:D3:871:G:H2'	56:D3:872:G:C8	2.41	0.56
57:D4:114:A:N7	57:D4:254:A:C6	2.74	0.56
56:D3:868:G:H2'	56:D3:869:A:H8	1.71	0.56
56:D3:1688:U:H2'	56:D3:1689:A:C8	2.41	0.56
20:UU:228:GLY:CA	20:UU:246:ILE:O	2.24	0.56
26:CE:431:ALA:HB3	55:D2:309:A:H61	1.71	0.56
55:D2:2:U:H2'	55:D2:3:G:H8	1.71	0.56
55:D2:193:G:H2'	55:D2:194:G:H8	1.71	0.56
55:D2:189:U:C2	55:D2:209:G:N1	2.74	0.56
55:D2:540:U:O2'	55:D2:542:U:OP2	2.23	0.56
56:D3:478:A:N1	56:D3:510:G:O6	2.39	0.56
56:D3:1655:A:N6	56:D3:1745:G:N1	2.32	0.56
4:UD:198:ASP:O	4:UD:215:ALA:O	2.24	0.56
28:CH:160:ILE:HA	28:CH:188:TYR:O	2.05	0.56
56:D3:23:G:C6	56:D3:603:U:N3	2.74	0.56
56:D3:1506:G:H2'	56:D3:1507:G:H8	1.71	0.56
13:UM:30:LYS:C	13:UM:45:LEU:H	2.09	0.56
55:D2:177:U:H3	55:D2:220:U:H3	1.53	0.55
56:D3:34:G:O6	56:D3:474:A:N7	2.39	0.55
12:UL:258:LYS:O	12:UL:274:ILE:HA	2.05	0.55
31:CK:328:GLY:N	56:D3:576:G:OP1	2.37	0.55
55:D2:117:G:H2'	55:D2:118:A:H8	1.71	0.55
55:D2:515:G:N2	55:D2:521:G:N7	2.54	0.55
28:CH:150:THR:O	28:CH:562:GLY:HA3	2.05	0.55
55:D2:467:A:N6	57:D4:49:C:H42	2.04	0.55
55:D2:554:G:N1	55:D2:583:U:C2	2.74	0.55
4:UD:265:TRP:HA	4:UD:272:LEU:HA	1.88	0.55
28:CH:424:LEU:O	28:CH:433:ILE:N	2.38	0.55
55:D2:2:U:H2'	55:D2:3:G:C8	2.42	0.55
28:CH:405:VAL:HA	28:CH:414:ILE:O	2.07	0.55
56:D3:976:G:N2	56:D3:978:A:H61	2.01	0.55
7:UG:132:GLY:HA2	7:UG:150:LEU:O	2.01	0.55
55:D2:24:U:N3	55:D2:56:G:N1	2.43	0.55
1:UA:482:SER:O	1:UA:486:SER:CA	2.55	0.55
56:D3:1270:G:H2'	56:D3:1271:G:H8	1.71	0.55
8:UH:209:PHE:CB	8:UH:222:PHE:O	2.55	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:CM:249:SER:O	33:CM:253:GLY:HA2	2.07	0.55
34:CN:200:GLU:O	34:CN:204:SER:CB	2.55	0.55
55:D2:238:G:C6	55:D2:275:A:C6	2.95	0.55
56:D3:1736:G:H2'	56:D3:1737:G:C8	2.42	0.55
4:UD:614:TRP:O	4:UD:618:ASN:CB	2.55	0.55
24:CA:201:HIS:O	24:CA:204:GLY:N	2.40	0.55
28:CH:442:ILE:HA	28:CH:472:PRO:HA	1.89	0.55
55:D2:22:A:H2'	55:D2:23:G:C8	2.41	0.55
56:D3:33:U:C2	56:D3:468:A:N7	2.75	0.55
43:DA:139:ALA:HA	43:DA:212:VAL:HA	1.89	0.54
55:D2:171:G:C6	55:D2:226:U:N3	2.75	0.54
55:D2:223:C:H2'	55:D2:224:G:C8	2.42	0.54
55:D2:271:G:H2'	55:D2:272:A:H8	1.71	0.54
55:D2:389:U:H2'	55:D2:390:C:C6	2.42	0.54
56:D3:884:A:H2'	56:D3:885:G:H8	1.72	0.54
56:D3:897:C:N4	56:D3:914:G:O2'	2.40	0.54
56:D3:1111:G:H2'	56:D3:1112:G:C8	2.43	0.54
56:D3:1274:C:C4	56:D3:1275:A:N6	2.75	0.54
56:D3:1582:U:C2	56:D3:1614:A:C8	2.94	0.54
56:D3:923:A:H2'	56:D3:924:A:C8	2.42	0.54
56:D3:938:G:N2	56:D3:941:A:OP2	2.35	0.54
19:US:171:ALA:HB1	19:US:217:GLY:HA2	1.90	0.54
4:UD:485:LYS:HA	4:UD:498:VAL:O	2.08	0.54
30:CJ:43:PRO:O	30:CJ:47:ALA:CB	2.56	0.54
30:CJ:189:LEU:O	31:CK:379:ASP:N	2.41	0.54
55:D2:210:U:H2'	55:D2:211:G:C8	2.43	0.54
56:D3:1512:G:H2'	56:D3:1513:G:C8	2.42	0.54
55:D2:503:C:H2'	55:D2:504:U:H6	1.72	0.54
56:D3:537:G:O2'	56:D3:543:C:N4	2.41	0.54
57:D4:114:A:C5	57:D4:254:A:N1	2.75	0.54
32:CL:281:PRO:HA	32:CL:782:GLY:HA3	1.89	0.54
41:JP:58:PHE:O	57:D4:32:G:N1	2.35	0.54
56:D3:1528:U:H2'	56:D3:1529:C:C6	2.43	0.54
55:D2:101:G:C8	55:D2:103:G:C2	2.94	0.54
56:D3:1044:U:O4	56:D3:1074:G:O6	2.25	0.54
56:D3:1057:U:O2'	56:D3:1058:U:O4'	2.26	0.54
56:D3:1202:A:H3'	56:D3:1203:A:C8	2.43	0.54
18:UR:358:PHE:HA	18:UR:376:LEU:O	2.08	0.54
56:D3:1267:G:H22	56:D3:1442:U:H2'	1.73	0.54
12:UL:284:PHE:HA	12:UL:329:PHE:H	1.72	0.53
55:D2:445:U:H2'	55:D2:446:U:C6	2.43	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:D4:77:U:H2'	57:D4:78:G:H8	1.72	0.53
1:UA:785:PHE:O	1:UA:789:SER:CB	2.57	0.53
10:UJ:407:PHE:O	10:UJ:410:ILE:C	2.47	0.53
55:D2:334:G:H2'	55:D2:335:G:C8	2.44	0.53
55:D2:467:A:H61	57:D4:49:C:H42	1.55	0.53
56:D3:1080:U:H2'	56:D3:1081:A:H8	1.74	0.53
55:D2:404:G:N2	55:D2:452:A:OP2	2.41	0.53
56:D3:477:A:C6	56:D3:539:G:N2	2.76	0.53
56:D3:1129:U:O4	56:D3:1140:G:O6	2.27	0.53
56:D3:1698:G:N1	56:D3:1704:U:N3	2.56	0.53
13:UM:438:THR:H	13:UM:458:SER:HA	1.73	0.53
28:CH:478:LEU:HA	28:CH:488:ILE:O	2.08	0.53
55:D2:411:A:H2'	55:D2:412:A:C8	2.44	0.53
55:D2:413:C:H2'	55:D2:414:G:H8	1.73	0.53
56:D3:32:U:C2	56:D3:595:G:N1	2.77	0.53
55:D2:249:G:H2'	55:D2:250:G:C8	2.44	0.53
21:UV:362:ALA:HB2	21:UV:418:SER:HA	1.90	0.53
37:JJ:268:SER:O	37:JJ:272:GLU:CB	2.57	0.53
55:D2:192:G:H2'	55:D2:193:G:H8	1.74	0.53
55:D2:546:G:O6	55:D2:592:U:C2	2.62	0.53
56:D3:931:C:H5''	56:D3:932:U:H2'	1.91	0.53
56:D3:1665:U:O2	56:D3:1737:G:C2	2.61	0.53
21:UV:467:LEU:O	21:UV:475:ASN:HA	2.09	0.53
56:D3:505:A:O2'	56:D3:585:A:N6	2.35	0.53
12:UL:938:VAL:HA	31:CK:467:ILE:HA	1.90	0.52
55:D2:101:G:C5	55:D2:103:G:N1	2.77	0.52
55:D2:136:U:H2'	55:D2:137:C:H6	1.74	0.52
55:D2:446:U:H2'	55:D2:447:G:H8	1.74	0.52
56:D3:862:A:O2'	56:D3:963:A:N1	2.34	0.52
25:CD:14:GLY:HA3	25:CD:55:PRO:HA	1.91	0.52
28:CH:423:CYS:HA	28:CH:434:PHE:O	2.10	0.52
56:D3:1450:U:H2'	56:D3:1451:C:C6	2.45	0.52
13:UM:30:LYS:HA	13:UM:45:LEU:C	2.18	0.52
55:D2:446:U:H2'	55:D2:447:G:C8	2.43	0.52
55:D2:524:U:O2'	55:D2:526:U:OP1	2.18	0.52
56:D3:1061:A:H2'	56:D3:1062:A:H4'	1.90	0.52
56:D3:1068:C:H2'	56:D3:1069:A:C8	2.43	0.52
8:UH:334:THR:HA	8:UH:345:LEU:HA	1.91	0.52
39:JN:293:ALA:N	56:D3:9:U:OP2	2.41	0.52
55:D2:494:C:H2'	55:D2:495:G:H8	1.74	0.52
56:D3:32:U:N3	56:D3:595:G:N1	2.57	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:D3:522:U:H2'	56:D3:523:G:C8	2.44	0.52
56:D3:1606:C:H2'	56:D3:1607:G:C8	2.45	0.52
5:UE:162:GLN:HA	5:UE:173:ILE:O	2.08	0.52
55:D2:182:G:H2'	55:D2:183:A:H8	1.74	0.52
56:D3:1151:A:H2'	56:D3:1152:A:H8	1.74	0.52
55:D2:182:G:H2'	55:D2:183:A:C8	2.44	0.52
56:D3:1270:G:N2	56:D3:1441:C:C2	2.78	0.52
56:D3:1582:U:O2	56:D3:1614:A:N7	2.43	0.52
57:D4:33:A:O2'	57:D4:34:A:O4'	2.24	0.52
2:UB:282:ARG:H	36:JH:381:ALA:HB1	1.74	0.52
55:D2:411:A:H2'	55:D2:412:A:H8	1.73	0.52
56:D3:1171:A:H2'	56:D3:1172:G:H8	1.75	0.52
4:UD:586:THR:O	4:UD:589:ASN:N	2.42	0.52
56:D3:1275:A:N1	56:D3:1435:G:C2	2.78	0.52
17:UQ:18:GLY:HA3	17:UQ:781:SER:O	2.10	0.52
19:US:285:ILE:O	19:US:289:PHE:N	2.43	0.52
35:JG:55:ILE:O	35:JG:63:ASP:N	2.43	0.52
56:D3:1080:U:H2'	56:D3:1081:A:C8	2.45	0.52
56:D3:1734:U:C2'	56:D3:1735:U:C5'	2.86	0.52
55:D2:217:C:H2'	55:D2:218:U:H6	1.73	0.51
55:D2:289:U:H2'	55:D2:290:G:H8	1.75	0.51
56:D3:540:G:O2'	56:D3:542:A:OP2	2.28	0.51
56:D3:483:A:H2'	56:D3:484:C:C6	2.45	0.51
56:D3:1746:A:O2'	56:D3:1747:G:O4'	2.29	0.51
20:UU:45:GLY:O	55:D2:308:A:O2'	2.28	0.51
55:D2:238:G:N1	55:D2:275:A:C5	2.78	0.51
55:D2:400:C:H2'	55:D2:401:A:H8	1.75	0.51
56:D3:1716:C:H2'	56:D3:1717:G:H5''	1.91	0.51
1:UA:308:VAL:HA	1:UA:318:ALA:O	2.10	0.51
2:UB:270:TYR:HA	36:JH:354:ALA:HB1	1.92	0.51
55:D2:184:U:O4	55:D2:213:G:O6	2.29	0.51
56:D3:1739:C:H2'	56:D3:1740:A:H8	1.75	0.51
56:D3:1775:U:H2'	56:D3:1776:A:C8	2.44	0.51
1:UA:501:SER:O	1:UA:507:GLN:HA	2.11	0.51
20:UU:142:LYS:HA	20:UU:150:PRO:HA	1.91	0.51
32:CL:846:VAL:HA	32:CL:855:GLN:HA	1.92	0.51
55:D2:378:C:H2'	55:D2:379:A:H8	1.75	0.51
55:D2:495:G:H2'	55:D2:496:G:C8	2.45	0.51
55:D2:513:G:N1	55:D2:523:U:N3	2.58	0.51
56:D3:590:C:H2'	56:D3:591:A:C8	2.46	0.51
57:D4:202:G:O6	57:D4:247:U:O2	2.27	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:UL:552:ASP:O	12:UL:554:THR:N	2.43	0.51
56:D3:924:A:H2'	56:D3:925:G:C8	2.45	0.51
56:D3:1144:U:O2'	56:D3:1146:G:OP2	2.21	0.51
8:UH:303:GLN:HA	8:UH:313:LYS:HA	1.93	0.51
56:D3:868:G:H2'	56:D3:869:A:C8	2.45	0.51
22:UX:50:ALA:HB1	22:UX:58:ALA:HB2	1.93	0.51
30:CJ:88:ILE:HA	30:CJ:138:ASP:O	2.10	0.51
55:D2:456:U:H2'	55:D2:457:G:H8	1.76	0.51
57:D4:95:A:H61	57:D4:321:C:N4	1.83	0.51
56:D3:1689:A:N6	56:D3:1690:G:O6	2.44	0.51
56:D3:1787:C:H2'	56:D3:1788:G:H8	1.76	0.51
4:UD:353:GLU:O	4:UD:355:THR:N	2.44	0.51
55:D2:145:A:H2'	55:D2:146:G:H8	1.74	0.51
55:D2:436:G:H2'	55:D2:437:G:H8	1.75	0.51
56:D3:1267:G:C5	56:D3:1442:U:N3	2.75	0.51
56:D3:1650:U:H2'	56:D3:1651:A:C8	2.45	0.51
56:D3:1683:C:O2'	56:D3:1684:U:O5'	2.29	0.51
55:D2:495:G:H2'	55:D2:496:G:H8	1.76	0.50
56:D3:1715:G:C5'	56:D3:1716:C:OP2	2.59	0.50
56:D3:1746:A:HO2'	56:D3:1747:G:H8	1.57	0.50
7:UG:356:GLY:HA3	55:D2:315:U:H5'	1.92	0.50
8:UH:295:TYR:HA	8:UH:302:LEU:HA	1.92	0.50
17:UQ:295:TRP:O	55:D2:84:G:O2'	2.30	0.50
55:D2:262:U:C4	55:D2:263:C:N4	2.79	0.50
12:UL:123:ALA:O	12:UL:141:LYS:N	2.45	0.50
13:UM:361:SER:HA	13:UM:384:TYR:O	2.11	0.50
15:UO:84:VAL:HA	15:UO:100:ASP:HA	1.93	0.50
55:D2:20:C:H2'	55:D2:21:A:C8	2.46	0.50
55:D2:24:U:O2	55:D2:56:G:N2	2.42	0.50
56:D3:1541:G:N2	56:D3:1569:A:N6	2.34	0.50
33:CM:114:PHE:O	33:CM:169:VAL:HA	2.11	0.50
56:D3:1594:G:N1	56:D3:1603:U:N3	2.60	0.50
56:D3:1735:U:C2	56:D3:1736:G:H1'	2.46	0.50
12:UL:49:VAL:O	12:UL:62:LYS:HA	2.11	0.50
17:UQ:318:GLU:O	17:UQ:320:VAL:N	2.43	0.50
21:UV:552:ARG:O	21:UV:556:ILE:HA	2.11	0.50
55:D2:533:G:H2'	55:D2:534:A:C8	2.47	0.50
56:D3:1170:G:O6	56:D3:1469:A:N1	2.45	0.50
56:D3:1692:G:C6	56:D3:1710:U:N3	2.79	0.50
55:D2:180:G:H2'	55:D2:181:A:H8	1.76	0.50
55:D2:205:C:H2'	55:D2:206:A:C8	2.47	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:D3:1140:G:H2'	56:D3:1141:G:C8	2.46	0.50
47:DN:10:GLY:HA3	56:D3:955:A:H5''	1.93	0.50
55:D2:22:A:H2'	55:D2:23:G:H8	1.77	0.50
55:D2:101:G:C6	55:D2:103:G:C6	3.00	0.50
55:D2:445:U:H2'	55:D2:446:U:H6	1.76	0.50
56:D3:1052:U:H2'	56:D3:1053:G:C8	2.47	0.50
12:UL:487:ARG:HA	12:UL:500:TRP:O	2.12	0.49
55:D2:145:A:H2'	55:D2:146:G:C8	2.47	0.49
55:D2:100:G:C2	55:D2:101:G:H1'	2.47	0.49
56:D3:1267:G:O6	56:D3:1442:U:C5	2.64	0.49
56:D3:1665:U:C2	56:D3:1737:G:C2	3.00	0.49
8:UH:341:LEU:CB	8:UH:358:VAL:O	2.57	0.49
45:DH:70:PHE:O	45:DH:74:GLN:CB	2.60	0.49
20:UU:760:LEU:O	20:UU:763:SER:N	2.45	0.49
55:D2:255:U:N3	55:D2:262:U:O2'	2.45	0.49
55:D2:398:A:H2'	55:D2:399:U:C6	2.47	0.49
56:D3:480:G:H2'	56:D3:481:A:C8	2.45	0.49
56:D3:566:C:H2'	56:D3:567:A:C8	2.47	0.49
56:D3:1698:G:O6	56:D3:1704:U:C4	2.65	0.49
24:CB:197:VAL:HA	24:CB:220:ILE:O	2.13	0.49
43:DA:138:PHE:O	43:DA:213:ARG:N	2.44	0.49
55:D2:249:G:H2'	55:D2:250:G:H8	1.76	0.49
57:D4:330:A:H2'	57:D4:331:A:H8	1.77	0.49
57:D4:315:A:H2'	57:D4:316:A:C8	2.47	0.49
55:D2:189:U:O2	55:D2:209:G:C2	2.66	0.49
56:D3:1163:A:H2'	56:D3:1164:G:O4'	2.13	0.49
56:D3:1698:G:N1	56:D3:1704:U:C2	2.81	0.49
56:D3:1706:C:H3'	56:D3:1706:C:H6	1.78	0.49
56:D3:1733:C:H2'	56:D3:1734:U:H6	1.78	0.49
56:D3:1744:A:H2'	56:D3:1745:G:C8	2.48	0.49
56:D3:634:G:C2	56:D3:966:A:C6	3.00	0.49
56:D3:1636:C:C4	56:D3:1637:C:N4	2.81	0.49
57:D4:10:C:H2'	57:D4:11:U:C6	2.48	0.49
55:D2:426:G:C2	55:D2:428:A:H5''	2.47	0.49
56:D3:1646:C:N3	56:D3:1754:A:N1	2.60	0.49
56:D3:1707:A:P	56:D3:1707:A:C8	3.05	0.49
55:D2:140:U:H2'	55:D2:143:A:H2	1.76	0.49
55:D2:186:C:H2'	55:D2:187:A:H8	1.78	0.49
