



## Full wwPDB EM Validation Report ⓘ

Dec 17, 2022 – 10:54 pm GMT

PDB ID : 6ZQG  
EMDB ID : EMD-11363  
Title : Cryo-EM structure of the 90S pre-ribosome from *Saccharomyces cerevisiae*, state Dis-C  
Authors : Cheng, J.; Lau, B.; Venuta, G.L.; Berninghausen, O.; Hurt, E.; Beckmann, R.  
Deposited on : 2020-07-09  
Resolution : 3.50 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:

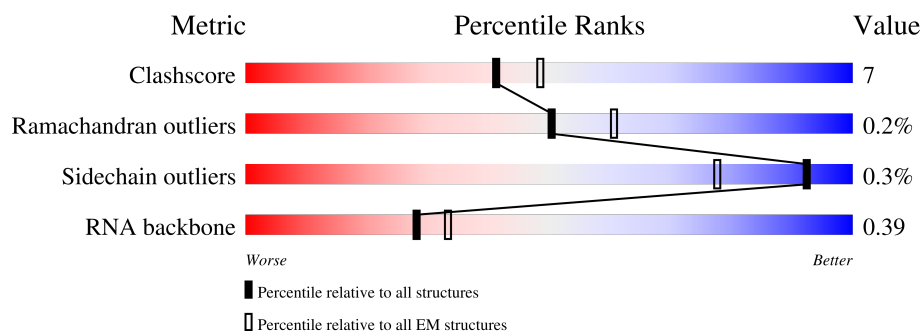
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (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 3.50 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.



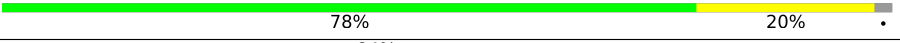




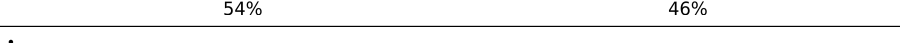

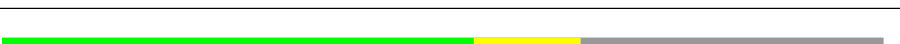








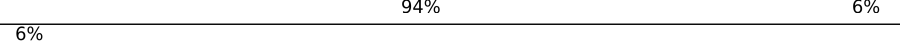
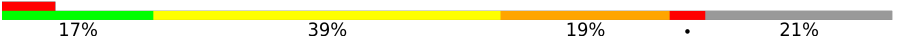

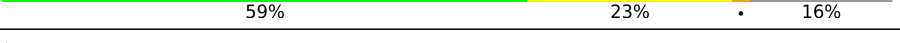




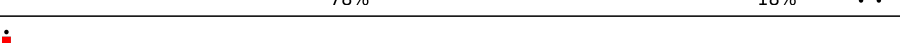





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	UB	810	
2	UC	610	
3	US	552	
4	UX	189	
5	CJ	290	
6	CK	593	
7	CL	1183	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	CM	367	
9	JF	252	
9	JG	252	
10	JH	483	
11	JL	318	
12	JJ	274	
13	DF	225	
14	DQ	143	
15	DS	147	
16	DT	144	
17	Dc	67	
18	D3	1758	
19	DA	255	
20	DE	261	
21	DG	236	
22	DH	190	
23	DI	200	
24	DJ	197	
25	DL	156	
26	DN	151	
27	DO	137	
28	DZ	108	
29	DW	130	
30	DX	145	
31	DY	135	
			
			
			
			
			

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
32	Db	82	<div><div></div><div>95%</div><div></div></div>
33	UN	899	<div><div></div><div>11%</div><div></div><div>88%</div><div></div></div>
34	JD	1267	<div><div></div><div>40%</div><div></div><div>60%</div><div></div><div>5%</div><div></div><div>35%</div><div></div></div>
35	D4	23	<div><div></div><div>61%</div><div></div><div>30%</div><div></div><div>9%</div><div></div></div>
36	D5	9	<div><div></div><div>33%</div><div></div><div>67%</div><div></div></div>

## 2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 80072 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 Nucleolar complex protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	UB	403	Total	C	N	O	S	0	0
			2207	1328	441	435	3		

- Molecule 2 is a protein called Something about silencing protein 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	UC	47	Total	C	N	O	0	0
			393	243	86	64		

- Molecule 3 is a protein called Noc4,Nucleolar complex protein 4,Noc4.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	US	484	Total	C	N	O	0	0
			2411	1443	484	484		

- Molecule 4 is a protein called rRNA-processing protein FCF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	UX	143	Total	C	N	O	S	0	0
			1132	729	199	194	10		

- Molecule 5 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	CJ	219	Total	C	N	O	0	0
			1083	645	219	219		

- Molecule 6 is a protein called U3 small nucleolar RNA-associated protein MPP10.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	CK	92	Total	C	N	O	0	0
			645	398	116	131		

- Molecule 7 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	CL	710	Total	C	N	O	S	0	0
			5758	3696	1019	1016	27		

- Molecule 8 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	CM	360	Total	C	N	O	S	0	0
			2781	1781	473	516	11		

- Molecule 9 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	JF	216	Total	C	N	O	0	0
			1071	639	216	216		
9	JG	221	Total	C	N	O	0	0
			1096	654	221	221		

- Molecule 10 is a protein called Essential nuclear protein 1.

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

- Molecule 11 is a protein called Dimethyladenosine transferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	JL	283	Total	C	N	O	S	0	0
			2262	1439	401	408	14		

- Molecule 12 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	JJ	181	Total	C	N	O	S	0	0
			1436	917	261	254	4		

- Molecule 13 is a protein called Rps5p.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	DF	196	Total	C	N	O	0	0
			970	578	196	196		

- Molecule 14 is a protein called 40S ribosomal protein S16-A.

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

- Molecule 15 is a protein called 40S ribosomal protein S18-A,40S ribosomal protein S18-A,Rps18.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	DS	77	Total	C	N	O	S	0	0
			630	403	115	110	2		

- Molecule 16 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	DT	143	Total	C	N	O	0	0
			700	414	143	143		

- Molecule 17 is a protein called 40S ribosomal protein S28-A.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	D3	1387	Total	C	N	O	P	0	0
			29536	13208	5223	9718	1387		

- Molecule 19 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	DA	214	Total	C	N	O	S	0	0
			1709	1084	310	311	4		

- Molecule 20 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	DE	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 21 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	DG	226	Total	C	N	O	S	0	0
			1799	1129	346	321	3		

- Molecule 22 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	DH	184	Total	C	N	O	S	0	0
			1481	951	265	265			

- Molecule 23 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	DI	188	Total	C	N	O	S	0	0
			1489	925	298	264	2		

- Molecule 24 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	DJ	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 25 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	DL	143	Total	C	N	O	S	0	0
			1154	739	218	194	3		

- Molecule 26 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	DN	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 27 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	DO	127	Total	C	N	O	S	0	0
			941	578	186	174	3		

- Molecule 28 is a protein called 40S ribosomal protein S25-A.



Mol	Chain	Residues	Atoms				AltConf	Trace
28	DZ	67	Total	C	N	O	0	0
			332	198	67	67		

- Molecule 29 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	DW	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 30 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	DX	143	Total	C	N	O	S	0	0
			1115	705	219	189	2		

- Molecule 31 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	DY	133	Total	C	N	O	0	0
			1067	673	207	187		

- Molecule 32 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Db	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 33 is a protein called U3 small nucleolar RNA-associated protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	UN	108	Total	C	N	O	S	0	0
			920	561	184	165	10		

- Molecule 34 is a protein called Probable ATP-dependent RNA helicase DHR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	JD	829	Total	C	N	O	S	0	0
			4600	2795	916	887	2		

- Molecule 35 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	D4	23	Total	C	N	O	P	0	0
			496	220	87	165	24		

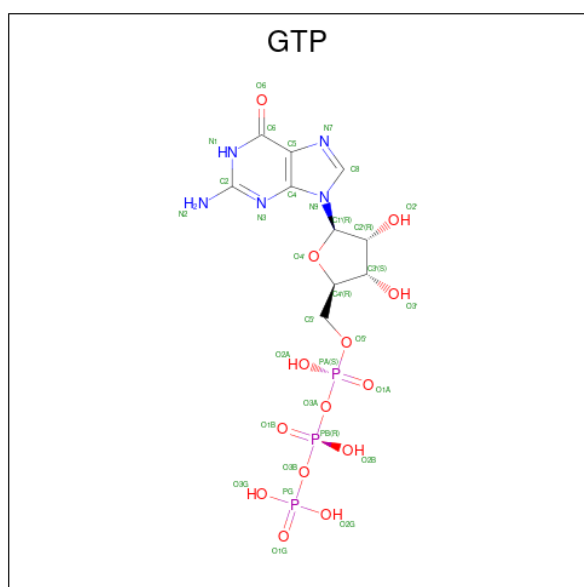
- Molecule 36 is a RNA chain called Poly-U RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	D5	9	Total	C	N	O	P	0	0
			180	81	18	72	9		

- Molecule 37 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 38 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
38	CL	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
39	CL	1	Total	Mg	0
			1	1	

*Continued on next page...*

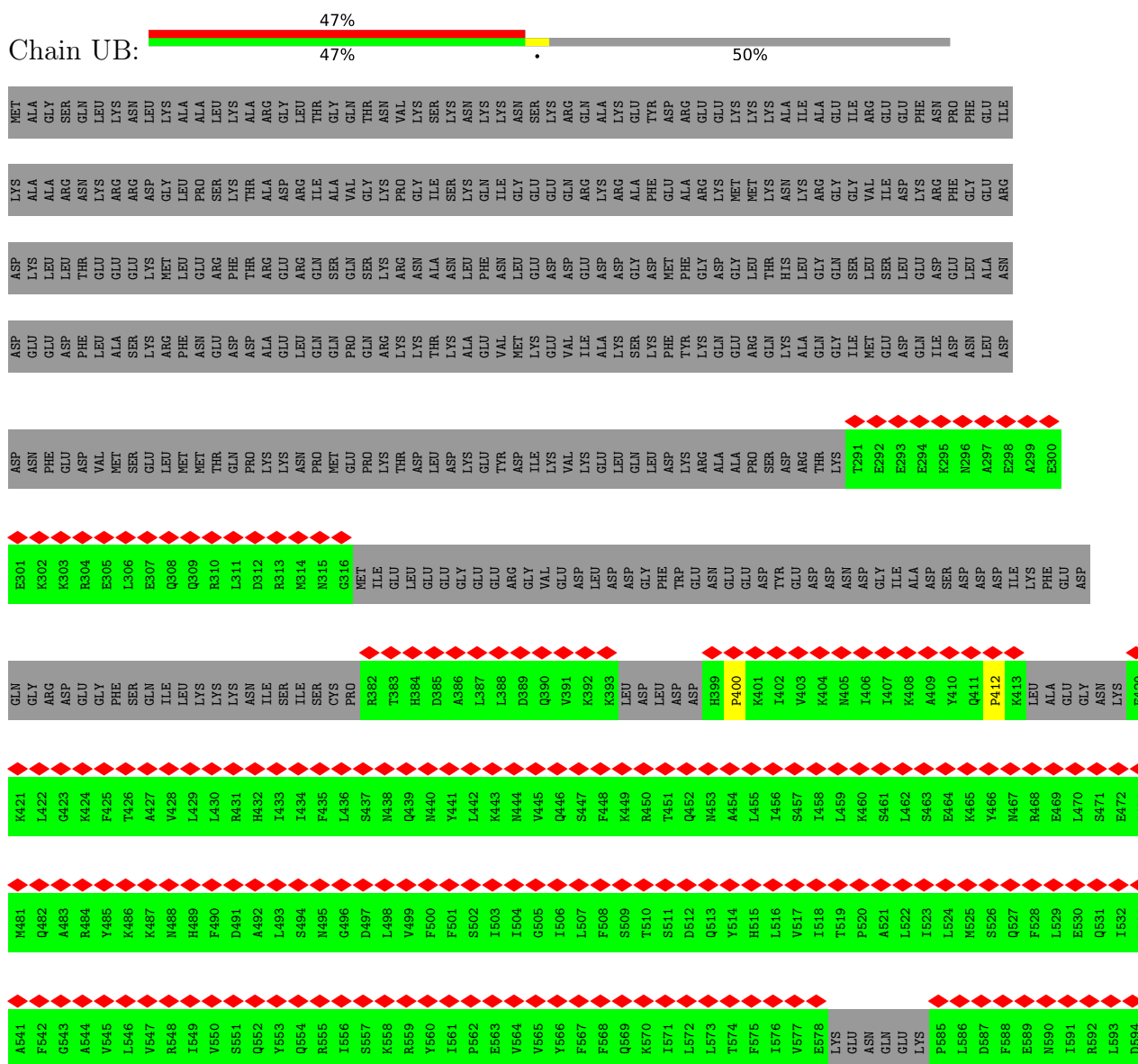
*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
39	D3	37	Total	Mg	0
			37	37	
39	DG	1	Total	Mg	0
			1	1	

### 3 Residue-property plots

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

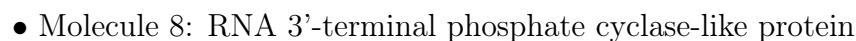
#### • Molecule 1: Nucleolar complex protein 14









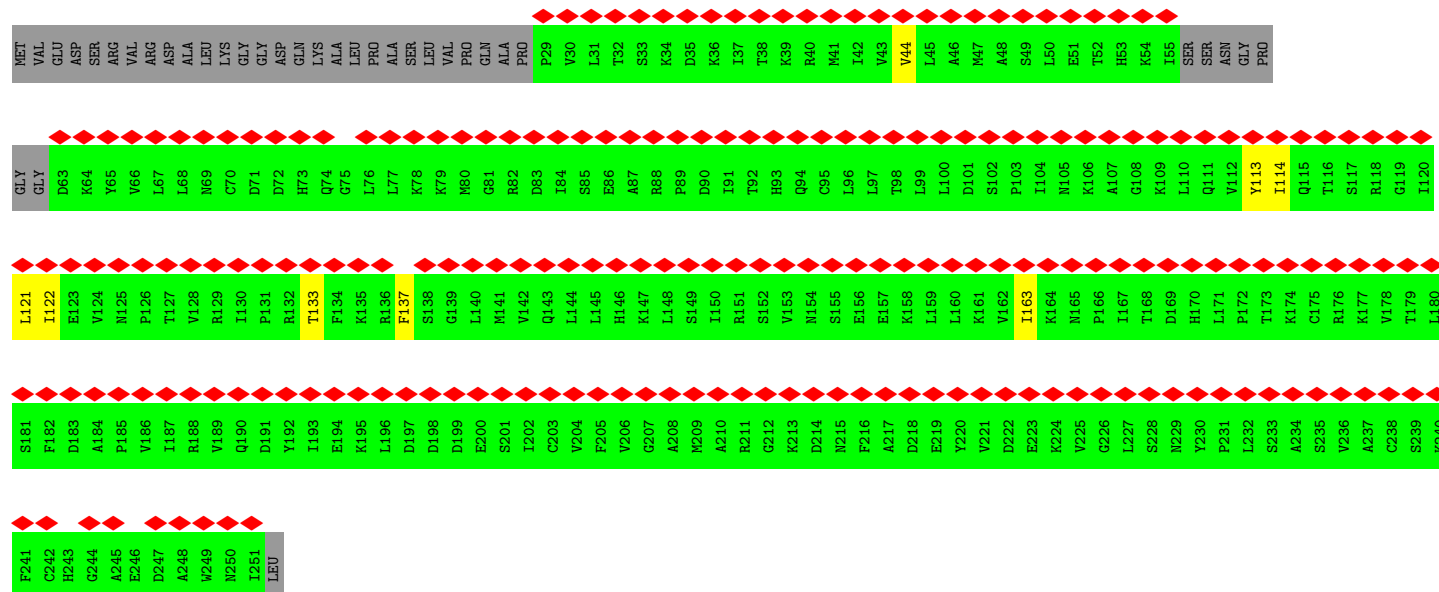
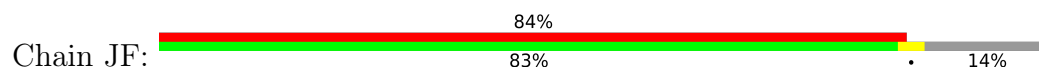


MET	SR8	SR9	SR10	SR11	SR12	SR13	SR14	SR15	SR16	SR17	SR18	SR19	SR20	SR21	SR22	SR23	SR24	SR25	SR26	SR27	SR28	SR29	SR30	SR31	SR32	SR33	SR34	SR35	SR36	SR37	SR38	SR39	SR40	SR41	SR42	SR43	SR44	SR45	SR46	SR47	SR48	SR49	SR50	SR51	SR52	SR53	SR54	SR55	SR56	SR57	SR58	SR59	SR60	SR61	SR62	SR63	SR64	SR65	SR66	SR67	SR68	SR69	SR70	SR71	SR72	SR73	SR74	SR75	SR76	SR77	SR78	SR79	SR80	SR81	SR82	SR83	SR84	SR85	SR86	SR87	SR88	SR89	SR90	SR91	SR92	SR93	SR94	SR95	SR96	SR97	SR98	SR99	SR100	SR101	SR102	SR103	SR104	SR105	SR106	SR107	SR108	SR109	SR110	SR111	SR112	SR113	SR114	SR115	SR116	SR117	SR118	SR119	SR120	SR121	SR122	SR123	SR124	SR125	SR126	SR127	SR128	SR129	SR130	SR131	SR132	SR133	SR134	SR135	SR136	SR137	SR138	SR139	SR140	SR141	SR142	SR143	SR144	SR145	SR146	SR147	SR148	SR149	SR150	SR151	SR152	SR153	SR154	SR155	SR156	SR157	SR158	SR159	SR160	SR161	SR162	SR163	SR164	SR165	SR166	SR167	SR168	SR169	SR170	SR171	SR172	SR173	SR174	SR175	SR176	SR177	SR178	SR179	SR180	SR181	SR182	SR183	SR184	SR185	SR186	SR187	SR188	SR189	SR190	SR191	SR192	SR193	SR194	SR195	SR196	SR197	SR198	SR199	SR200	SR201	SR202	SR203	SR204	SR205	SR206	SR207	SR208	SR209	SR210	SR211	SR212	SR213	SR214	SR215	SR216	SR217	SR218	SR219	SR220	SR221	SR222	SR223	SR224	SR225	SR226	SR227	SR228	SR229	SR230	SR231	SR232	SR233	SR234	SR235	SR236	SR237	SR238	SR239	SR240	SR241	SR242	SR243	SR244	SR245	SR246	SR247	SR248	SR249	SR250	SR251	SR252	SR253	SR254	SR255	SR256	SR257	SR258	SR259	SR260	SR261	SR262	SR263	SR264	SR265	SR266	SR267	SR268	SR269	SR270	SR271	SR272	SR273	SR274	SR275	SR276	SR277	SR278	SR279	SR280	SR281	SR282	SR283	SR284	SR285	SR286	SR287	SR288	SR289	SR290	SR291	SR292	SR293	SR294	SR295	SR296	SR297	SR298	SR299	SR300	SR301	SR302	SR303	SR304	SR305	SR306	SR307	SR308	SR309	SR310	SR311	SR312	SR313	SR314	SR315	SR316	SR317	SR318	SR319	SR320	SR321	SR322	SR323	SR324	SR325	SR326	SR327	SR328	SR329	SR330	SR331	SR332	SR333	SR334	SR335	SR336	SR337	SR338	SR339	SR340	SR341	SR342	SR343	SR344	SR345	SR346	SR347	SR348	SR349	SR350	SR351	SR352	SR353	SR354	SR355	SR356	SR357	SR358	SR359	SR360	SR361	SR362	SR363	SR364	SR365	SR366	SR367	SR368	SR369	SR370	SR371	SR372	SR373	SR374	SR375	SR376	SR377	SR378	SR379	SR380	SR381	SR382	SR383	SR384	SR385	SR386	SR387	SR388	SR389	SR390	SR391	SR392	SR393	SR394	SR395	SR396	SR397	SR398	SR399	SR400	SR401	SR402	SR403	SR404	SR405	SR406	SR407	SR408	SR409	SR410	SR411	SR412	SR413	SR414	SR415	SR416	SR417	SR418	SR419	SR420	SR421	SR422	SR423	SR424	SR425	SR426	SR427	SR428	SR429	SR430	SR431	SR432	SR433	SR434	SR435	SR436	SR437	SR438	SR439	SR440	SR441	SR442	SR443	SR444	SR445	SR446	SR447	SR448	SR449	SR450	SR451	SR452	SR453	SR454	SR455	SR456	SR457	SR458	SR459	SR460	SR461	SR462	SR463	SR464	SR465	SR466	SR467	SR468	SR469	SR470	SR471
-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------

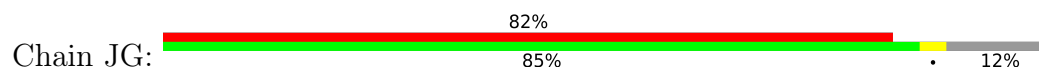




• Molecule 9: Ribosomal RNA small subunit methyltransferase NEP1

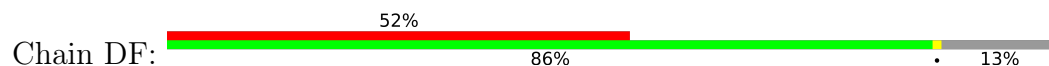


• Molecule 9: Ribosomal RNA small subunit methyltransferase NEP1

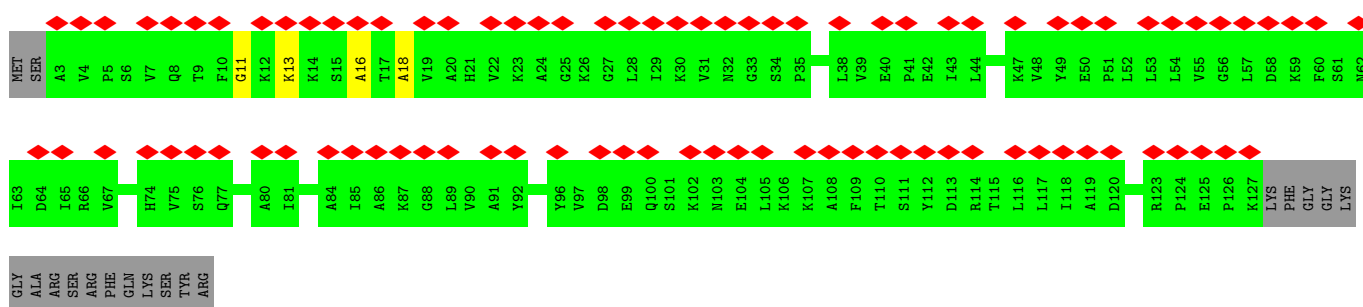
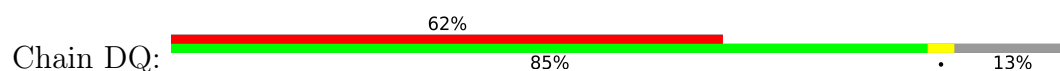




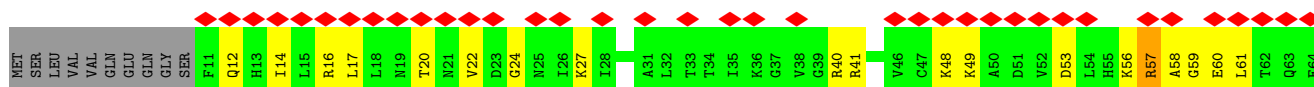
- Molecule 13: Rps5p

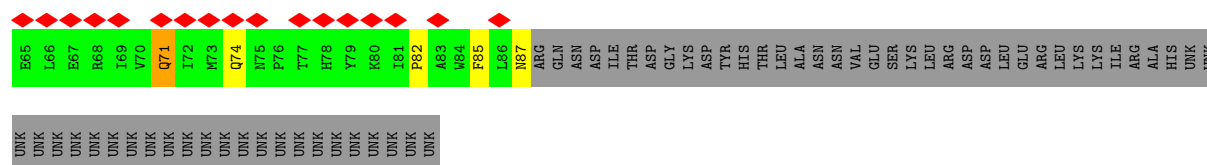


- Molecule 14: 40S ribosomal protein S16-A

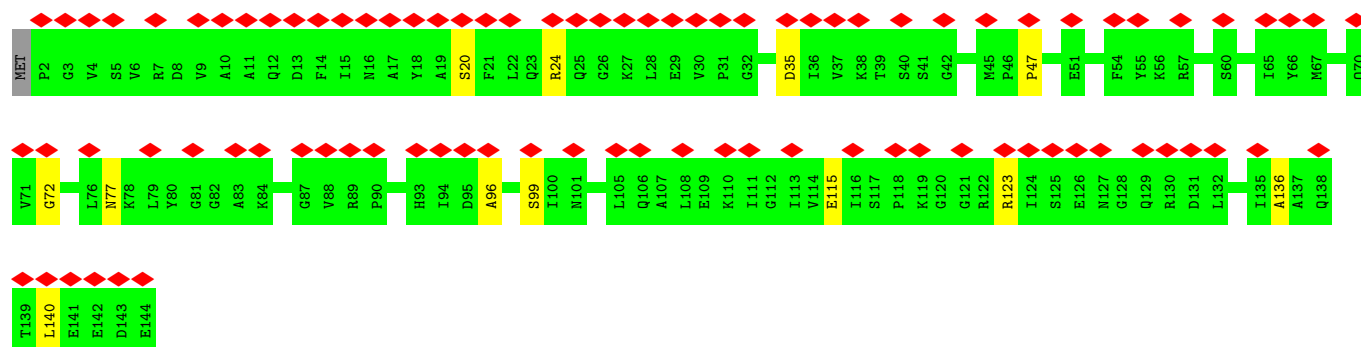


- Molecule 15: 40S ribosomal protein S18-A,40S ribosomal protein S18-A,Rps18

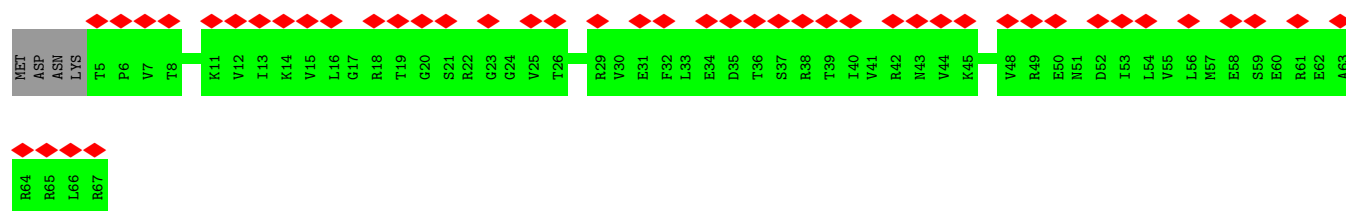




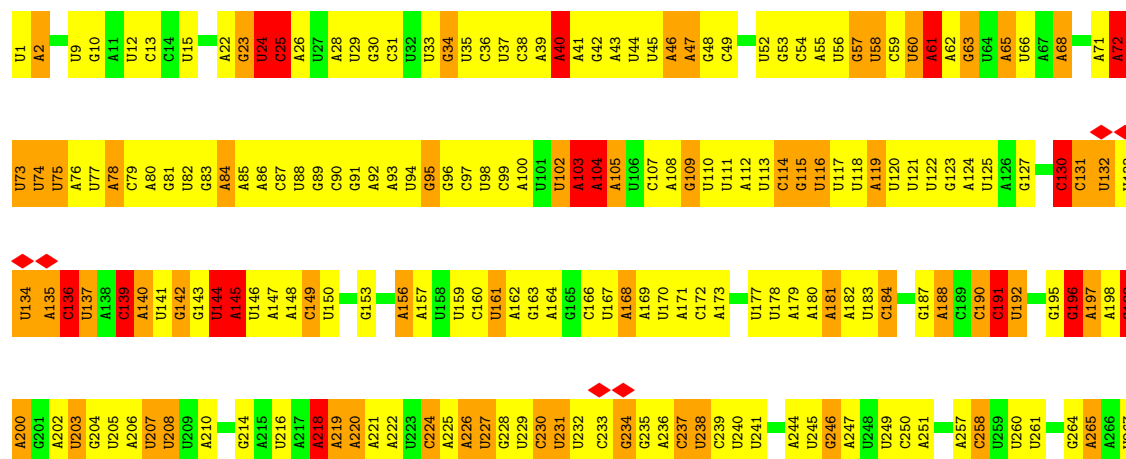
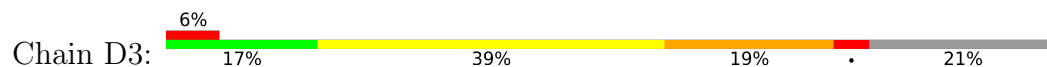
• Molecule 16: 40S ribosomal protein S19-A



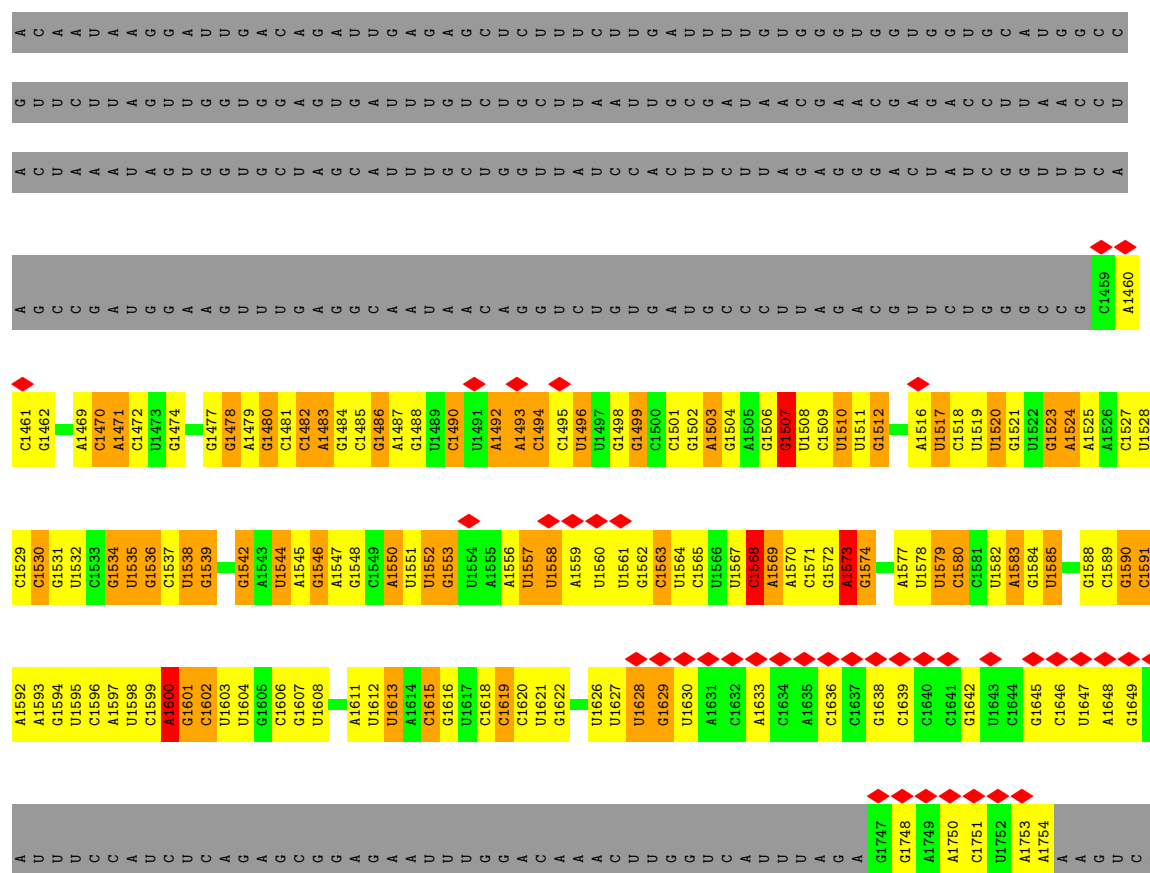
• Molecule 17: 40S ribosomal protein S28-A



• Molecule 18: 18S rRNA

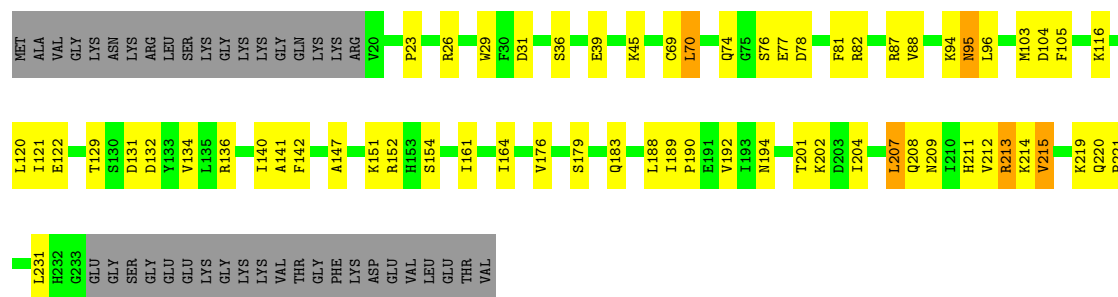


C1159	U1095	A1030	C962	G895	U767	A707	U640	A579	U513	A452	G392	G330	C268
A1160	C1096	U1031	A963	A898	C768	C708	G641	A580	G514	U453	C393	A331	G269
C1161	U1097	C1032	U964	A898	A769	C709	G647	U581	U517	U454	C394	A332	C270
C1162	U1098	C1033	U965	A898	A770	C710	G648	U582	U517	U455	C395	A333	A271
A1163	U1099	C1034	A966	G902	G834	G771	G649	C583	C519	A456	G396	A334	U272
G1164	G1100	G1035	A967	U903	G772	G712	U650	C584	C520	G457	U435	U335	G273
A1165	G1101	A1036	U968	G904	C773	G713	G651	C585	A521	G458	G397	G336	G274
G1166	G1102	C1037	C969	A905	A774	G714	G652	C586	U522	G459	A399	G337	C275
A1167	U1093	U1038	A970	U909	G775	G715	C653	C587	U523	A460	A401	C338	C276
G1170	C1104	G1040	A971	U912	C776	U715	C654	C588	U524	G462	C402	C339	U277
A1171	U106	G1041	A973	G913	G777	U716	G655	C589	A525	U463	G403	U340	U278
G1172	G1107	A1045	C975	G914	A780	C717	G656	A592	A526	A464	G404	C343	G279
C1173	G1108	U1044	A976	A915	U781	U718	U657	U593	A527	G465	C405	A344	U280
G1174	G1109	C1046	A977	U917	U782	U719	C658	A594	U528	U466	U407	U345	G281
C1177	U1109	G1047	A978	U918	G783	G720	C	C595	C530	A468	C408	U347	C282
A1178	G1110	U1048	G980	A919	C784	G721	A	C596	C531	A469	C409	U348	U283
G1179	U1115	C1048	C980	A920	A788	G722	U	G597	A534	A470	A410	U349	C286
A1180	U1117	G1051	U921	U920	A789	G723	U	U598	A535	A471	C411	U350	G287
U1181	G1118	U1052	G986	A922	U790	G724	U	A599	C536	A472	A412	U351	A288
U1182	G1119	G1053	A987	G923	U791	C725	U	U600	C537	A473	C413	A352	G290
A1183	U1120	U1054	U989	A924	U792	U725	U	A601	G537	A474	C414	A353	G291
A	C1121	U1055	C990	G925	U793	C726	U	U602	A538	A475	C415	C354	U292
U	G1122	U1056	G991	A926	U794	C727	C	A604	G539	U476	A416	G355	U293
U	C1123	U1057	A992	C927	U795	U727	G	A	G540	A477	A417	G356	C294
U	A1124	U1058	A993	U928	A796	U728	U	A	A541	A478	G418	C357	A295
G	U996	U1059	U996	U929	A797	G729	U	G	A542	C479	G419	U358	U296
A	G1127	U1060	U996	A930	A798	G730	U	U	C543	A480	A420	A359	U297
C	C1128	U1061	U996	C931	A799	G731	U	U	A544	A481	A421	A360	C298
C	U1129	A1065	U999	U932	U800	C732	A	U	A545	U482	G422	C361	A299
U	A1130	C1066	C1000	A933	G801	A733	U	G610	U546	A483	C423	G362	C300
A	A1131	C1067	A1001	C934	G802	C734	G676	U611	U547	C484	C424	G363	A301
A	A1132	C1068	G1002	U935	A803	A735	U681	U612	C548	A485	A425	G364	C308
C	A	A1069	G1002	U936	A804	C736	C677	G613	G549	A486	G426	G365	C309
C	C	C1070	C1006	C937	U805	A737	A678	C614	A550	G487	A367	A366	C310
C	U	U1071	C1007	C938	A806	A737	U679	A615	U558	A488	A428	C367	U304
C	U	C1072	G1008	U939	A807	G738	U680	G616	C559	C489	G429	U368	C305
G	A	G1073	U1009	A940	U808	A740	U681	U617	U563	C489	G430	A369	U306
G	A	C1074	C1010	A941	A809	A741	U682	U618	A555	C490	C431	A370	G307
G	A	G1075	G1011	G942	G810	U742	C682	A619	A556	C491	G432	G371	C308
G	A	U1076	U1012	C943	A811	U743	C683	A620	G557	C492	C433	G372	C309
A	G	C1077	A1013	A944	U812	U744	A684	A621	C558	U493	G434	U311	C310
A	A	C1078	G1014	U945	U813	U745	G687	A622	U560	U494	C435	A312	U311
A	A	U1079	U1015	G948	A814	A746	U687	A623	U563	C495	A436	U313	A312
A	U	U1080	C1016	G949	G815	C747	C691	A624	C564	C496	A437	C376	A313
A	U	C1081	U1017	C950	G816	U748	C692	U626	G564	G497	A378	G377	C314
C	A	G1082	U1018	A951	G817	U749	U693	C627	G565	G498	U379	A315	A315
C	C	A1083	A1019	A952	G818	U750	U694	G628	C566	U499	U380	A316	A316
C	C	U1084	U1020	G953	U820	G751	U695	U629	U567	C500	A441	C317	C317
C	C	G1085	C1021	G954	U821	A752	C696	A630	A570	C500	C442	C382	U318
G	G	A1086	C1022	A955	U822	A753	C697	G631	G571	U501	C443	G383	U319
U	U	A1087	A1023	G956	G823	A754	U698	U632	G572	U502	C444	G384	U320
C	C	C1090	U1024	G957	U824	A755	U699	G633	C573	G503	A445	A385	C321
C	C	A1091	A1025	U957	G825	A756	C700	U634	G573	U504	A446	G386	G322
A	A	A1092	A1026	U958	U826	A757	U701	A635	G575	A505	U447	A387	A323
A	A	U1093	A1027	U959	C827	U758	G702	A636	G576	U506	A448	G388	U324
A	A	G1094	C1028	U960	U828	U759	G703	C637	U577	U507	C449	G389	G325
A	A	C1157	U1029	U961	A829	A760	U705	U638	U578	U508	U450	G390	A328
C	C	C1158			A766	G765	A706	U639	U579	A512	A451	A391	G329



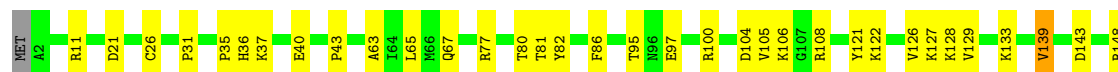
• Molecule 19: 40S ribosomal protein S1-A

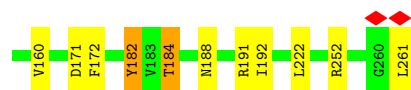
Chain DA:



• Molecule 20: 40S ribosomal protein S4-A

Chain DE:





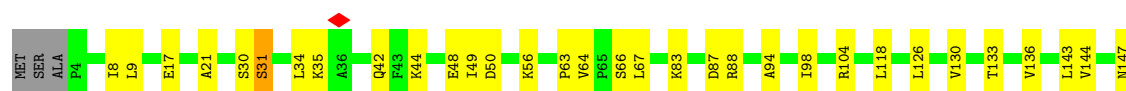
- Molecule 21: 40S ribosomal protein S6-A

Chain DG: 67% 28% . .