17:UQ:586:SER:O	17:UQ:594:TRP:HA	2.13	0.48
55:D2:549:G:N1	55:D2:589:U:N3	2.60	0.48
56:D3:1047:G:H2'	56:D3:1048:G:H8	1.78	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:UO:489:THR:O	15:UO:493:HIS:N	2.37	0.48
55:D2:208:A:H2'	55:D2:209:G:H8	1.78	0.48
56:D3:519:C:C4	56:D3:534:A:N7	2.81	0.48
56:D3:547:U:H2'	56:D3:548:G:C8	2.48	0.48
56:D3:600:U:H2'	56:D3:601:A:C8	2.49	0.48
56:D3:1735:U:C5'	56:D3:1735:U:H6	2.26	0.48
6:UF:155:TYR:HA	6:UF:159:ALA:HA	1.94	0.48
12:UL:937:ARG:O	31:CK:468:ARG:N	2.45	0.48
24:CB:264:GLN:CA	24:CB:320:TYR:O	2.61	0.48
28:CH:199:TYR:HA	28:CH:209:LYS:O	2.14	0.48
56:D3:1735:U:H5'	56:D3:1735:U:H6	1.79	0.48
32:CL:940:LYS:HA	56:D3:1492:A:C8	2.49	0.48
55:D2:238:G:C6	55:D2:275:A:C5	3.01	0.48
56:D3:891:A:H2'	56:D3:892:A:C8	2.48	0.48
8:UH:80:GLU:HA	8:UH:88:ASP:HA	1.95	0.48
56:D3:1505:A:C5	56:D3:1506:G:H1'	2.48	0.48
55:D2:21:A:H2'	55:D2:22:A:H8	1.79	0.48
55:D2:96:C:H2'	55:D2:97:G:C8	2.48	0.48
55:D2:186:C:H2'	55:D2:187:A:C8	2.48	0.48
56:D3:1666:U:O2	56:D3:1735:U:O4	2.32	0.48
57:D4:103:A:H2'	57:D4:104:C:C6	2.49	0.48
12:UL:486:LYS:O	12:UL:501:ASP:HA	2.14	0.48
32:CL:827:ALA:HA	32:CL:919:VAL:HA	1.95	0.48
55:D2:551:A:H2'	55:D2:552:G:H8	1.78	0.48
56:D3:35:U:H3	56:D3:474:A:H62	1.60	0.48
20:UU:759:PHE:O	20:UU:763:SER:CB	2.62	0.48
22:UX:154:ALA:HA	22:UX:173:MET:O	2.14	0.48
39:JN:257:ALA:O	39:JN:260:GLY:O	2.32	0.48
55:D2:289:U:H2'	55:D2:290:G:C8	2.49	0.48
6:UF:286:ILE:O	6:UF:290:LYS:HA	2.13	0.48
8:UH:229:TYR:HA	8:UH:240:LYS:O	2.14	0.48
56:D3:1151:A:H2'	56:D3:1152:A:C8	2.49	0.48
56:D3:1698:G:O6	56:D3:1704:U:O4	2.31	0.48
8:UH:182:THR:HA	8:UH:206:LEU:HA	1.95	0.47
55:D2:494:C:H2'	55:D2:495:G:C8	2.49	0.47
56:D3:1654:G:N2	56:D3:1746:A:C6	2.76	0.47
56:D3:1690:G:N1	56:D3:1711:C:C2	2.82	0.47
27:CF:56:ALA:HB3	27:CF:82:PRO:HA	1.95	0.47
56:D3:1704:U:H2'	56:D3:1705:C:C6	2.49	0.47
57:D4:41:C:H2'	57:D4:42:U:C6	2.50	0.47
55:D2:97:G:H1'	55:D2:155:A:N3	2.29	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:D2:166:U:H2'	55:D2:167:U:H6	1.79	0.47
57:D4:12:U:H2'	57:D4:13:C:C5	2.48	0.47
57:D4:104:C:H2'	57:D4:105:C:C6	2.49	0.47
35:JF:42:ILE:O	35:JF:203:CYS:HA	2.14	0.47
55:D2:101:G:N7	55:D2:103:G:N1	2.62	0.47
56:D3:32:U:C2	56:D3:595:G:C2	3.03	0.47
55:D2:60:G:H2'	55:D2:61:U:C6	2.49	0.47
56:D3:1592:A:H2'	56:D3:1593:A:C8	2.50	0.47
10:UJ:550:TYR:O	10:UJ:553:SER:O	2.32	0.47
12:UL:433:ALA:HA	12:UL:449:THR:HA	1.96	0.47
13:UM:418:ASN:O	13:UM:422:CYS:CA	2.63	0.47
55:D2:158:G:H2'	55:D2:159:A:C8	2.48	0.47
55:D2:180:G:H2'	55:D2:181:A:C8	2.50	0.47
55:D2:212:U:H2'	55:D2:213:G:H8	1.79	0.47
55:D2:237:A:N7	55:D2:274:C:O2'	2.47	0.47
55:D2:407:A:C6	55:D2:450:G:N1	2.82	0.47
56:D3:1158:C:N4	56:D3:1164:G:N1	2.63	0.47
56:D3:1524:A:H2'	56:D3:1525:A:C8	2.49	0.47
56:D3:924:A:H2'	56:D3:925:G:H8	1.80	0.47
30:CJ:157:PHE:O	30:CJ:159:HIS:N	2.47	0.47
52:DX:75:GLN:HA	52:DX:81:LYS:O	2.14	0.47
57:D4:205:G:C6	57:D4:245:U:N3	2.83	0.47
12:UL:412:GLY:HA3	12:UL:430:CYS:N	2.28	0.47
26:CE:319:ILE:O	26:CE:321:GLY:N	2.48	0.47
32:CL:69:PRO:HA	32:CL:114:ARG:O	2.14	0.47
55:D2:101:G:O6	55:D2:103:G:C6	2.69	0.47
55:D2:338:A:O2'	55:D2:339:A:N7	2.44	0.47
10:UJ:729:LYS:O	10:UJ:732:PHE:N	2.46	0.46
55:D2:400:C:H2'	55:D2:401:A:C8	2.50	0.46
56:D3:559:C:H2'	56:D3:560:U:H6	1.81	0.46
56:D3:1582:U:N3	56:D3:1614:A:C8	2.83	0.46
13:UM:39:GLU:HA	13:UM:56:ILE:O	2.15	0.46
55:D2:56:G:H2'	55:D2:57:C:C6	2.50	0.46
56:D3:34:G:C6	56:D3:474:A:N7	2.84	0.46
56:D3:1163:A:N6	56:D3:1164:G:C6	2.84	0.46
15:UO:237:TRP:HA	15:UO:244:LYS:HA	1.96	0.46
28:CH:496:LEU:O	28:CH:513:GLU:HA	2.15	0.46
56:D3:976:G:C2	56:D3:978:A:N6	2.83	0.46
56:D3:1752:U:H2'	56:D3:1753:A:H8	1.81	0.46
13:UM:538:ASP:O	13:UM:550:THR:HA	2.15	0.46
18:UR:382:GLY:CA	18:UR:400:ILE:O	2.30	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:D2:546:G:O6	55:D2:592:U:O2	2.31	0.46
56:D3:1043:A:N6	56:D3:1075:C:N4	2.36	0.46
56:D3:1169:G:N1	56:D3:1575:G:OP2	2.49	0.46
56:D3:1699:G:N2	56:D3:1702:A:N6	2.36	0.46
11:UK:7:ASP:O	11:UK:10:LYS:N	2.49	0.46
55:D2:195:A:H2'	55:D2:196:A:C8	2.51	0.46
55:D2:506:G:N2	55:D2:531:C:C2	2.83	0.46
55:D2:549:G:N1	55:D2:589:U:C4	2.84	0.46
56:D3:1663:G:N2	56:D3:1738:U:O2	2.49	0.46
3:UC:567:LYS:O	3:UC:571:LYS:N	2.46	0.46
12:UL:183:ASP:O	12:UL:185:MET:N	2.48	0.46
12:UL:939:PHE:O	31:CK:466:GLU:N	2.38	0.46
56:D3:519:C:N3	56:D3:534:A:C5	2.83	0.46
56:D3:521:A:N1	56:D3:531:C:N4	2.63	0.46
56:D3:1270:G:H2'	56:D3:1271:G:C8	2.49	0.46
55:D2:474:A:H2'	55:D2:475:G:H8	1.79	0.46
56:D3:502:U:H2'	56:D3:503:G:C8	2.50	0.46
56:D3:547:U:H2'	56:D3:548:G:H8	1.80	0.46
56:D3:591:A:H2'	56:D3:592:A:C8	2.50	0.46
2:UB:783:HIS:HA	56:D3:1119:G:H5''	1.98	0.46
45:DH:143:LEU:O	45:DH:146:GLY:N	2.47	0.46
56:D3:485:A:N1	56:D3:503:G:C6	2.84	0.46
56:D3:497:G:H2'	56:D3:498:G:H8	1.81	0.46
56:D3:884:A:H2'	56:D3:885:G:C8	2.51	0.46
56:D3:1736:G:H2'	56:D3:1737:G:H8	1.81	0.46
2:UB:396:LEU:O	2:UB:400:PRO:N	2.49	0.46
12:UL:577:LEU:N	12:UL:591:SER:O	2.39	0.46
55:D2:219:U:H2'	55:D2:220:U:H6	1.81	0.46
55:D2:452:A:H2'	55:D2:453:A:H8	1.80	0.46
56:D3:1124:A:H1'	57:D4:1:G:N1	2.31	0.46
57:D4:75:C:H2'	57:D4:76:U:C6	2.51	0.46
55:D2:217:C:H2'	55:D2:218:U:C6	2.50	0.46
55:D2:409:C:H2'	55:D2:410:A:C8	2.51	0.46
56:D3:592:A:H2'	56:D3:593:U:O4'	2.16	0.46
56:D3:1733:C:H2'	56:D3:1734:U:C6	2.51	0.46
2:UB:597:GLU:O	2:UB:599:GLY:N	2.49	0.45
35:JF:177:LYS:O	35:JF:222:ASP:N	2.49	0.45
56:D3:1530:C:H2'	56:D3:1531:G:C8	2.44	0.45
56:D3:1604:U:H2'	56:D3:1605:G:H8	1.80	0.45
57:D4:3:C:H2'	57:D4:4:G:C8	2.48	0.45
13:UM:507:ALA:HA	13:UM:516:LYS:O	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:CA:198:GLU:O	24:CA:221:ILE:HA	2.16	0.45
55:D2:212:U:H2'	55:D2:213:G:C8	2.52	0.45
55:D2:507:U:H2'	55:D2:508:C:C6	2.52	0.45
55:D2:514:U:N3	55:D2:521:G:N1	2.56	0.45
56:D3:1606:C:H2'	56:D3:1607:G:H8	1.80	0.45
56:D3:1665:U:N3	56:D3:1737:G:C6	2.84	0.45
57:D4:198:U:H3	57:D4:201:C:H41	1.64	0.45
57:D4:315:A:H2'	57:D4:316:A:H8	1.81	0.45
55:D2:262:U:N3	55:D2:263:C:N4	2.63	0.45
56:D3:23:G:C2	56:D3:603:U:C2	3.03	0.45
56:D3:1594:G:O2'	56:D3:1600:A:N6	2.35	0.45
8:UH:178:ILE:HA	8:UH:187:VAL:O	2.15	0.45
19:US:130:GLU:O	19:US:134:PHE:CB	2.65	0.45
55:D2:516:U:O2'	55:D2:519:A:N6	2.49	0.45
56:D3:1025:A:H2'	56:D3:1026:A:H8	1.80	0.45
56:D3:1437:U:H2'	56:D3:1438:G:C8	2.51	0.45
57:D4:17:G:H2'	57:D4:18:G:C8	2.51	0.45
12:UL:42:ILE:HA	12:UL:50:ASN:O	2.17	0.45
12:UL:148:TRP:HA	12:UL:156:LEU:H	1.81	0.45
20:UU:82:ALA:HB3	20:UU:93:ALA:HB3	1.98	0.45
20:UU:368:SER:O	20:UU:375:LEU:HA	2.15	0.45
32:CL:847:LEU:HA	32:CL:898:GLY:HA2	1.98	0.45
56:D3:953:G:H2'	56:D3:954:G:C8	2.52	0.45
57:D4:205:G:C6	57:D4:245:U:C4	3.05	0.45
19:US:188:PHE:HA	19:US:237:GLU:O	2.17	0.45
56:D3:1602:C:H2'	56:D3:1603:U:C6	2.52	0.45
56:D3:1677:C:N3	56:D3:1724:U:O2	2.50	0.45
57:D4:94:A:H2'	57:D4:95:A:H8	1.80	0.45
56:D3:1569:A:H2'	56:D3:1570:A:C8	2.52	0.45
55:D2:199:A:H2'	55:D2:200:A:C8	2.51	0.45
57:D4:95:A:H2'	57:D4:96:C:H6	1.82	0.45
55:D2:223:C:H2'	55:D2:224:G:H8	1.79	0.45
55:D2:409:C:H2'	55:D2:410:A:H8	1.82	0.45
55:D2:457:G:H2'	55:D2:458:A:C8	2.52	0.45
56:D3:961:U:H2'	56:D3:962:C:C6	2.52	0.45
56:D3:1666:U:C4	56:D3:1736:G:N1	2.85	0.45
56:D3:1272:U:O2	56:D3:1438:G:C6	2.70	0.45
56:D3:1583:A:N6	56:D3:1612:U:OP2	2.50	0.45
56:D3:1692:G:N1	56:D3:1710:U:N3	2.64	0.45
56:D3:1729:C:H2'	56:D3:1730:A:O4'	2.17	0.45
21:UV:587:GLY:HA3	21:UV:611:ASP:H	1.80	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:CI:137:ARG:HA	29:CI:142:LEU:HA	1.98	0.44
56:D3:1486:G:H21	56:D3:1592:A:H4'	1.82	0.44
56:D3:1592:A:H2'	56:D3:1593:A:H8	1.82	0.44
56:D3:1665:U:N3	56:D3:1737:G:N1	2.66	0.44
56:D3:1267:G:C2	56:D3:1442:U:C2	3.05	0.44
56:D3:1643:U:H2'	56:D3:1644:C:H6	1.82	0.44
57:D4:58:A:H2'	57:D4:59:G:C8	2.52	0.44
13:UM:170:GLY:O	13:UM:187:GLN:HA	2.17	0.44
32:CL:364:VAL:HA	32:CL:372:TYR:O	2.18	0.44
55:D2:287:G:H2'	55:D2:288:G:H8	1.82	0.44
55:D2:476:A:H2'	55:D2:477:G:H8	1.82	0.44
56:D3:516:G:O6	56:D3:537:G:C2	2.70	0.44
56:D3:1532:U:H2'	56:D3:1533:C:C6	2.52	0.44
56:D3:1699:G:N2	56:D3:1702:A:C5	2.85	0.44
17:UQ:216:SER:N	17:UQ:222:HIS:O	2.50	0.44
40:JO:163:TYR:O	40:JO:173:ALA:HA	2.17	0.44
55:D2:410:A:H2'	55:D2:411:A:C8	2.53	0.44
55:D2:464:G:H2'	55:D2:465:G:H8	1.82	0.44
55:D2:466:A:N6	57:D4:51:C:N4	2.66	0.44
56:D3:1707:A:C8	56:D3:1707:A:OP2	2.70	0.44
55:D2:21:A:H2'	55:D2:22:A:C8	2.53	0.44
55:D2:353:A:C6	55:D2:371:G:C6	3.05	0.44
55:D2:378:C:H2'	55:D2:379:A:C8	2.52	0.44
56:D3:1580:C:H2'	56:D3:1581:C:C6	2.52	0.44
4:UD:399:VAL:O	4:UD:419:LYS:HA	2.17	0.44
8:UH:351:SER:O	8:UH:353:ARG:N	2.51	0.44
55:D2:264:C:H2'	55:D2:265:A:C8	2.53	0.44
56:D3:900:A:H3'	56:D3:901:G:H21	1.82	0.44
56:D3:1625:C:H2'	56:D3:1626:U:C6	2.52	0.44
55:D2:182:G:O6	55:D2:215:U:O4	2.35	0.44
57:D4:202:G:H2'	57:D4:203:U:H6	1.82	0.44
35:JF:121:LEU:CB	35:JF:163:ILE:O	2.65	0.44
55:D2:161:A:N6	55:D2:233:G:C6	2.86	0.44
56:D3:1508:U:H2'	56:D3:1509:C:C6	2.53	0.44
21:UV:378:ASN:O	21:UV:387:GLY:N	2.51	0.44
28:CH:197:THR:HA	28:CH:212:LYS:O	2.18	0.44
32:CL:137:LEU:HA	32:CL:166:ARG:O	2.17	0.44
33:CM:196:TYR:HA	33:CM:228:ASP:O	2.18	0.44
55:D2:357:G:O6	55:D2:368:U:O2	2.36	0.44
56:D3:1050:G:H2'	56:D3:1051:G:C8	2.53	0.44
4:UD:573:VAL:HA	4:UD:583:VAL:O	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:UQ:780:GLU:O	17:UQ:782:THR:N	2.51	0.43
33:CM:118:PHE:O	33:CM:165:GLU:HA	2.18	0.43
55:D2:173:G:H2'	55:D2:174:U:C6	2.53	0.43
55:D2:208:A:H2'	55:D2:209:G:C8	2.52	0.43
55:D2:360:C:N3	55:D2:366:A:N1	2.66	0.43
55:D2:407:A:C6	55:D2:450:G:C2	3.06	0.43
56:D3:546:U:H2'	56:D3:547:U:C6	2.52	0.43
56:D3:568:G:H2'	56:D3:569:C:C6	2.53	0.43
4:UD:199:ASP:CA	4:UD:215:ALA:O	2.62	0.43
36:JH:430:ASN:HA	36:JH:465:SER:HA	1.99	0.43
55:D2:166:U:H2'	55:D2:167:U:C6	2.53	0.43
55:D2:324:U:H2'	55:D2:327:A:C8	2.53	0.43
55:D2:464:G:H2'	55:D2:465:G:C8	2.52	0.43
56:D3:953:G:H2'	56:D3:954:G:H8	1.82	0.43
56:D3:1156:C:H2'	56:D3:1157:A:C8	2.52	0.43
56:D3:881:A:H2'	56:D3:882:U:O4'	2.18	0.43
57:D4:95:A:H2'	57:D4:96:C:C6	2.52	0.43
57:D4:205:G:O6	57:D4:245:U:C4	2.71	0.43
56:D3:1152:A:H2'	56:D3:1153:G:C8	2.54	0.43
56:D3:1484:G:H1	56:D3:1591:C:H1'	1.82	0.43
56:D3:1752:U:H2'	56:D3:1753:A:C8	2.53	0.43
57:D4:98:U:H2'	57:D4:99:U:H6	1.82	0.43
10:UJ:559:ASN:O	10:UJ:599:PHE:N	2.34	0.43
43:DA:88:VAL:HA	43:DA:98:THR:HA	2.00	0.43
46:DJ:152:SER:O	46:DJ:155:HIS:N	2.42	0.43
1:UA:600:SER:HA	1:UA:615:PHE:O	2.19	0.43
13:UM:246:CYS:HA	13:UM:259:TYR:O	2.19	0.43
13:UM:623:LEU:HA	13:UM:633:VAL:O	2.19	0.43
51:DW:4:SER:O	56:D3:634:G:H5'	2.19	0.43
56:D3:1264:G:N2	56:D3:1265:G:N7	2.65	0.43
15:UO:127:THR:HA	15:UO:144:SER:HA	2.01	0.43
55:D2:415:U:H2'	55:D2:416:A:H8	1.84	0.43
55:D2:468:A:N6	57:D4:49:C:N3	2.67	0.43
56:D3:870:C:H2'	56:D3:871:G:C8	2.54	0.43
13:UM:418:ASN:CB	13:UM:423:LYS:O	2.67	0.43
56:D3:1736:G:H2'	56:D3:1736:G:N3	2.34	0.43
10:UJ:741:LEU:HA	10:UJ:742:ASN:HA	1.69	0.43
55:D2:188:A:H2	55:D2:209:G:H22	1.67	0.43
56:D3:939:A:H2'	56:D3:940:A:C8	2.53	0.43
8:UH:131:VAL:H	8:UH:145:ASP:C	2.22	0.43
10:UJ:705:SER:HA	10:UJ:708:ALA:HB3	1.99	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:D2:134:A:H2'	55:D2:135:G:H8	1.84	0.43
55:D2:476:A:H2'	55:D2:477:G:C8	2.53	0.43
55:D2:586:A:H2'	55:D2:587:G:H8	1.84	0.43
56:D3:891:A:H2'	56:D3:892:A:H8	1.84	0.43
56:D3:957:G:H2'	56:D3:958:U:C6	2.54	0.43
56:D3:1267:G:C2	56:D3:1442:U:O2	2.72	0.43
56:D3:1666:U:C2	56:D3:1735:U:O4	2.72	0.43
56:D3:1726:G:H2'	56:D3:1727:G:H8	1.84	0.43
56:D3:1739:C:H2'	56:D3:1740:A:C8	2.53	0.43
55:D2:478:U:H2'	55:D2:479:G:C8	2.54	0.42
56:D3:523:G:H21	56:D3:529:A:H62	1.66	0.42
56:D3:1111:G:H2'	56:D3:1112:G:H8	1.84	0.42
57:D4:331:A:H2'	57:D4:332:G:H8	1.83	0.42
45:DH:63:PRO:O	45:DH:67:LEU:CB	2.67	0.42
55:D2:554:G:C6	55:D2:583:U:N3	2.86	0.42
56:D3:1619:C:H2'	56:D3:1620:C:H6	1.85	0.42
57:D4:76:U:H2'	57:D4:77:U:C6	2.54	0.42
20:UU:515:ARG:O	20:UU:531:PHE:N	2.52	0.42
51:DW:48:GLY:HA3	51:DW:64:GLN:O	2.18	0.42
55:D2:2:U:O2'	55:D2:69:U:O2'	2.18	0.42
55:D2:247:U:H2'	55:D2:248:G:H8	1.83	0.42
55:D2:276:G:H2'	55:D2:277:C:H6	1.85	0.42
55:D2:362:C:H3'	55:D2:363:A:C8	2.55	0.42
55:D2:504:U:H2'	55:D2:505:G:C8	2.55	0.42
56:D3:887:A:H2'	56:D3:888:U:H6	1.85	0.42
56:D3:1047:G:H2'	56:D3:1048:G:C8	2.54	0.42
56:D3:1077:C:H2'	56:D3:1078:C:H6	1.84	0.42
55:D2:397:A:H2'	55:D2:398:A:C8	2.54	0.42
56:D3:485:A:C2	56:D3:503:G:N1	2.88	0.42
56:D3:601:A:H2'	56:D3:602:U:C6	2.54	0.42
56:D3:1483:A:C6	56:D3:1524:A:C5	3.07	0.42
26:CE:431:ALA:HB3	55:D2:309:A:N6	2.34	0.42
55:D2:227:U:H2'	55:D2:228:A:C8	2.55	0.42
55:D2:398:A:H2'	55:D2:399:U:H6	1.85	0.42
57:D4:263:A:N6	57:D4:309:G:C2	2.87	0.42
12:UL:148:TRP:HA	12:UL:155:GLY:HA2	2.00	0.42
41:JP:55:ALA:HA	41:JP:379:ALA:HB1	2.01	0.42
55:D2:134:A:H2'	55:D2:135:G:C8	2.55	0.42
55:D2:489:G:O2'	55:D2:490:G:H8	2.02	0.42
4:UD:548:GLY:O	4:UD:566:LEU:N	2.53	0.42
12:UL:450:ARG:O	12:UL:475:ALA:HA	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:D2:171:G:C6	55:D2:226:U:C4	3.07	0.42
56:D3:1643:U:H2'	56:D3:1644:C:C6	2.54	0.42
57:D4:104:C:H2'	57:D4:105:C:H6	1.85	0.42
57:D4:311:G:O2'	57:D4:312:U:O4'	2.35	0.42
24:CB:125:VAL:O	24:CB:138:LYS:HA	2.20	0.42
56:D3:1170:G:C6	56:D3:1574:G:N1	2.88	0.42
56:D3:1573:A:H5'	56:D3:1574:G:N3	2.34	0.42
57:D4:202:G:C6	57:D4:248:G:C5	3.07	0.42
12:UL:338:ILE:HA	12:UL:357:THR:HA	2.02	0.42
17:UQ:718:GLY:HA3	17:UQ:746:PHE:O	2.20	0.42
23:UZ:68:ARG:O	50:DS:82:PRO:HA	2.20	0.42
35:JG:121:LEU:CB	35:JG:163:ILE:O	2.67	0.42
55:D2:13:U:H1'	55:D2:70:A:N7	2.35	0.42
55:D2:174:U:H2'	55:D2:175:A:C8	2.55	0.42
55:D2:496:G:H2'	55:D2:497:A:C8	2.55	0.42
56:D3:1506:G:H2'	56:D3:1507:G:C8	2.53	0.42
57:D4:17:G:H2'	57:D4:18:G:H8	1.85	0.42
55:D2:453:A:H2'	55:D2:454:C:C6	2.55	0.42
56:D3:514:G:HO2'	56:D3:515:A:H8	1.68	0.42
56:D3:599:A:H2'	56:D3:600:U:C6	2.55	0.42
56:D3:1648:A:H2'	56:D3:1649:G:H8	1.84	0.42
12:UL:124:ILE:HA	12:UL:140:SER:HA	2.01	0.41
12:UL:619:MET:H	12:UL:634:SER:HA	1.85	0.41
32:CL:105:ILE:O	32:CL:117:PHE:N	2.50	0.41
56:D3:1525:A:H2'	56:D3:1526:A:C8	2.55	0.41
56:D3:1787:C:H2'	56:D3:1788:G:C8	2.55	0.41
50:DS:24:GLY:O	50:DS:59:GLY:N	2.52	0.41
56:D3:487:G:H2'	56:D3:488:G:H8	1.85	0.41
56:D3:1661:U:H2'	56:D3:1662:G:H8	1.85	0.41
56:D3:1692:G:C6	56:D3:1710:U:O4	2.73	0.41
56:D3:1693:A:O2'	56:D3:1694:A:O4'	2.21	0.41
14:UN:323:HIS:N	55:D2:534:A:O2'	2.53	0.41
20:UU:228:GLY:O	20:UU:245:LYS:HA	2.21	0.41
55:D2:147:C:H2'	55:D2:148:G:C8	2.55	0.41
55:D2:281:G:H2'	55:D2:282:G:H8	1.86	0.41
56:D3:1684:U:H2'	56:D3:1685:G:H8	1.85	0.41
57:D4:330:A:H2'	57:D4:331:A:C8	2.55	0.41
52:DX:103:LEU:N	52:DX:126:LYS:O	2.54	0.41
55:D2:547:C:H2'	55:D2:548:A:C8	2.54	0.41
56:D3:961:U:H2'	56:D3:962:C:H6	1.85	0.41
8:UH:309:PRO:O	8:UH:327:SER:N	2.53	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:US:456:THR:O	19:US:458:ALA:N	2.50	0.41
48:DO:82:LYS:HA	48:DO:116:GLU:O	2.21	0.41
55:D2:60:G:H2'	55:D2:61:U:H6	1.85	0.41
55:D2:192:G:H2'	55:D2:193:G:C8	2.53	0.41
56:D3:29:U:H2'	56:D3:30:G:C8	2.55	0.41
56:D3:1693:A:H2'	56:D3:1694:A:C8	2.55	0.41
56:D3:1723:U:H2'	56:D3:1724:U:C6	2.55	0.41
56:D3:1782:A:H3'	56:D3:1783:C:C6	2.55	0.41
43:DA:70:LEU:N	43:DA:82:ARG:O	2.47	0.41
55:D2:3:G:H2'	55:D2:4:C:C6	2.56	0.41
56:D3:504:U:HO2'	56:D3:506:A:H8	1.67	0.41
8:UH:55:ILE:HA	8:UH:72:ASN:HA	2.02	0.41
28:CH:153:GLY:O	57:D4:251:G:N1	2.48	0.41
55:D2:244:U:H2'	55:D2:245:C:C6	2.55	0.41
55:D2:353:A:N1	55:D2:371:G:C6	2.88	0.41
56:D3:33:U:O2	56:D3:468:A:N7	2.53	0.41
56:D3:472:U:H2'	56:D3:473:A:C8	2.55	0.41
56:D3:559:C:H2'	56:D3:560:U:C6	2.55	0.41
56:D3:1124:A:H1'	57:D4:1:G:C2	2.56	0.41
5:UE:359:GLY:HA2	55:D2:147:C:H4'	2.03	0.41
33:CM:159:PRO:HA	33:CM:160:PRO:HA	1.75	0.41
55:D2:376:U:H2'	55:D2:377:U:C6	2.56	0.41
56:D3:1602:C:H2'	56:D3:1603:U:H6	1.86	0.41
8:UH:142:THR:N	8:UH:157:TYR:O	2.35	0.41
13:UM:296:ILE:C	13:UM:298:SER:H	2.24	0.41
28:CH:551:ARG:O	28:CH:553:ILE:N	2.54	0.41
55:D2:262:U:H2'	55:D2:263:C:C6	2.55	0.41
55:D2:497:A:H2'	55:D2:498:G:C8	2.56	0.41
55:D2:528:G:H2'	55:D2:529:A:C8	2.56	0.41
56:D3:1707:A:O5'	56:D3:1707:A:C8	2.70	0.41
57:D4:263:A:N6	57:D4:309:G:N1	2.69	0.41
55:D2:397:A:H2'	55:D2:398:A:H8	1.86	0.41
55:D2:538:C:H2'	55:D2:539:A:C8	2.56	0.41
56:D3:1158:C:N4	56:D3:1164:G:H1	2.19	0.41
57:D4:101:G:C6	57:D4:315:A:C6	3.09	0.41
57:D4:205:G:N1	57:D4:245:U:O2	2.53	0.41
8:UH:54:TYR:O	8:UH:73:ILE:N	2.54	0.40
13:UM:63:GLU:O	13:UM:81:GLN:N	2.54	0.40
21:UV:304:GLU:O	21:UV:308:LEU:CB	2.69	0.40
28:CH:443:LEU:N	28:CH:471:GLN:O	2.41	0.40
55:D2:306:G:H2'	55:D2:307:C:C6	2.56	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:D2:307:C:O2'	55:D2:311:C:OP2	2.24	0.40
55:D2:552:G:H2'	55:D2:553:A:H8	1.85	0.40
56:D3:1504:G:H3'	56:D3:1505:A:H8	1.86	0.40
32:CL:169:GLY:O	32:CL:204:LEU:HA	2.21	0.40
35:JG:165:ASN:HA	35:JG:166:PRO:HA	1.80	0.40
55:D2:554:G:C2	55:D2:583:U:O2	2.74	0.40
56:D3:478:A:C6	56:D3:510:G:O6	2.73	0.40
56:D3:590:C:H2'	56:D3:591:A:H8	1.86	0.40
56:D3:1484:G:H22	56:D3:1591:C:H1'	1.86	0.40
56:D3:1723:U:H2'	56:D3:1724:U:H6	1.87	0.40
56:D3:1776:A:H2'	56:D3:1777:G:C8	2.55	0.40
8:UH:267:ILE:O	8:UH:284:LEU:HA	2.21	0.40
55:D2:96:C:H2'	55:D2:97:G:H8	1.85	0.40
55:D2:130:G:H2'	55:D2:131:C:C6	2.56	0.40
55:D2:147:C:H2'	55:D2:148:G:H8	1.85	0.40
55:D2:437:G:H2'	55:D2:438:U:C6	2.57	0.40
55:D2:543:C:H2'	55:D2:544:C:C6	2.56	0.40
56:D3:635:A:H2'	56:D3:636:A:H8	1.86	0.40
56:D3:1050:G:H2'	56:D3:1051:G:H8	1.87	0.40
56:D3:1684:U:H3	56:D3:1717:G:H1	1.69	0.40
57:D4:24:U:HO2'	57:D4:25:U:P	2.45	0.40
13:UM:591:ILE:HA	13:UM:600:LYS:O	2.21	0.40
55:D2:506:G:C2	55:D2:531:C:O2	2.75	0.40
55:D2:510:A:H2'	55:D2:511:G:H8	1.87	0.40
56:D3:34:G:H2'	56:D3:35:U:O4'	2.21	0.40
56:D3:1274:C:N3	56:D3:1275:A:N6	2.70	0.40
1:UA:219:GLU:O	1:UA:248:TRP:HA	2.21	0.40
1:UA:393:VAL:HA	1:UA:403:PHE:O	2.22	0.40
55:D2:68:U:H5	55:D2:70:A:H2'	1.87	0.40
55:D2:123:C:H3'	55:D2:124:A:C8	2.56	0.40
56:D3:878:G:H2'	56:D3:879:G:C8	2.56	0.40
56:D3:1035:G:H3'	56:D3:1037:C:H41	1.87	0.40
56:D3:1541:G:N3	56:D3:1570:A:N1	2.68	0.40
56:D3:1707:A:H8	56:D3:1707:A:OP2	2.03	0.40
57:D4:103:A:N1	57:D4:313:A:N6	2.70	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	UA	830/923 (90%)	750 (90%)	80 (10%)	0	100	100
2	UB	492/810 (61%)	451 (92%)	38 (8%)	3 (1%)	25	65
3	UC	124/610 (20%)	116 (94%)	8 (6%)	0	100	100
4	UD	663/776 (85%)	581 (88%)	81 (12%)	1 (0%)	47	81
5	UE	465/643 (72%)	407 (88%)	58 (12%)	0	100	100
6	UF	283/440 (64%)	277 (98%)	6 (2%)	0	100	100
7	UG	529/554 (96%)	472 (89%)	56 (11%)	1 (0%)	47	81
8	UH	426/713 (60%)	305 (72%)	84 (20%)	37 (9%)	1	13
9	UI	100/575 (17%)	94 (94%)	6 (6%)	0	100	100
10	UJ	720/1769 (41%)	665 (92%)	54 (8%)	1 (0%)	51	85
11	UK	238/250 (95%)	222 (93%)	16 (7%)	0	100	100
12	UL	828/943 (88%)	737 (89%)	91 (11%)	0	100	100
13	UM	750/817 (92%)	661 (88%)	87 (12%)	2 (0%)	41	76
14	UN	143/899 (16%)	130 (91%)	13 (9%)	0	100	100
15	UO	489/513 (95%)	435 (89%)	54 (11%)	0	100	100
16	UP	58/214 (27%)	55 (95%)	3 (5%)	0	100	100
17	UQ	820/896 (92%)	720 (88%)	100 (12%)	0	100	100
18	UR	474/594 (80%)	418 (88%)	56 (12%)	0	100	100
19	US	460/552 (83%)	419 (91%)	40 (9%)	1 (0%)	47	81
20	UU	842/939 (90%)	756 (90%)	86 (10%)	0	100	100
21	UV	1086/1237 (88%)	1037 (96%)	49 (4%)	0	100	100
22	UX	170/189 (90%)	160 (94%)	10 (6%)	0	100	100
23	UZ	245/274 (89%)	223 (91%)	22 (9%)	0	100	100
24	CA	238/327 (73%)	218 (92%)	20 (8%)	0	100	100
24	CB	224/327 (68%)	198 (88%)	26 (12%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	CD	376/504 (75%)	343 (91%)	31 (8%)	2 (0%)	29	68
26	CE	431/511 (84%)	392 (91%)	38 (9%)	1 (0%)	47	81
27	CF	121/126 (96%)	110 (91%)	11 (9%)	0	100	100
27	CG	121/126 (96%)	116 (96%)	5 (4%)	0	100	100
28	CH	434/573 (76%)	385 (89%)	46 (11%)	3 (1%)	22	62
29	CI	180/183 (98%)	163 (91%)	17 (9%)	0	100	100
30	CJ	278/290 (96%)	248 (89%)	29 (10%)	1 (0%)	34	72
31	CK	203/593 (34%)	192 (95%)	9 (4%)	2 (1%)	15	54
32	CL	771/1183 (65%)	716 (93%)	55 (7%)	0	100	100
33	CM	358/367 (98%)	328 (92%)	30 (8%)	0	100	100
34	CN	224/297 (75%)	215 (96%)	9 (4%)	0	100	100
35	JF	212/252 (84%)	199 (94%)	13 (6%)	0	100	100
35	JG	226/252 (90%)	209 (92%)	17 (8%)	0	100	100
36	JH	257/483 (53%)	234 (91%)	23 (9%)	0	100	100
37	JJ	180/274 (66%)	169 (94%)	11 (6%)	0	100	100
38	JM	129/217 (59%)	122 (95%)	7 (5%)	0	100	100
39	JN	178/346 (51%)	162 (91%)	11 (6%)	5 (3%)	5	33
40	JO	186/316 (59%)	177 (95%)	9 (5%)	0	100	100
41	JP	457/489 (94%)	412 (90%)	44 (10%)	1 (0%)	47	81
42	JQ	59/206 (29%)	54 (92%)	5 (8%)	0	100	100
43	DA	236/255 (92%)	217 (92%)	18 (8%)	1 (0%)	34	72
44	DF	211/225 (94%)	192 (91%)	19 (9%)	0	100	100
45	DH	182/190 (96%)	163 (90%)	19 (10%)	0	100	100
46	DJ	183/197 (93%)	169 (92%)	14 (8%)	0	100	100
47	DN	148/151 (98%)	132 (89%)	15 (10%)	1 (1%)	22	62
48	DO	118/137 (86%)	108 (92%)	10 (8%)	0	100	100
49	DQ	123/143 (86%)	110 (89%)	13 (11%)	0	100	100
50	DS	99/146 (68%)	88 (89%)	11 (11%)	0	100	100
51	DW	127/130 (98%)	107 (84%)	20 (16%)	0	100	100
52	DX	101/145 (70%)	86 (85%)	14 (14%)	1 (1%)	15	54
53	Db	79/82 (96%)	70 (89%)	9 (11%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	Dc	61/67 (91%)	52 (85%)	9 (15%)	0	100	100
All	All	18746/26240 (71%)	16947 (90%)	1735 (9%)	64 (0%)	44	76