- Molecule 22: 40S ribosomal protein S7-A

Chain DH: 78% 18% . .



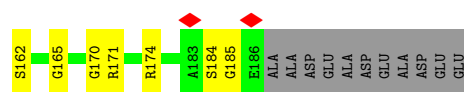
- Molecule 23: 40S ribosomal protein S8-A

Chain DI: 74% 20% 6%

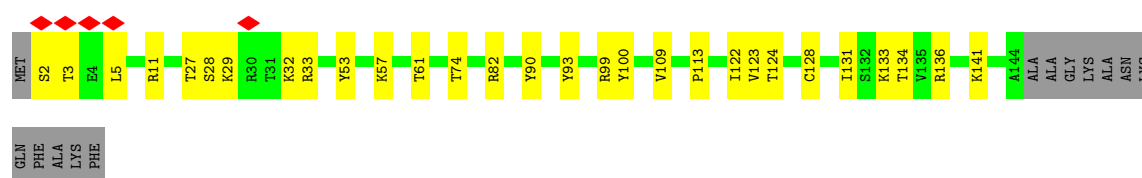


- Molecule 24: 40S ribosomal protein S9-A

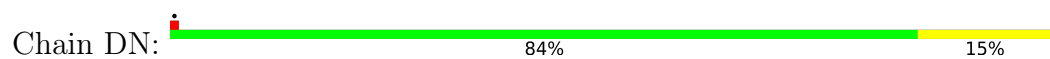
Chain DJ: 74% 19% 6%



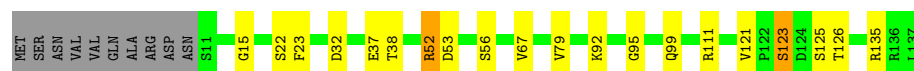
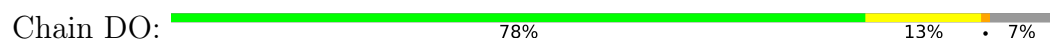
- Molecule 25: 40S ribosomal protein S11-A



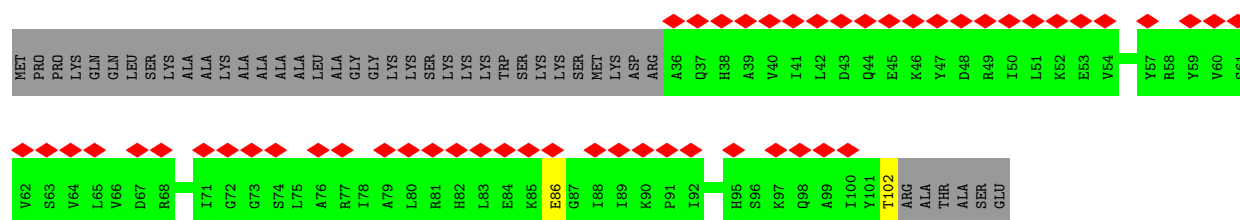
- Molecule 26: 40S ribosomal protein S13



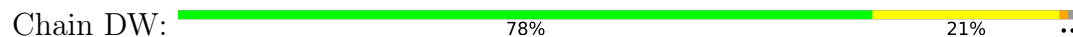
- Molecule 27: 40S ribosomal protein S14-A



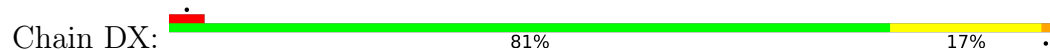
- Molecule 28: 40S ribosomal protein S25-A



- Molecule 29: 40S ribosomal protein S22-A

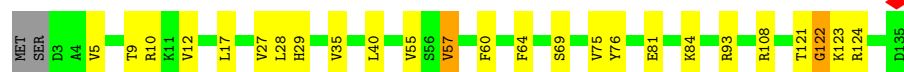


- Molecule 30: 40S ribosomal protein S23-A



- Molecule 31: 40S ribosomal protein S24-A



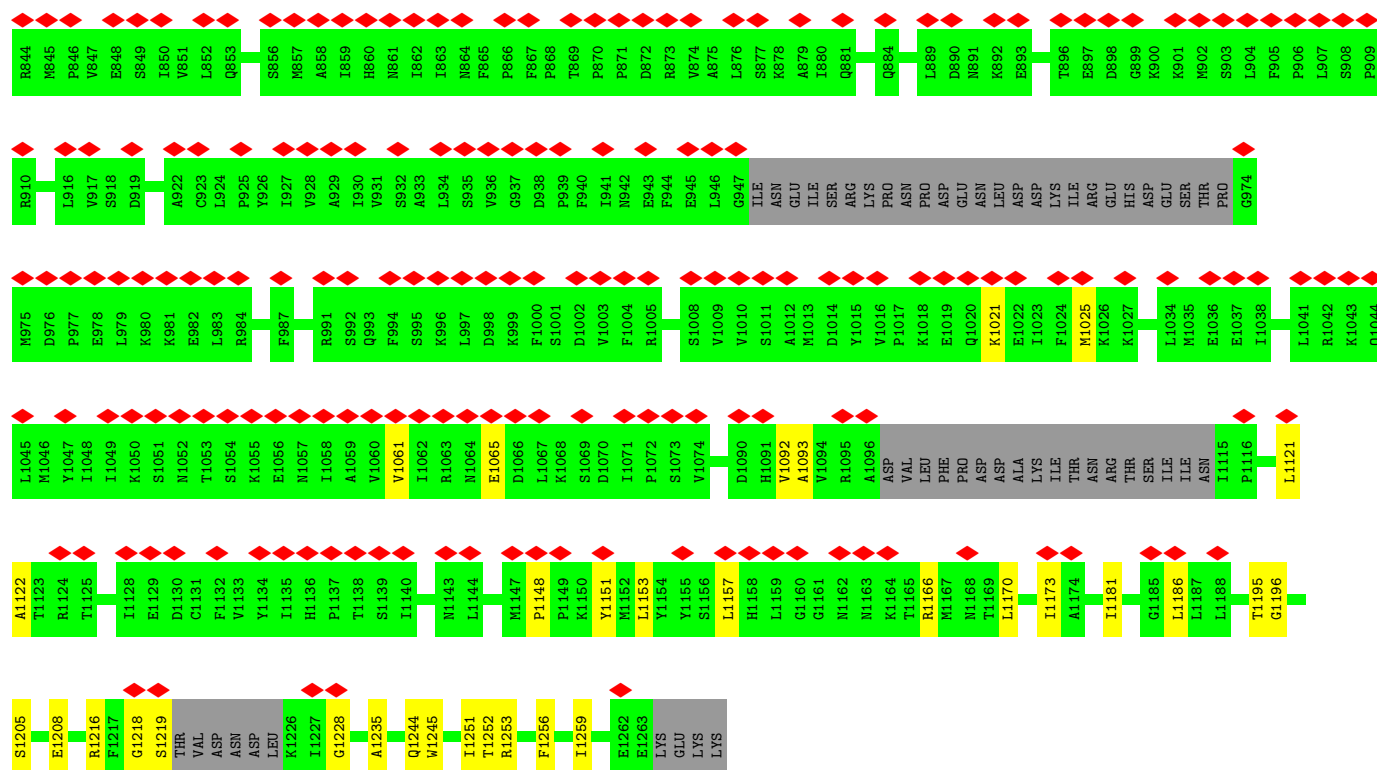


- 

- |     |     |     |     |     |     |     |      |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|------|-----|-----|-----|-----|-----|-----|
| ASN | GLY | VAL | SER | ASP | GLU | GLU | GLU  | TLE | LYS | GLU | ILE | ASN | MET |
| ASN | ASP | ILE | LYS | GLU | GLU | ASN | GLU  | VAL | LEU | GLU | ASP | SER | ALA |
| LYS | ASN | ASP | ASN | GLU | GLU | GLU | GLU  | GLN | SER | ASP | GLU | ASP | LYS |
| ARG | VAL | LYS | ALA | GLU | GLU | GLU | THR  | ASN | THR | PHE | PRO | GLU | LYS |
| LYS | PHE | ASP | THR | ASN | GLU | GLU | ALA  | ARG | ASP | ASP | LEU | ASP | SER |
| ILE | PHE | SER | ASN | GLY | GLU | ILE | GLU  | ARG | MET | GLU | MET | ILE | LYS |
| LYS | GLN | LYS | ASN | GLU | ILE | ASN | ASN  | ALA | MET | ILE | PRO | SER | ARG |
| VAL | GLN | VAL | GLY | ILE | SER | SER | THR  | HIS | ASN | GLU | LEU | SER | ARG |
| LYS | ASP | LYS | ALA | GLN | GLU | GLU | GLU  | LEU | ILE | ASP | GLN | SER | LYS |
| GLY | VAL | ALA | ILE | ILE | ALA | ILE | K375 | ILE | ASP | GLU | VAL | PHE | SER |
| VAL | ILE | MET | ILE | ASN | LEU | LEU | E379 | PHE | ASP | GLU | TRP | GLU | SER |
| VAL | ALA | ASN | VAL | LYS | SER | LYS | ASN  | PRO | ARG | ASP | ASP | GLU | ARG |
| ASN | GLU | LYS | GLU | GLY | GLU | GLU | L382 | LEU | GLN | ILE | MET | GLU | ARG |
| ALA | GLU | MET | GLU | ARG | GLU | LEU | ASN  | ASN | VAL | ASP | GLU | GLU | VAL |
| ASP | PHE | GLU | GLU | ARG | LEU | LEU | LYS  | LYS | ILE | LEU | GLU | LEU | LEU |
| LYS | ALA | LYS | SER | ILE | GLY | GLY | R389 | PRO | GLU | ASN | LYS | ASN | ASP |
| ARG | GLY | ALA | ASP | TYR | LYS | LYS | S402 | THR | GLU | ASN | THR | SER | ALA |
| ARG | ASP | GLU | GLY | PRO | THR | THR | ASN  | GLU | ALA | ILE | ALA | ASP | LEU |
| LYS | VAL | LYS | PRO | GLY | VAL | VAL | A421 | HIS | ASN | LEU | SER | ALA | GLN |
| ASN | VAL | GLN | LEU | SER | MET | MET | VAL  | HIS | LEU | LEU | ASN | GLY | ALA |
| LEU | ALA | LYS | GLN | LEU | ASN | ASN | SER  | ALA | LYS | LEU | GLY | GLY | GLU |
| GLN | GLU | LYS | ASP | GLU | MET | MET | SER  | SER | GLY | ILE | ASN | ILE | GLU |
| GLN | PHE | LYS | GLU | GLU | PHE | PHE | ASP  | ALA | LYS | ASP | ASP | SER | ARG |
| VAL | GLN | LYS | GLN | ASN | GLN | ASN | GLU  | PHE | SER | GLU | ASP | ASP | GLU |
| ILE | GLU | LYS | ASN | LYS | MET | MET | D427 | THR | SER | THR | GLU | GLU | TYR |
| ILE | GLU | GLY | ASN | ASP | LYS | LYS | ASN  | ARG | THR | LYS | ASP | TYR | GLY |
| ASN | LYS | LYS | GLN | MET | ASN | ASN | D430 | THR | TYR | SER | ALA | ASP | GLY |
| GLU | LYS | ASN | GLN | ASN | GLY | GLY | ASN  | GLN | TYR | LYS | ILE | ASP | PHE |
| ARG | ASN | ASN | ASP | GLU | GLU | GLU | R435 | GLN | VAL | ALA | PRO | ILE | LEU |
| VAL | VAL | ASP | GLU | LEU | ALA | ALA | ASN  | VAL | GLU | PRO | GLN | ASN | ASN |
| ASN | ILE | ASP | GLU | ASN | ARG | GLU | R439 | PRO | LEU | LYS | LEU | SER | ASN |
| LYS | ASP | GLU | ALA | ASP | GLU | GLU | ASN  | GLN | PRO | ARG | LYS | LYS | SER |
| LYS | ASP | ASP | LYS | HIS | ARG | ARG | R466 | THR | GLN | LEU | LEU | PHE | ASP |
| GLU | GLU | LEU | ASP | THR | GLU | GLU | ASN  | THR | GLN | ASP | GLN | ASN | ASN |
| LEU | ASP | LEU | VAL | THR | ARG | ASN | R480 | LEU | ARG | GLN | GLN | GLN | ASP |
| ASP | ASP | LEU | VAL | ARG | ASN | ASN | A481 | GLN | ILE | THR | THR | THR | GLN |
| LYS | LYS | THR | PRO | GLU | LYS | LYS | R482 | GLN | GLN | ASP | ASP | ILE | LYS |
| GLN | GLU | ALA | TRP | ASN | ASN | GLU | MET  | GLY | ARG | SER | ILE | ARG | HIS |
| VAL | VAL | ASP | LEU | LYS | THR | THR | LEU  | VAL | HIS | GLY | GLY | ASP | ASP |
| SER | ASP | ASP | ALA | VAL | GLU | LEU | ASP  | ASP | ASP | GLU | SER | ASP | ASP |
| THR | THR | SER | ASN | GLU | GLU | GLN | ASN  | GLN | LYS | ASN | GLU | GLU | LYS |
| LEU | LEU | ARG | SER | GLU | LEU | LEU | SER  | LEU | ALA | SER | SER | ASN | ASN |
| PRO | PRO | LEU | ASP | ARG | ARG | ARG | ASP  | GLN | ALA | TYR | SER | ALA | GLY |
| PHE | GLY | LYS | GLU | SER |     |     |      |     |     |     |     |     |     |

## Chain JD:





• Molecule 35: U3 snoRNA

Chain D4: 61% 30% 9%



• Molecule 36: Poly-U RNA

Chain D5: 33% 67% 67%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	102097	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	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.099	Depositor
Minimum map value	-0.043	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	508.32, 508.32, 508.32	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: GTP, M7G, MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	UB	0.27	0/2206	0.47	3/3035 (0.1%)
2	UC	0.85	0/395	0.83	1/517 (0.2%)
3	US	0.23	0/2406	0.38	2/3355 (0.1%)
4	UX	0.91	3/1154 (0.3%)	0.82	2/1557 (0.1%)
5	CJ	0.30	0/1082	0.62	0/1506
6	CK	0.47	0/649	0.67	0/877
7	CL	0.99	12/5887 (0.2%)	0.85	13/7931 (0.2%)
8	CM	0.92	0/2832	0.76	1/3825 (0.0%)
9	JF	0.24	0/1069	0.44	0/1488
9	JG	0.23	0/1094	0.45	0/1523
10	JH	0.24	0/1293	0.37	0/1801
11	JL	0.96	4/2305 (0.2%)	0.77	0/3116
12	JJ	0.86	0/1462	0.83	1/1969 (0.1%)
13	DF	0.24	0/969	0.44	0/1349
14	DQ	0.24	0/615	0.46	0/854
15	DS	0.26	0/641	0.56	0/866
16	DT	0.25	0/699	0.40	0/968
17	Dc	0.25	0/309	0.49	0/428
18	D3	2.08	1291/33028 (3.9%)	1.51	628/51447 (1.2%)
19	DA	0.91	1/1735 (0.1%)	0.84	2/2335 (0.1%)
20	DE	1.27	10/2109 (0.5%)	0.90	1/2839 (0.0%)
21	DG	0.78	0/1823	0.77	1/2439 (0.0%)
22	DH	0.74	1/1506 (0.1%)	0.77	1/2028 (0.0%)
23	DI	1.01	1/1514 (0.1%)	0.86	3/2021 (0.1%)
24	DJ	1.10	4/1519 (0.3%)	0.93	3/2035 (0.1%)
25	DL	1.38	8/1180 (0.7%)	0.85	1/1591 (0.1%)
26	DN	1.03	2/1215 (0.2%)	0.90	3/1638 (0.2%)
27	DO	0.94	1/952 (0.1%)	0.91	0/1279
28	DZ	0.27	0/331	0.56	0/460
29	DW	1.27	1/1038 (0.1%)	0.96	4/1395 (0.3%)
30	DX	1.17	3/1133 (0.3%)	0.94	3/1510 (0.2%)
31	DY	1.21	3/1081 (0.3%)	0.85	1/1441 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	Db	0.92	0/620	0.83	1/838 (0.1%)
33	UN	0.78	0/926	0.78	1/1213 (0.1%)
34	JD	0.45	0/4616	0.63	2/6348 (0.0%)
35	D4	1.78	2/521 (0.4%)	1.21	0/809
36	D5	0.28	0/197	1.00	0/302
All	All	1.46	1347/84111 (1.6%)	1.14	678/120933 (0.6%)

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	UB	0	1
7	CL	0	1
11	JL	0	1
19	DA	0	3
22	DH	0	4
23	DI	0	1
24	DJ	0	2
25	DL	0	1
26	DN	0	1
27	DO	0	2
31	DY	0	2
32	Db	0	2
33	UN	0	1
34	JD	0	3
All	All	0	25