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	UB	395	ASP
8	UH	67	PRO
8	UH	184	ASN
8	UH	234	CYS
8	UH	258	PRO
8	UH	267	ILE
8	UH	298	PRO
8	UH	309	PRO
8	UH	325	PRO
25	CD	265	GLU
28	CH	438	ILE
31	CK	454	VAL
39	JN	94	PRO
39	JN	97	ILE
8	UH	29	VAL
8	UH	127	TYR
8	UH	214	ASP
8	UH	235	PRO
8	UH	248	LEU
8	UH	268	GLU
8	UH	352	GLN
39	JN	107	VAL
39	JN	109	PRO
8	UH	128	THR
8	UH	174	LYS
8	UH	198	ILE
8	UH	205	LEU
8	UH	206	LEU
8	UH	217	LYS
8	UH	299	HIS
8	UH	308	PHE
8	UH	533	PRO
13	UM	420	ASN
26	CE	320	LEU
28	CH	437	ARG
28	CH	439	ALA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
39	JN	111	LYS
52	DX	90	ASP
8	UH	137	GLU
8	UH	138	ASP
8	UH	142	THR
8	UH	284	LEU
8	UH	341	LEU
30	CJ	93	SER
43	DA	81	PHE
2	UB	396	LEU
4	UD	759	PRO
8	UH	161	ASP
8	UH	249	THR
10	UJ	411	ASN
13	UM	37	LEU
19	US	106	ILE
25	CD	240	LEU
41	JP	284	HIS
2	UB	399	HIS
8	UH	57	ASN
8	UH	69	PRO
8	UH	193	ASN
8	UH	257	SER
8	UH	297	LEU
31	CK	460	PRO
47	DN	68	GLY
7	UG	385	PRO
8	UH	60	PRO

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
55	D2	519/700 (74%)	146 (28%)	6 (1%)
56	D3	770/1379 (55%)	264 (34%)	17 (2%)
57	D4	169/175 (96%)	51 (30%)	0
All	All	1458/2254 (64%)	461 (31%)	23 (1%)

All (461) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
55	D2	2	U
55	D2	6	A
55	D2	14	U
55	D2	15	G
55	D2	58	U
55	D2	63	G
55	D2	66	C
55	D2	68	U
55	D2	69	U
55	D2	70	A
55	D2	82	A
55	D2	83	U
55	D2	84	G
55	D2	85	G
55	D2	90	G
55	D2	98	G
55	D2	100	G
55	D2	101	G
55	D2	102	A
55	D2	103	G
55	D2	104	A
55	D2	105	G
55	D2	109	C
55	D2	110	G
55	D2	113	A
55	D2	124	A
55	D2	125	G
55	D2	129	U
55	D2	130	G
55	D2	141	A
55	D2	142	U
55	D2	144	C
55	D2	150	G
55	D2	151	U
55	D2	152	U
55	D2	153	U
55	D2	155	A
55	D2	163	G
55	D2	169	A
55	D2	170	U
55	D2	171	G
55	D2	176	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
55	D2	177	U
55	D2	190	U
55	D2	197	G
55	D2	198	A
55	D2	200	A
55	D2	201	U
55	D2	203	C
55	D2	207	G
55	D2	227	U
55	D2	228	A
55	D2	231	C
55	D2	234	A
55	D2	235	A
55	D2	236	C
55	D2	239	U
55	D2	240	C
55	D2	252	A
55	D2	253	U
55	D2	254	C
55	D2	256	U
55	D2	259	G
55	D2	261	U
55	D2	266	U
55	D2	267	U
55	D2	268	G
55	D2	270	U
55	D2	279	A
55	D2	280	A
55	D2	281	G
55	D2	294	U
55	D2	297	U
55	D2	303	A
55	D2	304	U
55	D2	305	A
55	D2	310	U
55	D2	311	C
55	D2	312	U
55	D2	313	A
55	D2	314	U
55	D2	315	U
55	D2	316	U
55	D2	324	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
55	D2	325	U
55	D2	327	A
55	D2	332	U
55	D2	337	G
55	D2	353	A
55	D2	354	G
55	D2	356	C
55	D2	365	G
55	D2	366	A
55	D2	368	U
55	D2	369	G
55	D2	370	U
55	D2	371	G
55	D2	372	A
55	D2	373	U
55	D2	382	U
55	D2	383	G
55	D2	385	A
55	D2	395	C
55	D2	399	U
55	D2	407	A
55	D2	418	C
55	D2	428	A
55	D2	430	C
55	D2	431	A
55	D2	432	C
55	D2	433	C
55	D2	440	U
55	D2	451	G
55	D2	452	A
55	D2	460	U
55	D2	461	A
55	D2	462	G
55	D2	468	A
55	D2	469	C
55	D2	470	U
55	D2	481	U
55	D2	482	A
55	D2	484	G
55	D2	485	G
55	D2	487	A
55	D2	488	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
55	D2	491	U
55	D2	492	G
55	D2	493	A
55	D2	494	C
55	D2	513	G
55	D2	526	U
55	D2	533	G
55	D2	535	G
55	D2	536	A
55	D2	537	G
55	D2	540	U
55	D2	541	U
55	D2	542	U
55	D2	546	G
55	D2	547	C
55	D2	548	A
55	D2	551	A
55	D2	555	A
55	D2	585	C
55	D2	586	A
56	D3	-6	A
56	D3	-5	G
56	D3	-4	A
56	D3	-3	U
56	D3	-2	A
56	D3	-1	G
56	D3	1	U
56	D3	2	A
56	D3	6	G
56	D3	7	G
56	D3	9	U
56	D3	10	G
56	D3	16	G
56	D3	17	C
56	D3	18	C
56	D3	25	C
56	D3	26	A
56	D3	33	U
56	D3	34	G
56	D3	36	C
56	D3	39	A
56	D3	468	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
56	D3	470	A
56	D3	473	A
56	D3	474	A
56	D3	475	A
56	D3	477	A
56	D3	482	U
56	D3	487	G
56	D3	496	G
56	D3	501	U
56	D3	505	A
56	D3	506	A
56	D3	511	A
56	D3	515	A
56	D3	520	A
56	D3	522	U
56	D3	525	A
56	D3	526	A
56	D3	527	A
56	D3	528	U
56	D3	529	A
56	D3	533	U
56	D3	534	A
56	D3	538	A
56	D3	539	G
56	D3	541	A
56	D3	542	A
56	D3	543	C
56	D3	544	A
56	D3	545	A
56	D3	546	U
56	D3	562	G
56	D3	564	G
56	D3	565	C
56	D3	570	A
56	D3	572	C
56	D3	576	G
56	D3	578	U
56	D3	579	A
56	D3	580	A
56	D3	584	C
56	D3	585	A
56	D3	586	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
56	D3	587	C
56	D3	594	A
56	D3	595	G
56	D3	597	G
56	D3	629	U
56	D3	631	G
56	D3	634	G
56	D3	635	A
56	D3	638	U
56	D3	860	U
56	D3	863	A
56	D3	864	U
56	D3	873	U
56	D3	876	G
56	D3	886	U
56	D3	898	A
56	D3	899	G
56	D3	906	A
56	D3	911	U
56	D3	912	U
56	D3	913	G
56	D3	914	G
56	D3	915	A
56	D3	921	U
56	D3	922	G
56	D3	926	A
56	D3	928	U
56	D3	929	A
56	D3	930	A
56	D3	931	C
56	D3	933	A
56	D3	934	C
56	D3	935	U
56	D3	942	G
56	D3	944	A
56	D3	952	A
56	D3	959	U
56	D3	966	A
56	D3	969	C
56	D3	970	A
56	D3	971	A
56	D3	972	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
56	D3	977	A
56	D3	978	A
56	D3	1029	U
56	D3	1031	U
56	D3	1032	G
56	D3	1033	C
56	D3	1035	G
56	D3	1036	A
56	D3	1038	U
56	D3	1040	G
56	D3	1041	G
56	D3	1043	A
56	D3	1044	U
56	D3	1053	G
56	D3	1054	U
56	D3	1058	U
56	D3	1061	A
56	D3	1062	A
56	D3	1063	U
56	D3	1064	G
56	D3	1072	C
56	D3	1076	A
56	D3	1079	U
56	D3	1118	G
56	D3	1119	G
56	D3	1122	G
56	D3	1124	A
56	D3	1125	A
56	D3	1126	G
56	D3	1127	G
56	D3	1128	C
56	D3	1130	G
56	D3	1133	A
56	D3	1134	C
56	D3	1136	U
56	D3	1143	A
56	D3	1145	U
56	D3	1146	G
56	D3	1147	A
56	D3	1149	G
56	D3	1150	G
56	D3	1158	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
56	D3	1159	C
56	D3	1160	A
56	D3	1202	A
56	D3	1203	A
56	D3	1204	A
56	D3	1205	C
56	D3	1207	C
56	D3	1208	A
56	D3	1212	G
56	D3	1214	U
56	D3	1217	A
56	D3	1218	G
56	D3	1219	A
56	D3	1259	U
56	D3	1261	G
56	D3	1267	G
56	D3	1268	G
56	D3	1269	U
56	D3	1270	G
56	D3	1276	U
56	D3	1434	U
56	D3	1436	A
56	D3	1437	U
56	D3	1438	G
56	D3	1442	U
56	D3	1443	U
56	D3	1454	G
56	D3	1465	C
56	D3	1466	G
56	D3	1470	C
56	D3	1471	A
56	D3	1472	C
56	D3	1473	U
56	D3	1474	G
56	D3	1483	A
56	D3	1486	G
56	D3	1488	G
56	D3	1489	U
56	D3	1490	C
56	D3	1491	U
56	D3	1492	A
56	D3	1493	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
56	D3	1498	G
56	D3	1504	G
56	D3	1506	G
56	D3	1509	C
56	D3	1516	A
56	D3	1526	A
56	D3	1571	C
56	D3	1572	G
56	D3	1573	A
56	D3	1574	G
56	D3	1575	G
56	D3	1583	A
56	D3	1584	G
56	D3	1590	G
56	D3	1595	U
56	D3	1596	C
56	D3	1601	G
56	D3	1602	C
56	D3	1618	C
56	D3	1619	C
56	D3	1621	U
56	D3	1622	G
56	D3	1627	U
56	D3	1628	U
56	D3	1629	G
56	D3	1630	U
56	D3	1631	A
56	D3	1633	A
56	D3	1637	C
56	D3	1638	G
56	D3	1639	C
56	D3	1645	G
56	D3	1651	A
56	D3	1655	A
56	D3	1657	U
56	D3	1658	G
56	D3	1663	G
56	D3	1666	U
56	D3	1667	A
56	D3	1670	G
56	D3	1671	A
56	D3	1672	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
56	D3	1676	U
56	D3	1680	G
56	D3	1681	A
56	D3	1682	U
56	D3	1683	C
56	D3	1684	U
56	D3	1690	G
56	D3	1692	G
56	D3	1695	G
56	D3	1696	G
56	D3	1697	G
56	D3	1699	G
56	D3	1703	C
56	D3	1706	C
56	D3	1707	A
56	D3	1710	U
56	D3	1711	C
56	D3	1712	A
56	D3	1713	G
56	D3	1714	A
56	D3	1717	G
56	D3	1735	U
56	D3	1736	G
56	D3	1742	U
56	D3	1746	A
56	D3	1747	G
56	D3	1769	U
56	D3	1770	U
56	D3	1773	C
56	D3	1780	G
56	D3	1782	A
56	D3	1783	C
57	D4	2	U
57	D4	4	G
57	D4	14	A
57	D4	15	U
57	D4	22	A
57	D4	23	U
57	D4	24	U
57	D4	25	U
57	D4	30	A
57	D4	32	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
57	D4	33	A
57	D4	34	A
57	D4	35	U
57	D4	37	G
57	D4	38	U
57	D4	39	C
57	D4	40	A
57	D4	55	A
57	D4	56	A
57	D4	60	A
57	D4	61	G
57	D4	62	C
57	D4	87	G
57	D4	88	U
57	D4	90	C
57	D4	91	C
57	D4	94	A
57	D4	100	U
57	D4	103	A
57	D4	104	C
57	D4	114	A
57	D4	115	G
57	D4	198	U
57	D4	199	G
57	D4	201	C
57	D4	246	A
57	D4	247	U
57	D4	248	G
57	D4	252	C
57	D4	254	A
57	D4	256	G
57	D4	259	C
57	D4	267	A
57	D4	305	G
57	D4	312	U
57	D4	313	A
57	D4	319	G
57	D4	322	A
57	D4	324	U
57	D4	325	C
57	D4	329	C