All (1347) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	621	A	N9-C4	-10.39	1.31	1.37
18	D3	387	A	N9-C4	-10.38	1.31	1.37
18	D3	387	A	N7-C5	-10.18	1.33	1.39
18	D3	621	A	N3-C4	-9.77	1.28	1.34
18	D3	1103	U	C2-N3	-9.54	1.31	1.37
18	D3	387	A	C5-C4	-9.39	1.32	1.38
18	D3	451	A	N9-C4	-9.33	1.32	1.37
18	D3	622	A	N9-C4	-9.30	1.32	1.37
18	D3	443	C	N1-C6	-9.29	1.31	1.37
18	D3	65	A	N9-C4	-9.02	1.32	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	426	G	N7-C5	-8.99	1.33	1.39
18	D3	1108	G	C5-C4	-8.86	1.32	1.38
18	D3	956	C	N1-C6	-8.77	1.31	1.37
18	D3	385	A	C5-C4	-8.77	1.32	1.38
18	D3	333	A	N9-C4	-8.73	1.32	1.37
18	D3	103	A	N3-C4	-8.67	1.29	1.34
18	D3	334	G	C5-C4	-8.67	1.32	1.38
18	D3	799	A	N9-C4	-8.63	1.32	1.37
18	D3	377	G	N7-C5	-8.59	1.34	1.39
18	D3	992	A	N9-C4	-8.59	1.32	1.37
18	D3	362	G	N9-C8	-8.55	1.31	1.37
18	D3	456	A	N7-C5	-8.49	1.34	1.39
18	D3	384	G	N9-C8	-8.49	1.31	1.37
18	D3	387	A	N3-C4	-8.49	1.29	1.34
18	D3	451	A	C5-C4	-8.44	1.32	1.38
18	D3	1788	G	N9-C8	-8.43	1.31	1.37
18	D3	87	C	N1-C6	-8.40	1.32	1.37
18	D3	385	A	N9-C4	-8.39	1.32	1.37
18	D3	399	A	N7-C5	-8.35	1.34	1.39
18	D3	396	G	N1-C2	-8.31	1.31	1.37
18	D3	1027	A	C5-C4	-8.25	1.32	1.38
18	D3	992	A	N3-C4	-8.24	1.29	1.34
18	D3	613	G	C5-C4	-8.23	1.32	1.38
18	D3	1047	G	C5-C4	-8.20	1.32	1.38
18	D3	377	G	C5-C4	-8.20	1.32	1.38
18	D3	378	A	N7-C5	-8.20	1.34	1.39
18	D3	429	G	N7-C5	-8.18	1.34	1.39
18	D3	809	A	N9-C4	-8.18	1.32	1.37
18	D3	770	A	C5-C4	-8.13	1.33	1.38
18	D3	1786	G	C5-C4	-8.11	1.32	1.38
18	D3	992	A	N7-C5	-8.08	1.34	1.39
18	D3	99	C	N3-C4	-8.07	1.28	1.33
18	D3	430	G	N7-C5	-8.06	1.34	1.39
18	D3	1035	G	C5-C4	-8.04	1.32	1.38
18	D3	1047	G	N9-C8	-7.96	1.32	1.37
18	D3	339	C	N1-C6	-7.92	1.32	1.37
18	D3	1025	A	C5-C4	-7.91	1.33	1.38
18	D3	599	A	N9-C4	-7.90	1.33	1.37
18	D3	96	G	C5-C4	-7.90	1.32	1.38
18	D3	461	G	N7-C5	-7.90	1.34	1.39
18	D3	451	A	C6-N1	-7.85	1.30	1.35
18	D3	362	G	C5-C4	-7.84	1.32	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	393	C	N3-C4	-7.84	1.28	1.33
18	D3	334	G	N1-C2	-7.83	1.31	1.37
18	D3	386	G	N9-C8	-7.82	1.32	1.37
18	D3	451	A	N3-C4	-7.82	1.30	1.34
18	D3	462	G	N9-C8	-7.81	1.32	1.37
18	D3	110	U	C2-N3	-7.81	1.32	1.37
18	D3	460	A	N3-C4	-7.79	1.30	1.34
18	D3	477	A	N9-C4	-7.78	1.33	1.37
18	D3	297	U	C2-N3	-7.77	1.32	1.37
18	D3	448	C	N3-C4	-7.74	1.28	1.33
18	D3	1773	C	N1-C6	-7.74	1.32	1.37
18	D3	610	G	N7-C5	-7.72	1.34	1.39
18	D3	89	G	C5-C4	-7.71	1.32	1.38
18	D3	103	A	C6-N1	-7.69	1.30	1.35
18	D3	769	A	N7-C5	-7.69	1.34	1.39
18	D3	359	A	N9-C4	-7.68	1.33	1.37
18	D3	430	G	C5-C4	-7.67	1.32	1.38
18	D3	377	G	N9-C8	-7.66	1.32	1.37
18	D3	47	A	N7-C5	-7.63	1.34	1.39
18	D3	123	G	C5-C4	-7.62	1.33	1.38
31	DY	57	VAL	CB-CG1	-7.61	1.36	1.52
18	D3	59	C	N1-C6	-7.60	1.32	1.37
18	D3	357	G	C5-C4	-7.58	1.33	1.38
18	D3	457	G	C5-C4	-7.58	1.33	1.38
18	D3	1034	C	N1-C6	-7.58	1.32	1.37
18	D3	429	G	C5-C4	-7.58	1.33	1.38
18	D3	1791	A	C5-C4	-7.57	1.33	1.38
18	D3	768	C	N1-C6	-7.56	1.32	1.37
18	D3	381	C	N1-C6	-7.56	1.32	1.37
18	D3	1103	U	N3-C4	-7.55	1.31	1.38
18	D3	1786	G	C6-N1	-7.55	1.34	1.39
18	D3	305	C	N1-C6	-7.53	1.32	1.37
18	D3	428	A	C5-C4	-7.52	1.33	1.38
18	D3	385	A	N3-C4	-7.52	1.30	1.34
18	D3	405	C	N1-C6	-7.50	1.32	1.37
18	D3	1791	A	N7-C5	-7.49	1.34	1.39
18	D3	429	G	N9-C8	-7.47	1.32	1.37
18	D3	383	G	C5-C4	-7.45	1.33	1.38
18	D3	362	G	N7-C5	-7.44	1.34	1.39
18	D3	622	A	N3-C4	-7.44	1.30	1.34
18	D3	310	C	N1-C6	-7.41	1.32	1.37
18	D3	331	A	N9-C4	-7.41	1.33	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	395	U	N1-C2	-7.40	1.31	1.38
18	D3	1108	G	N1-C2	-7.40	1.31	1.37
18	D3	468	A	C5-C4	-7.40	1.33	1.38
18	D3	1027	A	N7-C5	-7.39	1.34	1.39
18	D3	884	A	N9-C4	-7.39	1.33	1.37
18	D3	940	A	N7-C5	-7.39	1.34	1.39
18	D3	107	C	C4-C5	-7.38	1.37	1.43
18	D3	376	C	N1-C6	-7.38	1.32	1.37
18	D3	322	G	C5-C4	-7.38	1.33	1.38
18	D3	753	A	N9-C4	-7.38	1.33	1.37
18	D3	465	G	N7-C5	-7.37	1.34	1.39
18	D3	1792	G	C5-C4	-7.36	1.33	1.38
18	D3	976	G	C5-C4	-7.36	1.33	1.38
18	D3	331	A	C5-C4	-7.34	1.33	1.38
18	D3	1787	C	N1-C6	-7.31	1.32	1.37
18	D3	632	U	C4-C5	-7.31	1.36	1.43
18	D3	462	G	C5-C4	-7.31	1.33	1.38
18	D3	308	C	N1-C6	-7.30	1.32	1.37
18	D3	526	A	N9-C4	-7.29	1.33	1.37
18	D3	1084	A	N3-C4	-7.28	1.30	1.34
18	D3	931	C	N1-C6	-7.27	1.32	1.37
18	D3	628	G	C6-N1	-7.26	1.34	1.39
18	D3	363	G	N9-C8	-7.25	1.32	1.37
18	D3	47	A	N9-C4	-7.25	1.33	1.37
18	D3	173	A	N9-C4	-7.24	1.33	1.37
18	D3	427	C	N1-C6	-7.24	1.32	1.37
18	D3	115	G	N7-C5	-7.22	1.34	1.39
18	D3	444	C	N3-C4	-7.20	1.28	1.33
18	D3	804	A	N7-C5	-7.20	1.34	1.39
18	D3	613	G	N7-C5	-7.20	1.34	1.39
18	D3	55	A	C6-N1	-7.19	1.30	1.35
18	D3	446	A	N7-C5	-7.19	1.34	1.39
18	D3	444	C	C4-C5	-7.18	1.37	1.43
18	D3	89	G	C6-N1	-7.17	1.34	1.39
18	D3	1072	C	N1-C6	-7.17	1.32	1.37
18	D3	421	A	N9-C4	-7.17	1.33	1.37
18	D3	398	G	C5-C4	-7.17	1.33	1.38
18	D3	988	A	N7-C5	-7.15	1.34	1.39
18	D3	334	G	C6-N1	-7.15	1.34	1.39
18	D3	364	G	C5-C4	-7.14	1.33	1.38
18	D3	424	C	N3-C4	-7.14	1.28	1.33
18	D3	412	A	N9-C4	-7.13	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	389	G	N7-C5	-7.13	1.34	1.39
18	D3	628	G	N1-C2	-7.13	1.32	1.37
18	D3	91	G	N7-C5	-7.13	1.34	1.39
18	D3	54	C	N1-C6	-7.13	1.32	1.37
18	D3	442	C	N1-C6	-7.13	1.32	1.37
18	D3	937	C	N1-C6	-7.11	1.32	1.37
18	D3	407	A	N9-C4	-7.11	1.33	1.37
18	D3	966	A	N7-C5	-7.11	1.34	1.39
18	D3	300	A	N9-C4	-7.11	1.33	1.37
18	D3	1019	A	N9-C4	-7.11	1.33	1.37
18	D3	338	C	N1-C6	-7.10	1.32	1.37
18	D3	615	A	N9-C4	-7.08	1.33	1.37
18	D3	168	A	N9-C4	-7.08	1.33	1.37
18	D3	396	G	N9-C8	-7.08	1.32	1.37
18	D3	394	C	N3-C4	-7.08	1.28	1.33
18	D3	405	C	N3-C4	-7.07	1.29	1.33
18	D3	396	G	C6-N1	-7.07	1.34	1.39
18	D3	944	A	N9-C4	-7.07	1.33	1.37
18	D3	461	G	C5-C4	-7.06	1.33	1.38
18	D3	526	A	C5-C4	-7.06	1.33	1.38
18	D3	452	A	C5-C4	-7.04	1.33	1.38
18	D3	381	C	C4-C5	-7.04	1.37	1.43
18	D3	451	A	C5-C6	-7.03	1.34	1.41
18	D3	613	G	N9-C8	-7.03	1.32	1.37
18	D3	940	A	C5-C4	-7.03	1.33	1.38
18	D3	464	A	N3-C4	-7.03	1.30	1.34
18	D3	621	A	N7-C5	-7.03	1.35	1.39
18	D3	382	C	C4-C5	-7.02	1.37	1.43
18	D3	465	G	C5-C6	-7.02	1.35	1.42
18	D3	339	C	C4-C5	-7.01	1.37	1.43
18	D3	530	C	N1-C6	-7.01	1.32	1.37
18	D3	991	G	N9-C8	-7.01	1.32	1.37
18	D3	441	A	N7-C5	-7.00	1.35	1.39
18	D3	875	G	C5-C4	-7.00	1.33	1.38
18	D3	381	C	N3-C4	-7.00	1.29	1.33
18	D3	962	C	N1-C6	-7.00	1.32	1.37
18	D3	386	G	C5-C4	-6.99	1.33	1.38
18	D3	93	A	C6-N1	-6.98	1.30	1.35
18	D3	396	G	N7-C5	-6.98	1.35	1.39
18	D3	358	U	C2-N3	-6.97	1.32	1.37
18	D3	1046	G	C5-C4	-6.96	1.33	1.38
18	D3	1025	A	N7-C5	-6.96	1.35	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	384	G	C5-C4	-6.95	1.33	1.38
18	D3	797	G	N9-C8	-6.94	1.32	1.37
18	D3	312	A	N9-C4	-6.93	1.33	1.37
18	D3	364	G	N1-C2	-6.93	1.32	1.37
18	D3	477	A	N3-C4	-6.93	1.30	1.34
18	D3	305	C	C4-C5	-6.92	1.37	1.43
18	D3	523	G	C5-C4	-6.92	1.33	1.38
18	D3	1790	A	N3-C4	-6.92	1.30	1.34
18	D3	65	A	N3-C4	-6.92	1.30	1.34
18	D3	58	U	C2-N3	-6.91	1.32	1.37
18	D3	630	A	N7-C5	-6.91	1.35	1.39
18	D3	107	C	N1-C6	-6.91	1.33	1.37
18	D3	108	A	N3-C4	-6.91	1.30	1.34
18	D3	102	U	C4-C5	-6.90	1.37	1.43
18	D3	872	G	C5-C4	-6.90	1.33	1.38
18	D3	1778	G	C5-C4	-6.90	1.33	1.38
18	D3	877	G	C5-C4	-6.88	1.33	1.38
18	D3	99	C	N1-C6	-6.88	1.33	1.37
18	D3	1791	A	N9-C8	-6.87	1.32	1.37
18	D3	464	A	N9-C4	-6.87	1.33	1.37
18	D3	776	G	N7-C5	-6.87	1.35	1.39
18	D3	1788	G	C5-C4	-6.87	1.33	1.38
18	D3	312	A	C5-C4	-6.87	1.33	1.38
18	D3	448	C	N1-C6	-6.86	1.33	1.37
18	D3	308	C	N3-C4	-6.85	1.29	1.33
18	D3	55	A	N7-C5	-6.84	1.35	1.39
18	D3	1792	G	N9-C8	-6.84	1.33	1.37
18	D3	295	A	C5-C4	-6.84	1.33	1.38
18	D3	426	G	C8-N7	-6.84	1.26	1.30
18	D3	395	U	C4-C5	-6.84	1.37	1.43
18	D3	54	C	C4-C5	-6.83	1.37	1.43
18	D3	636	A	N9-C4	-6.83	1.33	1.37
18	D3	98	U	C4-C5	-6.81	1.37	1.43
18	D3	622	A	C5-C4	-6.80	1.33	1.38
18	D3	119	A	C5-C4	-6.80	1.33	1.38
20	DE	126	VAL	CB-CG2	-6.80	1.38	1.52
18	D3	95	G	C5-C4	-6.79	1.33	1.38
18	D3	396	G	C5-C4	-6.79	1.33	1.38
18	D3	246	G	C6-N1	-6.79	1.34	1.39
18	D3	97	C	N1-C6	-6.78	1.33	1.37
18	D3	939	A	N9-C4	-6.76	1.33	1.37
25	DL	100	TYR	CD1-CE1	-6.76	1.29	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	525	A	N9-C4	-6.75	1.33	1.37
18	D3	377	G	N1-C2	-6.75	1.32	1.37
18	D3	1776	A	C5-C4	-6.75	1.34	1.38
25	DL	109	VAL	CB-CG2	-6.75	1.38	1.52
18	D3	456	A	N3-C4	-6.74	1.30	1.34
18	D3	770	A	N9-C4	-6.74	1.33	1.37
18	D3	632	U	N1-C2	-6.73	1.32	1.38
18	D3	96	G	C6-N1	-6.72	1.34	1.39
18	D3	354	C	N1-C6	-6.72	1.33	1.37
18	D3	624	G	C5-C4	-6.72	1.33	1.38
18	D3	447	U	C4-C5	-6.71	1.37	1.43
18	D3	464	A	N9-C8	-6.70	1.32	1.37
18	D3	388	G	C5-C4	-6.70	1.33	1.38
18	D3	609	U	C2-N3	-6.70	1.33	1.37
18	D3	109	G	C5-C4	-6.70	1.33	1.38
18	D3	389	G	N9-C8	-6.70	1.33	1.37
18	D3	363	G	C5-C4	-6.69	1.33	1.38
18	D3	353	A	C5-C4	-6.69	1.34	1.38
18	D3	769	A	N9-C8	-6.68	1.32	1.37
18	D3	465	G	N1-C2	-6.68	1.32	1.37
18	D3	1047	G	C6-N1	-6.67	1.34	1.39
18	D3	1025	A	C5-C6	-6.67	1.35	1.41
18	D3	337	G	C5-C4	-6.67	1.33	1.38
18	D3	1105	C	C4-C5	-6.66	1.37	1.43
18	D3	621	A	C5-C4	-6.66	1.34	1.38
18	D3	89	G	N1-C2	-6.66	1.32	1.37
18	D3	446	A	N9-C8	-6.66	1.32	1.37
18	D3	394	C	N1-C6	-6.65	1.33	1.37
18	D3	386	G	C8-N7	-6.65	1.26	1.30
18	D3	1047	G	N1-C2	-6.64	1.32	1.37
18	D3	460	A	C5-C4	-6.64	1.34	1.38
18	D3	425	A	C5-C4	-6.64	1.34	1.38
18	D3	613	G	N1-C2	-6.64	1.32	1.37
18	D3	382	C	N1-C6	-6.63	1.33	1.37
18	D3	1788	G	N7-C5	-6.63	1.35	1.39
18	D3	1032	G	C5-C4	-6.62	1.33	1.38
18	D3	112	A	N3-C4	-6.62	1.30	1.34
18	D3	530	C	N3-C4	-6.62	1.29	1.33
18	D3	458	G	C5-C4	-6.62	1.33	1.38
18	D3	1108	G	N3-C4	-6.61	1.30	1.35
18	D3	96	G	N1-C2	-6.61	1.32	1.37
18	D3	459	G	C5-C4	-6.61	1.33	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	383	G	N9-C8	-6.60	1.33	1.37
18	D3	105	A	N7-C5	-6.60	1.35	1.39
18	D3	465	G	C6-N1	-6.60	1.34	1.39
18	D3	797	G	N7-C5	-6.58	1.35	1.39
18	D3	1775	U	N1-C2	-6.58	1.32	1.38
18	D3	357	G	C6-N1	-6.57	1.34	1.39
18	D3	768	C	N3-C4	-6.57	1.29	1.33
18	D3	635	A	C5-C4	-6.56	1.34	1.38
18	D3	1107	G	N1-C2	-6.55	1.32	1.37
18	D3	964	U	N1-C2	-6.55	1.32	1.38
18	D3	385	A	C6-N1	-6.54	1.30	1.35
18	D3	1035	G	N9-C8	-6.54	1.33	1.37
18	D3	634	G	N9-C8	-6.53	1.33	1.37
18	D3	1076	A	N9-C4	-6.53	1.33	1.37
18	D3	630	A	C5-C4	-6.53	1.34	1.38
25	DL	90	TYR	CD1-CE1	-6.53	1.29	1.39
18	D3	621	A	C6-N1	-6.53	1.30	1.35
11	JL	173	CYS	CB-SG	-6.53	1.71	1.82
18	D3	1073	G	N7-C5	-6.53	1.35	1.39
18	D3	1027	A	C5-C6	-6.52	1.35	1.41
18	D3	357	G	N9-C8	-6.51	1.33	1.37
18	D3	1028	C	N1-C6	-6.51	1.33	1.37
18	D3	1774	G	C5-C4	-6.51	1.33	1.38
18	D3	379	U	C2-N3	-6.50	1.33	1.37
18	D3	1107	G	C5-C4	-6.50	1.33	1.38
18	D3	109	G	N9-C8	-6.50	1.33	1.37
18	D3	362	G	C8-N7	-6.50	1.27	1.30
18	D3	455	C	N1-C6	-6.49	1.33	1.37
18	D3	465	G	C5-C4	-6.49	1.33	1.38
18	D3	1775	U	C2-N3	-6.49	1.33	1.37
18	D3	955	A	N9-C4	-6.48	1.33	1.37
18	D3	466	U	N3-C4	-6.48	1.32	1.38
18	D3	303	U	C2-N3	-6.48	1.33	1.37
18	D3	874	C	C4-C5	-6.47	1.37	1.43
18	D3	444	C	N1-C6	-6.47	1.33	1.37
18	D3	769	A	C6-N1	-6.47	1.31	1.35
18	D3	56	U	C2-N3	-6.46	1.33	1.37
18	D3	976	G	N1-C2	-6.46	1.32	1.37
18	D3	338	C	C4-C5	-6.45	1.37	1.43
18	D3	358	U	N3-C4	-6.45	1.32	1.38
18	D3	383	G	C2-N3	-6.45	1.27	1.32
18	D3	991	G	C6-N1	-6.45	1.35	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	34	G	C5-C4	-6.44	1.33	1.38
18	D3	939	A	N7-C5	-6.44	1.35	1.39
18	D3	445	A	N3-C4	-6.43	1.30	1.34
18	D3	872	G	N9-C8	-6.43	1.33	1.37
18	D3	246	G	C5-C4	-6.42	1.33	1.38
18	D3	404	G	N1-C2	-6.42	1.32	1.37
18	D3	968	U	N1-C2	-6.42	1.32	1.38
18	D3	108	A	C5-C4	-6.42	1.34	1.38
18	D3	387	A	C5-C6	-6.41	1.35	1.41
18	D3	323	A	N3-C4	-6.40	1.31	1.34
18	D3	47	A	C5-C6	-6.40	1.35	1.41
18	D3	425	A	C6-N1	-6.40	1.31	1.35
18	D3	339	C	N1-C2	-6.40	1.33	1.40
11	JL	207	VAL	CB-CG1	-6.40	1.39	1.52
18	D3	458	G	N1-C2	-6.40	1.32	1.37
18	D3	1087	A	N9-C4	-6.39	1.34	1.37
18	D3	974	A	C5-C4	-6.39	1.34	1.38
18	D3	1026	A	C5-C4	-6.38	1.34	1.38
18	D3	390	G	C5-C4	-6.38	1.33	1.38
18	D3	109	G	N7-C5	-6.38	1.35	1.39
18	D3	306	U	C4-C5	-6.37	1.37	1.43
18	D3	36	C	N1-C6	-6.37	1.33	1.37
18	D3	425	A	N3-C4	-6.37	1.31	1.34
18	D3	432	G	N7-C5	-6.37	1.35	1.39
18	D3	428	A	C6-N1	-6.37	1.31	1.35
18	D3	430	G	C8-N7	-6.37	1.27	1.30
18	D3	525	A	N7-C5	-6.37	1.35	1.39
18	D3	1101	G	C5-C4	-6.36	1.33	1.38
18	D3	756	A	N3-C4	-6.36	1.31	1.34
18	D3	1102	G	C5-C4	-6.36	1.33	1.38
18	D3	55	A	C5-C4	-6.36	1.34	1.38
18	D3	1033	C	N3-C4	-6.36	1.29	1.33
18	D3	358	U	N1-C2	-6.35	1.32	1.38
18	D3	1774	G	C6-N1	-6.35	1.35	1.39
18	D3	526	A	N3-C4	-6.35	1.31	1.34
18	D3	971	A	C6-N1	-6.35	1.31	1.35
18	D3	939	A	C5-C4	-6.34	1.34	1.38
18	D3	353	A	C6-N1	-6.34	1.31	1.35
18	D3	1012	U	C4-C5	-6.34	1.37	1.43
18	D3	361	C	C4-C5	-6.34	1.37	1.43
18	D3	968	U	C4-C5	-6.33	1.37	1.43
18	D3	408	C	N1-C6	-6.33	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	1011	G	C6-N1	-6.33	1.35	1.39
18	D3	615	A	N3-C4	-6.33	1.31	1.34
18	D3	395	U	C2-N3	-6.33	1.33	1.37
18	D3	41	A	C5-C4	-6.33	1.34	1.38
18	D3	938	G	C5-C4	-6.32	1.33	1.38
18	D3	361	C	N3-C4	-6.32	1.29	1.33
18	D3	988	A	N9-C4	-6.32	1.34	1.37
18	D3	1087	A	N3-C4	-6.32	1.31	1.34
18	D3	1788	G	C8-N7	-6.32	1.27	1.30
18	D3	443	C	N3-C4	-6.31	1.29	1.33
18	D3	112	A	N9-C4	-6.30	1.34	1.37
18	D3	615	A	N9-C8	-6.30	1.32	1.37
18	D3	403	G	C5-C4	-6.30	1.33	1.38
18	D3	599	A	N3-C4	-6.30	1.31	1.34
18	D3	89	G	N9-C8	-6.30	1.33	1.37
18	D3	99	C	C4-C5	-6.29	1.38	1.43
18	D3	988	A	C5-C4	-6.29	1.34	1.38
18	D3	404	G	C5-C4	-6.29	1.33	1.38
18	D3	465	G	N9-C8	-6.28	1.33	1.37
18	D3	434	G	C5-C4	-6.27	1.33	1.38
18	D3	89	G	N7-C5	-6.27	1.35	1.39
18	D3	757	A	C6-N1	-6.27	1.31	1.35
18	D3	423	G	N7-C5	-6.26	1.35	1.39
18	D3	614	C	C4-C5	-6.26	1.38	1.43
18	D3	739	G	C2-N3	-6.26	1.27	1.32
18	D3	930	A	N9-C4	-6.25	1.34	1.37
18	D3	943	C	N1-C6	-6.25	1.33	1.37
18	D3	449	C	N1-C6	-6.25	1.33	1.37
18	D3	462	G	N7-C5	-6.25	1.35	1.39
18	D3	115	G	C5-C4	-6.24	1.33	1.38
18	D3	399	A	C5-C4	-6.24	1.34	1.38
18	D3	445	A	C6-N1	-6.24	1.31	1.35
18	D3	871	G	C5-C4	-6.24	1.33	1.38
18	D3	398	G	N3-C4	-6.23	1.31	1.35
18	D3	783	G	C5-C4	-6.23	1.33	1.38
18	D3	633	U	C2-N3	-6.23	1.33	1.37
18	D3	102	U	N1-C2	-6.22	1.32	1.38
18	D3	249	U	C2-N3	-6.22	1.33	1.37
18	D3	942	G	N9-C8	-6.22	1.33	1.37
18	D3	756	A	C6-N1	-6.21	1.31	1.35
18	D3	97	C	C4-C5	-6.21	1.38	1.43
18	D3	1033	C	N1-C6	-6.21	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	538	A	N7-C5	-6.21	1.35	1.39
18	D3	973	A	N9-C4	-6.20	1.34	1.37
18	D3	954	G	N9-C8	-6.20	1.33	1.37
18	D3	438	A	C5-C4	-6.19	1.34	1.38
18	D3	1010	C	N1-C6	-6.19	1.33	1.37
18	D3	1024	U	C2-N3	-6.19	1.33	1.37
18	D3	401	A	C6-N1	-6.18	1.31	1.35
18	D3	799	A	N3-C4	-6.18	1.31	1.34
18	D3	1789	G	C2-N3	-6.18	1.27	1.32
18	D3	927	C	N1-C6	-6.18	1.33	1.37
18	D3	58	U	N1-C2	-6.18	1.32	1.38
18	D3	63	G	C6-N1	-6.18	1.35	1.39
18	D3	397	A	N9-C4	-6.17	1.34	1.37
18	D3	939	A	N9-C8	-6.17	1.32	1.37
18	D3	430	G	C6-N1	-6.17	1.35	1.39
18	D3	974	A	N3-C4	-6.17	1.31	1.34
4	UX	65	VAL	CB-CG2	-6.17	1.39	1.52
18	D3	424	C	N1-C6	-6.17	1.33	1.37
18	D3	451	A	N7-C5	-6.17	1.35	1.39
18	D3	346	G	C6-N1	-6.16	1.35	1.39
18	D3	884	A	C5-C4	-6.16	1.34	1.38
18	D3	442	C	C4-C5	-6.16	1.38	1.43
18	D3	455	C	N3-C4	-6.16	1.29	1.33
18	D3	339	C	N3-C4	-6.16	1.29	1.33
18	D3	776	G	C5-C4	-6.16	1.34	1.38
18	D3	634	G	C5-C4	-6.15	1.34	1.38
18	D3	1025	A	N9-C8	-6.15	1.32	1.37
18	D3	86	A	N3-C4	-6.15	1.31	1.34
18	D3	148	A	N3-C4	-6.15	1.31	1.34
18	D3	425	A	N7-C5	-6.15	1.35	1.39
18	D3	475	A	N9-C4	-6.15	1.34	1.37
18	D3	797	G	C5-C4	-6.15	1.34	1.38
18	D3	336	G	C5-C4	-6.15	1.34	1.38
18	D3	54	C	N3-C4	-6.14	1.29	1.33
18	D3	612	U	N1-C2	-6.14	1.33	1.38
18	D3	1108	G	C6-N1	-6.14	1.35	1.39
18	D3	328	A	N7-C5	-6.14	1.35	1.39
18	D3	524	U	N1-C2	-6.14	1.33	1.38
18	D3	958	U	C2-N3	-6.14	1.33	1.37
18	D3	757	A	C5-C4	-6.14	1.34	1.38
7	CL	170	VAL	CB-CG2	-6.13	1.40	1.52
18	D3	367	A	N9-C4	-6.13	1.34	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	902	G	N7-C5	-6.13	1.35	1.39
18	D3	1048	G	C5-C4	-6.13	1.34	1.38
18	D3	1073	G	C5-C4	-6.13	1.34	1.38
18	D3	86	A	N9-C4	-6.13	1.34	1.37
18	D3	930	A	N7-C5	-6.13	1.35	1.39
18	D3	531	C	N3-C4	-6.12	1.29	1.33
18	D3	1774	G	N9-C8	-6.12	1.33	1.37
18	D3	459	G	N1-C2	-6.12	1.32	1.37
18	D3	1033	C	C4-C5	-6.11	1.38	1.43
18	D3	414	C	N1-C6	-6.11	1.33	1.37
18	D3	767	U	N1-C6	-6.11	1.32	1.38
18	D3	59	C	N3-C4	-6.11	1.29	1.33
18	D3	168	A	C5-C4	-6.11	1.34	1.38
18	D3	41	A	N3-C4	-6.10	1.31	1.34
18	D3	247	A	N9-C4	-6.10	1.34	1.37
18	D3	988	A	C5-C6	-6.10	1.35	1.41
18	D3	40	A	C5-C4	-6.10	1.34	1.38
18	D3	300	A	N3-C4	-6.10	1.31	1.34
18	D3	377	G	C8-N7	-6.10	1.27	1.30
18	D3	767	U	N3-C4	-6.10	1.32	1.38
18	D3	399	A	C5-C6	-6.10	1.35	1.41
18	D3	65	A	C5-C6	-6.09	1.35	1.41
18	D3	992	A	C2-N3	-6.09	1.28	1.33
18	D3	121	U	N1-C6	-6.09	1.32	1.38
18	D3	398	G	N7-C5	-6.09	1.35	1.39
18	D3	613	G	C8-N7	-6.09	1.27	1.30
18	D3	931	C	N3-C4	-6.09	1.29	1.33
18	D3	367	A	C5-C4	-6.08	1.34	1.38
18	D3	974	A	N7-C5	-6.08	1.35	1.39
18	D3	306	U	N1-C2	-6.08	1.33	1.38
18	D3	1046	G	N9-C8	-6.08	1.33	1.37
18	D3	363	G	N7-C5	-6.07	1.35	1.39
18	D3	940	A	N9-C8	-6.07	1.32	1.37
30	DX	29	TYR	CD2-CE2	-6.07	1.30	1.39
18	D3	315	A	N3-C4	-6.07	1.31	1.34
18	D3	615	A	C5-C4	-6.07	1.34	1.38
18	D3	63	G	C5-C4	-6.07	1.34	1.38
18	D3	464	A	C5-C4	-6.07	1.34	1.38
18	D3	292	U	C2-N3	-6.06	1.33	1.37
18	D3	449	C	C4-C5	-6.06	1.38	1.43
18	D3	55	A	N3-C4	-6.06	1.31	1.34
18	D3	437	A	C5-C4	-6.06	1.34	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	409	C	N1-C6	-6.06	1.33	1.37
18	D3	92	A	C5-C4	-6.06	1.34	1.38
18	D3	475	A	C5-C4	-6.05	1.34	1.38
18	D3	957	G	N7-C5	-6.05	1.35	1.39
18	D3	52	U	C4-C5	-6.05	1.38	1.43
18	D3	456	A	C5-C4	-6.05	1.34	1.38
18	D3	1073	G	N9-C8	-6.05	1.33	1.37
18	D3	354	C	C4-C5	-6.04	1.38	1.43
18	D3	92	A	C6-N1	-6.04	1.31	1.35
18	D3	435	C	N3-C4	-6.04	1.29	1.33
18	D3	887	A	N9-C4	-6.04	1.34	1.37
18	D3	933	A	N7-C5	-6.04	1.35	1.39
18	D3	538	A	N9-C4	-6.04	1.34	1.37
18	D3	353	A	N3-C4	-6.04	1.31	1.34
18	D3	594	A	C5-C4	-6.03	1.34	1.38
18	D3	464	A	N7-C5	-6.03	1.35	1.39
18	D3	356	G	C5-C4	-6.03	1.34	1.38
18	D3	1104	U	N1-C6	-6.03	1.32	1.38
18	D3	407	A	N3-C4	-6.02	1.31	1.34
35	D4	7	G	C5-C4	-6.02	1.34	1.38
18	D3	112	A	C5-C4	-6.02	1.34	1.38
18	D3	965	U	C2-N3	-6.02	1.33	1.37
18	D3	1121	C	N1-C6	-6.02	1.33	1.37
18	D3	986	G	N7-C5	-6.02	1.35	1.39
18	D3	1084	A	C5-C4	-6.02	1.34	1.38
18	D3	1022	C	C4-C5	-6.01	1.38	1.43
18	D3	767	U	C2-N3	-6.01	1.33	1.37
18	D3	120	U	C4-C5	-6.00	1.38	1.43
18	D3	1100	G	C5-C4	-6.00	1.34	1.38
20	DE	126	VAL	CB-CG1	-6.00	1.40	1.52
7	CL	288	VAL	CB-CG1	-6.00	1.40	1.52
18	D3	346	G	C5-C4	-6.00	1.34	1.38
18	D3	875	G	C6-N1	-6.00	1.35	1.39
18	D3	954	G	C5-C4	-6.00	1.34	1.38
18	D3	306	U	N1-C6	-6.00	1.32	1.38
18	D3	1104	U	N1-C2	-6.00	1.33	1.38
18	D3	1094	G	N7-C5	-5.99	1.35	1.39
18	D3	95	G	N1-C2	-5.99	1.32	1.37
18	D3	299	A	C5-C4	-5.99	1.34	1.38
18	D3	1781	A	N3-C4	-5.99	1.31	1.34
18	D3	1786	G	N1-C2	-5.99	1.32	1.37
18	D3	334	G	N9-C8	-5.99	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	958	U	N1-C2	-5.99	1.33	1.38
18	D3	299	A	N7-C5	-5.98	1.35	1.39
18	D3	976	G	N3-C4	-5.98	1.31	1.35
18	D3	306	U	C5-C6	-5.98	1.28	1.34
18	D3	1791	A	N3-C4	-5.98	1.31	1.34
18	D3	427	C	N1-C2	-5.98	1.34	1.40
18	D3	430	G	N9-C8	-5.98	1.33	1.37
20	DE	184	THR	CA-CB	-5.98	1.37	1.53
18	D3	976	G	C6-N1	-5.98	1.35	1.39
18	D3	610	G	C6-N1	-5.97	1.35	1.39
18	D3	951	A	N9-C4	-5.97	1.34	1.37
18	D3	378	A	C5-C6	-5.97	1.35	1.41
25	DL	93	TYR	CE1-CZ	-5.97	1.30	1.38
18	D3	45	U	C2-N3	-5.97	1.33	1.37
18	D3	53	G	C5-C4	-5.97	1.34	1.38
18	D3	162	A	C5-C4	-5.97	1.34	1.38
18	D3	951	A	C5-C4	-5.97	1.34	1.38
18	D3	123	G	N1-C2	-5.96	1.32	1.37
18	D3	993	A	N9-C4	-5.96	1.34	1.37
18	D3	41	A	N9-C8	-5.96	1.32	1.37
18	D3	461	G	C8-N7	-5.95	1.27	1.30
18	D3	1108	G	N9-C8	-5.95	1.33	1.37
18	D3	246	G	N1-C2	-5.95	1.32	1.37
18	D3	364	G	C6-N1	-5.95	1.35	1.39
18	D3	397	A	C5-C4	-5.95	1.34	1.38
18	D3	400	A	N3-C4	-5.94	1.31	1.34
18	D3	461	G	N9-C8	-5.94	1.33	1.37
18	D3	448	C	C4-C5	-5.94	1.38	1.43
18	D3	336	G	N7-C5	-5.93	1.35	1.39
18	D3	512	A	C5-C4	-5.93	1.34	1.38
18	D3	330	G	N9-C8	-5.93	1.33	1.37
18	D3	116	U	N1-C2	-5.92	1.33	1.38
18	D3	990	C	C4-C5	-5.92	1.38	1.43
18	D3	1022	C	N1-C6	-5.92	1.33	1.37
18	D3	1024	U	N3-C4	-5.91	1.33	1.38
18	D3	91	G	C5-C4	-5.91	1.34	1.38
18	D3	1035	G	C6-N1	-5.91	1.35	1.39
18	D3	330	G	C5-C4	-5.91	1.34	1.38
18	D3	799	A	C5-C4	-5.91	1.34	1.38
18	D3	1028	C	C4-C5	-5.91	1.38	1.43
18	D3	925	G	C5-C4	-5.90	1.34	1.38
18	D3	60	U	N1-C2	-5.90	1.33	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	164	A	N7-C5	-5.89	1.35	1.39
18	D3	41	A	N7-C5	-5.89	1.35	1.39
18	D3	403	G	N1-C2	-5.89	1.33	1.37
18	D3	1094	G	C5-C4	-5.89	1.34	1.38
18	D3	1047	G	N7-C5	-5.89	1.35	1.39
18	D3	1130	A	C5-C6	-5.89	1.35	1.41
18	D3	55	A	N9-C4	-5.88	1.34	1.37
18	D3	473	A	C5-C4	-5.88	1.34	1.38
18	D3	638	U	C2-N3	-5.88	1.33	1.37
18	D3	955	A	N3-C4	-5.88	1.31	1.34
18	D3	116	U	C4-C5	-5.88	1.38	1.43
18	D3	312	A	N7-C5	-5.88	1.35	1.39
18	D3	428	A	N3-C4	-5.88	1.31	1.34
18	D3	1036	A	N3-C4	-5.87	1.31	1.34
20	DE	182	TYR	CE1-CZ	-5.87	1.30	1.38
18	D3	388	G	C8-N7	-5.87	1.27	1.30
18	D3	979	A	C5-C4	-5.87	1.34	1.38
18	D3	872	G	N1-C2	-5.87	1.33	1.37
18	D3	28	A	C5-C4	-5.87	1.34	1.38
18	D3	429	G	C6-N1	-5.87	1.35	1.39
18	D3	104	A	C5-C4	-5.86	1.34	1.38
18	D3	869	A	N9-C4	-5.86	1.34	1.37
18	D3	61	A	N7-C5	-5.86	1.35	1.39
18	D3	432	G	N9-C8	-5.86	1.33	1.37
18	D3	334	G	N7-C5	-5.86	1.35	1.39
18	D3	462	G	N9-C4	-5.86	1.33	1.38
18	D3	798	C	N3-C4	-5.86	1.29	1.33
18	D3	1773	C	C4-C5	-5.85	1.38	1.43
18	D3	332	U	N1-C2	-5.85	1.33	1.38
18	D3	456	A	C5-C6	-5.84	1.35	1.41
18	D3	393	C	N1-C6	-5.84	1.33	1.37
18	D3	865	A	N7-C5	-5.84	1.35	1.39
18	D3	1786	G	N9-C8	-5.84	1.33	1.37
18	D3	972	G	C5-C4	-5.83	1.34	1.38
18	D3	298	C	C4-C5	-5.83	1.38	1.43
18	D3	538	A	C5-C4	-5.83	1.34	1.38
18	D3	385	A	N9-C8	-5.83	1.33	1.37
18	D3	420	A	C5-C4	-5.83	1.34	1.38
18	D3	402	C	N1-C6	-5.82	1.33	1.37
18	D3	940	A	N3-C4	-5.82	1.31	1.34
25	DL	100	TYR	CD2-CE2	-5.82	1.30	1.39
18	D3	757	A	N7-C5	-5.82	1.35	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	110	U	N1-C2	-5.82	1.33	1.38
18	D3	757	A	N9-C4	-5.82	1.34	1.37
18	D3	47	A	C5-C4	-5.82	1.34	1.38
18	D3	246	G	C5-C6	-5.82	1.36	1.42
18	D3	356	G	C6-N1	-5.82	1.35	1.39
18	D3	634	G	C8-N7	-5.82	1.27	1.30
18	D3	293	U	N1-C2	-5.81	1.33	1.38
18	D3	352	A	C5-C4	-5.81	1.34	1.38
18	D3	124	A	C5-C4	-5.81	1.34	1.38
18	D3	875	G	N1-C2	-5.80	1.33	1.37
18	D3	1084	A	N9-C4	-5.80	1.34	1.37
18	D3	109	G	N1-C2	-5.80	1.33	1.37
18	D3	1107	G	N9-C8	-5.80	1.33	1.37
18	D3	443	C	C4-C5	-5.80	1.38	1.43
20	DE	160	VAL	CB-CG1	-5.80	1.40	1.52
18	D3	756	A	C5-C4	-5.79	1.34	1.38
18	D3	386	G	C6-N1	-5.79	1.35	1.39
18	D3	545	A	C5-C4	-5.79	1.34	1.38
18	D3	886	U	C2-N3	-5.79	1.33	1.37
18	D3	357	G	N7-C5	-5.79	1.35	1.39
18	D3	347	G	N9-C8	-5.78	1.33	1.37
18	D3	375	U	C2-N3	-5.78	1.33	1.37
18	D3	631	G	N9-C8	-5.78	1.33	1.37
18	D3	294	C	N1-C6	-5.78	1.33	1.37
18	D3	99	C	C2-N3	-5.78	1.31	1.35
18	D3	634	G	N1-C2	-5.78	1.33	1.37
18	D3	300	A	C5-C4	-5.78	1.34	1.38
18	D3	404	G	C6-N1	-5.78	1.35	1.39
23	DI	46	VAL	CB-CG2	-5.78	1.40	1.52
18	D3	173	A	N3-C4	-5.77	1.31	1.34
18	D3	122	U	N1-C2	-5.77	1.33	1.38
18	D3	446	A	C5-C4	-5.77	1.34	1.38
18	D3	631	G	N7-C5	-5.77	1.35	1.39
18	D3	953	G	N7-C5	-5.77	1.35	1.39
18	D3	1776	A	N9-C4	-5.77	1.34	1.37
18	D3	98	U	N1-C2	-5.77	1.33	1.38
18	D3	755	A	N7-C5	-5.77	1.35	1.39
18	D3	866	G	C6-N1	-5.77	1.35	1.39
18	D3	164	A	C5-C4	-5.76	1.34	1.38
18	D3	418	G	C6-N1	-5.76	1.35	1.39
18	D3	434	G	C6-N1	-5.76	1.35	1.39
18	D3	377	G	C5-C6	-5.76	1.36	1.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	103	A	N7-C5	-5.75	1.35	1.39
24	DJ	113	VAL	CB-CG2	-5.75	1.40	1.52
18	D3	402	C	N3-C4	-5.75	1.29	1.33
18	D3	365	G	N9-C8	-5.75	1.33	1.37
18	D3	296	U	N1-C2	-5.75	1.33	1.38
18	D3	449	C	N3-C4	-5.75	1.29	1.33
18	D3	1108	G	C8-N7	-5.75	1.27	1.30
18	D3	311	U	N1-C2	-5.74	1.33	1.38
18	D3	961	U	N1-C2	-5.74	1.33	1.38
18	D3	316	A	N3-C4	-5.74	1.31	1.34
18	D3	1772	C	N3-C4	-5.74	1.29	1.33
18	D3	147	A	C5-C4	-5.74	1.34	1.38
18	D3	597	G	C5-C4	-5.73	1.34	1.38
18	D3	310	C	C4-C5	-5.73	1.38	1.43
18	D3	333	A	N9-C8	-5.73	1.33	1.37
18	D3	364	G	N3-C4	-5.73	1.31	1.35
18	D3	877	G	N1-C2	-5.73	1.33	1.37
18	D3	378	A	C5-C4	-5.73	1.34	1.38
18	D3	398	G	N9-C8	-5.73	1.33	1.37
18	D3	1103	U	N1-C2	-5.73	1.33	1.38
18	D3	1790	A	C5-C4	-5.73	1.34	1.38
18	D3	969	C	N1-C6	-5.72	1.33	1.37
24	DJ	108	ARG	CB-CG	-5.72	1.37	1.52
18	D3	322	G	N9-C8	-5.72	1.33	1.37
18	D3	543	C	N1-C6	-5.72	1.33	1.37
18	D3	1074	G	N1-C2	-5.72	1.33	1.37
18	D3	90	C	C4-C5	-5.72	1.38	1.43
18	D3	755	A	C5-C4	-5.72	1.34	1.38
18	D3	1069	A	N9-C4	-5.72	1.34	1.37
18	D3	97	C	N3-C4	-5.71	1.29	1.33
18	D3	96	G	N3-C4	-5.71	1.31	1.35
18	D3	247	A	C5-C4	-5.71	1.34	1.38
18	D3	389	G	C5-C4	-5.71	1.34	1.38
18	D3	346	G	N3-C4	-5.71	1.31	1.35
18	D3	529	A	N7-C5	-5.71	1.35	1.39
18	D3	317	C	N1-C6	-5.71	1.33	1.37
18	D3	1094	G	C5-C6	-5.71	1.36	1.42
18	D3	797	G	N1-C2	-5.70	1.33	1.37
18	D3	865	A	N9-C4	-5.70	1.34	1.37
18	D3	295	A	N9-C4	-5.70	1.34	1.37
18	D3	157	A	N9-C4	-5.70	1.34	1.37
18	D3	382	C	N3-C4	-5.70	1.29	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	1019	A	N3-C4	-5.70	1.31	1.34
18	D3	384	G	N1-C2	-5.70	1.33	1.37
18	D3	974	A	N9-C4	-5.70	1.34	1.37
18	D3	251	A	C5-C4	-5.70	1.34	1.38
18	D3	298	C	N1-C2	-5.69	1.34	1.40
18	D3	386	G	N3-C4	-5.69	1.31	1.35
18	D3	392	G	N9-C8	-5.69	1.33	1.37
18	D3	747	C	C4-C5	-5.68	1.38	1.43
18	D3	1789	G	N3-C4	-5.68	1.31	1.35
18	D3	47	A	N9-C8	-5.68	1.33	1.37
18	D3	387	A	C8-N7	-5.68	1.27	1.31
18	D3	1067	C	N1-C6	-5.68	1.33	1.37
18	D3	1105	C	N1-C6	-5.68	1.33	1.37
18	D3	392	G	N7-C5	-5.68	1.35	1.39
18	D3	595	G	C6-N1	-5.68	1.35	1.39
18	D3	625	C	C4-C5	-5.68	1.38	1.43
18	D3	764	U	C2-N3	-5.67	1.33	1.37
18	D3	1130	A	N7-C5	-5.67	1.35	1.39
18	D3	1035	G	N7-C5	-5.67	1.35	1.39
18	D3	1013	A	C5-C4	-5.67	1.34	1.38
18	D3	1124	A	N9-C4	-5.67	1.34	1.37
18	D3	513	U	N1-C2	-5.67	1.33	1.38
18	D3	147	A	N3-C4	-5.66	1.31	1.34
18	D3	531	C	N1-C6	-5.66	1.33	1.37
18	D3	756	A	N9-C8	-5.66	1.33	1.37
18	D3	145	A	N7-C5	-5.66	1.35	1.39
18	D3	796	A	N9-C4	-5.66	1.34	1.37
18	D3	44	U	N3-C4	-5.66	1.33	1.38
18	D3	383	G	C6-N1	-5.66	1.35	1.39
18	D3	115	G	C5-C6	-5.65	1.36	1.42
18	D3	98	U	N3-C4	-5.65	1.33	1.38
18	D3	948	G	C6-N1	-5.65	1.35	1.39
18	D3	1792	G	N7-C5	-5.65	1.35	1.39
18	D3	52	U	N1-C2	-5.65	1.33	1.38
18	D3	298	C	N3-C4	-5.65	1.29	1.33
18	D3	442	C	N3-C4	-5.65	1.29	1.33
18	D3	875	G	N7-C5	-5.65	1.35	1.39
18	D3	295	A	N7-C5	-5.65	1.35	1.39
18	D3	757	A	C5-C6	-5.64	1.35	1.41
18	D3	1035	G	N9-C4	-5.64	1.33	1.38
18	D3	54	C	C2-N3	-5.64	1.31	1.35
18	D3	966	A	C5-C6	-5.64	1.35	1.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	111	U	C2-N3	-5.64	1.33	1.37
18	D3	481	A	N9-C4	-5.64	1.34	1.37
18	D3	609	U	N1-C2	-5.64	1.33	1.38
18	D3	1023	A	C5-C4	-5.63	1.34	1.38
18	D3	113	U	C2-N3	-5.63	1.33	1.37
18	D3	257	A	N3-C4	-5.63	1.31	1.34
18	D3	980	G	N3-C4	-5.63	1.31	1.35
18	D3	328	A	C5-C4	-5.62	1.34	1.38
7	CL	109	SER	CA-CB	-5.62	1.44	1.52
18	D3	386	G	N9-C4	-5.62	1.33	1.38
18	D3	514	G	C5-C4	-5.62	1.34	1.38
18	D3	338	C	N3-C4	-5.62	1.30	1.33
18	D3	34	G	N7-C5	-5.62	1.35	1.39
18	D3	91	G	C8-N7	-5.62	1.27	1.30
18	D3	115	G	N9-C8	-5.62	1.33	1.37
18	D3	610	G	N1-C2	-5.62	1.33	1.37
18	D3	988	A	N3-C4	-5.62	1.31	1.34
18	D3	305	C	N3-C4	-5.61	1.30	1.33
18	D3	941	A	N3-C4	-5.61	1.31	1.34
18	D3	91	G	N9-C8	-5.61	1.33	1.37
18	D3	364	G	N9-C8	-5.61	1.33	1.37
18	D3	375	U	N1-C2	-5.61	1.33	1.38
18	D3	628	G	N7-C5	-5.61	1.35	1.39
18	D3	622	A	C5-C6	-5.61	1.36	1.41
18	D3	378	A	N9-C4	-5.60	1.34	1.37
18	D3	425	A	N9-C8	-5.60	1.33	1.37
18	D3	940	A	C6-N1	-5.60	1.31	1.35
18	D3	473	A	N7-C5	-5.60	1.35	1.39
18	D3	766	U	C4-O4	-5.60	1.19	1.23
18	D3	1048	G	N7-C5	-5.60	1.35	1.39
18	D3	1071	U	C2-N3	-5.60	1.33	1.37
18	D3	119	A	N3-C4	-5.60	1.31	1.34
18	D3	247	A	N3-C4	-5.59	1.31	1.34
18	D3	251	A	N3-C4	-5.59	1.31	1.34
18	D3	344	A	C5-C4	-5.59	1.34	1.38
18	D3	142	G	C2-N3	-5.59	1.28	1.32
18	D3	941	A	C5-C4	-5.59	1.34	1.38
18	D3	1774	G	N1-C2	-5.59	1.33	1.37
18	D3	757	A	N9-C8	-5.59	1.33	1.37
18	D3	950	C	N3-C4	-5.58	1.30	1.33
18	D3	427	C	C4-C5	-5.58	1.38	1.43
18	D3	1104	U	C4-C5	-5.58	1.38	1.43