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
55	D2	82	A
55	D2	311	C
55	D2	314	U
55	D2	370	U
55	D2	451	G
55	D2	492	G
56	D3	0	U
56	D3	474	A
56	D3	579	A
56	D3	586	G
56	D3	912	U
56	D3	925	G
56	D3	934	C
56	D3	1057	U
56	D3	1525	A
56	D3	1573	A
56	D3	1594	G
56	D3	1620	C
56	D3	1638	G
56	D3	1657	U
56	D3	1669	U
56	D3	1706	C
56	D3	1746	A

## 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 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	$\# Z  > 2$
60	GTP	CL	2001	59	26,34,34	0.93	1 (3%)	32,54,54	1.49	5 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	GTP	CL	2001	59	-	3/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	CL	2001	GTP	C6-N1	-2.43	1.34	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	CL	2001	GTP	PB-O3B-PG	-3.79	119.82	132.83
60	CL	2001	GTP	PA-O3A-PB	-3.57	120.58	132.83
60	CL	2001	GTP	C3'-C2'-C1'	3.18	105.77	100.98
60	CL	2001	GTP	C8-N7-C5	2.42	107.60	102.99
60	CL	2001	GTP	C5-C6-N1	2.31	118.03	113.95

There are no chirality outliers.

All (3) torsion outliers are listed below:

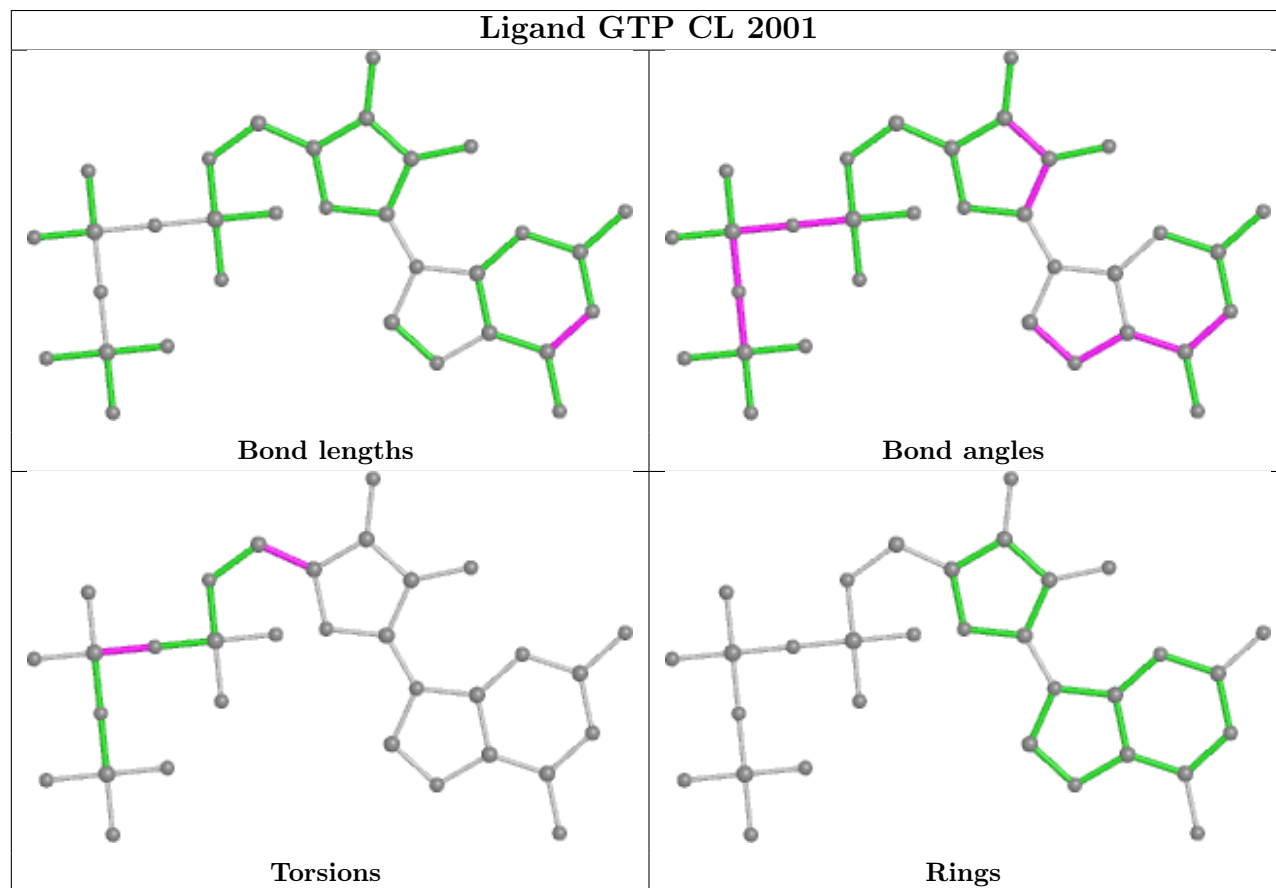
Mol	Chain	Res	Type	Atoms
60	CL	2001	GTP	O4'-C4'-C5'-O5'
60	CL	2001	GTP	C3'-C4'-C5'-O5'
60	CL	2001	GTP	PA-O3A-PB-O2B

There are no ring outliers.

No monomer is involved in short contacts.

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

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
57	D4	5
56	D3	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D4	118:A	O3'	197:G	P	26.63
1	D4	106:C	O3'	111:G	P	20.40
1	D3	40:A	O3'	467:G	P	18.14
1	D4	267:A	O3'	304:U	P	18.02
1	D4	206:C	O3'	245:U	P	17.13
1	D4	260:U	O3'	263:A	P	9.74
1	D3	18:C	O3'	22:A	P	8.80

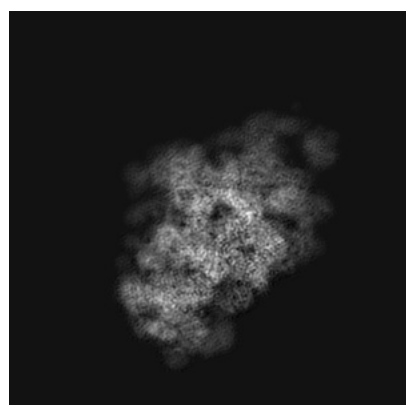
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11357. These allow visual inspection of the internal detail of the map and identification of artifacts.

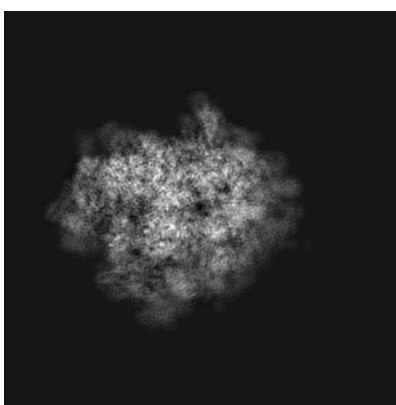
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

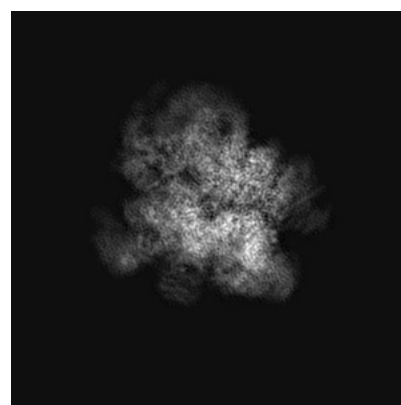
#### 6.1.1 Primary map



X



Y

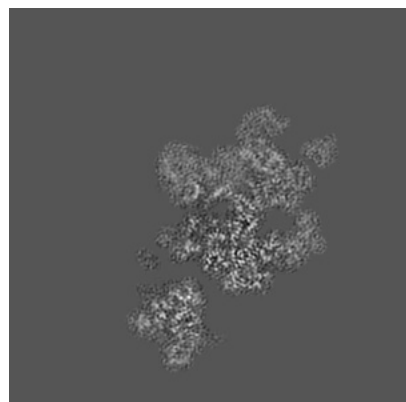


Z

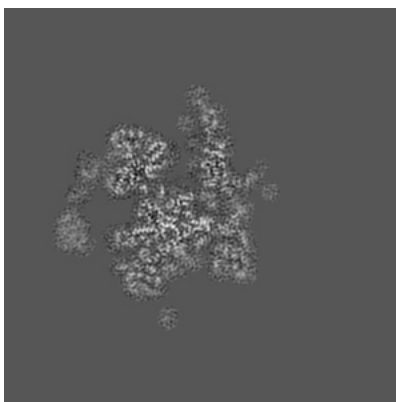
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

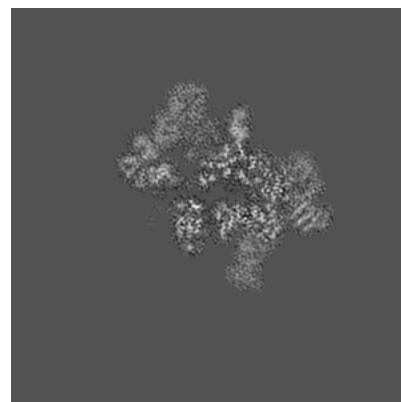
#### 6.2.1 Primary map



X Index: 240



Y Index: 240

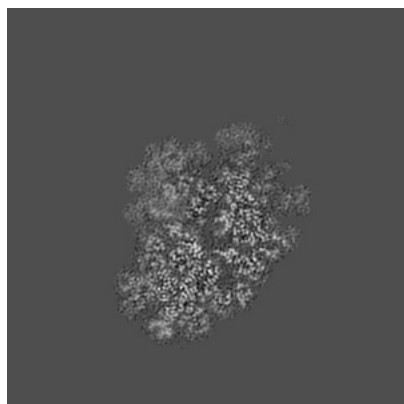


Z Index: 240

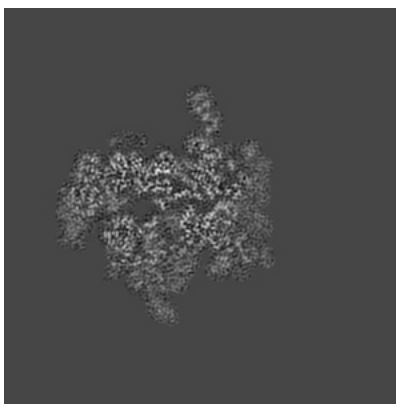
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

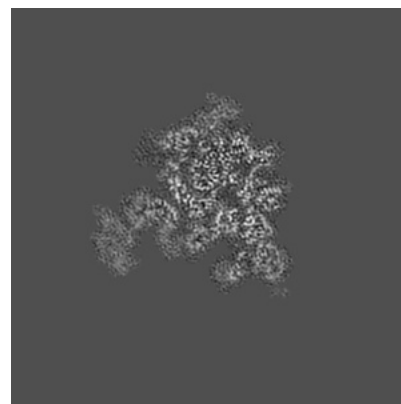
### 6.3.1 Primary map



X Index: 283



Y Index: 225



Z Index: 187

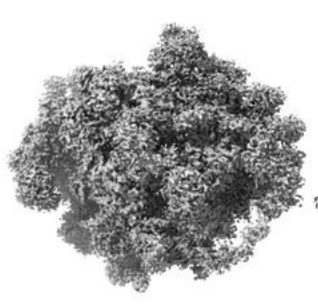
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