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	258	C	N1-C6	-5.58	1.33	1.37
18	D3	383	G	N1-C2	-5.58	1.33	1.37
18	D3	875	G	C2-N3	-5.58	1.28	1.32
18	D3	1792	G	C8-N7	-5.58	1.27	1.30
18	D3	467	G	C5-C4	-5.58	1.34	1.38
18	D3	1093	A	N9-C4	-5.58	1.34	1.37
18	D3	149	C	N1-C6	-5.58	1.33	1.37
18	D3	404	G	N7-C5	-5.57	1.35	1.39
18	D3	432	G	C6-N1	-5.57	1.35	1.39
18	D3	336	G	N1-C2	-5.57	1.33	1.37
18	D3	1782	A	N9-C4	-5.57	1.34	1.37
18	D3	776	G	N9-C8	-5.56	1.33	1.37
18	D3	871	G	C6-N1	-5.56	1.35	1.39
18	D3	957	G	C5-C4	-5.56	1.34	1.38
18	D3	305	C	N1-C2	-5.56	1.34	1.40
18	D3	517	U	C2-N3	-5.56	1.33	1.37
18	D3	116	U	N3-C4	-5.56	1.33	1.38
18	D3	633	U	N1-C2	-5.56	1.33	1.38
18	D3	862	A	C5-C4	-5.55	1.34	1.38
18	D3	614	C	N1-C6	-5.55	1.33	1.37
18	D3	125	U	C2-N3	-5.55	1.33	1.37
18	D3	409	C	N3-C4	-5.55	1.30	1.33
18	D3	102	U	N1-C6	-5.55	1.32	1.38
18	D3	306	U	N3-C4	-5.55	1.33	1.38
18	D3	868	G	C5-C4	-5.55	1.34	1.38
18	D3	87	C	C4-C5	-5.54	1.38	1.43
18	D3	35	U	C2-N3	-5.54	1.33	1.37
18	D3	980	G	C2-N3	-5.54	1.28	1.32
18	D3	354	C	N3-C4	-5.54	1.30	1.33
18	D3	98	U	C5-C6	-5.54	1.29	1.34
18	D3	318	U	N1-C2	-5.54	1.33	1.38
18	D3	616	G	N9-C8	-5.54	1.33	1.37
18	D3	801	G	N7-C5	-5.54	1.35	1.39
18	D3	461	G	C6-N1	-5.53	1.35	1.39
25	DL	123	VAL	CB-CG2	-5.53	1.41	1.52
18	D3	531	C	C4-C5	-5.53	1.38	1.43
11	JL	185	VAL	CB-CG1	-5.53	1.41	1.52
18	D3	475	A	N3-C4	-5.53	1.31	1.34
18	D3	547	U	N1-C6	-5.53	1.32	1.38
18	D3	937	C	C4-C5	-5.53	1.38	1.43
18	D3	338	C	N1-C2	-5.53	1.34	1.40
18	D3	426	G	N9-C8	-5.53	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	1037	C	N3-C4	-5.53	1.30	1.33
18	D3	1094	G	N9-C8	-5.53	1.33	1.37
18	D3	301	A	C5-C4	-5.52	1.34	1.38
18	D3	991	G	C5-C4	-5.52	1.34	1.38
18	D3	426	G	C5-C6	-5.52	1.36	1.42
18	D3	37	U	N3-C4	-5.51	1.33	1.38
18	D3	611	U	C4-C5	-5.51	1.38	1.43
18	D3	1065	A	N3-C4	-5.51	1.31	1.34
18	D3	47	A	C6-N1	-5.51	1.31	1.35
18	D3	103	A	C5-C4	-5.51	1.34	1.38
18	D3	863	A	C5-C4	-5.51	1.34	1.38
18	D3	460	A	C6-N1	-5.51	1.31	1.35
18	D3	65	A	N7-C5	-5.51	1.35	1.39
18	D3	310	C	N3-C4	-5.51	1.30	1.33
18	D3	1068	C	N1-C2	-5.51	1.34	1.40
18	D3	1076	A	C5-C4	-5.51	1.34	1.38
18	D3	246	G	N7-C5	-5.50	1.35	1.39
18	D3	304	U	C2-N3	-5.50	1.33	1.37
18	D3	323	A	N7-C5	-5.50	1.35	1.39
18	D3	403	G	N7-C5	-5.50	1.35	1.39
18	D3	1097	U	N1-C6	-5.50	1.32	1.38
18	D3	613	G	C5-C6	-5.50	1.36	1.42
18	D3	865	A	C5-C4	-5.50	1.34	1.38
18	D3	1116	A	N7-C5	-5.50	1.35	1.39
18	D3	311	U	C2-N3	-5.50	1.33	1.37
18	D3	1093	A	N3-C4	-5.50	1.31	1.34
18	D3	105	A	C5-C4	-5.50	1.34	1.38
18	D3	324	U	C4-C5	-5.50	1.38	1.43
18	D3	1793	G	C5-C4	-5.50	1.34	1.38
18	D3	1107	G	C6-N1	-5.49	1.35	1.39
18	D3	390	G	N9-C8	-5.49	1.34	1.37
18	D3	394	C	C2-N3	-5.49	1.31	1.35
18	D3	617	U	C4-C5	-5.49	1.38	1.43
18	D3	980	G	C6-N1	-5.49	1.35	1.39
18	D3	118	U	N1-C2	-5.49	1.33	1.38
18	D3	331	A	N9-C8	-5.49	1.33	1.37
18	D3	45	U	C2-O2	-5.49	1.17	1.22
18	D3	297	U	C4-C5	-5.48	1.38	1.43
18	D3	428	A	N7-C5	-5.48	1.35	1.39
18	D3	333	A	N3-C4	-5.48	1.31	1.34
18	D3	445	A	C5-C4	-5.48	1.34	1.38
18	D3	547	U	N1-C2	-5.48	1.33	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	123	G	C6-N1	-5.48	1.35	1.39
18	D3	612	U	C2-N3	-5.48	1.33	1.37
18	D3	895	G	N3-C4	-5.48	1.31	1.35
18	D3	385	A	N7-C5	-5.47	1.35	1.39
18	D3	756	A	N7-C5	-5.47	1.35	1.39
18	D3	967	A	C5-C4	-5.47	1.34	1.38
18	D3	1095	U	N1-C2	-5.47	1.33	1.38
18	D3	447	U	N1-C6	-5.47	1.33	1.38
18	D3	450	U	N1-C2	-5.47	1.33	1.38
18	D3	599	A	C5-C4	-5.47	1.34	1.38
18	D3	322	G	N3-C4	-5.47	1.31	1.35
7	CL	74	VAL	CB-CG1	-5.47	1.41	1.52
18	D3	111	U	C4-C5	-5.47	1.38	1.43
18	D3	971	A	N3-C4	-5.47	1.31	1.34
18	D3	400	A	N7-C5	-5.47	1.35	1.39
18	D3	631	G	C5-C4	-5.47	1.34	1.38
18	D3	884	A	N3-C4	-5.47	1.31	1.34
18	D3	329	G	C6-N1	-5.46	1.35	1.39
18	D3	363	G	C8-N7	-5.46	1.27	1.30
18	D3	427	C	C2-N3	-5.46	1.31	1.35
18	D3	763	G	C5-C4	-5.46	1.34	1.38
18	D3	362	G	N1-C2	-5.46	1.33	1.37
18	D3	450	U	N1-C6	-5.46	1.33	1.38
18	D3	769	A	C5-C4	-5.46	1.34	1.38
18	D3	57	G	N9-C8	-5.46	1.34	1.37
18	D3	36	C	C4-C5	-5.46	1.38	1.43
18	D3	53	G	N9-C8	-5.46	1.34	1.37
18	D3	772	G	N1-C2	-5.46	1.33	1.37
18	D3	1776	A	N9-C8	-5.46	1.33	1.37
18	D3	246	G	N3-C4	-5.45	1.31	1.35
18	D3	356	G	C8-N7	-5.45	1.27	1.30
18	D3	939	A	C6-N1	-5.45	1.31	1.35
18	D3	1037	C	N1-C6	-5.45	1.33	1.37
18	D3	927	C	N3-C4	-5.45	1.30	1.33
18	D3	95	G	C6-N1	-5.45	1.35	1.39
18	D3	172	C	N1-C6	-5.45	1.33	1.37
18	D3	315	A	C5-C4	-5.45	1.34	1.38
18	D3	631	G	N1-C2	-5.45	1.33	1.37
18	D3	478	A	N9-C4	-5.45	1.34	1.37
18	D3	760	A	C5-C4	-5.45	1.34	1.38
18	D3	458	G	C6-N1	-5.45	1.35	1.39
18	D3	1778	G	N3-C4	-5.45	1.31	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	306	U	C2-N3	-5.44	1.33	1.37
18	D3	459	G	C6-N1	-5.44	1.35	1.39
18	D3	53	G	C8-N7	-5.44	1.27	1.30
18	D3	391	A	N7-C5	-5.44	1.35	1.39
18	D3	1102	G	N9-C8	-5.44	1.34	1.37
18	D3	87	C	C2-N3	-5.43	1.31	1.35
18	D3	364	G	N9-C4	-5.43	1.33	1.38
18	D3	926	A	N7-C5	-5.43	1.35	1.39
18	D3	966	A	C6-N1	-5.43	1.31	1.35
18	D3	625	C	N1-C2	-5.43	1.34	1.40
18	D3	1040	G	C5-C4	-5.43	1.34	1.38
18	D3	1076	A	N3-C4	-5.43	1.31	1.34
18	D3	1103	U	C4-O4	-5.43	1.19	1.23
18	D3	92	A	N3-C4	-5.43	1.31	1.34
18	D3	1069	A	C5-C4	-5.43	1.34	1.38
35	D4	9	A	N9-C4	-5.43	1.34	1.37
18	D3	955	A	C5-C4	-5.42	1.34	1.38
18	D3	1787	C	C4-C5	-5.42	1.38	1.43
18	D3	758	U	C4-C5	-5.42	1.38	1.43
18	D3	1072	C	N1-C2	-5.42	1.34	1.40
18	D3	322	G	C6-N1	-5.42	1.35	1.39
18	D3	383	G	N3-C4	-5.42	1.31	1.35
18	D3	628	G	N9-C8	-5.42	1.34	1.37
18	D3	776	G	C5-C6	-5.42	1.36	1.42
18	D3	365	G	C5-C4	-5.42	1.34	1.38
18	D3	161	U	C2-N3	-5.41	1.33	1.37
18	D3	164	A	N9-C4	-5.41	1.34	1.37
18	D3	887	A	N7-C5	-5.41	1.36	1.39
18	D3	974	A	C6-N1	-5.41	1.31	1.35
18	D3	627	C	C4-C5	-5.41	1.38	1.43
18	D3	977	A	C5-C4	-5.41	1.34	1.38
18	D3	1786	G	N7-C5	-5.41	1.36	1.39
18	D3	931	C	C4-C5	-5.41	1.38	1.43
18	D3	953	G	N9-C8	-5.41	1.34	1.37
20	DE	105	VAL	CB-CG1	-5.41	1.41	1.52
18	D3	390	G	N9-C4	-5.40	1.33	1.38
18	D3	525	A	C5-C6	-5.40	1.36	1.41
18	D3	788	A	N7-C5	-5.40	1.36	1.39
18	D3	751	G	N1-C2	-5.40	1.33	1.37
18	D3	1028	C	N3-C4	-5.40	1.30	1.33
4	UX	80	VAL	CB-CG2	-5.39	1.41	1.52
18	D3	40	A	N9-C4	-5.39	1.34	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	108	A	N7-C5	-5.39	1.36	1.39
18	D3	610	G	C5-C4	-5.39	1.34	1.38
18	D3	875	G	N3-C4	-5.39	1.31	1.35
27	DO	67	VAL	CB-CG2	-5.39	1.41	1.52
18	D3	1105	C	N1-C2	-5.39	1.34	1.40
18	D3	42	G	C5-C4	-5.39	1.34	1.38
18	D3	426	G	C2-N3	-5.39	1.28	1.32
18	D3	957	G	N9-C8	-5.39	1.34	1.37
18	D3	1092	A	N3-C4	-5.38	1.31	1.34
18	D3	94	U	N3-C4	-5.38	1.33	1.38
18	D3	761	G	N1-C2	-5.38	1.33	1.37
18	D3	149	C	C4-C5	-5.38	1.38	1.43
18	D3	337	G	C6-N1	-5.38	1.35	1.39
18	D3	357	G	C8-N7	-5.38	1.27	1.30
18	D3	378	A	C8-N7	-5.38	1.27	1.31
18	D3	434	G	N1-C2	-5.38	1.33	1.37
18	D3	429	G	C5-C6	-5.38	1.36	1.42
18	D3	628	G	C5-C4	-5.38	1.34	1.38
18	D3	773	C	N1-C6	-5.38	1.33	1.37
18	D3	37	U	C2-N3	-5.38	1.33	1.37
18	D3	96	G	N7-C5	-5.38	1.36	1.39
18	D3	350	U	C2-N3	-5.38	1.33	1.37
18	D3	594	A	N3-C4	-5.38	1.31	1.34
18	D3	1015	U	C2-N3	-5.38	1.33	1.37
18	D3	1036	A	N9-C4	-5.38	1.34	1.37
18	D3	46	A	C6-N1	-5.37	1.31	1.35
18	D3	387	A	N9-C8	-5.37	1.33	1.37
18	D3	1074	G	C6-N1	-5.37	1.35	1.39
18	D3	423	G	C5-C4	-5.37	1.34	1.38
18	D3	471	A	N7-C5	-5.37	1.36	1.39
18	D3	1011	G	C5-C4	-5.37	1.34	1.38
18	D3	1789	G	C5-C4	-5.37	1.34	1.38
18	D3	245	U	C2-N3	-5.37	1.33	1.37
18	D3	409	C	C4-C5	-5.37	1.38	1.43
18	D3	926	A	N9-C4	-5.37	1.34	1.37
18	D3	297	U	N3-C4	-5.37	1.33	1.38
18	D3	943	C	N3-C4	-5.37	1.30	1.33
18	D3	55	A	N9-C8	-5.37	1.33	1.37
18	D3	93	A	C5-C4	-5.37	1.34	1.38
18	D3	57	G	C5-C4	-5.36	1.34	1.38
18	D3	98	U	N1-C6	-5.36	1.33	1.38
18	D3	434	G	N9-C8	-5.36	1.34	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	31	C	C4-C5	-5.36	1.38	1.43
18	D3	118	U	C4-C5	-5.36	1.38	1.43
18	D3	459	G	C2-N3	-5.36	1.28	1.32
18	D3	529	A	C5-C6	-5.36	1.36	1.41
18	D3	356	G	N7-C5	-5.35	1.36	1.39
18	D3	960	U	N1-C2	-5.35	1.33	1.38
18	D3	160	C	C4-C5	-5.35	1.38	1.43
18	D3	439	U	C4-C5	-5.35	1.38	1.43
18	D3	804	A	C5-C4	-5.35	1.35	1.38
18	D3	473	A	N9-C8	-5.35	1.33	1.37
18	D3	863	A	N3-C4	-5.35	1.31	1.34
18	D3	977	A	N9-C8	-5.35	1.33	1.37
18	D3	405	C	C4-C5	-5.35	1.38	1.43
18	D3	925	G	N3-C4	-5.35	1.31	1.35
18	D3	251	A	N9-C4	-5.34	1.34	1.37
18	D3	108	A	N9-C4	-5.34	1.34	1.37
18	D3	446	A	C6-N1	-5.34	1.31	1.35
18	D3	943	C	C4-C5	-5.34	1.38	1.43
18	D3	763	G	N9-C8	-5.34	1.34	1.37
18	D3	936	G	C6-N1	-5.34	1.35	1.39
18	D3	299	A	C5-C6	-5.34	1.36	1.41
18	D3	43	A	N9-C4	-5.34	1.34	1.37
18	D3	397	A	N9-C8	-5.34	1.33	1.37
18	D3	805	U	C4-C5	-5.33	1.38	1.43
18	D3	344	A	N7-C5	-5.33	1.36	1.39
18	D3	63	G	N1-C2	-5.33	1.33	1.37
18	D3	102	U	N3-C4	-5.33	1.33	1.38
18	D3	1085	G	C5-C4	-5.33	1.34	1.38
18	D3	806	A	N9-C4	-5.33	1.34	1.37
18	D3	1074	G	C5-C4	-5.33	1.34	1.38
18	D3	108	A	C6-N1	-5.33	1.31	1.35
18	D3	96	G	C8-N7	-5.32	1.27	1.30
18	D3	768	C	C4-C5	-5.32	1.38	1.43
18	D3	867	G	C5-C4	-5.32	1.34	1.38
11	JL	223	TRP	CB-CG	-5.32	1.40	1.50
18	D3	399	A	N9-C8	-5.32	1.33	1.37
18	D3	521	A	N9-C4	-5.32	1.34	1.37
18	D3	731	C	O3'-P	5.32	1.67	1.61
18	D3	878	G	N7-C5	-5.32	1.36	1.39
18	D3	545	A	N3-C4	-5.32	1.31	1.34
7	CL	195	TRP	CB-CG	-5.31	1.40	1.50
18	D3	616	G	C6-N1	-5.31	1.35	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	386	G	N1-C2	-5.31	1.33	1.37
18	D3	477	A	C5-C4	-5.31	1.35	1.38
18	D3	936	G	N9-C8	-5.31	1.34	1.37
18	D3	1106	U	N1-C2	-5.31	1.33	1.38
18	D3	356	G	N9-C8	-5.31	1.34	1.37
18	D3	408	C	C4-C5	-5.30	1.38	1.43
18	D3	797	G	C6-N1	-5.30	1.35	1.39
18	D3	265	A	C5-C4	-5.30	1.35	1.38
20	DE	26	CYS	CB-SG	-5.30	1.73	1.81
18	D3	46	A	N7-C5	-5.30	1.36	1.39
18	D3	258	C	N3-C4	-5.30	1.30	1.33
18	D3	410	A	N3-C4	-5.29	1.31	1.34
18	D3	523	G	C6-N1	-5.29	1.35	1.39
18	D3	964	U	C4-C5	-5.29	1.38	1.43
18	D3	1778	G	N9-C4	-5.29	1.33	1.38
18	D3	315	A	N9-C8	-5.29	1.33	1.37
18	D3	417	A	N7-C5	-5.29	1.36	1.39
18	D3	456	A	N9-C4	-5.29	1.34	1.37
18	D3	950	C	N1-C6	-5.29	1.33	1.37
20	DE	182	TYR	CD1-CE1	-5.29	1.31	1.39
18	D3	388	G	N9-C8	-5.29	1.34	1.37
18	D3	424	C	C2-N3	-5.29	1.31	1.35
18	D3	975	C	N1-C6	-5.29	1.33	1.37
18	D3	635	A	N9-C8	-5.29	1.33	1.37
18	D3	1104	U	N3-C4	-5.29	1.33	1.38
18	D3	366	A	N3-C4	-5.29	1.31	1.34
18	D3	923	A	N7-C5	-5.29	1.36	1.39
18	D3	109	G	C8-N7	-5.29	1.27	1.30
18	D3	616	G	C5-C4	-5.29	1.34	1.38
18	D3	157	A	N3-C4	-5.28	1.31	1.34
18	D3	1026	A	N3-C4	-5.28	1.31	1.34
18	D3	102	U	C2-N3	-5.28	1.34	1.37
18	D3	930	A	N3-C4	-5.28	1.31	1.34
18	D3	377	G	C6-N1	-5.28	1.35	1.39
18	D3	400	A	C5-C6	-5.28	1.36	1.41
18	D3	938	G	C6-N1	-5.28	1.35	1.39
18	D3	951	A	N3-C4	-5.28	1.31	1.34
25	DL	128	CYS	CB-SG	-5.28	1.73	1.81
18	D3	297	U	N1-C2	-5.27	1.33	1.38
18	D3	298	C	N1-C6	-5.27	1.33	1.37
18	D3	396	G	N3-C4	-5.27	1.31	1.35
18	D3	615	A	N7-C5	-5.27	1.36	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	1101	G	C8-N7	-5.27	1.27	1.30
18	D3	527	A	N9-C8	-5.27	1.33	1.37
18	D3	1116	A	C5-C4	-5.27	1.35	1.38
18	D3	953	G	C5-C4	-5.27	1.34	1.38
18	D3	990	C	N1-C2	-5.27	1.34	1.40
18	D3	382	C	C2-N3	-5.27	1.31	1.35
18	D3	423	G	N9-C8	-5.27	1.34	1.37
18	D3	955	A	N9-C8	-5.27	1.33	1.37
18	D3	288	A	N7-C5	-5.26	1.36	1.39
18	D3	979	A	N7-C5	-5.26	1.36	1.39
18	D3	1026	A	N9-C8	-5.26	1.33	1.37
18	D3	536	C	C4-C5	-5.26	1.38	1.43
20	DE	82	TYR	CD1-CE1	-5.26	1.31	1.39
18	D3	542	A	N9-C4	-5.26	1.34	1.37
18	D3	790	U	N1-C2	-5.26	1.33	1.38
18	D3	468	A	C5-C6	-5.26	1.36	1.41
18	D3	329	G	N9-C8	-5.26	1.34	1.37
18	D3	400	A	C6-N1	-5.26	1.31	1.35
18	D3	468	A	N7-C5	-5.26	1.36	1.39
18	D3	599	A	N7-C5	-5.26	1.36	1.39
7	CL	897	CYS	CB-SG	-5.25	1.73	1.81
18	D3	431	C	N1-C6	-5.25	1.33	1.37
18	D3	807	A	N3-C4	-5.25	1.31	1.34
18	D3	1094	G	N1-C2	-5.25	1.33	1.37
18	D3	472	U	C2-N3	-5.25	1.34	1.37
18	D3	626	U	N1-C2	-5.25	1.33	1.38
18	D3	340	U	N1-C2	-5.24	1.33	1.38
18	D3	432	G	N1-C2	-5.24	1.33	1.37
18	D3	452	A	N7-C5	-5.24	1.36	1.39
18	D3	1039	A	N7-C5	-5.24	1.36	1.39
18	D3	609	U	N1-C6	-5.24	1.33	1.38
18	D3	866	G	C5-C4	-5.24	1.34	1.38
18	D3	593	U	C2-N3	-5.23	1.34	1.37
18	D3	1777	G	C5-C4	-5.23	1.34	1.38
18	D3	462	G	C2-N3	-5.23	1.28	1.32
18	D3	877	G	N7-C5	-5.23	1.36	1.39
7	CL	75	VAL	CB-CG2	-5.23	1.41	1.52
18	D3	1021	C	N1-C6	-5.23	1.34	1.37
18	D3	117	U	N1-C6	-5.23	1.33	1.38
18	D3	214	G	C6-N1	-5.22	1.35	1.39
18	D3	307	G	C5-C4	-5.22	1.34	1.38
18	D3	318	U	C2-N3	-5.22	1.34	1.37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	365	G	C2-N3	-5.22	1.28	1.32
18	D3	396	G	C5-C6	-5.22	1.37	1.42
18	D3	437	A	N9-C4	-5.22	1.34	1.37
18	D3	874	C	N1-C6	-5.22	1.34	1.37
18	D3	1014	G	C5-C4	-5.22	1.34	1.38
18	D3	1791	A	C8-N7	-5.22	1.27	1.31
18	D3	404	G	N9-C8	-5.22	1.34	1.37
18	D3	449	C	N1-C2	-5.22	1.34	1.40
18	D3	65	A	C6-N1	-5.22	1.31	1.35
18	D3	424	C	C5-C6	-5.22	1.30	1.34
18	D3	439	U	N1-C2	-5.22	1.33	1.38
18	D3	1022	C	N3-C4	-5.22	1.30	1.33
18	D3	343	C	N3-C4	-5.22	1.30	1.33
18	D3	362	G	C6-N1	-5.22	1.35	1.39
18	D3	457	G	N1-C2	-5.22	1.33	1.37
18	D3	1077	C	N1-C6	-5.22	1.34	1.37
18	D3	468	A	N9-C4	-5.21	1.34	1.37
18	D3	1117	U	C2-N3	-5.21	1.34	1.37
18	D3	333	A	N7-C5	-5.21	1.36	1.39
18	D3	390	G	N7-C5	-5.21	1.36	1.39
18	D3	457	G	N7-C5	-5.21	1.36	1.39
18	D3	1044	U	C2-N3	-5.21	1.34	1.37
18	D3	100	A	N7-C5	-5.20	1.36	1.39
18	D3	429	G	N1-C2	-5.20	1.33	1.37
18	D3	600	U	C2-N3	-5.20	1.34	1.37
18	D3	993	A	C5-C4	-5.20	1.35	1.38
18	D3	431	C	C4-C5	-5.20	1.38	1.43
18	D3	592	A	N7-C5	-5.20	1.36	1.39
18	D3	1096	C	N3-C4	-5.20	1.30	1.33
24	DJ	8	TYR	CD2-CE2	-5.20	1.31	1.39
18	D3	92	A	N9-C4	-5.20	1.34	1.37
18	D3	462	G	C5-C6	-5.20	1.37	1.42
18	D3	637	C	N1-C2	-5.20	1.34	1.40
18	D3	1107	G	C8-N7	-5.20	1.27	1.30
18	D3	634	G	N7-C5	-5.19	1.36	1.39
18	D3	208	U	N1-C2	-5.19	1.33	1.38
18	D3	428	A	C6-N6	-5.19	1.29	1.33
18	D3	115	G	C8-N7	-5.19	1.27	1.30
18	D3	1012	U	C2-N3	-5.19	1.34	1.37
18	D3	527	A	N7-C5	-5.19	1.36	1.39
22	DH	64	VAL	CB-CG1	-5.19	1.42	1.52
7	CL	789	VAL	CB-CG1	-5.19	1.42	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	87	C	N3-C4	-5.19	1.30	1.33
18	D3	316	A	C5-C4	-5.19	1.35	1.38
18	D3	376	C	C2-N3	-5.19	1.31	1.35
18	D3	530	C	C4-C5	-5.19	1.38	1.43
18	D3	423	G	C6-N1	-5.18	1.35	1.39
18	D3	441	A	N9-C4	-5.18	1.34	1.37
18	D3	511	A	N9-C4	-5.18	1.34	1.37
18	D3	943	C	N1-C2	-5.18	1.34	1.40
18	D3	1100	G	C6-N1	-5.18	1.35	1.39
18	D3	317	C	C4-C5	-5.18	1.38	1.43
18	D3	360	A	N9-C8	-5.18	1.33	1.37
18	D3	1793	G	N9-C4	-5.18	1.33	1.38
18	D3	40	A	N7-C5	-5.18	1.36	1.39
18	D3	245	U	N1-C2	-5.18	1.33	1.38
18	D3	789	A	N3-C4	-5.18	1.31	1.34
18	D3	1070	C	N1-C6	-5.18	1.34	1.37
18	D3	1095	U	N1-C6	-5.18	1.33	1.38
18	D3	1787	C	N3-C4	-5.18	1.30	1.33
19	DA	215	VAL	CB-CG1	-5.18	1.42	1.52
18	D3	592	A	N3-C4	-5.17	1.31	1.34
18	D3	868	G	N9-C8	-5.17	1.34	1.37
18	D3	1774	G	C8-N7	-5.17	1.27	1.30
18	D3	360	A	N3-C4	-5.17	1.31	1.34
18	D3	942	G	C5-C4	-5.17	1.34	1.38
18	D3	1027	A	N9-C8	-5.17	1.33	1.37
18	D3	973	A	N7-C5	-5.17	1.36	1.39
18	D3	312	A	N3-C4	-5.17	1.31	1.34
18	D3	389	G	C6-N1	-5.16	1.35	1.39
18	D3	1792	G	C5-C6	-5.16	1.37	1.42
18	D3	1044	U	N1-C2	-5.16	1.33	1.38
18	D3	424	C	C4-C5	-5.16	1.38	1.43
18	D3	461	G	N3-C4	-5.16	1.31	1.35
18	D3	879	G	C5-C4	-5.16	1.34	1.38
18	D3	463	U	N1-C2	-5.16	1.33	1.38
18	D3	531	C	C2-O2	-5.16	1.19	1.24
18	D3	929	A	N7-C5	-5.16	1.36	1.39
18	D3	1083	G	C5-C4	-5.16	1.34	1.38
18	D3	798	C	C4-C5	-5.16	1.38	1.43
18	D3	1078	C	N1-C6	-5.16	1.34	1.37
18	D3	595	G	C5-C4	-5.16	1.34	1.38
18	D3	156	A	N9-C4	-5.15	1.34	1.37
18	D3	613	G	C6-N1	-5.15	1.35	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	936	G	N7-C5	-5.15	1.36	1.39
18	D3	102	U	C4-O4	-5.15	1.19	1.23
18	D3	357	G	C5-C6	-5.15	1.37	1.42
18	D3	610	G	N9-C8	-5.15	1.34	1.37
18	D3	775	G	N7-C5	-5.15	1.36	1.39
31	DY	76	TYR	CD1-CE1	-5.15	1.31	1.39
18	D3	113	U	N1-C2	-5.15	1.33	1.38
18	D3	751	G	C5-C4	-5.15	1.34	1.38
18	D3	372	G	N7-C5	-5.15	1.36	1.39
18	D3	381	C	C5-C6	-5.14	1.30	1.34
18	D3	990	C	N1-C6	-5.14	1.34	1.37
7	CL	107	VAL	CB-CG2	-5.14	1.42	1.52
18	D3	96	G	N9-C8	-5.14	1.34	1.37
18	D3	634	G	C6-N1	-5.14	1.35	1.39
18	D3	953	G	N3-C4	-5.14	1.31	1.35
18	D3	304	U	C4-C5	-5.14	1.39	1.43
18	D3	451	A	N1-C2	-5.14	1.29	1.34
18	D3	459	G	N7-C5	-5.14	1.36	1.39
18	D3	1019	A	C5-C4	-5.14	1.35	1.38
18	D3	524	U	C2-N3	-5.14	1.34	1.37
18	D3	775	G	C5-C4	-5.14	1.34	1.38
7	CL	751	TYR	CE2-CZ	-5.13	1.31	1.38
18	D3	170	U	N1-C2	-5.13	1.33	1.38
18	D3	384	G	C8-N7	-5.13	1.27	1.30
18	D3	62	A	C5-C4	-5.13	1.35	1.38
18	D3	336	G	C8-N7	-5.13	1.27	1.30
18	D3	1787	C	C2-N3	-5.13	1.31	1.35
18	D3	41	A	N9-C4	-5.12	1.34	1.37
18	D3	967	A	N9-C4	-5.12	1.34	1.37
18	D3	1036	A	C5-C4	-5.12	1.35	1.38
18	D3	986	G	C5-C4	-5.12	1.34	1.38
18	D3	462	G	N3-C4	-5.12	1.31	1.35
26	DN	18	TYR	CD1-CE1	-5.12	1.31	1.39
18	D3	244	A	N3-C4	-5.12	1.31	1.34
18	D3	324	U	N1-C6	-5.12	1.33	1.38
18	D3	375	U	N1-C6	-5.12	1.33	1.38
18	D3	751	G	N9-C8	-5.12	1.34	1.37
18	D3	1035	G	C8-N7	-5.12	1.27	1.30
18	D3	85	A	N7-C5	-5.12	1.36	1.39
18	D3	111	U	N3-C4	-5.12	1.33	1.38
18	D3	621	A	N9-C8	-5.12	1.33	1.37
7	CL	61	ARG	C-N	-5.11	1.22	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	302	U	N3-C4	-5.11	1.33	1.38
18	D3	872	G	C8-N7	-5.11	1.27	1.30
18	D3	168	A	C5-C6	-5.11	1.36	1.41
18	D3	169	A	N9-C4	-5.11	1.34	1.37
18	D3	301	A	C6-N1	-5.11	1.31	1.35
18	D3	461	G	N1-C2	-5.11	1.33	1.37
18	D3	969	C	N3-C4	-5.11	1.30	1.33
18	D3	330	G	C6-N1	-5.11	1.35	1.39
18	D3	360	A	P-O5'	-5.11	1.54	1.59
18	D3	437	A	N3-C4	-5.11	1.31	1.34
18	D3	872	G	N7-C5	-5.11	1.36	1.39
18	D3	977	A	C6-N1	-5.11	1.31	1.35
18	D3	748	U	C2-N3	-5.10	1.34	1.37
18	D3	381	C	C2-N3	-5.10	1.31	1.35
18	D3	614	C	N3-C4	-5.10	1.30	1.33
18	D3	1104	U	C2-N3	-5.10	1.34	1.37
18	D3	529	A	N9-C4	-5.10	1.34	1.37
18	D3	48	G	N9-C8	-5.10	1.34	1.37
18	D3	357	G	N9-C4	-5.10	1.33	1.38
18	D3	401	A	N9-C8	-5.10	1.33	1.37
18	D3	450	U	C4-C5	-5.10	1.39	1.43
18	D3	1130	A	C5-C4	-5.10	1.35	1.38
25	DL	90	TYR	CD2-CE2	-5.09	1.31	1.39
18	D3	148	A	N9-C4	-5.09	1.34	1.37
18	D3	315	A	C6-N1	-5.09	1.31	1.35
18	D3	525	A	C5-C4	-5.09	1.35	1.38
18	D3	344	A	N9-C4	-5.09	1.34	1.37
18	D3	361	C	N1-C2	-5.09	1.35	1.40
18	D3	1031	U	N1-C6	-5.09	1.33	1.38
18	D3	1107	G	C5-C6	-5.09	1.37	1.42
18	D3	973	A	N3-C4	-5.09	1.31	1.34
18	D3	119	A	N9-C4	-5.09	1.34	1.37
18	D3	123	G	C8-N7	-5.09	1.27	1.30
18	D3	244	A	N9-C4	-5.09	1.34	1.37
18	D3	148	A	C6-N1	-5.08	1.31	1.35
18	D3	30	G	C6-N1	-5.08	1.35	1.39
18	D3	210	A	N7-C5	-5.08	1.36	1.39
18	D3	770	A	N3-C4	-5.08	1.31	1.34
18	D3	1102	G	C6-N1	-5.08	1.35	1.39
18	D3	1796	C	N1-C6	-5.08	1.34	1.37
18	D3	88	U	N1-C6	-5.08	1.33	1.38
18	D3	399	A	N3-C4	-5.08	1.31	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	328	A	N9-C8	-5.08	1.33	1.37
18	D3	766	U	C4-C5	-5.08	1.39	1.43
18	D3	347	G	C5-C4	-5.07	1.34	1.38
18	D3	78	A	N3-C4	-5.07	1.31	1.34
30	DX	53	VAL	CB-CG2	-5.07	1.42	1.52
18	D3	944	A	N3-C4	-5.07	1.31	1.34
18	D3	1026	A	C6-N1	-5.07	1.32	1.35
20	DE	139	VAL	CB-CG1	-5.07	1.42	1.52
18	D3	360	A	N9-C4	-5.07	1.34	1.37
18	D3	518	A	N3-C4	-5.07	1.31	1.34
18	D3	544	A	N9-C4	-5.07	1.34	1.37
18	D3	513	U	C4-C5	-5.06	1.39	1.43
18	D3	33	U	C2-N3	-5.06	1.34	1.37
18	D3	303	U	N3-C4	-5.06	1.33	1.38
18	D3	758	U	C2-N3	-5.06	1.34	1.37
18	D3	962	C	N3-C4	-5.06	1.30	1.33
18	D3	445	A	N7-C5	-5.06	1.36	1.39
18	D3	110	U	N3-C4	-5.06	1.33	1.38
31	DY	76	TYR	CD2-CE2	-5.06	1.31	1.39
18	D3	119	A	C6-N1	-5.06	1.32	1.35
18	D3	162	A	N7-C5	-5.06	1.36	1.39
29	DW	72	CYS	CB-SG	-5.06	1.73	1.81
18	D3	162	A	N3-C4	-5.06	1.31	1.34
18	D3	98	U	C2-N3	-5.05	1.34	1.37
18	D3	474	A	C6-N1	-5.05	1.32	1.35
18	D3	446	A	C5-C6	-5.05	1.36	1.41
18	D3	875	G	N9-C8	-5.05	1.34	1.37
18	D3	924	A	C5-C4	-5.05	1.35	1.38
18	D3	83	G	C5-C4	-5.05	1.34	1.38
18	D3	884	A	N7-C5	-5.05	1.36	1.39
18	D3	1120	U	N1-C2	-5.05	1.34	1.38
18	D3	770	A	N9-C8	-5.05	1.33	1.37
18	D3	806	A	N3-C4	-5.05	1.31	1.34
18	D3	976	G	N7-C5	-5.05	1.36	1.39
18	D3	1772	C	N1-C6	-5.05	1.34	1.37
18	D3	1048	G	N9-C8	-5.04	1.34	1.37
18	D3	1066	C	N1-C6	-5.04	1.34	1.37
18	D3	322	G	N1-C2	-5.04	1.33	1.37
18	D3	1023	A	N7-C5	-5.04	1.36	1.39
18	D3	304	U	N1-C6	-5.04	1.33	1.38
18	D3	142	G	N9-C4	-5.04	1.33	1.38
18	D3	348	U	N1-C6	-5.04	1.33	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D3	937	C	C2-N3	-5.04	1.31	1.35
18	D3	639	U	C2-N3	-5.04	1.34	1.37
18	D3	971	A	C5-C4	-5.04	1.35	1.38
18	D3	1071	U	N1-C2	-5.04	1.34	1.38
18	D3	451	A	C2-N3	-5.04	1.29	1.33
18	D3	442	C	C5-C6	-5.03	1.30	1.34
18	D3	467	G	N1-C2	-5.03	1.33	1.37
18	D3	425	A	N9-C4	-5.03	1.34	1.37
30	DX	29	TYR	CD1-CE1	-5.03	1.31	1.39
18	D3	63	G	N9-C8	-5.03	1.34	1.37
18	D3	339	C	C2-N3	-5.03	1.31	1.35
18	D3	624	G	N9-C8	-5.03	1.34	1.37
18	D3	38	C	N1-C6	-5.03	1.34	1.37
18	D3	170	U	N1-C6	-5.03	1.33	1.38
18	D3	48	G	C6-N1	-5.02	1.36	1.39
18	D3	796	A	C6-N1	-5.02	1.32	1.35
18	D3	44	U	N1-C2	-5.02	1.34	1.38
18	D3	986	G	N9-C8	-5.02	1.34	1.37
24	DJ	8	TYR	CE2-CZ	-5.02	1.32	1.38
18	D3	403	G	N9-C8	-5.02	1.34	1.37
26	DN	128	TYR	CD2-CE2	-5.02	1.31	1.39
18	D3	746	A	N3-C4	-5.02	1.31	1.34
7	CL	751	TYR	CD2-CE2	-5.02	1.31	1.39
18	D3	49	C	N3-C4	-5.02	1.30	1.33
18	D3	523	G	N3-C4	-5.02	1.31	1.35
18	D3	1025	A	C8-N7	-5.02	1.28	1.31
18	D3	359	A	C5-C6	-5.01	1.36	1.41
18	D3	527	A	N9-C4	-5.01	1.34	1.37
4	UX	89	CYS	CB-SG	-5.01	1.73	1.81
18	D3	167	U	C2-N3	-5.01	1.34	1.37
18	D3	357	G	N3-C4	-5.01	1.31	1.35
18	D3	1093	A	C6-N1	-5.01	1.32	1.35
18	D3	1011	G	N1-C2	-5.00	1.33	1.37
18	D3	1065	A	N7-C5	-5.00	1.36	1.39
18	D3	969	C	C4-C5	-5.00	1.39	1.43

All (678) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D3	44	U	N3-C4-O4	-13.16	110.19	119.40
18	D3	453	U	N1-C2-O2	12.13	131.29	122.80
18	D3	507	U	N3-C2-O2	-11.72	113.99	122.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D3	44	U	C5-C4-O4	11.71	132.93	125.90
18	D3	453	U	C2-N1-C1'	11.62	131.64	117.70
18	D3	314	C	C2-N1-C1'	-11.38	106.28	118.80
18	D3	190	C	N3-C2-O2	-11.31	113.98	121.90
18	D3	638	U	N3-C2-O2	-11.28	114.31	122.20
18	D3	45	U	N3-C2-O2	-11.22	114.35	122.20
18	D3	992	A	C8-N9-C4	-10.94	101.42	105.80
18	D3	1129	U	C2-N1-C1'	10.93	130.82	117.70
18	D3	435	C	N3-C2-O2	-10.91	114.27	121.90
18	D3	453	U	N3-C2-O2	-10.77	114.66	122.20
18	D3	1129	U	N3-C2-O2	-10.68	114.73	122.20
18	D3	191	C	O4'-C1'-N1	10.50	116.60	108.20
18	D3	314	C	C6-N1-C1'	10.41	133.29	120.80
18	D3	191	C	C2-N1-C1'	-10.40	107.36	118.80
7	CL	223	LEU	CB-CG-CD2	-10.23	93.60	111.00
18	D3	107	C	C5-C6-N1	10.18	126.09	121.00
18	D3	1128	C	N1-C2-O2	10.16	125.00	118.90
18	D3	638	U	N1-C2-O2	10.05	129.83	122.80
18	D3	320	U	N1-C2-O2	9.96	129.78	122.80
18	D3	1129	U	N1-C2-O2	9.92	129.75	122.80
18	D3	320	U	C2-N1-C1'	9.64	129.27	117.70
18	D3	1068	C	N3-C2-O2	-9.64	115.15	121.90
18	D3	739	G	N9-C4-C5	9.61	109.25	105.40
18	D3	739	G	N3-C4-N9	-9.36	120.38	126.00
30	DX	9	LEU	CA-CB-CG	9.31	136.72	115.30
18	D3	1501	C	N3-C2-O2	-9.30	115.39	121.90
18	D3	864	U	N3-C2-O2	-9.25	115.72	122.20
18	D3	1086	A	N3-C4-N9	9.25	134.80	127.40
18	D3	1653	C	N3-C2-O2	-9.23	115.44	121.90
18	D3	676	G	N3-C4-N9	-9.14	120.52	126.00
18	D3	959	U	N3-C2-O2	-9.08	115.84	122.20
18	D3	507	U	C2-N1-C1'	9.06	128.57	117.70
18	D3	638	U	C2-N1-C1'	8.97	128.46	117.70
18	D3	632	U	C5-C6-N1	8.93	127.17	122.70
18	D3	539	G	N9-C4-C5	-8.85	101.86	105.40
18	D3	1103	U	N3-C4-O4	-8.83	113.22	119.40
18	D3	334	G	N1-C6-O6	-8.78	114.63	119.90
18	D3	435	C	C2-N1-C1'	8.77	128.45	118.80
18	D3	435	C	N1-C2-O2	8.77	124.16	118.90
18	D3	276	C	O4'-C1'-N1	8.74	115.19	108.20
18	D3	385	A	N1-C6-N6	-8.70	113.38	118.60
18	D3	191	C	C6-N1-C1'	8.65	131.19	120.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D3	878	G	C8-N9-C4	-8.64	102.94	106.40
18	D3	336	G	C4-C5-N7	8.62	114.25	110.80
18	D3	1509	C	N3-C2-O2	-8.62	115.86	121.90
18	D3	453	U	C6-N1-C1'	-8.47	109.33	121.20
18	D3	990	C	C5-C6-N1	8.47	125.23	121.00
7	CL	141	LEU	CA-CB-CG	8.37	134.54	115.30
18	D3	320	U	N3-C2-O2	-8.35	116.36	122.20
18	D3	1000	C	N1-C2-O2	8.32	123.89	118.90
18	D3	1636	C	N1-C2-O2	8.31	123.88	118.90
18	D3	377	G	N3-C4-N9	8.24	130.95	126.00
18	D3	992	A	N7-C8-N9	8.24	117.92	113.80
18	D3	1530	C	N3-C2-O2	-8.24	116.13	121.90
18	D3	507	U	N1-C2-O2	8.21	128.55	122.80
18	D3	190	C	N1-C2-O2	8.17	123.80	118.90
18	D3	676	G	C8-N9-C1'	8.16	137.61	127.00
18	D3	739	G	C8-N9-C4	-8.12	103.15	106.40
18	D3	1096	C	N3-C2-O2	-8.11	116.22	121.90
18	D3	1096	C	N1-C2-O2	8.08	123.75	118.90
18	D3	1086	A	C6-N1-C2	-8.08	113.75	118.60
18	D3	311	U	O5'-P-OP1	-8.07	98.44	105.70
18	D3	482	U	C2-N1-C1'	8.07	127.38	117.70
18	D3	61	A	C5-N7-C8	-8.05	99.88	103.90
18	D3	276	C	N3-C2-O2	-8.04	116.27	121.90
18	D3	1024	U	N3-C2-O2	-8.02	116.59	122.20
18	D3	676	G	C6-C5-N7	8.00	135.20	130.40
18	D3	136	C	N1-C2-O2	7.92	123.65	118.90
18	D3	1773	C	C6-N1-C2	-7.92	117.13	120.30
18	D3	683	C	N3-C2-O2	-7.89	116.38	121.90
18	D3	1128	C	C6-N1-C2	-7.88	117.15	120.30
18	D3	909	U	N3-C2-O2	-7.87	116.69	122.20
18	D3	1128	C	N3-C2-O2	-7.87	116.39	121.90
18	D3	65	A	C2-N3-C4	-7.86	106.67	110.60
18	D3	1128	C	C2-N1-C1'	7.85	127.44	118.80
18	D3	955	A	O5'-P-OP1	-7.84	98.65	105.70
18	D3	676	G	N1-C6-O6	-7.81	115.21	119.90
18	D3	1086	A	N3-C4-C5	-7.81	121.33	126.80
18	D3	956	C	N1-C2-O2	7.79	123.57	118.90
18	D3	676	G	C5-C6-O6	7.78	133.27	128.60
24	DJ	108	ARG	NE-CZ-NH1	-7.78	116.41	120.30
18	D3	676	G	C4-N9-C1'	-7.78	116.39	126.50
18	D3	507	U	C5-C4-O4	7.77	130.56	125.90
18	D3	739	G	C5-C6-O6	7.75	133.25	128.60

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D3	1636	C	N3-C2-O2	-7.74	116.48	121.90
18	D3	230	C	C5-C6-N1	7.73	124.87	121.00
18	D3	184	C	C5-C6-N1	7.72	124.86	121.00
18	D3	1082	C	N1-C2-O2	7.70	123.52	118.90
18	D3	695	U	N1-C2-N3	7.70	119.52	114.90
23	DI	6	ASP	CB-CG-OD2	7.68	125.21	118.30
18	D3	45	U	N1-C2-N3	7.63	119.48	114.90
18	D3	739	G	C8-N9-C1'	7.63	136.92	127.00
18	D3	246	G	C4-C5-N7	7.62	113.85	110.80
18	D3	992	A	N1-C2-N3	7.61	133.10	129.30
18	D3	1128	C	C5-C6-N1	7.60	124.80	121.00
18	D3	831	U	N3-C2-O2	-7.57	116.90	122.20
18	D3	969	C	C6-N1-C2	-7.55	117.28	120.30
18	D3	676	G	N9-C4-C5	7.55	108.42	105.40
18	D3	1180	C	C6-N1-C2	-7.54	117.28	120.30
18	D3	539	G	C4-C5-N7	7.54	113.82	110.80
18	D3	1086	A	C5-C6-N1	7.54	121.47	117.70
18	D3	479	C	N3-C2-O2	-7.53	116.63	121.90
18	D3	360	A	O5'-P-OP2	-7.52	98.93	105.70
18	D3	1560	U	N1-C2-O2	7.51	128.06	122.80
18	D3	618	U	C2-N3-C4	-7.48	122.51	127.00
18	D3	144	U	C2-N1-C1'	7.46	126.65	117.70
18	D3	469	C	N1-C2-O2	7.42	123.35	118.90
18	D3	267	U	N3-C2-O2	-7.40	117.02	122.20
18	D3	625	C	C5-C6-N1	7.40	124.70	121.00
18	D3	587	C	C5-C6-N1	7.37	124.68	121.00
18	D3	747	C	C5-C6-N1	7.34	124.67	121.00
18	D3	23	G	N9-C4-C5	-7.34	102.46	105.40
18	D3	700	C	C6-N1-C2	-7.34	117.36	120.30
18	D3	739	G	N1-C6-O6	-7.34	115.50	119.90
18	D3	531	C	C6-N1-C2	-7.32	117.37	120.30
18	D3	144	U	C6-N1-C1'	-7.29	111.00	121.20
18	D3	1060	U	N1-C2-O2	7.26	127.88	122.80
18	D3	1568	C	OP2-P-O3'	7.26	121.18	105.20
18	D3	874	C	C6-N1-C2	-7.25	117.40	120.30
18	D3	336	G	C5-N7-C8	-7.25	100.67	104.30
18	D3	1509	C	N1-C2-O2	7.25	123.25	118.90
18	D3	831	U	C6-N1-C2	-7.24	116.66	121.00
18	D3	610	G	C4-N9-C1'	7.19	135.85	126.50
18	D3	286	C	C6-N1-C2	-7.18	117.43	120.30
18	D3	861	U	C2-N1-C1'	7.16	126.29	117.70
18	D3	107	C	C6-N1-C2	-7.16	117.44	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D3	1026	A	N1-C6-N6	-7.16	114.31	118.60
18	D3	992	A	C5-N7-C8	-7.16	100.32	103.90
18	D3	652	G	C5-C6-O6	7.15	132.89	128.60
18	D3	46	A	N1-C6-N6	-7.14	114.31	118.60
18	D3	465	G	C4-C5-N7	7.13	113.65	110.80
18	D3	1461	C	N1-C2-O2	7.12	123.17	118.90
18	D3	831	U	C5-C6-N1	7.12	126.26	122.70
18	D3	767	U	C2-N1-C1'	7.12	126.24	117.70
18	D3	114	C	N3-C4-C5	7.11	124.75	121.90
18	D3	1021	C	C6-N1-C2	-7.10	117.46	120.30
18	D3	334	G	C5-C6-N1	7.08	115.04	111.50
18	D3	45	U	C6-N1-C2	-7.08	116.75	121.00
18	D3	226	A	N9-C4-C5	7.07	108.63	105.80
18	D3	1483	A	N1-C6-N6	-7.07	114.36	118.60
18	D3	874	C	C5-C6-N1	7.07	124.53	121.00
7	CL	1021	LEU	CA-CB-CG	7.07	131.56	115.30
18	D3	115	G	O5'-P-OP2	-7.07	99.34	105.70
18	D3	482	U	C5-C6-N1	7.07	126.23	122.70
18	D3	54	C	C6-N1-C2	-7.07	117.47	120.30
18	D3	990	C	C4-C5-C6	-7.04	113.88	117.40
18	D3	57	G	O5'-P-OP2	-7.04	99.36	105.70
18	D3	1060	U	C2-N1-C1'	7.02	126.12	117.70
18	D3	1082	C	N3-C2-O2	-7.01	116.99	121.90
18	D3	377	G	C5-C6-O6	-7.01	124.39	128.60
18	D3	747	C	C6-N1-C2	-7.00	117.50	120.30
18	D3	45	U	C2-N1-C1'	6.98	126.08	117.70
24	DJ	118	LEU	CA-CB-CG	6.98	131.36	115.30
2	UC	544	ILE	CG1-CB-CG2	-6.98	96.05	111.40
18	D3	236	A	N9-C4-C5	-6.98	103.01	105.80
18	D3	738	G	O4'-C1'-N9	6.97	113.78	108.20
18	D3	1501	C	C6-N1-C2	-6.97	117.51	120.30
18	D3	1560	U	C2-N1-C1'	6.96	126.05	117.70
18	D3	1461	C	N3-C2-O2	-6.94	117.04	121.90
18	D3	61	A	C4-C5-N7	6.93	114.17	110.70
18	D3	700	C	N3-C2-O2	-6.93	117.05	121.90
18	D3	468	A	C5-C6-N6	-6.93	118.16	123.70
18	D3	837	G	N3-C4-N9	6.91	130.15	126.00
19	DA	70	LEU	CA-CB-CG	6.89	131.16	115.30
18	D3	935	U	N1-C2-O2	6.88	127.62	122.80
18	D3	1105	C	C5-C6-N1	6.88	124.44	121.00
18	D3	767	U	N3-C2-O2	-6.86	117.40	122.20
18	D3	1068	C	N1-C2-N3	6.86	124.00	119.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D3	1086	A	C4-N9-C1'	6.85	138.64	126.30
18	D3	1024	U	N1-C2-O2	6.85	127.59	122.80
18	D3	61	A	N7-C8-N9	6.84	117.22	113.80
18	D3	13	C	C5-C6-N1	6.83	124.42	121.00
18	D3	1129	U	C6-N1-C1'	-6.83	111.64	121.20
18	D3	795	U	N3-C2-O2	-6.82	117.42	122.20
19	DA	207	LEU	CB-CG-CD1	-6.82	99.42	111.00
18	D3	1068	C	C6-N1-C1'	6.81	128.97	120.80
18	D3	848	C	N3-C2-O2	-6.79	117.15	121.90
18	D3	337	G	C5-C6-N1	6.79	114.89	111.50
18	D3	381	C	C6-N1-C2	-6.79	117.58	120.30
18	D3	638	U	C6-N1-C1'	-6.79	111.70	121.20
18	D3	377	G	C6-C5-N7	-6.78	126.33	130.40
18	D3	1086	A	C8-N9-C1'	-6.77	115.51	127.70
18	D3	539	G	N1-C6-O6	6.76	123.96	119.90
33	UN	430	ASP	CB-CG-OD1	6.76	124.38	118.30
7	CL	141	LEU	CB-CG-CD2	-6.75	99.52	111.00
18	D3	224	C	N3-C2-O2	-6.74	117.18	121.90
12	JJ	130	MET	CG-SD-CE	-6.73	89.44	100.20
18	D3	207	U	N3-C2-O2	-6.72	117.49	122.20
18	D3	909	U	C2-N1-C1'	6.72	125.77	117.70
18	D3	23	G	C6-C5-N7	-6.72	126.37	130.40
18	D3	102	U	O5'-P-OP1	-6.71	99.67	105.70
18	D3	1573	A	OP2-P-O3'	6.69	119.93	105.20
18	D3	54	C	C5-C6-N1	6.69	124.35	121.00
18	D3	648	G	C4-N9-C1'	6.69	135.20	126.50
18	D3	190	C	C6-N1-C2	-6.69	117.62	120.30
18	D3	458	G	N1-C6-O6	-6.68	115.89	119.90
18	D3	226	A	O4'-C1'-N9	6.67	113.54	108.20
18	D3	1080	U	C5-C6-N1	6.67	126.04	122.70
18	D3	503	G	C2'-C3'-O3'	6.67	124.36	113.70
18	D3	849	C	C6-N1-C1'	6.66	128.79	120.80
18	D3	829	A	P-O3'-C3'	6.66	127.69	119.70
18	D3	909	U	N1-C2-O2	6.65	127.46	122.80
18	D3	23	G	C4-C5-N7	6.65	113.46	110.80
18	D3	103	A	P-O3'-C3'	6.65	127.68	119.70
18	D3	587	C	C2-N1-C1'	6.63	126.09	118.80
18	D3	1021	C	C2-N1-C1'	6.63	126.09	118.80
18	D3	320	U	C6-N1-C1'	-6.62	111.92	121.20
18	D3	584	C	O5'-P-OP1	6.62	118.65	110.70
18	D3	1027	A	C5-C6-N1	6.62	121.01	117.70
18	D3	226	A	N3-C4-N9	-6.61	122.11	127.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D3	864	U	C2-N1-C1'	6.60	125.62	117.70
18	D3	359	A	N3-C4-C5	6.60	131.42	126.80
18	D3	465	G	N9-C4-C5	-6.59	102.76	105.40
18	D3	893	U	N3-C2-O2	-6.59	117.59	122.20
18	D3	396	G	C6-N1-C2	-6.58	121.16	125.10
18	D3	498	G	P-O3'-C3'	6.56	127.57	119.70
18	D3	382	C	N3-C4-C5	6.56	124.52	121.90
18	D3	442	C	C5-C6-N1	6.55	124.28	121.00
7	CL	168	LEU	CB-CG-CD1	-6.54	99.89	111.00
18	D3	648	G	C8-N9-C1'	-6.54	118.50	127.00
18	D3	1068	C	C6-N1-C2	-6.52	117.69	120.30
18	D3	935	U	C2-N1-C1'	6.51	125.51	117.70
18	D3	992	A	N9-C4-C5	6.51	108.40	105.80
18	D3	1470	C	N3-C2-O2	-6.51	117.34	121.90
18	D3	878	G	N7-C8-N9	6.51	116.36	113.10
18	D3	579	A	P-O3'-C3'	6.50	127.50	119.70
18	D3	1000	C	N3-C2-O2	-6.50	117.35	121.90
18	D3	236	A	N3-C4-N9	6.49	132.59	127.40
18	D3	751	G	N1-C6-O6	-6.49	116.00	119.90
18	D3	433	C	C6-N1-C2	-6.48	117.71	120.30
18	D3	613	G	N3-C4-N9	6.48	129.89	126.00
18	D3	589	C	N1-C2-O2	6.47	122.78	118.90
18	D3	935	U	N3-C2-O2	-6.47	117.67	122.20
18	D3	959	U	C6-N1-C2	-6.47	117.12	121.00
18	D3	1017	U	C5-C6-N1	6.47	125.93	122.70
18	D3	778	G	C4-C5-N7	6.43	113.37	110.80
18	D3	144	U	C5-C4-O4	-6.42	122.05	125.90
18	D3	739	G	N3-C2-N2	-6.42	115.40	119.90
18	D3	902	G	C6-C5-N7	-6.42	126.55	130.40
18	D3	873	U	N3-C2-O2	-6.42	117.70	122.20
18	D3	218	A	P-O3'-C3'	6.42	127.41	119.70
18	D3	824	G	C5-C6-O6	6.42	132.45	128.60
18	D3	99	C	C6-N1-C2	-6.42	117.73	120.30
18	D3	794	U	N1-C2-O2	6.40	127.28	122.80
18	D3	795	U	C6-N1-C2	-6.39	117.17	121.00
18	D3	632	U	C6-N1-C2	-6.38	117.17	121.00
18	D3	426	G	C4-C5-N7	6.38	113.35	110.80
18	D3	837	G	C8-N9-C1'	-6.38	118.71	127.00
18	D3	13	C	C2-N1-C1'	6.37	125.81	118.80
18	D3	1012	U	C5-C4-O4	-6.37	122.08	125.90
18	D3	1560	U	N3-C2-O2	-6.34	117.76	122.20
18	D3	954	G	C6-N1-C2	-6.34	121.30	125.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D3	116	U	C6-N1-C2	-6.34	117.20	121.00
18	D3	93	A	N1-C6-N6	-6.33	114.80	118.60
18	D3	1573	A	P-O3'-C3'	6.32	127.29	119.70
18	D3	961	U	C6-N1-C2	-6.31	117.22	121.00
18	D3	1786	G	C5-C6-N1	6.30	114.65	111.50
18	D3	625	C	C6-N1-C2	-6.30	117.78	120.30
18	D3	498	G	OP1-P-O3'	6.30	119.06	105.20
18	D3	132	U	P-O3'-C3'	6.30	127.26	119.70
18	D3	295	A	C5-C6-N1	6.30	120.85	117.70
18	D3	426	G	C6-C5-N7	-6.29	126.62	130.40
18	D3	230	C	C6-N1-C2	-6.29	117.78	120.30
18	D3	23	G	N1-C6-O6	6.29	123.67	119.90
18	D3	1072	C	C5-C6-N1	6.28	124.14	121.00
18	D3	610	G	C8-N9-C1'	-6.26	118.86	127.00
18	D3	286	C	C5-C6-N1	6.26	124.13	121.00
18	D3	377	G	C4-C5-N7	6.26	113.30	110.80
18	D3	1748	G	N1-C6-O6	-6.26	116.15	119.90
18	D3	268	C	C6-N1-C2	-6.24	117.80	120.30
18	D3	824	G	N1-C6-O6	-6.22	116.17	119.90
18	D3	758	U	N3-C2-O2	-6.22	117.85	122.20
18	D3	1563	C	N1-C2-O2	6.22	122.63	118.90
18	D3	795	U	C2-N1-C1'	6.21	125.16	117.70
18	D3	625	C	C4-C5-C6	-6.21	114.30	117.40
18	D3	351	C	O5'-P-OP2	-6.19	100.13	105.70
18	D3	652	G	N1-C6-O6	-6.19	116.19	119.90
4	UX	152	ILE	CG1-CB-CG2	-6.18	97.80	111.40
18	D3	1773	C	N3-C4-C5	-6.18	119.43	121.90
1	UB	400	PRO	N-CA-CB	6.17	110.70	103.30
18	D3	676	G	C4-C5-N7	-6.16	108.34	110.80
18	D3	873	U	N1-C2-O2	6.15	127.11	122.80
18	D3	830	U	O4'-C1'-N1	6.15	113.12	108.20
18	D3	584	C	C6-N1-C2	-6.15	117.84	120.30
18	D3	1052	U	C5-C6-N1	6.14	125.77	122.70
18	D3	647	G	N3-C2-N2	-6.13	115.61	119.90
3	US	75	PRO	N-CA-CB	6.12	110.65	103.30
18	D3	831	U	N1-C2-O2	6.12	127.08	122.80
18	D3	236	A	C6-C5-N7	-6.12	128.02	132.30
18	D3	956	C	N3-C2-O2	-6.09	117.63	121.90
18	D3	976	G	N1-C6-O6	-6.09	116.24	119.90
18	D3	435	C	C6-N1-C1'	-6.09	113.49	120.80
18	D3	852	C	C2-N1-C1'	-6.09	112.11	118.80
18	D3	1800	A	P-O3'-C3'	6.09	127.00	119.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D3	693	U	C2-N1-C1'	6.08	125.00	117.70
18	D3	861	U	C6-N1-C1'	-6.08	112.69	121.20
18	D3	379	U	O5'-P-OP1	-6.07	100.23	105.70
18	D3	831	U	O4'-C1'-N1	6.07	113.06	108.20
18	D3	39	A	C5-N7-C8	-6.06	100.87	103.90
18	D3	648	G	C6-C5-N7	-6.06	126.76	130.40
18	D3	746	A	N9-C4-C5	6.06	108.22	105.80
18	D3	428	A	C5-C6-N1	6.05	120.73	117.70
18	D3	1086	A	C6-C5-N7	-6.05	128.06	132.30
18	D3	864	U	N1-C2-O2	6.05	127.03	122.80
3	US	37	PRO	N-CA-CB	6.04	110.55	103.30
18	D3	1527	C	N1-C2-O2	6.04	122.53	118.90
18	D3	23	G	C5-C6-O6	-6.04	124.98	128.60
18	D3	783	G	O4'-C1'-N9	6.04	113.03	108.20
18	D3	650	U	C5-C6-N1	6.02	125.71	122.70
18	D3	113	U	C2-N3-C4	-6.02	123.39	127.00
18	D3	402	C	O4'-C1'-N1	6.01	113.01	108.20
18	D3	517	U	C2-N1-C1'	-6.01	110.49	117.70
18	D3	1653	C	N1-C2-O2	6.01	122.51	118.90
18	D3	1082	C	C2-N1-C1'	6.01	125.41	118.80
18	D3	468	A	N1-C6-N6	6.00	122.20	118.60
18	D3	613	G	C5-C6-O6	-6.00	125.00	128.60
18	D3	613	G	C4-C5-N7	6.00	113.20	110.80
18	D3	1103	U	C2-N1-C1'	-6.00	110.50	117.70
29	DW	28	ARG	C-N-CD	-6.00	107.41	120.60
18	D3	1086	A	C4-C5-C6	5.99	120.00	117.00
31	DY	57	VAL	CG1-CB-CG2	-5.99	101.31	110.90
8	CM	301	MET	CG-SD-CE	-5.99	90.62	100.20
18	D3	510	G	N1-C6-O6	-5.99	116.31	119.90
18	D3	1591	C	N1-C2-O2	5.97	122.48	118.90
18	D3	166	C	N3-C2-O2	-5.97	117.72	121.90
18	D3	1748	G	C5-C6-O6	5.96	132.18	128.60
18	D3	479	C	N1-C2-O2	5.95	122.47	118.90
18	D3	442	C	C6-N1-C2	-5.95	117.92	120.30
29	DW	104	LEU	CA-CB-CG	5.95	128.97	115.30
18	D3	353	A	N1-C6-N6	-5.94	115.03	118.60
18	D3	794	U	OP1-P-OP2	-5.94	110.69	119.60
18	D3	1083	G	N9-C4-C5	-5.94	103.02	105.40
18	D3	482	U	N1-C2-O2	5.94	126.96	122.80
18	D3	39	A	C4-C5-N7	5.94	113.67	110.70
21	DG	31	ARG	NE-CZ-NH1	5.94	123.27	120.30
18	D3	641	G	C5-C6-O6	5.93	132.16	128.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D3	136	C	C2-N1-C1'	5.92	125.31	118.80
18	D3	835	U	C2-N1-C1'	-5.92	110.59	117.70
18	D3	1800	A	C2-N3-C4	5.92	113.56	110.60
18	D3	139	C	P-O3'-C3'	5.92	126.80	119.70
18	D3	377	G	N3-C4-C5	-5.92	125.64	128.60
18	D3	587	C	N1-C2-O2	5.91	122.45	118.90
18	D3	837	G	C4-N9-C1'	5.91	134.18	126.50
18	D3	610	G	O4'-C1'-N9	5.90	112.92	108.20
18	D3	275	C	N1-C2-O2	5.90	122.44	118.90
18	D3	380	U	C5-C6-N1	-5.89	119.75	122.70
18	D3	396	G	C5-C6-N1	5.89	114.44	111.50
18	D3	196	G	N1-C2-N2	-5.89	110.90	116.20
18	D3	1091	A	N1-C6-N6	-5.88	115.07	118.60
18	D3	136	C	N3-C2-O2	-5.88	117.78	121.90
18	D3	933	A	C4-C5-N7	5.88	113.64	110.70
18	D3	932	U	O5'-P-OP2	-5.88	100.41	105.70
18	D3	142	G	N3-C2-N2	-5.87	115.79	119.90
18	D3	28	A	N1-C6-N6	-5.87	115.08	118.60
18	D3	614	C	C5-C6-N1	5.87	123.93	121.00
18	D3	795	U	O4'-C1'-N1	5.87	112.89	108.20
18	D3	855	A	O4'-C1'-N9	5.87	112.89	108.20
18	D3	1023	A	O5'-P-OP1	-5.87	100.42	105.70
18	D3	274	G	N3-C4-N9	5.86	129.52	126.00
18	D3	226	A	C6-C5-N7	5.85	136.40	132.30
18	D3	849	C	N1-C2-O2	-5.85	115.39	118.90
18	D3	118	U	C5-C6-N1	5.85	125.62	122.70
18	D3	308	C	C2-N3-C4	-5.85	116.98	119.90
18	D3	378	A	C4-C5-N7	5.85	113.62	110.70
18	D3	505	A	N3-C4-N9	5.84	132.07	127.40
18	D3	992	A	N3-C4-N9	-5.84	122.73	127.40
23	DI	58	LEU	CA-CB-CG	5.84	128.72	115.30
18	D3	772	G	C4-C5-N7	5.83	113.13	110.80
18	D3	693	U	N3-C2-O2	-5.83	118.12	122.20
18	D3	184	C	C6-N1-C2	-5.83	117.97	120.30
18	D3	115	G	C4-C5-N7	5.83	113.13	110.80
7	CL	183	LEU	CB-CG-CD1	-5.83	101.09	111.00
18	D3	1086	A	C2-N3-C4	5.83	113.51	110.60
18	D3	798	C	C6-N1-C2	-5.82	117.97	120.30
18	D3	120	U	C2-N1-C1'	5.81	124.67	117.70
34	JD	1181	ILE	CG1-CB-CG2	-5.81	98.63	111.40
18	D3	236	A	C4-N9-C1'	5.80	136.75	126.30
30	DX	33	LEU	CB-CG-CD1	-5.80	101.13	111.00

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D3	1051	G	C2-N3-C4	-5.80	109.00	111.90
18	D3	539	G	C8-N9-C4	5.79	108.72	106.40
18	D3	621	A	N9-C4-C5	5.79	108.11	105.80
18	D3	842	C	C6-N1-C2	-5.78	117.99	120.30
18	D3	1129	U	C6-N1-C2	-5.78	117.53	121.00
18	D3	759	U	C6-N1-C2	-5.78	117.53	121.00
18	D3	695	U	C4-C5-C6	5.78	123.17	119.70
18	D3	236	A	C4-C5-N7	5.77	113.58	110.70
1	UB	412	PRO	N-CA-CB	5.77	110.22	103.30
18	D3	1082	C	C6-N1-C2	-5.76	118.00	120.30
18	D3	835	U	C6-N1-C1'	5.76	129.27	121.20
18	D3	687	G	N3-C2-N2	-5.76	115.87	119.90
18	D3	58	U	O5'-P-OP1	-5.75	100.53	105.70
18	D3	1591	C	C5-C6-N1	5.75	123.87	121.00
18	D3	609	U	C2-N3-C4	-5.74	123.56	127.00
18	D3	1530	C	C6-N1-C2	-5.74	118.00	120.30
18	D3	1507	G	C5-C6-O6	5.74	132.04	128.60
24	DJ	108	ARG	CB-CG-CD	5.73	126.50	111.60
18	D3	765	G	C5-C6-O6	-5.73	125.16	128.60
18	D3	52	U	C5-C6-N1	5.73	125.56	122.70
18	D3	184	C	C2-N1-C1'	5.72	125.09	118.80
18	D3	746	A	N1-C6-N6	-5.71	115.17	118.60
18	D3	388	G	C8-N9-C4	5.71	108.68	106.40
18	D3	772	G	N3-C4-N9	5.71	129.42	126.00
18	D3	1060	U	N3-C2-O2	-5.70	118.21	122.20
18	D3	99	C	O5'-P-OP1	-5.69	100.58	105.70
18	D3	695	U	C5-C4-O4	5.69	129.31	125.90
18	D3	1108	G	C8-N9-C1'	-5.67	119.62	127.00
18	D3	281	G	N1-C2-N2	-5.67	111.10	116.20
18	D3	115	G	C5-C6-O6	-5.67	125.20	128.60
18	D3	359	A	C4-C5-C6	-5.67	114.17	117.00
18	D3	196	G	N9-C1'-C2'	-5.66	105.77	112.00
18	D3	435	C	C6-N1-C2	-5.66	118.04	120.30
18	D3	926	A	N9-C4-C5	-5.66	103.54	105.80
7	CL	85	LEU	CA-CB-CG	-5.65	102.30	115.30
18	D3	849	C	C2-N1-C1'	-5.65	112.58	118.80
18	D3	123	G	N1-C6-O6	-5.64	116.51	119.90
34	JD	1186	LEU	CA-CB-CG	5.64	128.27	115.30
18	D3	425	A	O5'-P-OP2	-5.63	100.63	105.70
18	D3	1568	C	P-O3'-C3'	5.63	126.46	119.70
18	D3	676	G	O4'-C1'-N9	5.63	112.71	108.20
18	D3	759	U	C5-C6-N1	5.62	125.51	122.70