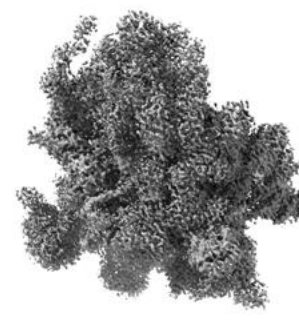
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

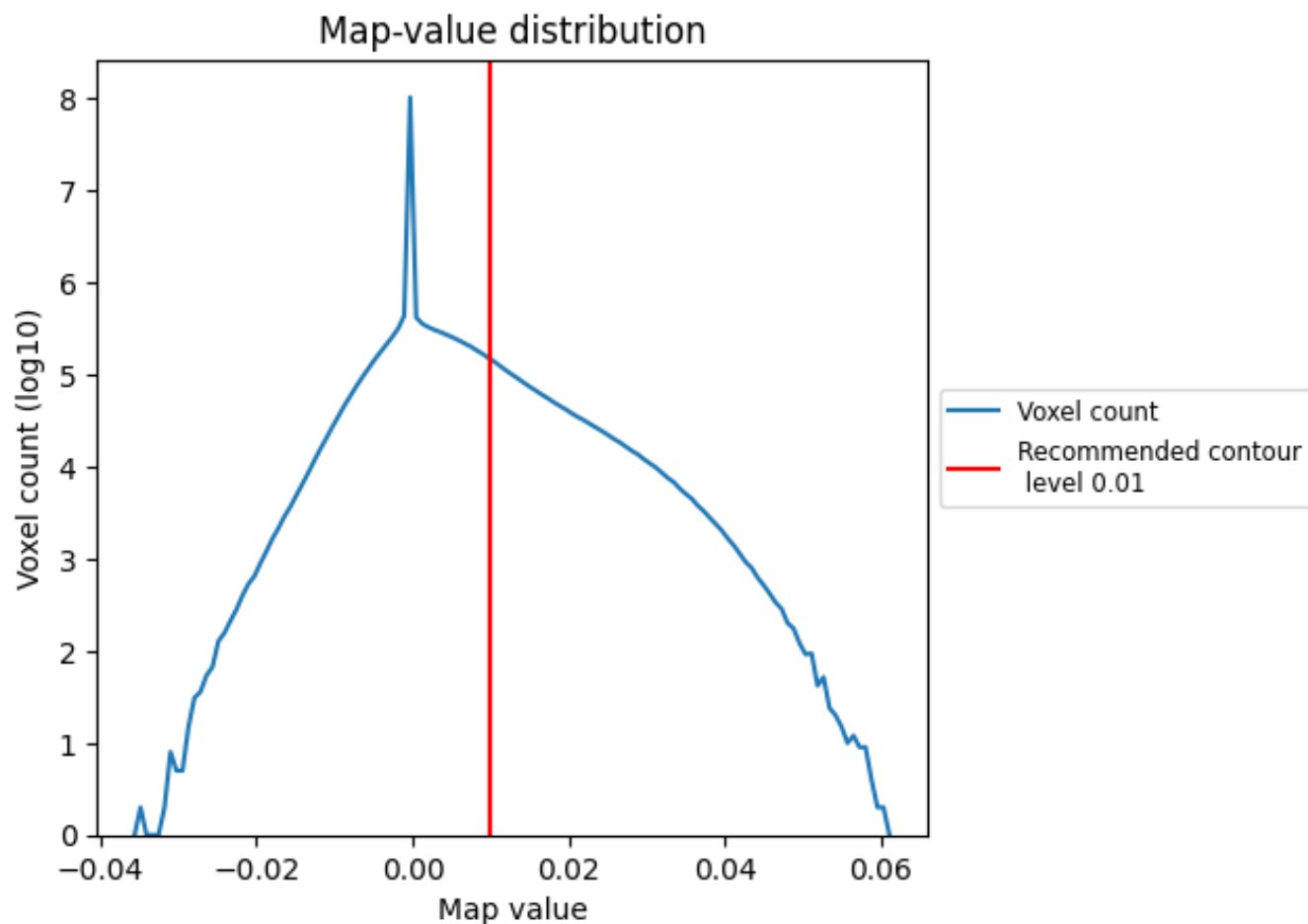
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

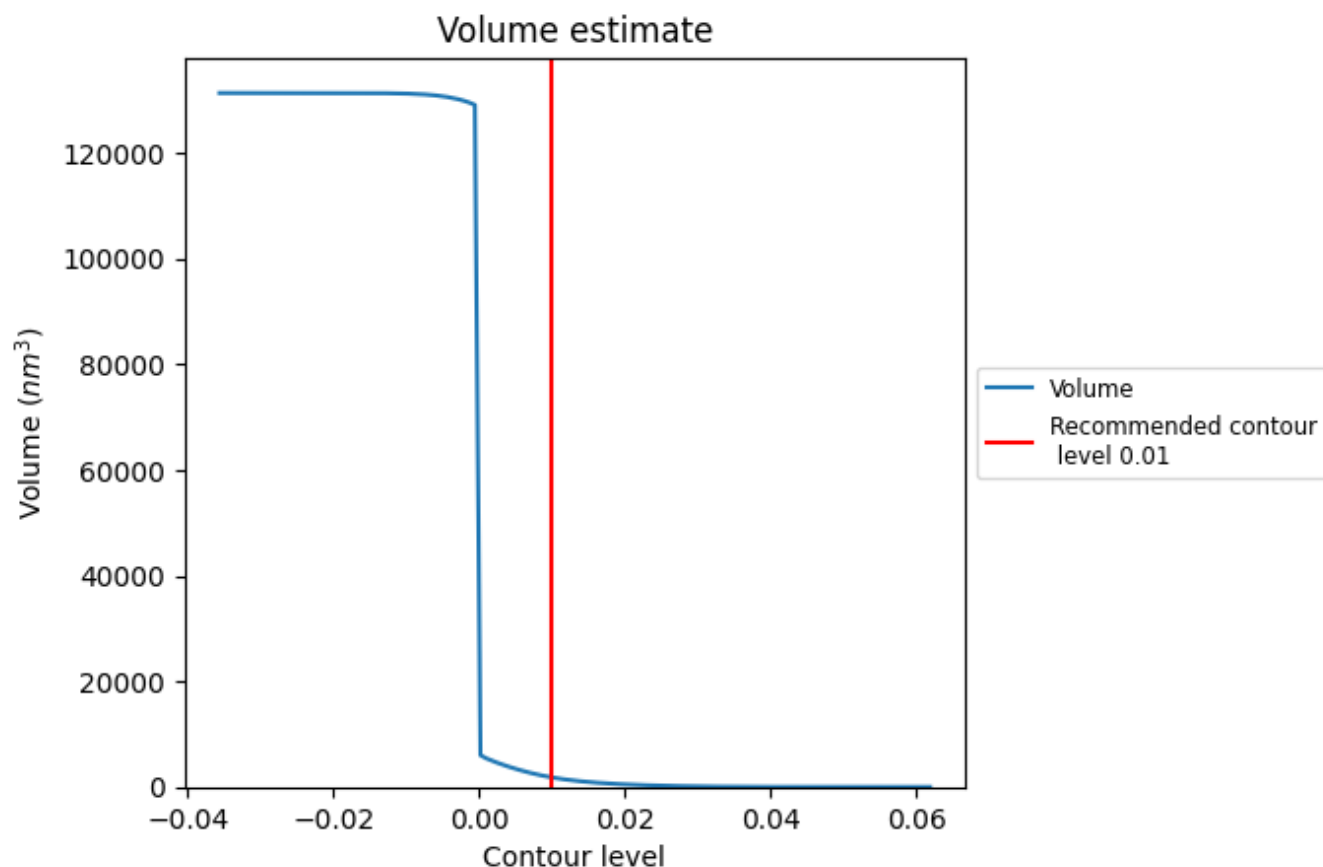
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

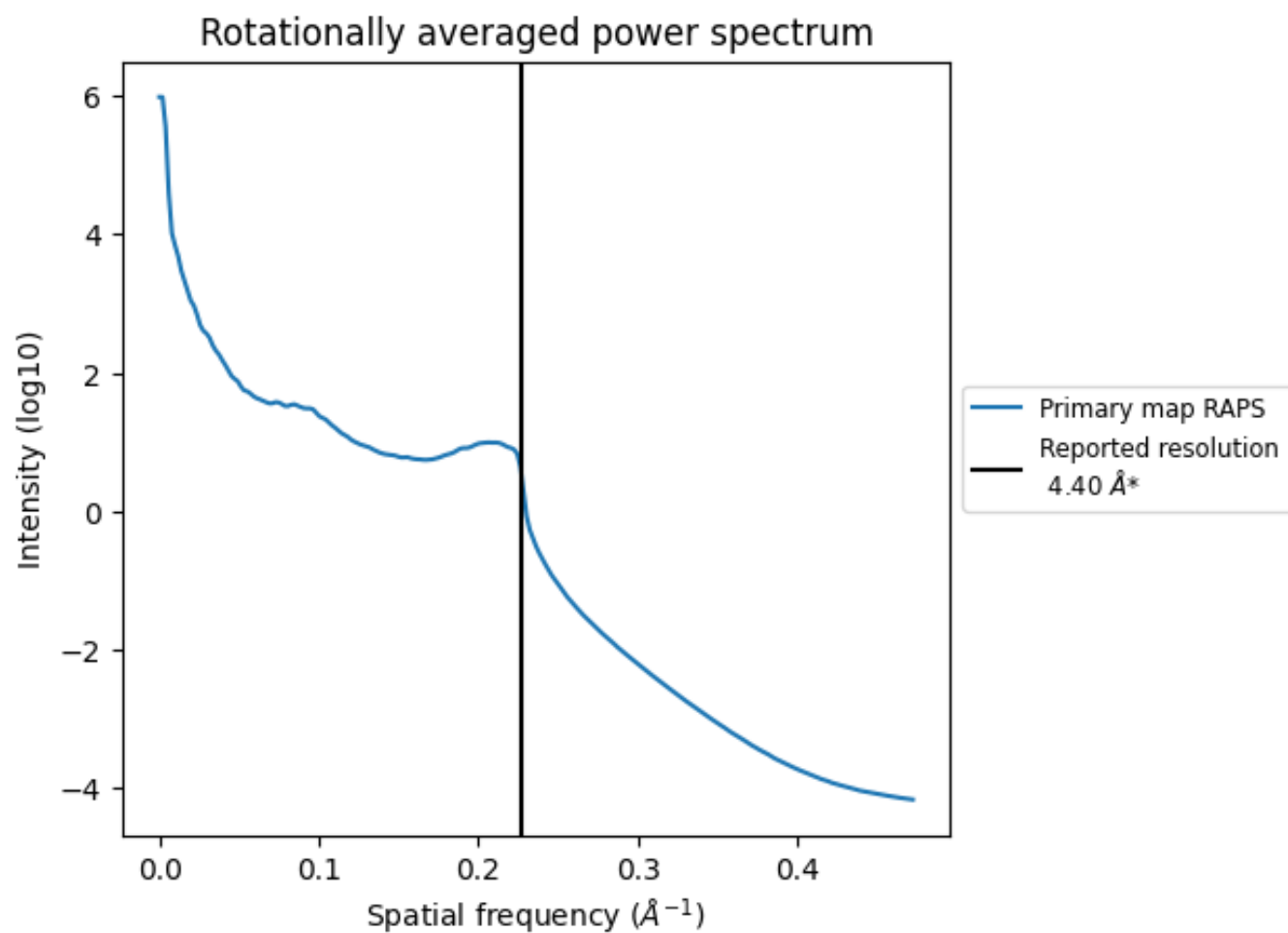
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1809 nm<sup>3</sup>; this corresponds to an approximate mass of 1634 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 ⓘ

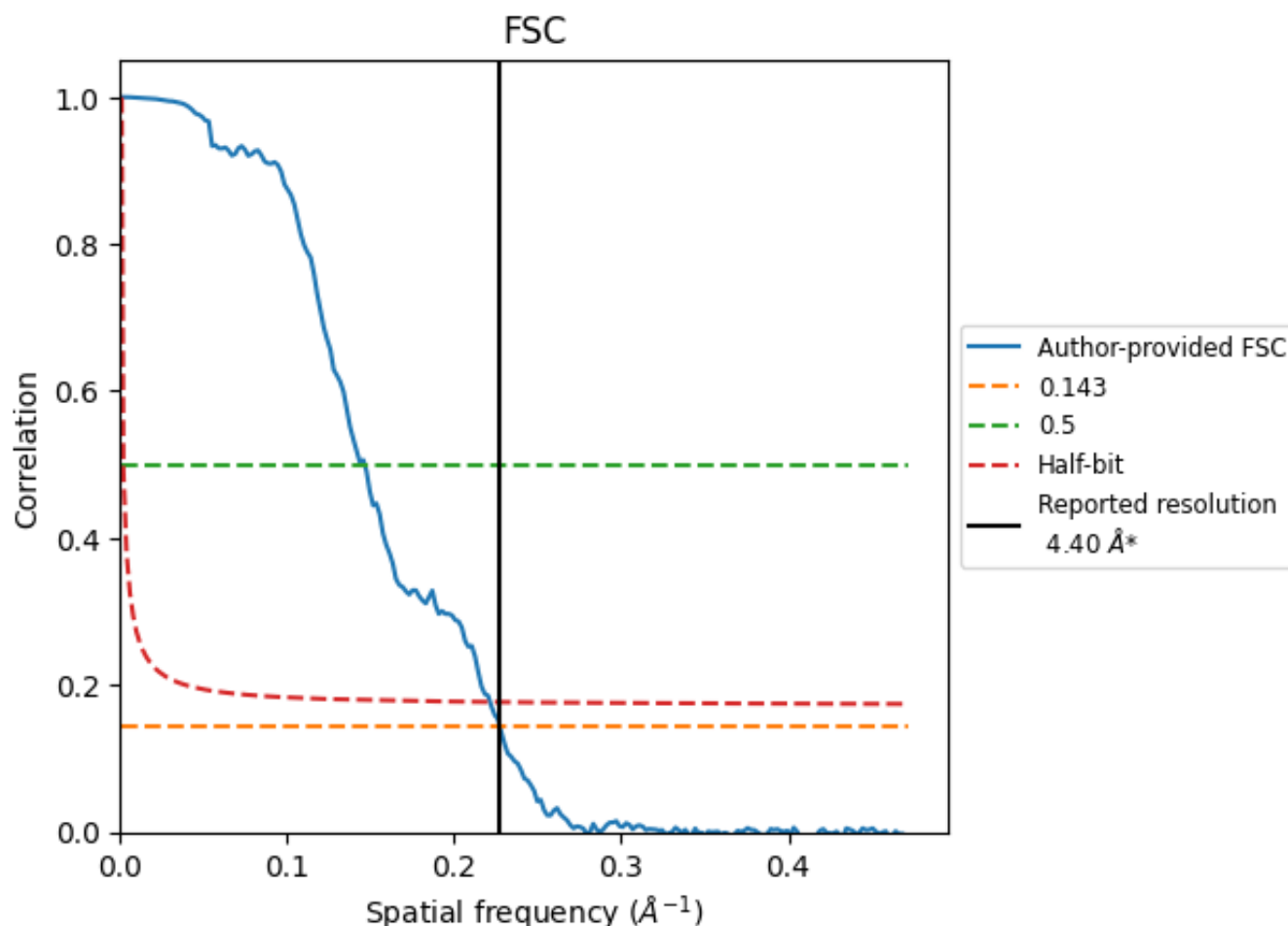


\*Reported resolution corresponds to spatial frequency of 0.227 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.227 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