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	CL	847	LEU	CA-CB-CG	5.62	128.22	115.30
18	D3	65	A	N3-C4-C5	5.62	130.73	126.80
18	D3	23	G	N3-C4-N9	5.61	129.37	126.00
18	D3	95	G	O5'-P-OP1	-5.61	100.65	105.70
18	D3	426	G	C4-N9-C1'	5.61	133.80	126.50
18	D3	191	C	N3-C4-N4	-5.60	114.08	118.00
18	D3	739	G	C6-C5-N7	5.60	133.76	130.40
18	D3	236	A	C8-N9-C1'	-5.60	117.63	127.70
18	D3	758	U	N1-C2-O2	5.59	126.72	122.80
18	D3	428	A	N1-C6-N6	-5.59	115.25	118.60
7	CL	204	LEU	CA-CB-CG	5.58	128.15	115.30
18	D3	166	C	C6-N1-C2	-5.58	118.07	120.30
18	D3	1629	G	N3-C2-N2	5.58	123.81	119.90
18	D3	830	U	C2-N1-C1'	5.58	124.39	117.70
18	D3	90	C	C6-N1-C2	-5.57	118.07	120.30
18	D3	135	A	OP2-P-O3'	5.57	117.45	105.20
18	D3	1046	G	O5'-P-OP1	-5.57	100.69	105.70
18	D3	834	G	O4'-C1'-N9	5.56	112.65	108.20
18	D3	639	U	N3-C2-O2	-5.55	118.31	122.20
18	D3	149	C	C5-C6-N1	5.55	123.78	121.00
18	D3	976	G	C5-C6-N1	5.55	114.28	111.50
18	D3	264	G	C6-C5-N7	-5.54	127.07	130.40
18	D3	426	G	O5'-P-OP1	-5.54	100.71	105.70
18	D3	1792	G	N9-C4-C5	-5.54	103.18	105.40
18	D3	488	G	C8-N9-C4	-5.54	104.18	106.40
18	D3	1483	A	C5-C6-N6	5.54	128.13	123.70
18	D3	46	A	C5-C6-N6	5.54	128.13	123.70
18	D3	1090	C	C6-N1-C2	-5.54	118.09	120.30
18	D3	94	U	N3-C2-O2	-5.53	118.33	122.20
18	D3	622	A	N3-C4-N9	-5.53	122.98	127.40
18	D3	913	G	P-O3'-C3'	5.52	126.33	119.70
18	D3	834	G	N9-C1'-C2'	5.52	121.17	114.00
29	DW	28	ARG	C-N-CA	5.52	145.17	122.00
18	D3	1790	A	N9-C4-C5	5.52	108.01	105.80
1	UB	744	LEU	CA-CB-CG	5.50	127.96	115.30
18	D3	29	U	N3-C2-O2	-5.50	118.35	122.20
18	D3	338	C	C6-N1-C2	-5.50	118.10	120.30
18	D3	37	U	N3-C2-O2	-5.50	118.35	122.20
18	D3	927	C	N3-C2-O2	-5.50	118.05	121.90
18	D3	1072	C	C4-C5-C6	-5.50	114.65	117.40
30	DX	93	LEU	CB-CG-CD1	-5.50	101.65	111.00
18	D3	758	U	C5-C6-N1	5.50	125.45	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D3	207	U	C6-N1-C2	-5.49	117.70	121.00
18	D3	883	C	C6-N1-C2	-5.49	118.10	120.30
18	D3	469	C	N3-C2-O2	-5.49	118.06	121.90
18	D3	691	C	C2-N1-C1'	5.49	124.83	118.80
26	DN	11	ILE	CG1-CB-CG2	-5.49	99.33	111.40
18	D3	652	G	N1-C2-N2	-5.48	111.27	116.20
18	D3	772	G	O5'-P-OP1	-5.48	100.77	105.70
18	D3	885	G	N3-C4-C5	-5.48	125.86	128.60
18	D3	283	U	N1-C2-O2	5.47	126.63	122.80
18	D3	404	G	C5-C6-N1	5.47	114.24	111.50
18	D3	726	C	N3-C2-O2	-5.46	118.07	121.90
18	D3	144	U	C2-N3-C4	-5.46	123.72	127.00
18	D3	795	U	N1-C2-N3	5.46	118.18	114.90
18	D3	1036	A	C6-N1-C2	-5.46	115.33	118.60
18	D3	799	A	C4-C5-C6	-5.45	114.27	117.00
18	D3	631	G	N1-C2-N3	5.45	127.17	123.90
18	D3	269	G	N3-C4-N9	5.45	129.27	126.00
18	D3	489	C	N1-C2-N3	5.45	123.01	119.20
18	D3	226	A	C8-N9-C1'	5.45	137.50	127.70
18	D3	433	C	O4'-C1'-N1	5.45	112.56	108.20
18	D3	1103	U	C5-C4-O4	5.44	129.16	125.90
18	D3	109	G	N3-C4-C5	-5.43	125.88	128.60
18	D3	142	G	N1-C2-N2	5.43	121.09	116.20
18	D3	507	U	C6-N1-C1'	-5.43	113.60	121.20
18	D3	1055	U	N3-C2-O2	-5.43	118.40	122.20
18	D3	721	U	P-O3'-C3'	5.43	126.21	119.70
18	D3	1129	U	C5-C6-N1	5.43	125.41	122.70
23	DI	196	LEU	CA-CB-CG	5.43	127.78	115.30
18	D3	539	G	C6-C5-N7	-5.42	127.15	130.40
18	D3	49	C	N3-C4-C5	5.42	124.07	121.90
18	D3	783	G	C8-N9-C4	5.42	108.57	106.40
18	D3	809	A	N3-C4-N9	-5.42	123.07	127.40
18	D3	364	G	C5-C6-N1	5.41	114.21	111.50
18	D3	778	G	C6-C5-N7	-5.41	127.15	130.40
7	CL	190	LEU	CA-CB-CG	5.41	127.74	115.30
18	D3	1083	G	C4-C5-N7	5.41	112.96	110.80
18	D3	89	G	N1-C6-O6	-5.41	116.66	119.90
18	D3	746	A	C8-N9-C4	-5.40	103.64	105.80
18	D3	388	G	N9-C4-C5	-5.40	103.24	105.40
18	D3	687	G	C8-N9-C4	-5.40	104.24	106.40
18	D3	852	C	N1-C2-O2	-5.40	115.66	118.90
18	D3	410	A	N1-C6-N6	-5.40	115.36	118.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D3	196	G	C2-N3-C4	-5.40	109.20	111.90
18	D3	482	U	C6-N1-C2	-5.40	117.76	121.00
18	D3	1790	A	C8-N9-C4	-5.39	103.64	105.80
18	D3	1786	G	N1-C6-O6	-5.39	116.67	119.90
20	DE	222	LEU	CB-CG-CD1	-5.39	101.84	111.00
18	D3	589	C	C2-N1-C1'	5.38	124.72	118.80
18	D3	992	A	C2-N3-C4	-5.38	107.91	110.60
18	D3	1552	U	C2-N1-C1'	5.38	124.16	117.70
18	D3	505	A	N9-C4-C5	-5.37	103.65	105.80
18	D3	246	G	C5-N7-C8	-5.37	101.62	104.30
18	D3	320	U	C5-C6-N1	5.36	125.38	122.70
18	D3	359	A	C4-N9-C1'	-5.36	116.66	126.30
18	D3	398	G	N9-C4-C5	5.36	107.54	105.40
18	D3	1027	A	C5-C6-N6	-5.36	119.42	123.70
18	D3	447	U	C5-C4-O4	-5.36	122.69	125.90
18	D3	1055	U	N1-C2-O2	5.36	126.55	122.80
18	D3	751	G	N3-C4-C5	-5.35	125.92	128.60
18	D3	529	A	C5-N7-C8	-5.35	101.22	103.90
18	D3	628	G	N1-C2-N3	5.35	127.11	123.90
18	D3	103	A	C4-N9-C1'	5.35	135.93	126.30
18	D3	496	G	P-O3'-C3'	5.35	126.12	119.70
18	D3	90	C	C5-C6-N1	5.35	123.67	121.00
18	D3	61	A	C6-C5-N7	-5.34	128.56	132.30
18	D3	482	U	N3-C2-O2	-5.34	118.46	122.20
18	D3	1796	C	C6-N1-C2	-5.34	118.16	120.30
18	D3	959	U	C2-N1-C1'	5.33	124.10	117.70
18	D3	131	C	C6-N1-C2	-5.33	118.17	120.30
18	D3	1012	U	N3-C4-O4	5.33	123.13	119.40
32	Db	34	ASP	CB-CG-OD1	5.32	123.09	118.30
18	D3	631	G	C6-N1-C2	-5.32	121.91	125.10
22	DH	130	VAL	CG1-CB-CG2	-5.32	102.39	110.90
18	D3	31	C	C6-N1-C2	-5.31	118.18	120.30
18	D3	961	U	C5-C6-N1	5.31	125.35	122.70
18	D3	130	C	P-O3'-C3'	5.30	126.06	119.70
18	D3	507	U	C6-N1-C2	-5.29	117.82	121.00
18	D3	142	G	N3-C4-N9	-5.29	122.83	126.00
18	D3	622	A	N3-C4-C5	5.29	130.50	126.80
18	D3	715	U	N1-C2-O2	5.29	126.50	122.80
18	D3	464	A	N1-C6-N6	-5.28	115.43	118.60
18	D3	104	A	N9-C4-C5	-5.28	103.69	105.80
18	D3	589	C	N3-C2-O2	-5.28	118.20	121.90
18	D3	1748	G	N1-C2-N2	-5.28	111.45	116.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D3	772	G	N1-C2-N2	-5.28	111.45	116.20
18	D3	123	G	C5-C6-N1	5.27	114.14	111.50
18	D3	1040	G	N1-C6-O6	-5.27	116.74	119.90
18	D3	104	A	C8-N9-C4	5.27	107.91	105.80
18	D3	959	U	N1-C2-N3	5.27	118.06	114.90
18	D3	264	G	C4-N9-C1'	5.26	133.34	126.50
18	D3	996	U	C5-C6-N1	5.26	125.33	122.70
18	D3	114	C	OP1-P-O3'	5.26	116.77	105.20
18	D3	274	G	C8-N9-C1'	-5.26	120.16	127.00
7	CL	74	VAL	CG1-CB-CG2	-5.25	102.50	110.90
18	D3	116	U	N1-C2-N3	5.25	118.05	114.90
18	D3	418	G	N3-C2-N2	5.25	123.57	119.90
18	D3	95	G	C5-C6-N1	5.24	114.12	111.50
18	D3	926	A	C4-C5-N7	5.24	113.32	110.70
18	D3	767	U	C6-N1-C1'	-5.23	113.87	121.20
18	D3	274	G	C6-C5-N7	-5.23	127.26	130.40
18	D3	926	A	N1-C6-N6	5.23	121.74	118.60
18	D3	41	A	OP2-P-O3'	5.23	116.70	105.20
18	D3	852	C	C6-N1-C1'	5.22	127.06	120.80
18	D3	683	C	N1-C2-O2	5.22	122.03	118.90
18	D3	968	U	O5'-P-OP1	-5.22	101.00	105.70
18	D3	363	G	N1-C6-O6	-5.21	116.77	119.90
18	D3	1108	G	C4-N9-C1'	5.21	133.28	126.50
18	D3	1585	U	N1-C2-O2	5.21	126.45	122.80
18	D3	460	A	C5-C6-N1	5.20	120.30	117.70
7	CL	263	LEU	CA-CB-CG	5.20	127.26	115.30
18	D3	848	C	N1-C2-O2	5.20	122.02	118.90
18	D3	459	G	C8-N9-C4	-5.20	104.32	106.40
18	D3	747	C	C2-N1-C1'	5.19	124.51	118.80
4	UX	106	LEU	CA-CB-CG	5.19	127.24	115.30
18	D3	226	A	C4-N9-C1'	-5.19	116.95	126.30
18	D3	1115	U	C5-C6-N1	5.19	125.30	122.70
18	D3	1025	A	N9-C4-C5	-5.19	103.72	105.80
18	D3	611	U	C2-N1-C1'	5.19	123.92	117.70
18	D3	1096	C	N3-C4-N4	-5.18	114.37	118.00
18	D3	1629	G	N1-C2-N2	-5.18	111.54	116.20
18	D3	876	G	C8-N9-C1'	-5.18	120.27	127.00
18	D3	348	U	N1-C2-N3	5.18	118.01	114.90
18	D3	401	A	N1-C6-N6	-5.18	115.49	118.60
18	D3	45	U	O4'-C1'-N1	5.17	112.34	108.20
18	D3	868	G	N1-C6-O6	-5.17	116.80	119.90
29	DW	126	LEU	CB-CG-CD1	-5.17	102.21	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D3	229	U	C5-C4-O4	-5.17	122.80	125.90
18	D3	650	U	N1-C2-O2	5.17	126.42	122.80
18	D3	426	G	C8-N9-C1'	-5.17	120.28	127.00
18	D3	465	G	C6-C5-N7	-5.17	127.30	130.40
18	D3	449	C	C5-C6-N1	5.17	123.58	121.00
18	D3	756	A	O5'-P-OP1	-5.17	101.05	105.70
18	D3	72	A	C8-N9-C4	5.16	107.86	105.80
18	D3	136	C	O5'-P-OP2	-5.16	101.05	105.70
25	DL	99	ARG	NE-CZ-NH1	-5.16	117.72	120.30
18	D3	684	A	C4-C5-N7	5.16	113.28	110.70
18	D3	739	G	O4'-C1'-N9	5.16	112.33	108.20
18	D3	171	A	C6-N1-C2	-5.16	115.51	118.60
18	D3	338	C	O5'-P-OP2	-5.16	101.06	105.70
18	D3	641	G	N1-C6-O6	-5.16	116.81	119.90
18	D3	166	C	C2-N1-C1'	5.16	124.47	118.80
18	D3	264	G	C8-N9-C1'	-5.16	120.30	127.00
18	D3	902	G	C4-C5-N7	5.15	112.86	110.80
18	D3	888	U	C6-N1-C2	-5.15	117.91	121.00
18	D3	75	U	C5-C6-N1	5.14	125.27	122.70
18	D3	807	A	C6-N1-C2	-5.14	115.51	118.60
18	D3	364	G	C6-N1-C2	-5.14	122.02	125.10
18	D3	378	A	C5-N7-C8	-5.14	101.33	103.90
18	D3	610	G	N3-C4-C5	-5.14	126.03	128.60
18	D3	739	G	C4-N9-C1'	-5.14	119.82	126.50
18	D3	1081	A	C5-N7-C8	-5.14	101.33	103.90
18	D3	1600	A	P-O3'-C3'	5.14	125.86	119.70
18	D3	61	A	N1-C6-N6	5.13	121.68	118.60
18	D3	878	G	N9-C4-C5	5.13	107.45	105.40
18	D3	1527	C	N3-C2-O2	-5.13	118.31	121.90
18	D3	291	G	N1-C6-O6	-5.13	116.82	119.90
18	D3	79	C	C6-N1-C2	-5.12	118.25	120.30
18	D3	517	U	N3-C4-O4	-5.12	115.81	119.40
18	D3	613	G	C6-C5-N7	-5.12	127.33	130.40
18	D3	864	U	C6-N1-C2	-5.12	117.92	121.00
18	D3	386	G	N1-C6-O6	-5.12	116.83	119.90
18	D3	65	A	C5-N7-C8	-5.11	101.34	103.90
7	CL	118	LEU	CB-CG-CD2	-5.11	102.31	111.00
18	D3	1012	U	N1-C2-O2	5.11	126.38	122.80
18	D3	1772	C	C6-N1-C2	-5.11	118.26	120.30
18	D3	1060	U	C6-N1-C1'	-5.10	114.05	121.20
18	D3	658	C	C5-C4-N4	5.10	123.77	120.20
18	D3	968	U	C5-C4-O4	-5.10	122.84	125.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D3	89	G	C5-C6-N1	5.10	114.05	111.50
18	D3	595	G	N3-C4-N9	5.10	129.06	126.00
18	D3	1792	G	C8-N9-C4	5.09	108.44	106.40
18	D3	199	G	C3'-C2'-C1'	5.09	105.57	101.50
18	D3	604	A	C2-N3-C4	5.09	113.14	110.60
18	D3	618	U	N1-C2-N3	5.09	117.95	114.90
18	D3	41	A	P-O3'-C3'	5.09	125.80	119.70
18	D3	352	A	C5-C6-N1	5.08	120.24	117.70
18	D3	715	U	N3-C2-O2	-5.08	118.64	122.20
18	D3	726	C	C6-N1-C2	-5.08	118.27	120.30
18	D3	48	G	N3-C4-N9	5.08	129.05	126.00
18	D3	417	A	P-O3'-C3'	5.08	125.80	119.70
18	D3	496	G	C8-N9-C1'	5.08	133.60	127.00
18	D3	613	G	C8-N9-C1'	-5.08	120.40	127.00
18	D3	356	G	C8-N9-C1'	-5.08	120.40	127.00
18	D3	621	A	N3-C4-N9	-5.07	123.34	127.40
18	D3	933	A	C5-N7-C8	-5.07	101.37	103.90
26	DN	88	LEU	CB-CG-CD2	-5.07	102.39	111.00
18	D3	103	A	C6-N1-C2	-5.06	115.56	118.60
18	D3	430	G	C6-C5-N7	-5.06	127.36	130.40
18	D3	337	G	N3-C4-C5	-5.05	126.07	128.60
18	D3	107	C	C4-C5-C6	-5.05	114.88	117.40
18	D3	610	G	N3-C4-N9	5.05	129.03	126.00
18	D3	1535	U	P-O3'-C3'	5.05	125.76	119.70
18	D3	24	U	C2-N1-C1'	5.05	123.76	117.70
18	D3	171	A	C4-N9-C1'	5.05	135.38	126.30
18	D3	1585	U	C2-N1-C1'	5.05	123.76	117.70
18	D3	460	A	C6-N1-C2	-5.04	115.57	118.60
18	D3	378	A	C6-C5-N7	-5.04	128.77	132.30
18	D3	305	C	C5-C6-N1	5.04	123.52	121.00
26	DN	115	LEU	CB-CG-CD2	-5.04	102.43	111.00
18	D3	25	C	O4'-C1'-N1	5.04	112.23	108.20
18	D3	609	U	N3-C4-C5	5.03	117.62	114.60
18	D3	1470	C	N1-C2-O2	5.03	121.92	118.90
18	D3	1560	U	C6-N1-C1'	-5.03	114.16	121.20
18	D3	396	G	N1-C2-N3	5.03	126.92	123.90
18	D3	1103	U	N3-C4-C5	5.02	117.61	114.60
18	D3	1552	U	N1-C2-O2	5.02	126.31	122.80
18	D3	542	A	C5-N7-C8	-5.02	101.39	103.90
18	D3	610	G	C6-C5-N7	-5.02	127.39	130.40
18	D3	695	U	C6-N1-C2	-5.01	117.99	121.00
18	D3	517	U	N3-C2-O2	-5.01	118.69	122.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D3	1002	G	C4-N9-C1'	5.01	133.01	126.50
18	D3	377	G	N9-C4-C5	-5.01	103.40	105.40
18	D3	354	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	CL	51	GLU	Peptide
19	DA	147	ALA	Peptide
19	DA	151	LYS	Peptide
19	DA	69	CYS	Peptide
22	DH	133	THR	Peptide
22	DH	154	LEU	Peptide
22	DH	30	SER	Peptide
22	DH	31	SER	Peptide
23	DI	51	GLY	Peptide
24	DJ	137	GLY	Peptide
24	DJ	20	GLU	Peptide
25	DL	5	LEU	Peptide
26	DN	58	HIS	Peptide
27	DO	123	SER	Peptide
27	DO	52	ARG	Peptide
31	DY	122	GLY	Peptide
31	DY	17	LEU	Peptide
32	Db	3	LEU	Peptide
32	Db	4	VAL	Peptide
34	JD	1148	PRO	Peptide
34	JD	501	MET	Peptide
34	JD	588	PHE	Peptide
11	JL	233	ARG	Peptide
1	UB	784	ILE	Peptide
33	UN	402	SER	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	UB	2207	0	1231	22	0
2	UC	393	0	444	10	0
3	US	2411	0	1035	7	0
4	UX	1132	0	1186	16	0
5	CJ	1083	0	478	11	0
6	CK	645	0	541	18	0
7	CL	5758	0	5885	119	0
8	CM	2781	0	2878	49	0
9	JF	1071	0	467	5	0
9	JG	1096	0	478	4	0
10	JH	1295	0	570	0	0
11	JL	2262	0	2330	30	0
12	JJ	1436	0	1515	22	0
13	DF	970	0	462	2	0
14	DQ	616	0	285	3	0
15	DS	630	0	652	16	0
16	DT	700	0	334	8	0
17	Dc	310	0	134	0	0
18	D3	29536	0	14872	424	0
19	DA	1709	0	1784	42	0
20	DE	2068	0	2154	26	0
21	DG	1799	0	1879	49	0
22	DH	1481	0	1572	23	0
23	DI	1489	0	1525	25	0
24	DJ	1494	0	1573	23	0
25	DL	1154	0	1220	14	0
26	DN	1192	0	1255	10	0
27	DO	941	0	979	13	0
28	DZ	332	0	149	1	0
29	DW	1021	0	1060	22	0
30	DX	1115	0	1191	16	0
31	DY	1067	0	1127	19	0
32	Db	610	0	633	0	0
33	UN	920	0	972	6	0
34	JD	4600	0	2789	36	0
35	D4	496	0	253	2	0
36	D5	180	0	91	0	0
37	UX	1	0	0	0	0
38	CL	32	0	12	1	0
39	CL	1	0	0	0	0
39	D3	37	0	0	0	0
39	DG	1	0	0	0	0
All	All	80072	0	57995	973	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 7.

All (973) 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)
1:UB:701:ALA:HB2	3:US:417:HIS:HA	1.27	1.14
18:D3:187:G:N2	18:D3:198:A:N7	2.04	1.06
18:D3:736:C:H6	18:D3:736:C:H5'	1.24	1.02
1:UB:701:ALA:CB	3:US:417:HIS:HA	1.91	1.00
18:D3:895:G:H1	18:D3:917:U:H3	1.02	0.99
18:D3:1588:G:H1	18:D3:1608:U:H3	0.99	0.93
1:UB:701:ALA:CB	3:US:417:HIS:CB	2.47	0.92
1:UB:701:ALA:HB1	3:US:417:HIS:CB	2.00	0.92
7:CL:943:LYS:HG2	18:D3:1594:G:H5'	1.49	0.91
13:DF:149:VAL:O	13:DF:155:ALA:HA	1.71	0.90
18:D3:736:C:H5'	18:D3:736:C:C6	2.06	0.89
18:D3:1471:A:N6	18:D3:1538:U:H3	1.70	0.89
34:JD:1153:LEU:O	34:JD:1170:LEU:HA	1.74	0.88
18:D3:1504:G:N2	18:D3:1563:C:O2	2.09	0.86
18:D3:1471:A:H62	18:D3:1538:U:H3	0.87	0.85
18:D3:737:A:OP2	18:D3:737:A:H2'	1.75	0.85
18:D3:488:G:C6	18:D3:498:G:N2	2.45	0.85
34:JD:445:VAL:HA	34:JD:512:SER:O	1.77	0.84
18:D3:1646:C:N4	18:D3:1754:A:N6	2.25	0.83
1:UB:701:ALA:CB	3:US:417:HIS:CA	2.56	0.83
18:D3:488:G:O6	18:D3:498:G:N2	2.13	0.82
18:D3:505:A:N1	18:D3:507:U:C4	2.48	0.81
1:UB:701:ALA:HB2	3:US:417:HIS:CA	2.11	0.79
18:D3:496:G:H3'	18:D3:497:G:H4'	1.65	0.79
34:JD:1218:GLY:HA3	34:JD:1228:GLY:HA3	1.65	0.79
5:CJ:225:ALA:O	5:CJ:231:ILE:HA	1.84	0.77
18:D3:187:G:H21	18:D3:198:A:H62	1.32	0.77
18:D3:824:G:N2	18:D3:849:C:O2	2.18	0.76
18:D3:1583:A:H61	18:D3:1611:A:H3'	1.51	0.76
18:D3:1550:A:C6	18:D3:1562:G:C6	2.74	0.75
34:JD:733:PRO:HA	34:JD:759:VAL:O	1.87	0.74
7:CL:174:LEU:HD23	7:CL:206:TYR:HB3	1.67	0.74
7:CL:267:ARG:HH12	7:CL:798:MET:HG2	1.52	0.74
18:D3:868:G:H1	18:D3:960:U:H3	1.35	0.74
21:DG:74:LYS:HA	21:DG:95:LYS:O	1.86	0.74
23:DI:57:ALA:HB2	23:DI:177:GLY:HA2	1.69	0.74
18:D3:693:U:C2	18:D3:695:U:O4	2.40	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D3:933:A:OP1	19:DA:116:LYS:NZ	2.20	0.73
5:CJ:223:THR:O	5:CJ:233:VAL:HA	1.88	0.73
18:D3:826:U:H4'	18:D3:826:U:OP1	1.87	0.72
18:D3:1646:C:N4	18:D3:1754:A:H61	1.86	0.72
20:DE:122:LYS:NZ	20:DE:143:ASP:OD2	2.19	0.72
18:D3:708:C:N3	18:D3:710:U:C5	2.57	0.72
18:D3:1556:A:H4'	18:D3:1557:U:H2'	1.72	0.72
18:D3:736:C:H6	18:D3:736:C:C5'	2.01	0.71
18:D3:1096:C:N4	29:DW:18:GLU:OE1	2.23	0.71
11:JL:235:ASN:O	11:JL:294:ARG:NH2	2.23	0.71
21:DG:162:VAL:O	21:DG:168:THR:HA	1.90	0.71
19:DA:208:GLN:HG3	19:DA:209:ASN:HB2	1.71	0.71
18:D3:195:G:O6	23:DI:137:LYS:NZ	2.23	0.71
18:D3:227:U:C2	18:D3:834:G:C6	2.77	0.71
18:D3:1498:G:N2	18:D3:1510:U:O2	2.24	0.71
27:DO:15:GLY:O	27:DO:79:VAL:HA	1.91	0.70
18:D3:486:G:H5''	18:D3:497:G:H1	1.56	0.70
18:D3:23:G:C6	18:D3:603:U:O2	2.45	0.70
18:D3:104:A:OP2	18:D3:308:C:N4	2.23	0.70
18:D3:177:U:O2	21:DG:191:ARG:NH1	2.26	0.69
21:DG:162:VAL:HB	21:DG:169:TYR:HB2	1.74	0.69
18:D3:188:A:OP2	23:DI:138:ASN:ND2	2.25	0.69
22:DH:143:LEU:O	29:DW:42:GLN:NE2	2.26	0.69
18:D3:1484:G:H1	18:D3:1591:C:H1'	1.56	0.69
18:D3:1484:G:N2	18:D3:1591:C:O2	2.26	0.69
19:DA:82:ARG:HA	19:DA:104:ASP:O	1.92	0.69
34:JD:621:ALA:HB3	34:JD:773:VAL:HA	1.75	0.69
18:D3:220:A:C8	18:D3:832:U:C2	2.81	0.69
18:D3:68:A:OP1	21:DG:160:ARG:NH2	2.25	0.69
18:D3:905:A:O3'	27:DO:52:ARG:NH2	2.27	0.68
18:D3:1471:A:N7	18:D3:1538:U:O4	2.26	0.68
27:DO:125:SER:OG	27:DO:126:THR:N	2.26	0.68
18:D3:1646:C:H42	18:D3:1754:A:N6	1.90	0.68
22:DH:31:SER:HB3	22:DH:35:LYS:HD2	1.73	0.68
21:DG:164:LYS:HB3	21:DG:167:LYS:HB2	1.76	0.68
31:DY:27:VAL:HG11	31:DY:35:VAL:HG11	1.74	0.68
18:D3:821:U:N3	18:D3:852:C:O2	2.26	0.68
18:D3:23:G:O6	18:D3:603:U:O2	2.12	0.68
34:JD:1157:LEU:HA	34:JD:1166:ARG:O	1.94	0.68
18:D3:496:G:H5'	18:D3:497:G:H5''	1.76	0.67
18:D3:195:G:N7	23:DI:141:ARG:NH2	2.43	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:JL:181:MET:SD	11:JL:300:GLN:NE2	2.68	0.67
18:D3:821:U:O4	18:D3:852:C:N3	2.28	0.67
24:DJ:17:ARG:HD2	24:DJ:18:PRO:HD2	1.76	0.67
18:D3:1480:G:C2	18:D3:1528:U:O2	2.48	0.66
18:D3:1573:A:H4'	18:D3:1574:G:H5'	1.77	0.66
2:UC:538:ARG:NH1	7:CL:151:GLU:OE2	2.28	0.66
18:D3:187:G:H21	18:D3:198:A:N6	1.94	0.66
18:D3:207:U:O2	23:DI:178:ARG:NH1	2.25	0.66
18:D3:230:C:N4	18:D3:231:U:C4	2.64	0.66
26:DN:130:ARG:NH2	26:DN:139:TRP:O	2.29	0.66
18:D3:715:U:H3	18:D3:723:G:H1	1.43	0.66
26:DN:20:ARG:HH21	29:DW:56:HIS:CG	2.14	0.66
24:DJ:139:GLN:NE2	31:DY:64:PHE:O	2.28	0.65
11:JL:299:ASP:OD2	34:JD:106:LYS:NZ	2.28	0.65
18:D3:76:A:N6	18:D3:80:A:O2'	2.27	0.65
18:D3:789:A:O2'	20:DE:106:LYS:NZ	2.27	0.65
7:CL:166:ARG:NH2	18:D3:435:C:OP1	2.29	0.65
7:CL:248:ARG:HG2	7:CL:272:TYR:HB2	1.77	0.65
7:CL:889:LEU:HD22	7:CL:922:ILE:HG23	1.78	0.65
11:JL:162:ARG:O	11:JL:176:SER:OG	2.14	0.65
18:D3:218:A:C6	18:D3:830:U:N3	2.64	0.65
18:D3:1550:A:N1	18:D3:1562:G:C6	2.65	0.65
26:DN:4:MET:SD	26:DN:124:ARG:NH1	2.70	0.65
4:UX:56:ASN:ND2	4:UX:169:GLY:O	2.29	0.65
7:CL:830:ARG:NH1	30:DX:138:GLU:OE2	2.29	0.65
23:DI:84:HIS:NE2	23:DI:97:THR:OG1	2.29	0.65
18:D3:1498:G:H1	18:D3:1510:U:H3	1.45	0.65
18:D3:396:G:N2	18:D3:399:A:OP2	2.30	0.64
18:D3:1170:G:N2	18:D3:1571:C:O2'	2.30	0.64
7:CL:309:PRO:HB3	7:CL:313:TYR:HD2	1.61	0.64
12:JJ:193:LEU:HD22	12:JJ:197:HIS:HB3	1.78	0.64
23:DI:48:THR:OG1	23:DI:52:ASN:O	2.15	0.64
23:DI:67:TRP:NE1	23:DI:185:GLU:OE2	2.29	0.64
2:UC:553:LYS:HB3	18:D3:586:G:H21	1.62	0.64
34:JD:1151:TYR:CB	34:JD:1173:ILE:O	2.46	0.64
7:CL:736:GLU:OE2	7:CL:739:LYS:NZ	2.30	0.64
18:D3:710:U:C4	18:D3:730:G:C6	2.86	0.64
11:JL:208:ARG:NH2	35:D4:2:U:OP1	2.21	0.64
12:JJ:95:GLU:OE1	27:DO:111:ARG:NH1	2.30	0.64
18:D3:140:A:OP2	21:DG:187:LYS:NZ	2.26	0.64
19:DA:82:ARG:NH2	19:DA:188:LEU:O	2.31	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D3:698:U:OP1	18:D3:733:A:N6	2.31	0.64
18:D3:227:U:C2	18:D3:834:G:O6	2.51	0.63
18:D3:729:G:N2	18:D3:730:G:O2'	2.31	0.63
4:UX:149:LYS:NZ	4:UX:168:PRO:O	2.32	0.63
18:D3:187:G:N2	18:D3:198:A:H62	1.96	0.63
7:CL:64:GLU:OE2	7:CL:766:ASN:ND2	2.32	0.63
18:D3:1498:G:C2	18:D3:1510:U:O2	2.52	0.63
18:D3:66:U:OP1	21:DG:136:LYS:NZ	2.32	0.63
7:CL:193:ARG:NH2	7:CL:197:GLU:OE2	2.30	0.63
19:DA:154:SER:OG	19:DA:154:SER:O	2.15	0.63
18:D3:485:A:C8	18:D3:485:A:H5''	2.34	0.62
18:D3:324:U:OP1	25:DL:133:LYS:NZ	2.27	0.62
18:D3:224:C:H2'	18:D3:225:A:H8	1.63	0.62
18:D3:647:G:H2'	18:D3:648:G:H8	1.63	0.62
18:D3:1477:G:O6	18:D3:1531:G:C6	2.53	0.62
7:CL:996:LEU:HD23	7:CL:998:SER:H	1.65	0.62
8:CM:158:SER:H	8:CM:162:GLY:HA2	1.65	0.62
25:DL:133:LYS:O	25:DL:136:ARG:NH1	2.32	0.62
12:JJ:259:VAL:O	12:JJ:263:LEU:HB2	1.99	0.62
19:DA:76:SER:OG	19:DA:78:ASP:OD1	2.17	0.62
24:DJ:170:GLY:O	24:DJ:174:ARG:NE	2.32	0.62
18:D3:227:U:O2	18:D3:834:G:C6	2.53	0.62
18:D3:846:G:H5''	18:D3:846:G:N3	2.14	0.62
22:DH:9:LEU:HD21	22:DH:21:ALA:HB2	1.80	0.62
18:D3:803:A:N3	22:DH:104:ARG:NH2	2.46	0.62
18:D3:1057:U:H3	18:D3:1060:U:H3'	1.65	0.62
30:DX:46:SER:OG	30:DX:48:HIS:O	2.16	0.62
34:JD:1092:VAL:H	34:JD:1122:ALA:HB2	1.65	0.62
5:CJ:154:ILE:O	5:CJ:162:THR:HA	2.00	0.62
18:D3:488:G:O6	18:D3:498:G:C2	2.52	0.62
6:CK:298:SER:OG	6:CK:301:GLU:OE1	2.16	0.62
18:D3:258:C:O2	23:DI:178:ARG:NH2	2.33	0.62
8:CM:286:SER:HA	8:CM:317:GLN:HE21	1.65	0.61
15:DS:40:ARG:HH11	18:D3:1539:G:H4'	1.65	0.61
7:CL:819:GLU:O	7:CL:852:ARG:NH2	2.34	0.61
6:CK:344:GLU:OE2	7:CL:960:ARG:NH2	2.33	0.61
18:D3:504:U:H2'	18:D3:505:A:H4'	1.82	0.61
18:D3:1530:C:H2'	18:D3:1531:G:H8	1.64	0.61
20:DE:63:ALA:O	20:DE:67:GLN:NE2	2.33	0.61
29:DW:87:GLU:HA	29:DW:90:THR:HG22	1.81	0.61
1:UB:785:VAL:HG11	30:DX:119:GLY:HA2	1.82	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D3:500:C:O5'	18:D3:500:C:H6	1.83	0.61
7:CL:71:ILE:HD12	7:CL:245:LEU:HD22	1.82	0.61
7:CL:943:LYS:CG	18:D3:1594:G:H5'	2.27	0.61
18:D3:709:C:H5	18:D3:730:G:H21	1.49	0.61
18:D3:40:A:N6	18:D3:466:U:O4	2.33	0.61
25:DL:57:LYS:HD2	25:DL:131:ILE:HG23	1.83	0.61
18:D3:1470:C:H3'	18:D3:1573:A:H62	1.66	0.61
9:JF:44:VAL:HA	9:JF:113:TYR:O	2.01	0.60
34:JD:1235:ALA:HB3	34:JD:1251:ILE:O	2.00	0.60
2:UC:580:ARG:NH2	4:UX:49:SER:O	2.35	0.60
18:D3:283:U:H5''	21:DG:188:ARG:HD2	1.82	0.60
18:D3:647:G:H22	18:D3:687:G:H1	1.49	0.60
18:D3:405:C:O2'	21:DG:92:ARG:O	2.18	0.60
23:DI:152:ILE:HG13	23:DI:153:GLU:H	1.66	0.60
29:DW:112:ASP:OD1	29:DW:112:ASP:N	2.28	0.60
30:DX:9:LEU:O	30:DX:10:ASN:ND2	2.31	0.60
1:UB:787:THR:HG23	18:D3:1116:A:H4'	1.82	0.60
18:D3:1163:A:N3	18:D3:1613:U:O2'	2.31	0.60
7:CL:134:ILE:HG21	7:CL:811:VAL:HG21	1.83	0.60
18:D3:976:G:H1	18:D3:1023:A:HO2'	1.45	0.60
18:D3:780:A:H62	31:DY:10:ARG:HH21	1.48	0.60
30:DX:27:ASN:O	30:DX:31:LYS:HB2	2.01	0.60
11:JL:156:GLN:NE2	11:JL:158:GLU:OE2	2.31	0.60
18:D3:738:G:H2'	18:D3:739:G:C8	2.37	0.60
18:D3:1160:A:O2'	18:D3:1620:C:N3	2.30	0.60
7:CL:831:ARG:NH2	7:CL:835:HIS:O	2.34	0.60
33:UN:466:ARG:NH1	35:D4:15:U:OP1	2.33	0.60
34:JD:514:ILE:HA	34:JD:556:ILE:O	2.02	0.60
20:DE:129:VAL:HG12	20:DE:139:VAL:HG12	1.83	0.59
23:DI:137:LYS:HZ3	23:DI:141:ARG:HH22	1.50	0.59
8:CM:193:GLY:O	8:CM:225:ILE:HA	2.02	0.59
24:DJ:87:SER:HG	24:DJ:90:LYS:H	1.50	0.59
18:D3:1472:C:N3	18:D3:1534:G:C2	2.71	0.59
24:DJ:145:SER:OG	24:DJ:145:SER:O	2.16	0.59
18:D3:504:U:H6	18:D3:504:U:O5'	1.86	0.59
18:D3:717:C:N3	18:D3:720:G:N1	2.51	0.59
18:D3:781:U:OP2	31:DY:9:THR:OG1	2.19	0.59
11:JL:285:LEU:HB3	11:JL:291:GLY:HA3	1.84	0.59
34:JD:1092:VAL:O	34:JD:1121:LEU:N	2.34	0.59
7:CL:14:LYS:HG2	7:CL:19:LYS:HD3	1.84	0.59
19:DA:121:ILE:HG12	19:DA:161:ILE:HG23	1.84	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:DG:67:VAL:HG23	21:DG:99:GLY:HA2	1.84	0.59
7:CL:210:VAL:O	7:CL:210:VAL:HG13	2.01	0.59
7:CL:130:ASP:OD1	7:CL:853:ARG:NH2	2.35	0.59
18:D3:485:A:C8	18:D3:485:A:C5'	2.86	0.59
18:D3:1477:G:C6	18:D3:1531:G:C6	2.90	0.59
18:D3:1550:A:C6	18:D3:1562:G:N1	2.71	0.59
18:D3:1583:A:H62	18:D3:1612:U:H5	1.50	0.59
18:D3:549:G:HO2'	18:D3:550:A:H8	1.51	0.59
18:D3:1588:G:N2	18:D3:1608:U:O2	2.30	0.59
25:DL:57:LYS:HD2	25:DL:131:ILE:HD12	1.85	0.59
7:CL:135:ALA:O	7:CL:238:ARG:NH2	2.29	0.58
18:D3:149:C:OP1	31:DY:121:THR:OG1	2.20	0.58
7:CL:105:ILE:HD11	7:CL:354:ILE:HD11	1.86	0.58
18:D3:1627:U:H5''	18:D3:1628:U:H5'	1.85	0.58
7:CL:562:GLU:OE2	7:CL:566:ARG:NH1	2.36	0.58
7:CL:826:LYS:HE3	7:CL:926:ILE:HD13	1.85	0.58
20:DE:148:ARG:NH1	21:DG:201:GLN:OE1	2.36	0.58
21:DG:57:ASP:HA	21:DG:106:LEU:HA	1.85	0.58
18:D3:23:G:O6	18:D3:603:U:C2	2.57	0.58
18:D3:1127:G:OP2	34:JD:107:ARG:NH1	2.36	0.58
18:D3:1478:G:H2'	18:D3:1479:A:H8	1.68	0.58
18:D3:1480:G:N1	18:D3:1528:U:C2	2.72	0.58
6:CK:345:LEU:HD13	7:CL:1005:SER:HB2	1.85	0.58
11:JL:271:GLY:N	11:JL:275:ASP:OD2	2.36	0.58
18:D3:717:C:C4	18:D3:720:G:N2	2.72	0.58
18:D3:130:C:N4	18:D3:177:U:OP1	2.37	0.57
7:CL:1018:VAL:O	7:CL:1029:TRP:NE1	2.37	0.57
18:D3:428:A:N3	18:D3:440:U:O2'	2.33	0.57
18:D3:1122:G:OP2	34:JD:95:LYS:NZ	2.35	0.57
26:DN:132:VAL:HG13	26:DN:134:VAL:HG23	1.87	0.57
18:D3:505:A:N1	18:D3:507:U:O4	2.36	0.57
18:D3:1542:G:H1	18:D3:1568:C:HO2'	1.49	0.57
5:CJ:144:GLU:HA	5:CJ:149:PRO:HA	1.85	0.57
18:D3:1164:G:H2'	18:D3:1165:G:H8	1.69	0.57
29:DW:41:MET:HG2	29:DW:129:VAL:HG11	1.86	0.57
18:D3:163:G:OP2	18:D3:163:G:N2	2.35	0.57
18:D3:640:U:O2	22:DH:179:LYS:NZ	2.29	0.57
18:D3:656:G:H1	18:D3:679:U:H1'	1.69	0.57
7:CL:228:SER:O	7:CL:228:SER:OG	2.15	0.57
18:D3:683:C:H2'	18:D3:684:A:H8	1.68	0.57
19:DA:29:TRP:O	19:DA:94:LYS:NZ	2.36	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:DS:14:ILE:HA	15:DS:22:VAL:O	2.05	0.57
18:D3:65:A:H2	18:D3:84:A:H62	1.51	0.57
18:D3:1542:G:O2'	18:D3:1544:U:O4	2.22	0.57
19:DA:104:ASP:OD1	19:DA:105:PHE:N	2.37	0.57
31:DY:29:HIS:O	31:DY:29:HIS:ND1	2.38	0.57
24:DJ:27:GLU:OE1	24:DJ:39:LYS:NZ	2.37	0.57
34:JD:1195:THR:OG1	34:JD:1196:GLY:N	2.35	0.57
8:CM:285:LYS:NZ	8:CM:316:GLU:OE1	2.38	0.56
8:CM:289:VAL:HG21	8:CM:294:LEU:HD13	1.87	0.56
34:JD:536:VAL:O	34:JD:540:ALA:N	2.38	0.56
18:D3:195:G:H2'	18:D3:196:G:C8	2.40	0.56
18:D3:651:G:H2'	18:D3:652:G:C8	2.39	0.56
2:UC:562:ARG:NH2	18:D3:476:U:OP2	2.38	0.56
7:CL:282:SER:O	7:CL:282:SER:OG	2.22	0.56
18:D3:144:U:O4	21:DG:137:ARG:NH1	2.39	0.56
18:D3:1472:C:C2	18:D3:1534:G:C2	2.93	0.56
21:DG:116:LYS:NZ	21:DG:117:GLY:O	2.34	0.56
7:CL:170:VAL:HG12	7:CL:205:PHE:HB2	1.87	0.56
7:CL:954:SER:N	7:CL:957:GLU:OE1	2.34	0.56
18:D3:482:U:N3	18:D3:507:U:O4	2.38	0.56
18:D3:706:A:N6	18:D3:731:C:O3'	2.38	0.56
4:UX:89:CYS:SG	4:UX:90:LEU:N	2.78	0.56
18:D3:1550:A:N6	18:D3:1562:G:O6	2.39	0.56
26:DN:12:SER:O	26:DN:12:SER:OG	2.19	0.56
7:CL:984:GLU:OE1	18:D3:1558:U:O2'	2.24	0.56
18:D3:438:A:O2'	18:D3:465:G:N2	2.39	0.56
18:D3:1498:G:N1	18:D3:1510:U:N3	2.52	0.56
6:CK:304:GLN:HB3	6:CK:308:ARG:HH22	1.71	0.55
9:JG:175:CYS:HA	9:JG:201:SER:H	1.72	0.55
19:DA:76:SER:OG	19:DA:77:GLU:N	2.40	0.55
1:UB:749:LYS:NZ	18:D3:1177:C:O3'	2.40	0.55
12:JJ:96:SER:OG	12:JJ:97:ARG:N	2.37	0.55
15:DS:12:GLN:HG2	15:DS:59:GLY:HA2	1.88	0.55
7:CL:970:SER:OG	7:CL:999:ASP:OD1	2.22	0.55
15:DS:82:PRO:HG2	15:DS:85:PHE:HB2	1.89	0.55
18:D3:976:G:N1	18:D3:1023:A:O2'	2.38	0.55
18:D3:1127:G:N7	34:JD:107:ARG:NH2	2.53	0.55
15:DS:87:ASN:O	18:D3:1546:G:N2	2.40	0.55
18:D3:1588:G:O6	18:D3:1608:U:O4	2.25	0.55
29:DW:6:VAL:HG12	29:DW:34:ILE:HD11	1.89	0.55
6:CK:311:ILE:HG23	7:CL:1032:LEU:HD23	1.88	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:CL:9:ARG:NH1	18:D3:619:A:O4'	2.40	0.55
18:D3:712:G:O6	18:D3:727:U:O4	2.24	0.55
30:DX:90:ASP:OD1	30:DX:90:ASP:N	2.39	0.55
8:CM:260:ASP:OD1	8:CM:261:ILE:N	2.39	0.55
18:D3:61:A:H8	18:D3:269:G:HO2'	1.55	0.55
18:D3:715:U:O2	18:D3:723:G:N2	2.38	0.55
18:D3:1484:G:N2	18:D3:1591:C:C2	2.73	0.55
21:DG:147:LEU:HD13	21:DG:151:ASP:HB2	1.89	0.55
7:CL:952:PHE:HD2	7:CL:958:VAL:HG22	1.72	0.55
8:CM:110:SER:OG	8:CM:112:LYS:O	2.25	0.55
12:JJ:107:THR:O	12:JJ:111:ASN:HB2	2.07	0.55
18:D3:830:U:O2'	18:D3:831:U:O4'	2.25	0.54
18:D3:218:A:H2'	18:D3:219:A:H5''	1.89	0.54
21:DG:148:SER:N	21:DG:151:ASP:OD2	2.40	0.54
12:JJ:98:LYS:HB2	12:JJ:138:GLU:HG2	1.89	0.54
18:D3:269:G:C6	18:D3:287:G:C2	2.96	0.54
18:D3:777:C:H4'	20:DE:261:LEU:HD11	1.88	0.54
7:CL:166:ARG:NH1	7:CL:231:LYS:O	2.40	0.54
7:CL:281:PRO:HG2	7:CL:286:THR:HG21	1.89	0.54
8:CM:68:SER:HB2	8:CM:73:THR:HB	1.89	0.54
18:D3:840:U:HO2'	18:D3:841:U:H6	1.54	0.54
18:D3:220:A:N7	18:D3:832:U:N3	2.55	0.54
18:D3:237:C:H4'	18:D3:238:U:H5'	1.89	0.54
18:D3:802:G:N2	29:DW:107:SER:HG	2.05	0.54
18:D3:912:U:OP1	18:D3:913:G:O2'	2.21	0.54
18:D3:1647:U:H2'	18:D3:1648:A:H8	1.72	0.54
27:DO:92:LYS:HD3	27:DO:121:VAL:HG22	1.88	0.54
5:CJ:188:HIS:N	5:CJ:220:ARG:O	2.36	0.54
8:CM:361:ASN:O	8:CM:364:LYS:NZ	2.29	0.54
18:D3:620:A:N7	18:D3:1109:G:C2	2.76	0.54
19:DA:88:VAL:HG11	19:DA:96:LEU:HD12	1.89	0.54
22:DH:144:VAL:HA	29:DW:42:GLN:HE21	1.72	0.54
24:DJ:65:LYS:HA	24:DJ:70:LEU:HD11	1.89	0.54
7:CL:607:ASP:OD1	7:CL:607:ASP:N	2.39	0.54
22:DH:63:PRO:O	22:DH:66:SER:OG	2.19	0.54
34:JD:1061:VAL:O	34:JD:1065:GLU:N	2.36	0.54
2:UC:580:ARG:NH1	4:UX:51:LEU:O	2.41	0.54
5:CJ:238:TYR:HA	5:CJ:246:GLU:O	2.07	0.54
18:D3:220:A:H3'	18:D3:832:U:H1'	1.88	0.54
18:D3:734:A:C8	18:D3:734:A:H3'	2.43	0.54
18:D3:1164:G:H2'	18:D3:1165:G:C8	2.43	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D3:319:U:H4'	18:D3:323:A:C8	2.43	0.54
19:DA:78:ASP:OD1	19:DA:78:ASP:N	2.40	0.54
22:DH:67:LEU:HD11	22:DH:94:ALA:HB2	1.90	0.54
12:JJ:216:ILE:HA	12:JJ:263:LEU:HD21	1.90	0.54
16:DT:72:GLY:HA3	18:D3:1498:G:H5''	1.89	0.54
27:DO:53:ASP:HB2	27:DO:56:SER:HB2	1.90	0.54
7:CL:977:LYS:NZ	18:D3:1597:A:OP1	2.30	0.53
18:D3:852:C:H2'	18:D3:853:G:C8	2.43	0.53
18:D3:895:G:H21	27:DO:38:THR:HG21	1.73	0.53
7:CL:960:ARG:HD3	7:CL:961:PHE:HE1	1.73	0.53
18:D3:704:C:H3'	18:D3:705:U:H4'	1.90	0.53
19:DA:31:ASP:OD1	19:DA:31:ASP:N	2.41	0.53
8:CM:306:GLU:OE2	8:CM:355:LYS:NZ	2.41	0.53
9:JF:113:TYR:HA	9:JF:122:ILE:O	2.09	0.53
23:DI:89:GLU:OE2	23:DI:92:ARG:NH2	2.38	0.53
30:DX:109:ARG:NE	30:DX:111:GLY:O	2.40	0.53
18:D3:717:C:N4	18:D3:720:G:N2	2.56	0.53
19:DA:132:ASP:OD1	19:DA:132:ASP:N	2.36	0.53
24:DJ:17:ARG:NH2	24:DJ:19:TYR:H	2.06	0.53
34:JD:731:VAL:HA	34:JD:757:CYS:O	2.09	0.53
18:D3:134:U:H4'	18:D3:136:C:H41	1.73	0.53
18:D3:585:A:H3'	18:D3:586:G:H2'	1.89	0.53
28:DZ:86:GLU:HA	28:DZ:102:THR:HA	1.91	0.53
18:D3:704:C:H2'	18:D3:734:A:H2	1.74	0.53
8:CM:124:SER:OG	8:CM:125:HIS:N	2.39	0.53
25:DL:27:THR:HG22	25:DL:28:SER:H	1.73	0.53
16:DT:136:ALA:O	16:DT:140:LEU:N	2.42	0.53
7:CL:843:ASP:OD1	7:CL:1035:THR:OG1	2.26	0.52
18:D3:1506:G:H2'	18:D3:1507:G:C8	2.44	0.52
18:D3:1518:C:H2'	18:D3:1519:U:C6	2.44	0.52
19:DA:81:PHE:HD2	19:DA:82:ARG:HG3	1.75	0.52
20:DE:104:ASP:N	20:DE:104:ASP:OD1	2.41	0.52
7:CL:923:ASP:OD1	7:CL:923:ASP:N	2.42	0.52
8:CM:312:ARG:NH2	8:CM:344:GLU:OE1	2.34	0.52
18:D3:513:U:O4	24:DJ:171:ARG:NH2	2.43	0.52
18:D3:741:C:O2'	18:D3:742:U:O4'	2.27	0.52
24:DJ:119:ALA:O	24:DJ:124:HIS:ND1	2.42	0.52
1:UB:784:ILE:HD11	30:DX:73:ARG:HH12	1.74	0.52
18:D3:218:A:C6	18:D3:830:U:C4	2.97	0.52
18:D3:1477:G:H2'	18:D3:1478:G:C8	2.45	0.52
23:DI:85:PRO:O	25:DL:11:ARG:NH2	2.34	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UB:734:ARG:NH1	18:D3:1173:C:OP1	2.43	0.52
18:D3:895:G:O6	18:D3:917:U:O4	2.28	0.52
7:CL:729:GLN:NE2	7:CL:733:GLU:OE2	2.39	0.52
8:CM:204:LEU:HD23	8:CM:268:PRO:HG3	1.92	0.52
18:D3:1157:A:N6	18:D3:1618:C:O2	2.43	0.52
19:DA:87:ARG:NH1	19:DA:220:GLN:OE1	2.43	0.52
18:D3:434:G:O2'	18:D3:435:C:O2	2.27	0.52
18:D3:846:G:N3	18:D3:846:G:C5'	2.73	0.52
18:D3:992:A:OP2	18:D3:1011:G:N1	2.30	0.52
1:UB:657:PHE:O	1:UB:661:ILE:N	2.42	0.51
18:D3:1056:U:O3'	19:DA:202:LYS:NZ	2.41	0.51
18:D3:1511:U:H2'	18:D3:1512:G:H8	1.75	0.51
29:DW:30:SER:O	29:DW:30:SER:OG	2.26	0.51
7:CL:14:LYS:HE2	7:CL:19:LYS:HB3	1.92	0.51
9:JF:114:ILE:O	9:JF:121:LEU:HA	2.09	0.51
11:JL:55:ARG:N	11:JL:58:ASP:OD2	2.36	0.51
18:D3:1594:G:N1	18:D3:1603:U:N3	2.58	0.51
18:D3:487:G:H1	18:D3:500:C:H42	1.59	0.51
18:D3:1486:G:O6	18:D3:1520:U:C4	2.64	0.51
19:DA:103:MET:HB3	19:DA:215:VAL:HG12	1.93	0.51
19:DA:134:VAL:HB	19:DA:219:LYS:HB2	1.91	0.51
21:DG:43:ASP:OD1	21:DG:43:ASP:N	2.43	0.51
18:D3:168:A:OP1	21:DG:140:ASN:ND2	2.44	0.51
18:D3:1583:A:N1	18:D3:1611:A:H5''	2.26	0.51
24:DJ:113:VAL:HG12	24:DJ:119:ALA:HB2	1.92	0.51
18:D3:23:G:C2	18:D3:24:U:H1'	2.46	0.51
18:D3:1483:A:H2'	18:D3:1484:G:C8	2.45	0.51
21:DG:50:PHE:HE1	21:DG:113:ILE:HG12	1.76	0.51
21:DG:52:ILE:HA	21:DG:111:LEU:HD23	1.91	0.51
7:CL:174:LEU:CD2	7:CL:206:TYR:HB3	2.39	0.51
11:JL:75:LEU:HD22	11:JL:81:VAL:HG21	1.93	0.51
18:D3:503:G:H3'	18:D3:504:U:H5	1.75	0.51
18:D3:1504:G:H21	18:D3:1563:C:H1'	1.74	0.51
20:DE:31:PRO:HG3	20:DE:43:PRO:HG3	1.93	0.51
22:DH:8:ILE:HA	22:DH:42:GLN:HG3	1.92	0.51
7:CL:773:THR:O	7:CL:776:GLN:N	2.40	0.51
11:JL:233:ARG:HG2	11:JL:236:ARG:HD3	1.92	0.51
15:DS:27:LYS:HA	15:DS:57:ARG:HA	1.92	0.51
18:D3:1484:G:O2'	18:D3:1606:C:O3'	2.28	0.51
21:DG:160:ARG:O	21:DG:170:THR:HA	2.10	0.51
18:D3:738:G:H2'	18:D3:739:G:H8	1.73	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:CL:844:PRO:HG3	7:CL:1032:LEU:HB2	1.93	0.51
19:DA:141:ALA:HB1	19:DA:207:LEU:HD11	1.93	0.51
19:DA:194:ASN:HD21	19:DA:211:HIS:HA	1.76	0.51
6:CK:337:GLU:OE2	7:CL:954:SER:OG	2.27	0.50
18:D3:734:A:H2'	18:D3:735:C:C2	2.46	0.50
20:DE:182:TYR:HD1	20:DE:192:ILE:HG12	1.76	0.50
9:JF:121:LEU:CB	9:JF:163:ILE:O	2.59	0.50
18:D3:824:G:H2'	18:D3:825:U:H6	1.77	0.50
23:DI:104:ILE:HG13	23:DI:105:ASP:H	1.76	0.50
7:CL:244:MET:HB3	7:CL:812:MET:HB3	1.93	0.50
7:CL:934:LEU:O	7:CL:1002:ILE:HA	2.11	0.50
11:JL:299:ASP:OD1	11:JL:299:ASP:N	2.44	0.50
18:D3:1585:U:O2	18:D3:1611:A:N7	2.44	0.50
7:CL:905:SER:OG	7:CL:906:ASP:N	2.45	0.50
9:JF:133:THR:O	9:JF:137:PHE:N	2.42	0.50
18:D3:1486:G:H2'	18:D3:1487:A:C8	2.46	0.50
2:UC:535:ASP:HB3	2:UC:537:LYS:H	1.77	0.50
2:UC:557:ASP:OD2	2:UC:567:LYS:NZ	2.27	0.50
7:CL:719:ASN:N	7:CL:719:ASN:OD1	2.44	0.50
18:D3:824:G:H2'	18:D3:825:U:C6	2.46	0.50
30:DX:109:ARG:HH12	30:DX:116:ASP:HB2	1.77	0.50
1:UB:756:ARG:NH1	6:CK:353:PRO:O	2.45	0.50
18:D3:394:C:O2'	21:DG:90:GLY:O	2.26	0.50
18:D3:636:A:H5''	29:DW:31:SER:HB3	1.93	0.50
18:D3:1008:G:OP1	27:DO:135:ARG:NH1	2.45	0.50
34:JD:1244:GLN:OE1	34:JD:1245:TRP:N	2.44	0.50
7:CL:125:LEU:HD22	7:CL:912:ARG:HH21	1.77	0.50
7:CL:198:VAL:HG12	7:CL:199:TYR:H	1.77	0.50
11:JL:60:VAL:HG11	11:JL:74:ILE:HG21	1.93	0.50
18:D3:1480:G:C2	18:D3:1528:U:C2	2.99	0.50
25:DL:124:THR:HB	25:DL:141:LYS:HG2	1.92	0.50
18:D3:1800:A:O2'	18:D3:1801:A:O5'	2.25	0.50
11:JL:280:LYS:O	11:JL:283:THR:OG1	2.29	0.50
18:D3:1538:U:HO2'	18:D3:1539:G:H8	1.60	0.50
4:UX:106:LEU:HA	4:UX:109:LEU:HD23	1.94	0.49
7:CL:267:ARG:NH1	7:CL:798:MET:HG2	2.22	0.49
18:D3:225:A:N6	18:D3:837:G:O6	2.45	0.49
18:D3:720:G:O2'	18:D3:722:G:N7	2.34	0.49
23:DI:135:LYS:N	23:DI:140:GLU:OE1	2.45	0.49
8:CM:85:ALA:HA	8:CM:115:SER:O	2.12	0.49
15:DS:53:ASP:HB3	15:DS:56:LYS:HG3	1.93	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D3:834:G:H2'	18:D3:835:U:C2	2.47	0.49
22:DH:49:ILE:HD11	22:DH:172:VAL:HG22	1.94	0.49
24:DJ:20:GLU:O	24:DJ:23:ARG:N	2.35	0.49
7:CL:921:GLU:HB3	8:CM:365:LYS:HG3	1.95	0.49
34:JD:788:ASN:N	34:JD:793:VAL:O	2.38	0.49
18:D3:150:U:O4	31:DY:124:ARG:NH2	2.45	0.49
18:D3:827:C:H2'	18:D3:828:U:C6	2.47	0.49
7:CL:719:ASN:HA	7:CL:722:LYS:HE2	1.93	0.49
7:CL:831:ARG:HD3	7:CL:838:ILE:HG22	1.92	0.49
18:D3:1564:U:H2'	18:D3:1565:C:C6	2.48	0.49
7:CL:87:ARG:NH2	7:CL:99:ASN:OD1	2.46	0.49
15:DS:17:LEU:O	15:DS:20:THR:OG1	2.25	0.49
7:CL:105:ILE:HG13	7:CL:356:ALA:HB2	1.95	0.49
7:CL:870:ARG:NH1	18:D3:574:G:OP1	2.45	0.49
4:UX:72:ILE:O	4:UX:76:ILE:HG12	2.13	0.49
8:CM:190:SER:OG	8:CM:191:ILE:N	2.46	0.49
7:CL:140:LEU:HD11	7:CL:152:THR:HG23	1.95	0.49
18:D3:142:G:H5''	21:DG:139:ASN:HD21	1.78	0.49
18:D3:647:G:N2	18:D3:687:G:H22	2.11	0.49
18:D3:649:U:O2'	18:D3:650:U:O5'	2.26	0.49
18:D3:734:A:H3'	18:D3:734:A:H8	1.77	0.49
21:DG:10:ASN:OD1	21:DG:128:THR:OG1	2.23	0.49
7:CL:983:PRO:HB2	7:CL:986:HIS:HB2	1.94	0.48
8:CM:148:GLU:HB2	8:CM:171:ASP:HB2	1.95	0.48
22:DH:48:GLU:OE2	22:DH:88:ARG:NH2	2.46	0.48
8:CM:233:GLU:OE2	8:CM:233:GLU:N	2.46	0.48
14:DQ:11:GLY:N	14:DQ:18:ALA:O	2.43	0.48
18:D3:734:A:C8	18:D3:734:A:C3'	2.96	0.48
20:DE:100:ARG:NH2	20:DE:121:TYR:O	2.45	0.48
15:DS:71:GLN:HA	15:DS:74:GLN:HG2	1.95	0.48
18:D3:828:U:O4	18:D3:829:A:N6	2.36	0.48
18:D3:1498:G:H2'	18:D3:1499:G:C8	2.48	0.48
5:CJ:157:PHE:O	5:CJ:159:HIS:N	2.47	0.48
8:CM:47:ASP:OD1	8:CM:47:ASP:N	2.45	0.48
18:D3:269:G:C5	18:D3:287:G:C2	3.01	0.48
18:D3:693:U:N3	18:D3:695:U:O4	2.46	0.48
18:D3:1041:G:H2'	18:D3:1042:G:C8	2.48	0.48
21:DG:24:ILE:HG22	21:DG:28:PHE:HE1	1.78	0.48
23:DI:12:SER:OG	23:DI:13:ALA:N	2.47	0.48
16:DT:20:SER:O	16:DT:24:ARG:N	2.42	0.48
18:D3:1001:A:H3'	18:D3:1002:G:C8	2.48	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D3:1490:C:N3	18:D3:1492:A:N6	2.60	0.48
7:CL:549:ILE:HB	7:CL:567:TRP:CD1	2.49	0.48
7:CL:968:THR:OG1	7:CL:972:ILE:N	2.45	0.48
18:D3:220:A:OP2	18:D3:831:U:O2'	2.18	0.48
18:D3:851:U:H2'	18:D3:852:C:C2	2.48	0.48
20:DE:35:PRO:HB2	20:DE:36:HIS:CD2	2.49	0.48
5:CJ:165:PHE:HA	5:CJ:258:LEU:HA	1.94	0.48
21:DG:173:PRO:HB2	21:DG:174:LYS:H	1.47	0.48
22:DH:136:VAL:HG23	22:DH:155:ASP:HA	1.95	0.48
6:CK:347:PHE:HE2	6:CK:349:ARG:HH11	1.61	0.48
12:JJ:224:ILE:HG12	12:JJ:233:ILE:HG12	1.95	0.48
18:D3:220:A:N7	18:D3:832:U:C4	2.81	0.48
18:D3:1472:C:C2	18:D3:1534:G:N1	2.82	0.48
31:DY:57:VAL:HG13	31:DY:60:PHE:HE2	1.79	0.48
18:D3:237:C:H2'	18:D3:834:G:H4'	1.95	0.48
20:DE:252:ARG:HD3	24:DJ:71:PHE:HE1	1.77	0.48
6:CK:337:GLU:HG3	7:CL:953:SER:HB3	1.95	0.48
18:D3:320:U:H3'	18:D3:321:C:H2'	1.96	0.48
18:D3:577:G:N2	18:D3:581:U:O2'	2.46	0.48
18:D3:849:C:H2'	18:D3:850:A:C8	2.49	0.48
29:DW:30:SER:HA	29:DW:34:ILE:HD12	1.96	0.48
1:UB:753:LYS:NZ	6:CK:356:VAL:H	2.12	0.47
6:CK:341:LEU:HD23	7:CL:960:ARG:HD2	1.96	0.47
11:JL:157:ARG:NH2	11:JL:203:GLU:OE1	2.46	0.47
21:DG:39:GLU:HG3	21:DG:46:LYS:HG2	1.95	0.47
7:CL:280:LEU:HD12	7:CL:281:PRO:HD2	1.96	0.47
8:CM:113:LYS:HD2	8:CM:171:ASP:HA	1.97	0.47
18:D3:433:C:N4	18:D3:436:A:OP1	2.46	0.47
18:D3:844:A:H2'	18:D3:845:G:C8	2.49	0.47
7:CL:933:LYS:HA	7:CL:1003:LEU:O	2.14	0.47
18:D3:78:A:H1'	21:DG:175:ILE:HG12	1.96	0.47
18:D3:219:A:C5	18:D3:843:U:H1'	2.49	0.47
18:D3:351:C:O4'	30:DX:13:ARG:NH1	2.47	0.47
18:D3:739:G:H2'	18:D3:740:A:C8	2.50	0.47
21:DG:2:LYS:HB3	21:DG:108:VAL:HG22	1.96	0.47
31:DY:122:GLY:O	31:DY:124:ARG:N	2.47	0.47
8:CM:83:GLY:HA2	8:CM:114:PHE:CE1	2.50	0.47
12:JJ:102:PRO:HD2	12:JJ:163:THR:HG23	1.97	0.47
18:D3:1542:G:N2	18:D3:1569:A:C8	2.76	0.47
18:D3:1603:U:H2'	18:D3:1604:U:C6	2.49	0.47
19:DA:39:GLU:N	19:DA:74:GLN:OE1	2.40	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:DE:171:ASP:OD1	20:DE:172:PHE:N	2.47	0.47
11:JL:41:ASN:HB2	11:JL:195:ASN:HB3	1.96	0.47
18:D3:710:U:N3	18:D3:730:G:C6	2.83	0.47
18:D3:1548:G:N1	18:D3:1564:U:N3	2.63	0.47
18:D3:1753:A:H2'	18:D3:1754:A:C8	2.49	0.47
22:DH:50:ASP:OD1	22:DH:50:ASP:N	2.47	0.47
12:JJ:110:ARG:HD3	12:JJ:130:MET:HE3	1.97	0.47
18:D3:22:A:H2'	18:D3:23:G:C8	2.49	0.47
18:D3:358:U:O2'	18:D3:360:A:OP1	2.26	0.47
18:D3:1486:G:N2	18:D3:1592:A:H4'	2.30	0.47
20:DE:81:THR:O	20:DE:81:THR:OG1	2.28	0.47
21:DG:159:ARG:HA	21:DG:171:LYS:O	2.14	0.47
30:DX:86:PHE:HB2	30:DX:120:VAL:HG11	1.95	0.47
8:CM:123:ALA:HB1	8:CM:261:ILE:HG21	1.96	0.47
18:D3:150:U:OP1	31:DY:123:LYS:NZ	2.48	0.47
18:D3:840:U:O2'	18:D3:841:U:O4'	2.33	0.47
15:DS:48:LYS:HE2	16:DT:35:ASP:HA	1.96	0.47
21:DG:191:ARG:HA	21:DG:191:ARG:HD3	1.68	0.47
25:DL:74:THR:HG22	25:DL:122:ILE:HG12	1.97	0.47
9:JG:208:ALA:HB2	9:JG:234:ALA:H	1.80	0.47
15:DS:16:ARG:HA	15:DS:20:THR:O	2.15	0.47
18:D3:1471:A:C6	18:D3:1536:G:O6	2.68	0.47
18:D3:1594:G:HO2'	18:D3:1600:A:H61	1.58	0.47
34:JD:1021:LYS:O	34:JD:1025:MET:N	2.48	0.47
6:CK:348:ASP:OD1	6:CK:349:ARG:N	2.41	0.46
25:DL:33:ARG:HH11	25:DL:61:THR:HG21	1.80	0.46
1:UB:764:ARG:O	1:UB:767:ILE:N	2.46	0.46
7:CL:748:ASP:OD1	7:CL:748:ASP:N	2.46	0.46
18:D3:1494:C:H2'	18:D3:1495:C:C6	2.50	0.46
20:DE:37:LYS:HB2	20:DE:40:GLU:HG2	1.96	0.46
20:DE:188:ASN:HB3	20:DE:191:ARG:HD3	1.97	0.46
21:DG:71:THR:OG1	21:DG:72:ARG:N	2.48	0.46
34:JD:1205:SER:HB2	34:JD:1208:GLU:HB3	1.97	0.46
18:D3:196:G:H2'	18:D3:197:A:H8	1.80	0.46
18:D3:1592:A:H2'	18:D3:1593:A:C8	2.50	0.46
7:CL:56:VAL:HG22	30:DX:52:ILE:HG12	1.96	0.46
18:D3:487:G:O5'	18:D3:487:G:H8	1.98	0.46
18:D3:1152:A:H2'	18:D3:1153:G:H8	1.79	0.46
23:DI:42:ARG:NH1	23:DI:59:ARG:HE	2.13	0.46
24:DJ:112:GLN:O	24:DJ:116:LEU:HD23	2.16	0.46
1:UB:753:LYS:HD2	1:UB:753:LYS:HA	1.62	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D3:453:U:H2'	18:D3:454:U:H5''	1.96	0.46
18:D3:726:C:N4	18:D3:727:U:O4	2.48	0.46
18:D3:814:A:N6	18:D3:816:G:C6	2.84	0.46
18:D3:1472:C:C2	18:D3:1534:G:N2	2.84	0.46
7:CL:548:ASN:HB3	7:CL:551:LYS:HG2	1.96	0.46
18:D3:1545:A:N1	18:D3:1567:U:N3	2.63	0.46
19:DA:74:GLN:HE21	19:DA:189:ILE:HG21	1.80	0.46
24:DJ:45:ILE:HG13	24:DJ:105:LEU:HD11	1.97	0.46
1:UB:701:ALA:HB2	3:US:416:LEU:O	2.16	0.46
4:UX:81:ASP:OD1	4:UX:82:ILE:N	2.49	0.46
20:DE:95:THR:O	20:DE:97:GLU:HG3	2.16	0.46
16:DT:115:GLU:O	16:DT:123:ARG:N	2.46	0.46
18:D3:202:A:H2'	18:D3:203:U:O4'	2.15	0.46
19:DA:212:VAL:O	19:DA:214:LYS:N	2.46	0.46
18:D3:734:A:C8	18:D3:734:A:O5'	2.69	0.46
11:JL:99:ARG:NH1	11:JL:104:GLU:OE2	2.41	0.46
21:DG:3:LEU:O	21:DG:15:THR:HA	2.16	0.46
7:CL:636:LEU:HA	7:CL:636:LEU:HD23	1.80	0.45
18:D3:231:U:O2	18:D3:234:G:N1	2.31	0.45
18:D3:504:U:C6	18:D3:504:U:H3'	2.52	0.45
18:D3:1495:C:O5'	18:D3:1495:C:H6	1.99	0.45
18:D3:1496:U:H1'	18:D3:1512:G:N2	2.31	0.45
7:CL:88:SER:HB3	7:CL:214:ARG:HB2	1.98	0.45
7:CL:629:ASP:O	7:CL:632:LYS:HB2	2.15	0.45
8:CM:225:ILE:N	18:D3:1130:A:H61	2.14	0.45
12:JJ:221:ARG:HE	12:JJ:271:LYS:NZ	2.13	0.45
18:D3:1512:G:C8	18:D3:1512:G:OP2	2.70	0.45
23:DI:76:THR:HG22	23:DI:108:PRO:HG2	1.98	0.45
34:JD:1256:PHE:HA	34:JD:1259:ILE:HG22	1.97	0.45
7:CL:81:GLY:HA2	38:CL:2001:GTP:O3A	2.16	0.45
7:CL:611:PHE:HZ	8:CM:137:LEU:HD11	1.81	0.45
16:DT:77:ASN:HA	16:DT:96:ALA:HB3	1.98	0.45
18:D3:73:U:O2	18:D3:74:U:N3	2.50	0.45
18:D3:191:C:O2'	18:D3:192:U:O5'	2.32	0.45
18:D3:485:A:C5'	18:D3:485:A:H8	2.28	0.45
18:D3:1594:G:HO2'	18:D3:1600:A:N6	2.15	0.45
4:UX:51:LEU:HG	4:UX:52:PHE:O	2.17	0.45
5:CJ:74:ASP:O	5:CJ:78:ALA:N	2.50	0.45
7:CL:606:VAL:HG22	7:CL:607:ASP:H	1.81	0.45
18:D3:221:A:H2'	18:D3:222:A:C8	2.51	0.45
19:DA:31:ASP:HB3	19:DA:45:LYS:HD3	1.99	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:DG:73:ILE:O	21:DG:96:SER:HA	2.16	0.45
11:JL:51:LYS:HA	11:JL:51:LYS:HD2	1.76	0.45
18:D3:24:U:H2'	18:D3:25:C:C4	2.51	0.45
18:D3:754:A:N6	18:D3:793:A:N7	2.64	0.45
18:D3:855:A:O2'	18:D3:856:A:H3'	2.16	0.45
18:D3:1511:U:H2'	18:D3:1512:G:C8	2.51	0.45
18:D3:802:G:H21	29:DW:107:SER:HG	1.61	0.45
30:DX:46:SER:OG	30:DX:47:SER:N	2.50	0.45
1:UB:774:SER:O	1:UB:778:HIS:ND1	2.50	0.45
8:CM:201:SER:HA	8:CM:202:PRO:HD3	1.81	0.45
11:JL:259:LEU:O	11:JL:263:ASN:N	2.50	0.45
13:DF:78:ALA:O	18:D3:1615:C:N4	2.35	0.45
18:D3:329:G:H5''	23:DI:98:LYS:HB3	1.97	0.45
18:D3:814:A:C6	18:D3:816:G:C6	3.05	0.45
21:DG:21:GLU:O	21:DG:25:ARG:N	2.48	0.45
6:CK:295:LYS:HD2	6:CK:296:ASN:HB2	1.99	0.45
12:JJ:169:ASP:N	12:JJ:169:ASP:OD1	2.49	0.45
18:D3:218:A:C6	18:D3:830:U:C2	3.05	0.45
18:D3:712:G:C6	18:D3:727:U:C4	3.05	0.45
18:D3:1174:C:O2'	18:D3:1601:G:O2'	2.33	0.45
18:D3:1545:A:C2	18:D3:1567:U:C2	3.05	0.45
19:DA:122:GLU:OE2	19:DA:213:ARG:NH2	2.50	0.45
20:DE:133:LYS:HB2	20:DE:133:LYS:HE3	1.74	0.45
34:JD:804:ALA:N	34:JD:836:GLN:O	2.50	0.45
6:CK:304:GLN:HB3	6:CK:308:ARG:NH2	2.30	0.45
8:CM:23:LEU:HD23	8:CM:23:LEU:HA	1.83	0.45
18:D3:782:U:H4'	31:DY:12:VAL:HG11	1.99	0.45
18:D3:1492:A:O2'	18:D3:1493:A:O4'	2.35	0.45
18:D3:1528:U:O4	18:D3:1529:C:N4	2.50	0.45
26:DN:39:LYS:HE3	26:DN:39:LYS:HB2	1.78	0.45
7:CL:9:ARG:NH1	18:D3:619:A:N3	2.66	0.44
18:D3:1479:A:H2'	18:D3:1480:G:C8	2.52	0.44
19:DA:70:LEU:O	19:DA:74:GLN:N	2.51	0.44
11:JL:63:VAL:HG12	11:JL:129:THR:HG21	1.99	0.44
11:JL:72:VAL:O	11:JL:76:GLU:HG2	2.16	0.44
16:DT:47:PRO:HA	18:D3:1477:G:H4'	2.00	0.44
18:D3:601:A:H2'	18:D3:602:U:O4'	2.17	0.44
18:D3:736:C:C6	18:D3:736:C:C4'	3.00	0.44
18:D3:884:A:OP1	19:DA:136:ARG:NH2	2.50	0.44
18:D3:1506:G:H4'	18:D3:1551:U:H5'	1.99	0.44
19:DA:94:LYS:C	19:DA:95:ASN:HD22	2.19	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:DA:129:THR:OG1	19:DA:131:ASP:O	2.31	0.44
8:CM:301:MET:HE3	8:CM:311:LEU:HD22	1.99	0.44
12:JJ:159:ILE:HD12	12:JJ:159:ILE:HG23	1.80	0.44
18:D3:1:U:O2'	18:D3:2:A:H5''	2.17	0.44
18:D3:600:U:H2'	18:D3:601:A:O4'	2.18	0.44
20:DE:21:ASP:OD1	20:DE:21:ASP:N	2.49	0.44
4:UX:105:GLU:OE1	33:UN:439:ARG:NH1	2.49	0.44
18:D3:1552:U:H3'	18:D3:1553:G:C8	2.53	0.44
27:DO:22:SER:OG	27:DO:23:PHE:O	2.25	0.44
4:UX:76:ILE:HD11	4:UX:119:LEU:HG	2.00	0.44
8:CM:54:ARG:HD3	8:CM:54:ARG:HA	1.80	0.44
18:D3:25:C:H42	18:D3:601:A:H61	1.65	0.44
18:D3:119:A:H1'	18:D3:397:A:C5	2.53	0.44
18:D3:208:U:O2'	23:DI:180:ASP:OD2	2.23	0.44
18:D3:496:G:H8	18:D3:498:G:O5'	2.00	0.44
18:D3:701:U:C6	18:D3:701:U:O5'	2.70	0.44
18:D3:835:U:H2'	18:D3:836:U:C6	2.52	0.44
18:D3:1162:C:H2'	18:D3:1163:A:C8	2.52	0.44
18:D3:1477:G:C6	18:D3:1531:G:N1	2.86	0.44
18:D3:1503:A:H3'	18:D3:1504:G:H8	1.82	0.44
18:D3:1517:U:H2'	18:D3:1518:C:H5	1.83	0.44
19:DA:120:LEU:HD12	19:DA:142:PHE:CE2	2.53	0.44
21:DG:150:GLU:OE1	21:DG:150:GLU:N	2.51	0.44
8:CM:95:PRO:HG3	8:CM:124:SER:HB3	1.99	0.44
15:DS:49:LYS:HD2	15:DS:49:LYS:HA	1.83	0.44
18:D3:504:U:C6	18:D3:504:U:C3'	3.00	0.44
18:D3:699:U:H3	18:D3:739:G:H1	1.64	0.44
7:CL:137:LEU:HD12	7:CL:166:ARG:O	2.18	0.44
7:CL:350:LYS:HB3	7:CL:350:LYS:HE2	1.82	0.44
18:D3:218:A:N6	18:D3:830:U:C2	2.85	0.44
30:DX:130:VAL:HG21	30:DX:135:LEU:HD21	1.99	0.44
8:CM:198:THR:O	8:CM:239:PRO:HA	2.18	0.44
11:JL:167:PRO:HG2	11:JL:299:ASP:HB3	2.00	0.44
18:D3:58:U:O2'	18:D3:451:A:N3	2.49	0.44
18:D3:224:C:H2'	18:D3:225:A:C8	2.50	0.44
18:D3:740:A:N6	18:D3:741:C:N4	2.66	0.44
1:UB:667:LEU:O	1:UB:670:ALA:HB3	2.18	0.44
7:CL:156:LEU:HD23	7:CL:156:LEU:HA	1.78	0.44
8:CM:291:ARG:HH11	8:CM:291:ARG:HD3	1.68	0.44
18:D3:416:A:H5'	18:D3:417:A:N7	2.33	0.44
18:D3:1546:G:H2'	18:D3:1547:A:C8	2.53	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D3:1548:G:C2	18:D3:1564:U:C2	3.06	0.44
24:DJ:184:SER:OG	24:DJ:185:GLY:N	2.50	0.44
7:CL:943:LYS:HB3	7:CL:943:LYS:HE2	1.60	0.43
18:D3:736:C:C6	18:D3:736:C:C5'	2.85	0.43
18:D3:885:G:N2	27:DO:123:SER:O	2.51	0.43
18:D3:1589:C:H2'	18:D3:1590:G:C8	2.53	0.43
19:DA:219:LYS:HB3	19:DA:219:LYS:HE3	1.70	0.43
21:DG:20:ASP:HB3	21:DG:23:ARG:HD3	2.00	0.43
22:DH:87:ASP:O	22:DH:88:ARG:NH1	2.43	0.43
26:DN:61:THR:OG1	26:DN:62:GLN:N	2.51	0.43
7:CL:977:LYS:NZ	18:D3:1598:U:OP2	2.34	0.43
14:DQ:11:GLY:O	14:DQ:18:ALA:N	2.51	0.43
18:D3:1173:C:H2'	18:D3:1174:C:H6	1.83	0.43
18:D3:1482:C:OP2	18:D3:1521:G:N2	2.51	0.43
24:DJ:110:GLN:NE2	24:DJ:126:ARG:HB2	2.33	0.43
7:CL:301:ILE:HD12	7:CL:783:PHE:CE2	2.53	0.43
7:CL:830:ARG:NH2	7:CL:831:ARG:O	2.51	0.43
18:D3:218:A:N6	18:D3:830:U:N3	2.65	0.43
18:D3:593:U:HO2'	18:D3:595:G:HO2'	1.53	0.43
18:D3:834:G:H3'	18:D3:835:U:C5	2.53	0.43
26:DN:84:ILE:HD13	26:DN:149:LEU:HD21	1.99	0.43
29:DW:61:ILE:HG21	29:DW:61:ILE:HD13	1.73	0.43
34:JD:5:ARG:HH21	34:JD:7:ARG:NE	2.15	0.43
7:CL:126:ASN:OD1	7:CL:853:ARG:NE	2.51	0.43
7:CL:230:MET:HB3	7:CL:230:MET:HE2	1.84	0.43
7:CL:748:ASP:OD1	7:CL:749:THR:N	2.50	0.43
7:CL:859:ILE:HG21	7:CL:1011:VAL:HG12	2.01	0.43
8:CM:83:GLY:HA2	8:CM:114:PHE:HE1	1.84	0.43
11:JL:275:ASP:O	11:JL:278:LYS:HB3	2.19	0.43
18:D3:136:C:H4'	18:D3:137:U:H5'	2.00	0.43
18:D3:486:G:H4'	18:D3:486:G:OP1	2.18	0.43
18:D3:1523:G:OP2	18:D3:1523:G:N2	2.39	0.43
21:DG:75:LEU:HA	21:DG:75:LEU:HD23	1.80	0.43
22:DH:44:LYS:HG3	22:DH:63:PRO:HD3	2.00	0.43
24:DJ:97:LEU:HD23	24:DJ:97:LEU:HA	1.86	0.43
8:CM:106:LEU:HA	8:CM:106:LEU:HD23	1.84	0.43
8:CM:337:VAL:HG13	8:CM:354:ILE:HG13	2.01	0.43
8:CM:338:PHE:CE2	8:CM:340:LYS:HB3	2.53	0.43
11:JL:58:ASP:O	11:JL:79:LYS:HG2	2.19	0.43
14:DQ:13:LYS:N	14:DQ:16:ALA:O	2.52	0.43
18:D3:692:C:H2'	18:D3:693:U:H6	1.84	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D3:1477:G:C5	18:D3:1531:G:C2	3.07	0.43
18:D3:1478:G:H2'	18:D3:1479:A:C8	2.50	0.43
18:D3:1524:A:H2'	18:D3:1525:A:C8	2.52	0.43
18:D3:1551:U:H2'	18:D3:1552:U:C6	2.54	0.43
18:D3:1552:U:N3	18:D3:1556:A:C8	2.73	0.43
7:CL:143:ASP:OD1	7:CL:146:PHE:N	2.36	0.43
7:CL:157:ASN:HD22	7:CL:911:PHE:HZ	1.65	0.43
7:CL:855:GLN:HE22	7:CL:1031:GLY:HA3	1.83	0.43
8:CM:176:GLN:HE21	8:CM:305:LYS:HB3	1.83	0.43
9:JG:114:ILE:O	9:JG:121:LEU:HA	2.18	0.43
18:D3:992:A:O2'	18:D3:1785:U:O2	2.30	0.43
18:D3:1579:U:H2'	18:D3:1580:C:C6	2.54	0.43
20:DE:128:LYS:HB3	20:DE:128:LYS:HE2	1.81	0.43
22:DH:50:ASP:HA	22:DH:56:LYS:HD3	2.00	0.43
22:DH:83:LYS:HE3	22:DH:83:LYS:HB3	1.77	0.43
34:JD:827:SER:O	34:JD:831:GLU:N	2.44	0.43
34:JD:1216:ARG:HH12	34:JD:1219:SER:C	2.22	0.43
7:CL:626:LYS:HB2	7:CL:626:LYS:HE2	1.70	0.43
7:CL:940:LYS:HB3	7:CL:947:PHE:HB2	2.01	0.43
11:JL:289:ASP:OD2	11:JL:293:LYS:NZ	2.38	0.43
18:D3:1519:U:H3'	18:D3:1520:U:H2'	1.99	0.43
34:JD:447:ILE:HA	34:JD:514:ILE:O	2.19	0.43
7:CL:869:THR:O	7:CL:869:THR:OG1	2.30	0.43
7:CL:870:ARG:NH2	18:D3:573:C:O2'	2.39	0.43
7:CL:871:MET:HB2	7:CL:928:ILE:HG22	2.00	0.43
18:D3:485:A:H8	18:D3:485:A:O5'	2.02	0.43
18:D3:1173:C:H2'	18:D3:1174:C:C6	2.54	0.43
18:D3:1511:U:C2'	18:D3:1512:G:H5'	2.49	0.43
18:D3:1529:C:C4	18:D3:1530:C:N4	2.87	0.43
33:UN:382:LEU:HD23	33:UN:382:LEU:HA	1.89	0.43
7:CL:321:GLU:C	7:CL:322:ARG:HD2	2.39	0.43
29:DW:29:PRO:HB3	29:DW:58:SER:HB3	2.00	0.43
18:D3:218:A:N1	18:D3:830:U:C4	2.87	0.43
18:D3:1542:G:N2	18:D3:1569:A:OP1	2.48	0.43
19:DA:190:PRO:HG2	19:DA:192:VAL:HG23	2.01	0.43
12:JJ:204:ARG:HH12	12:JJ:253:GLY:HA2	1.84	0.42
18:D3:1161:C:H1'	18:D3:1619:C:H42	1.84	0.42
19:DA:201:THR:HG23	19:DA:204:ILE:HD12	2.01	0.42
21:DG:32:ILE:HG12	21:DG:100:ALA:HB1	2.00	0.42
31:DY:29:HIS:NE2	31:DY:69:SER:OG	2.43	0.42
31:DY:81:GLU:HA	31:DY:84:LYS:HG2	2.00	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:CM:312:ARG:NE	8:CM:349:ASP:OD2	2.31	0.42
12:JJ:131:ASN:OD1	12:JJ:133:LYS:N	2.53	0.42
18:D3:570:A:H2'	18:D3:571:G:C8	2.55	0.42
18:D3:780:A:H62	31:DY:10:ARG:NH2	2.13	0.42
18:D3:1484:G:H2'	18:D3:1485:C:C6	2.54	0.42
24:DJ:162:SER:HG	24:DJ:165:GLY:H	1.65	0.42
29:DW:55:ASP:OD1	29:DW:55:ASP:N	2.28	0.42
34:JD:826:SER:O	34:JD:830:PHE:N	2.46	0.42
8:CM:274:LYS:O	8:CM:278:GLN:HG3	2.18	0.42
11:JL:75:LEU:HD12	11:JL:103:VAL:HB	2.01	0.42
12:JJ:225:VAL:HG12	12:JJ:232:HIS:HB2	2.00	0.42
18:D3:95:G:O2'	18:D3:460:A:O2'	2.32	0.42
18:D3:500:C:C6	18:D3:500:C:H3'	2.53	0.42
2:UC:542:TYR:OH	2:UC:548:LYS:NZ	2.52	0.42
4:UX:77:GLN:O	18:D3:1098:U:O2'	2.25	0.42
12:JJ:263:LEU:HD12	12:JJ:263:LEU:HA	1.75	0.42
18:D3:501:U:H1'	18:D3:502:U:C5	2.54	0.42
18:D3:1545:A:H2'	18:D3:1546:G:C8	2.54	0.42
19:DA:36:SER:HB2	19:DA:231:LEU:O	2.18	0.42
19:DA:94:LYS:O	19:DA:95:ASN:ND2	2.45	0.42
22:DH:9:LEU:HD13	22:DH:17:GLU:HB3	2.01	0.42
7:CL:838:ILE:HD11	18:D3:578:U:N3	2.35	0.42
11:JL:253:LYS:HB2	11:JL:253:LYS:HE3	1.75	0.42
12:JJ:102:PRO:HA	12:JJ:103:PRO:HD3	1.91	0.42
18:D3:199:G:H2'	18:D3:200:A:C8	2.55	0.42
18:D3:712:G:N1	18:D3:727:U:C4	2.87	0.42
18:D3:734:A:H8	18:D3:734:A:O5'	2.03	0.42
18:D3:1150:G:H2'	18:D3:1151:A:C8	2.54	0.42
21:DG:121:LEU:HD23	21:DG:121:LEU:HA	1.88	0.42
22:DH:147:ASN:OD1	22:DH:147:ASN:N	2.52	0.42
25:DL:29:LYS:NZ	25:DL:32:LYS:HA	2.35	0.42
34:JD:117:LEU:HA	34:JD:117:LEU:HD23	1.81	0.42
4:UX:102:VAL:HG22	4:UX:137:ALA:HB1	2.00	0.42
18:D3:72:A:N7	21:DG:169:TYR:OH	2.45	0.42
18:D3:205:U:H2'	18:D3:206:A:H8	1.85	0.42
18:D3:504:U:C2'	18:D3:505:A:H4'	2.48	0.42
18:D3:886:U:O2	27:DO:123:SER:N	2.49	0.42
18:D3:1479:A:H2'	18:D3:1480:G:H8	1.84	0.42
18:D3:1538:U:H2'	18:D3:1539:G:H2'	2.01	0.42
20:DE:86:PHE:CE2	20:DE:184:THR:HG21	2.55	0.42
21:DG:199:GLN:O	21:DG:203:GLU:HG2	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:JD:26:ILE:O	34:JD:29:LYS:HG2	2.19	0.42
8:CM:191:ILE:HB	8:CM:223:VAL:HG22	2.02	0.42
18:D3:182:A:H2'	18:D3:183:U:C6	2.55	0.42
18:D3:559:C:H2'	18:D3:560:U:C6	2.54	0.42
18:D3:922:G:H2'	18:D3:923:A:H8	1.85	0.42
18:D3:1152:A:H2'	18:D3:1153:G:C8	2.54	0.42
18:D3:1545:A:N1	18:D3:1567:U:C4	2.88	0.42
18:D3:1619:C:H2'	18:D3:1620:C:C6	2.54	0.42
24:DJ:86:LEU:HD12	24:DJ:87:SER:H	1.84	0.42
29:DW:78:ARG:HE	29:DW:126:LEU:HD23	1.85	0.42
2:UC:576:LEU:HG	2:UC:580:ARG:HD3	2.02	0.42
12:JJ:124:LEU:HD12	12:JJ:124:LEU:HA	1.87	0.42
12:JJ:125:LYS:O	12:JJ:146:THR:HG22	2.19	0.42
18:D3:710:U:N3	18:D3:730:G:C5	2.87	0.42
22:DH:126:LEU:HA	22:DH:126:LEU:HD23	1.78	0.42
33:UN:435:ARG:NH1	33:UN:480:LYS:O	2.53	0.42
7:CL:78:PRO:HD3	7:CL:122:ALA:HB1	2.01	0.42
7:CL:879:THR:HB	7:CL:880:TYR:H	1.66	0.42
16:DT:99:SER:N	18:D3:1502:G:O6	2.53	0.42
18:D3:139:C:HO2'	18:D3:140:A:P	2.42	0.42
18:D3:1486:G:H2'	18:D3:1487:A:H8	1.84	0.42
18:D3:1517:U:O2	18:D3:1517:U:O2'	2.32	0.42
18:D3:1583:A:N6	18:D3:1612:U:OP2	2.53	0.42
23:DI:138:ASN:HB3	23:DI:142:LYS:NZ	2.34	0.42
25:DL:2:SER:N	25:DL:82:ARG:HG2	2.34	0.42
25:DL:53:TYR:CD1	25:DL:113:PRO:HG2	2.55	0.42
29:DW:103:ILE:HG22	29:DW:126:LEU:HD12	2.00	0.42
30:DX:107:PHE:CE2	30:DX:109:ARG:HD2	2.55	0.42
34:JD:1093:ALA:HA	34:JD:1121:LEU:H	1.85	0.42
5:CJ:261:LEU:O	5:CJ:274:GLU:N	2.53	0.42
6:CK:332:ALA:HA	6:CK:335:ARG:HG2	2.02	0.42
8:CM:202:PRO:HG3	8:CM:229:VAL:HG11	2.01	0.42
12:JJ:141:THR:OG1	12:JJ:146:THR:HG21	2.20	0.42
18:D3:924:A:H2'	18:D3:925:G:C8	2.55	0.42
21:DG:92:ARG:HE	21:DG:92:ARG:HB2	1.63	0.42
22:DH:34:LEU:HD12	22:DH:34:LEU:HA	1.93	0.42
34:JD:33:ARG:HD3	34:JD:33:ARG:HA	1.77	0.42
2:UC:544:ILE:HD13	2:UC:544:ILE:HG21	1.72	0.41
7:CL:613:PRO:HD3	8:CM:292:ASN:HD22	1.84	0.41
18:D3:739:G:O2'	18:D3:740:A:H5'	2.21	0.41
19:DA:164:ILE:HG23	19:DA:201:THR:HG21	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:CM:351:ILE:HD13	8:CM:351:ILE:HA	1.91	0.41
18:D3:494:U:O2'	18:D3:495:C:O5'	2.31	0.41
26:DN:121:ARG:HH11	26:DN:121:ARG:HD2	1.70	0.41
7:CL:142:ILE:HG21	7:CL:142:ILE:HD13	1.84	0.41
11:JL:270:LYS:N	11:JL:275:ASP:OD2	2.53	0.41
18:D3:500:C:C6	18:D3:500:C:C3'	3.03	0.41
18:D3:583:C:H2'	18:D3:584:C:H5''	2.02	0.41
18:D3:1602:C:H2'	18:D3:1603:U:C6	2.55	0.41
19:DA:152:ARG:H	19:DA:152:ARG:HG2	1.64	0.41
31:DY:108:ARG:HH11	31:DY:108:ARG:HD2	1.72	0.41
34:JD:411:ILE:O	34:JD:580:VAL:HA	2.20	0.41
18:D3:280:U:O2'	18:D3:281:G:OP2	2.34	0.41
18:D3:330:G:OP2	23:DI:172:ARG:NH1	2.53	0.41
18:D3:584:C:OP1	18:D3:584:C:H4'	2.20	0.41
18:D3:703:G:H2'	18:D3:704:C:H5'	2.02	0.41
23:DI:165:LEU:HD22	23:DI:183:ILE:HD13	2.02	0.41
24:DJ:107:ARG:HA	24:DJ:107:ARG:HD2	1.69	0.41
24:DJ:150:LEU:HA	24:DJ:150:LEU:HD12	1.85	0.41
11:JL:39:LEU:HD11	11:JL:44:VAL:HG11	2.02	0.41
18:D3:199:G:O2'	18:D3:200:A:O4'	2.32	0.41
18:D3:325:G:OP1	25:DL:134:THR:OG1	2.36	0.41
20:DE:77:ARG:HD3	20:DE:77:ARG:HA	1.78	0.41
21:DG:193:LEU:HA	21:DG:193:LEU:HD23	1.82	0.41
25:DL:3:THR:OG1	25:DL:113:PRO:HG3	2.20	0.41
7:CL:830:ARG:HG3	7:CL:831:ARG:O	2.20	0.41
15:DS:60:GLU:HG3	15:DS:61:LEU:HD12	2.02	0.41
18:D3:483:A:N1	18:D3:505:A:H1'	2.35	0.41
18:D3:793:A:H4'	18:D3:794:U:C5	2.56	0.41
20:DE:127:LYS:HA	20:DE:127:LYS:HD2	1.89	0.41
21:DG:48:TYR:OH	21:DG:119:GLN:O	2.26	0.41
23:DI:152:ILE:HG13	23:DI:153:GLU:N	2.32	0.41
29:DW:38:LEU:HD23	29:DW:38:LEU:HA	1.80	0.41
34:JD:1252:THR:OG1	34:JD:1253:ARG:N	2.53	0.41
5:CJ:279:ARG:N	18:D3:1596:C:O2	2.44	0.41
7:CL:552:LEU:HB3	7:CL:563:CYS:SG	2.60	0.41
8:CM:18:ARG:HD3	8:CM:98:TYR:CZ	2.55	0.41
15:DS:17:LEU:HD12	15:DS:22:VAL:HB	2.03	0.41
18:D3:788:A:OP2	20:DE:108:ARG:NH1	2.54	0.41
26:DN:99:ARG:O	26:DN:103:GLU:HG2	2.20	0.41
29:DW:14:ILE:HD13	29:DW:14:ILE:HG21	1.86	0.41
4:UX:158:ALA:O	4:UX:162:GLN:HG2	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:CL:561:GLU:O	7:CL:565:ARG:HG3	2.20	0.41
7:CL:720:ALA:O	7:CL:724:GLU:HG2	2.19	0.41
8:CM:60:THR:O	8:CM:60:THR:OG1	2.38	0.41
18:D3:143:G:P	21:DG:139:ASN:HD22	2.44	0.41
18:D3:584:C:H5'	18:D3:586:G:H3'	2.03	0.41
18:D3:1057:U:O2	18:D3:1058:U:O2'	2.36	0.41
4:UX:65:VAL:HG12	4:UX:152:ILE:CG1	2.51	0.41
7:CL:227:ILE:HD13	7:CL:227:ILE:HG21	1.82	0.41
7:CL:237:TRP:CZ2	7:CL:850:GLY:HA2	2.56	0.41
7:CL:631:ILE:HD12	7:CL:631:ILE:HA	1.92	0.41
8:CM:104:LEU:HD22	8:CM:141:MET:SD	2.60	0.41
8:CM:217:LYS:HE3	8:CM:217:LYS:HB3	1.92	0.41
8:CM:298:ILE:HD13	8:CM:298:ILE:HA	1.94	0.41
18:D3:103:A:H8	18:D3:103:A:H2'	1.63	0.41
18:D3:144:U:HO2'	18:D3:145:A:H8	1.65	0.41
18:D3:650:U:H2'	18:D3:651:G:C8	2.56	0.41
18:D3:736:C:C6	18:D3:736:C:C3'	3.04	0.41
18:D3:848:C:H2'	18:D3:849:C:C6	2.55	0.41
18:D3:914:G:H5''	18:D3:914:G:H8	1.86	0.41
18:D3:919:A:H2'	18:D3:920:U:C6	2.56	0.41
20:DE:65:LEU:HD22	20:DE:80:THR:HA	2.02	0.41
21:DG:75:LEU:O	21:DG:94:ARG:HA	2.21	0.41
21:DG:159:ARG:HH21	21:DG:170:THR:HG23	1.86	0.41
22:DH:98:ILE:HD13	22:DH:118:LEU:HD12	2.02	0.41
29:DW:27:ILE:HD13	29:DW:27:ILE:HG21	1.84	0.41
33:UN:375:LYS:O	33:UN:379:GLU:HG2	2.20	0.41
1:UB:767:ILE:HD13	1:UB:767:ILE:HA	1.90	0.41
12:JJ:231:ILE:HD13	12:JJ:247:VAL:HG11	2.02	0.41
15:DS:41:ARG:HG3	15:DS:85:PHE:CZ	2.56	0.41
18:D3:829:A:H2	18:D3:830:U:H3	1.67	0.41
27:DO:32:ASP:OD2	27:DO:37:GLU:HB2	2.21	0.41
31:DY:5:VAL:HA	31:DY:28:LEU:O	2.21	0.41
6:CK:335:ARG:NH2	7:CL:957:GLU:OE2	2.48	0.40
6:CK:370:ARG:O	6:CK:374:GLN:CB	2.69	0.40
7:CL:177:PHE:CD2	7:CL:183:LEU:HD12	2.56	0.40
7:CL:632:LYS:HB2	7:CL:632:LYS:HE2	1.84	0.40
8:CM:26:LEU:HD23	8:CM:26:LEU:HA	1.83	0.40
11:JL:131:TYR:CD2	11:JL:156:GLN:HB2	2.56	0.40
18:D3:1570:A:H2'	18:D3:1571:C:O4'	2.21	0.40
18:D3:1615:C:H4'	18:D3:1616:G:H8	1.85	0.40
22:DH:31:SER:O	22:DH:34:LEU:N	2.52	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:DJ:100:LYS:H	24:DJ:100:LYS:HG2	1.70	0.40
7:CL:89:LEU:HD23	7:CL:89:LEU:HA	1.87	0.40
7:CL:906:ASP:N	7:CL:906:ASP:OD1	2.40	0.40
18:D3:701:U:O5'	18:D3:701:U:H6	2.04	0.40
18:D3:855:A:N1	18:D3:857:U:O2	2.55	0.40
18:D3:1506:G:N1	18:D3:1507:G:C6	2.89	0.40
18:D3:1571:C:H3'	18:D3:1572:G:H21	1.86	0.40
19:DA:176:VAL:O	19:DA:179:SER:OG	2.27	0.40
23:DI:136:SER:O	23:DI:139:ALA:N	2.41	0.40
1:UB:753:LYS:HZ1	6:CK:356:VAL:H	1.69	0.40
8:CM:103:MET:O	8:CM:107:ALA:HB2	2.21	0.40
18:D3:81:G:C6	18:D3:82:U:C4	3.10	0.40
18:D3:655:G:C6	18:D3:677:G:C6	3.09	0.40
18:D3:1547:A:H2'	18:D3:1548:G:C8	2.56	0.40
19:DA:23:PRO:HA	19:DA:26:ARG:NH1	2.36	0.40
27:DO:95:GLY:O	27:DO:99:GLN:NE2	2.54	0.40
30:DX:69:ARG:O	30:DX:93:LEU:HD11	2.21	0.40
31:DY:40:LEU:HA	31:DY:40:LEU:HD23	1.89	0.40
4:UX:90:LEU:HD12	4:UX:94:CYS:SG	2.61	0.40
7:CL:948:ILE:O	7:CL:986:HIS:HA	2.21	0.40
9:JG:176:ARG:O	9:JG:203:CYS:N	2.52	0.40
18:D3:180:A:H2'	18:D3:181:A:O4'	2.21	0.40
18:D3:526:A:OP2	31:DY:93:ARG:NH2	2.54	0.40
18:D3:1799:U:C4	33:UN:389:ARG:HD3	2.56	0.40
19:DA:179:SER:HB2	19:DA:183:GLN:HB2	2.03	0.40
29:DW:25:VAL:O	29:DW:62:VAL:HA	2.21	0.40
1:UB:734:ARG:HH12	18:D3:1173:C:P	2.44	0.40
15:DS:24:GLY:O	15:DS:58:ALA:N	2.55	0.40
18:D3:182:A:H2'	18:D3:183:U:H6	1.86	0.40
18:D3:369:A:H2'	18:D3:371:G:OP2	2.21	0.40
18:D3:683:C:H2'	18:D3:684:A:C8	2.51	0.40
19:DA:140:ILE:HB	19:DA:213:ARG:HD2	2.04	0.40
20:DE:11:ARG:HE	20:DE:11:ARG:HB2	1.75	0.40
31:DY:55:VAL:HG22	31:DY:75:VAL:HG23	2.02	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	UB	391/810 (48%)	372 (95%)	14 (4%)	5 (1%)	12	48
2	UC	45/610 (7%)	40 (89%)	5 (11%)	0	100	100
3	US	474/552 (86%)	463 (98%)	11 (2%)	0	100	100
4	UX	141/189 (75%)	124 (88%)	17 (12%)	0	100	100
5	CJ	217/290 (75%)	195 (90%)	22 (10%)	0	100	100
6	CK	90/593 (15%)	83 (92%)	7 (8%)	0	100	100
7	CL	698/1183 (59%)	633 (91%)	64 (9%)	1 (0%)	51	84
8	CM	358/367 (98%)	326 (91%)	32 (9%)	0	100	100
9	JF	212/252 (84%)	211 (100%)	1 (0%)	0	100	100
9	JG	217/252 (86%)	209 (96%)	8 (4%)	0	100	100
10	JH	257/483 (53%)	252 (98%)	5 (2%)	0	100	100
11	JL	281/318 (88%)	260 (92%)	21 (8%)	0	100	100
12	JJ	179/274 (65%)	167 (93%)	12 (7%)	0	100	100
13	DF	194/225 (86%)	185 (95%)	9 (5%)	0	100	100
14	DQ	123/143 (86%)	114 (93%)	9 (7%)	0	100	100
15	DS	75/147 (51%)	67 (89%)	8 (11%)	0	100	100
16	DT	141/144 (98%)	136 (96%)	5 (4%)	0	100	100
17	Dc	61/67 (91%)	60 (98%)	1 (2%)	0	100	100
19	DA	212/255 (83%)	170 (80%)	40 (19%)	2 (1%)	17	56
20	DE	258/261 (99%)	229 (89%)	29 (11%)	0	100	100
21	DG	224/236 (95%)	202 (90%)	19 (8%)	3 (1%)	12	48
22	DH	182/190 (96%)	158 (87%)	23 (13%)	1 (0%)	29	68
23	DI	184/200 (92%)	154 (84%)	30 (16%)	0	100	100
24	DJ	183/197 (93%)	163 (89%)	19 (10%)	1 (0%)	29	68
25	DL	141/156 (90%)	125 (89%)	16 (11%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	DN	148/151 (98%)	129 (87%)	18 (12%)	1 (1%)	22	61
27	DO	125/137 (91%)	102 (82%)	23 (18%)	0	100	100
28	DZ	65/108 (60%)	51 (78%)	14 (22%)	0	100	100
29	DW	127/130 (98%)	116 (91%)	11 (9%)	0	100	100
30	DX	141/145 (97%)	123 (87%)	18 (13%)	0	100	100
31	DY	131/135 (97%)	120 (92%)	11 (8%)	0	100	100
32	Db	79/82 (96%)	72 (91%)	7 (9%)	0	100	100
33	UN	104/899 (12%)	100 (96%)	4 (4%)	0	100	100
34	JD	815/1267 (64%)	743 (91%)	72 (9%)	0	100	100
All	All	7273/11448 (64%)	6654 (92%)	605 (8%)	14 (0%)	50	81