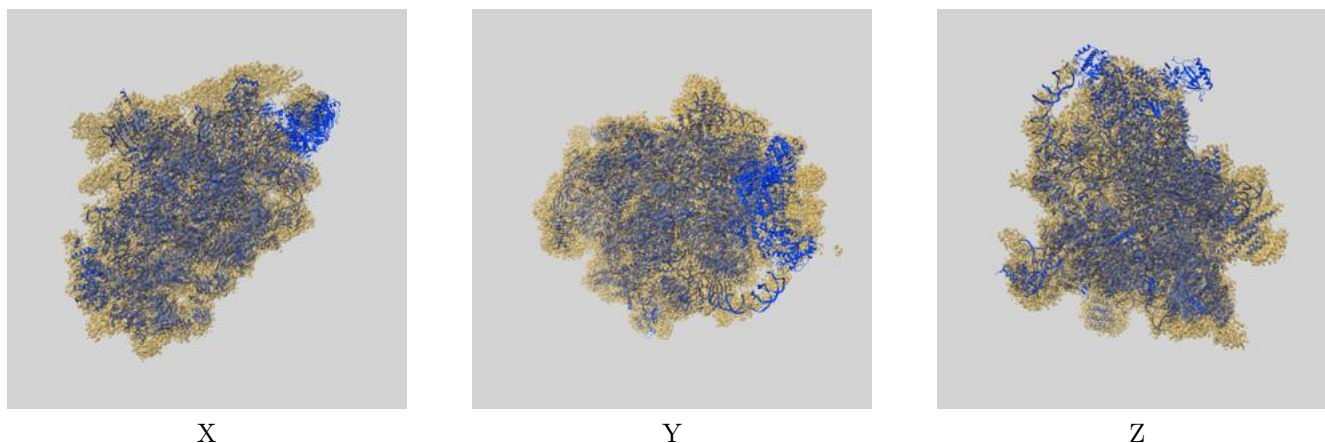
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.40	6.83	4.51
Unmasked-calculated*	-	-	-

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

## 9 Map-model fit [i](#)

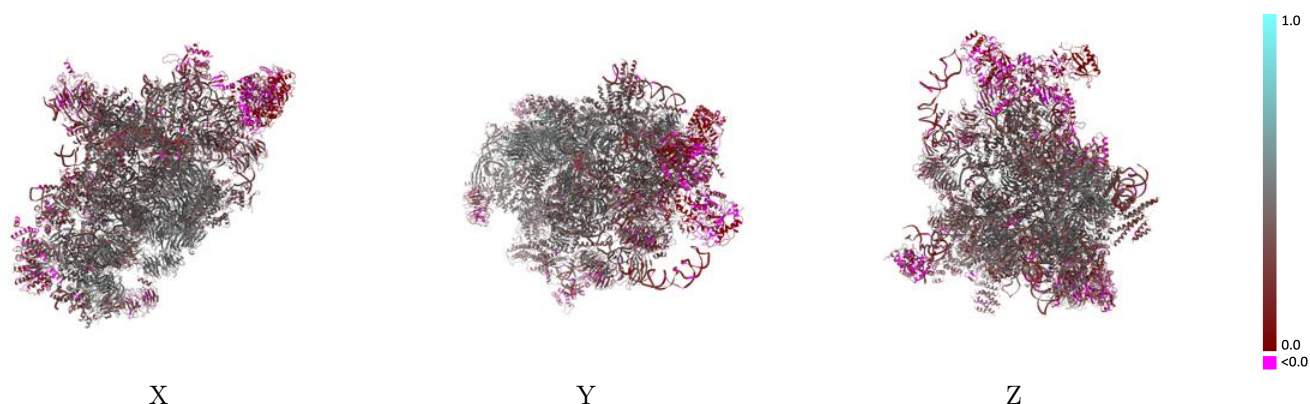
This section contains information regarding the fit between EMDB map EMD-11357 and PDB model 6ZQA. Per-residue inclusion information can be found in section 3 on page 16.

### 9.1 Map-model overlay [i](#)



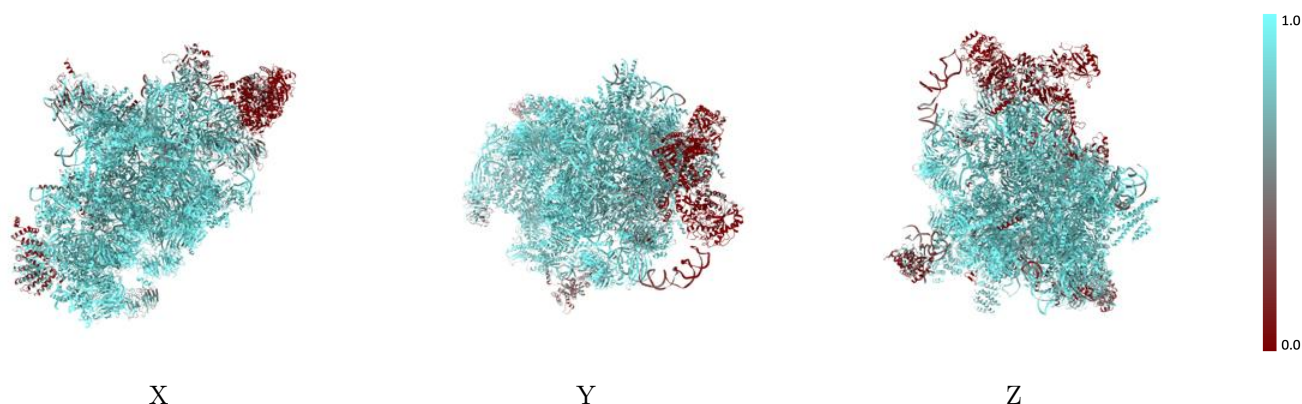
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



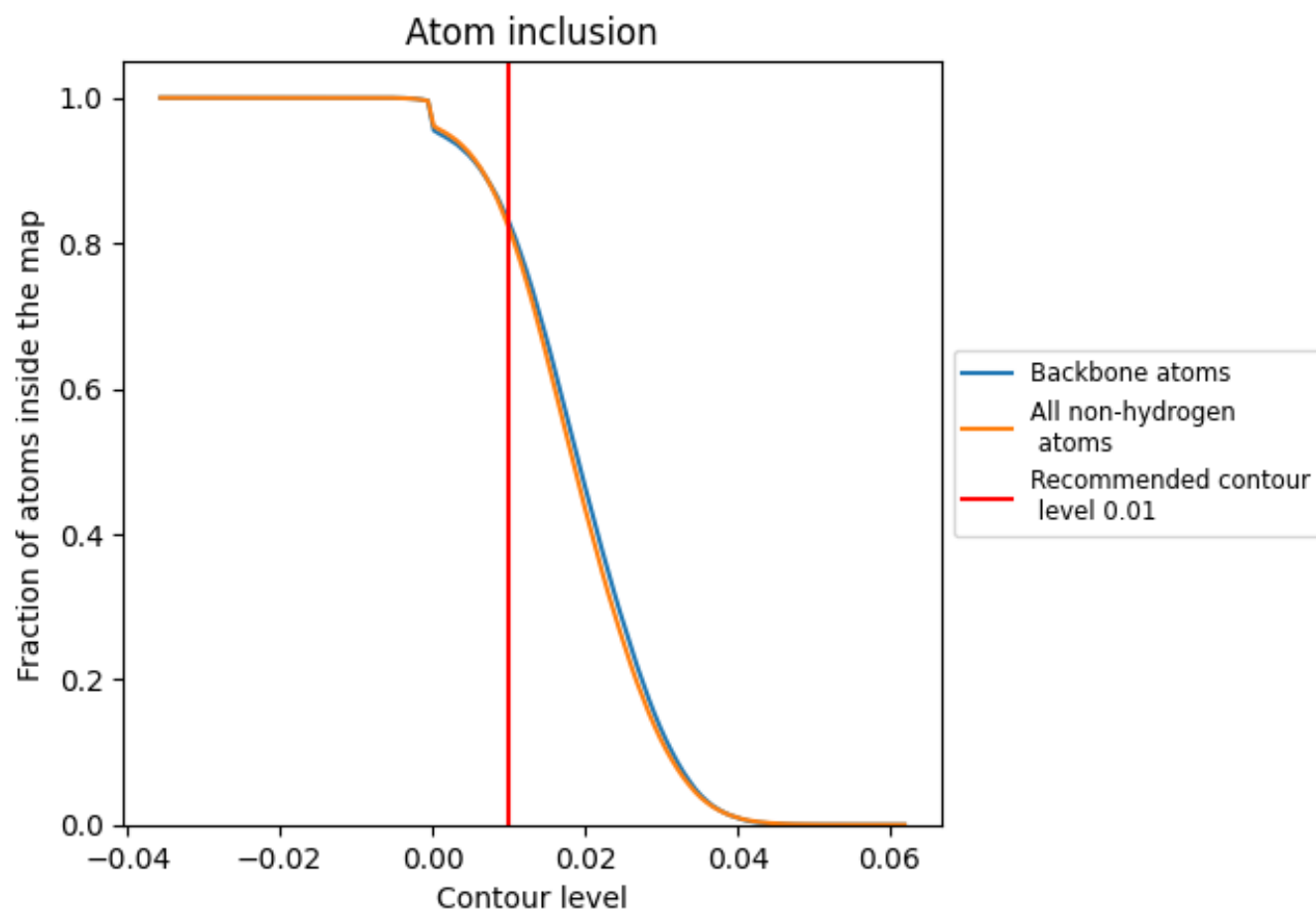
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 82% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8227	 0.3460
CA	 0.9454	 0.4470
CB	 0.9439	 0.4010
CD	 0.9186	 0.3530
CE	 0.9012	 0.3480
CF	 0.9640	 0.4440
CG	 0.9198	 0.3700
CH	 0.6664	 0.2100
CI	 0.9624	 0.4390
CJ	 0.9356	 0.4310
CK	 0.9340	 0.4060
CL	 0.8939	 0.3820
CM	 0.9281	 0.3770
CN	 0.0719	 0.0340
D2	 0.9094	 0.3450
D3	 0.8026	 0.3160
D4	 0.9046	 0.3430
DA	 0.6706	 0.3100
DF	 0.9374	 0.4280
DH	 0.4830	 0.2050
DJ	 0.8721	 0.3550
DN	 0.5863	 0.2760
DO	 0.8416	 0.3740
DQ	 0.9497	 0.4520
DS	 0.4031	 0.2190
DW	 0.8502	 0.3970
DX	 0.9085	 0.4270
Db	 0.1222	 0.1760
Dc	 0.9774	 0.4680
JF	 0.9141	 0.3620
JG	 0.9334	 0.4250
JH	 0.2780	 0.0800
JJ	 0.8552	 0.3440
JM	 0.9061	 0.3970
JN	 0.8377	 0.3820



*Continued on next page...*

Continued from previous page...

Chain	Atom inclusion	Q-score
JO	 0.8950	 0.3890
JP	 0.9466	 0.4470
JQ	 0.3910	 0.2500
UA	 0.9624	 0.4620
UB	 0.7938	 0.2880
UC	 0.9315	 0.3950
UD	 0.9533	 0.4240
UE	 0.9707	 0.4420
UF	 0.9457	 0.3420
UG	 0.9022	 0.4350
UH	 0.7553	 0.2660
UI	 0.9497	 0.3370
UJ	 0.6940	 0.2990
UK	 0.9551	 0.4010
UL	 0.9282	 0.3590
UM	 0.7186	 0.2860
UN	 0.8349	 0.3770
UO	 0.9648	 0.4470
UP	 0.9195	 0.3510
UQ	 0.9522	 0.4320
UR	 0.9600	 0.4600
US	 0.8935	 0.3210
UU	 0.9668	 0.4630
UV	 0.0722	 0.0420
UX	 0.9699	 0.4540
UZ	 0.9330	 0.3770