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	UB	698	ILE
1	UB	699	PRO
1	UB	706	LYS
19	DA	213	ARG
21	DG	173	PRO
7	CL	208	SER
22	DH	155	ASP
26	DN	28	LEU
1	UB	702	LEU
1	UB	707	PRO
21	DG	174	LYS
24	DJ	98	ALA
21	DG	21	GLU
19	DA	221	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	UB	52/732 (7%)	51 (98%)	1 (2%)	57	80
2	UC	42/538 (8%)	41 (98%)	1 (2%)	49	76
4	UX	126/169 (75%)	126 (100%)	0	100	100
6	CK	51/535 (10%)	51 (100%)	0	100	100
7	CL	624/1039 (60%)	619 (99%)	5 (1%)	81	91
8	CM	307/312 (98%)	307 (100%)	0	100	100
11	JL	255/283 (90%)	253 (99%)	2 (1%)	81	91
12	JJ	158/238 (66%)	158 (100%)	0	100	100
15	DS	69/110 (63%)	67 (97%)	2 (3%)	42	71
19	DA	191/224 (85%)	190 (100%)	1 (0%)	88	94
20	DE	221/222 (100%)	221 (100%)	0	100	100
21	DG	188/201 (94%)	187 (100%)	1 (0%)	88	94
22	DH	165/170 (97%)	165 (100%)	0	100	100
23	DI	150/161 (93%)	150 (100%)	0	100	100
24	DJ	158/166 (95%)	158 (100%)	0	100	100
25	DL	129/137 (94%)	129 (100%)	0	100	100
26	DN	127/128 (99%)	127 (100%)	0	100	100
27	DO	96/105 (91%)	96 (100%)	0	100	100
29	DW	110/111 (99%)	110 (100%)	0	100	100
30	DX	118/120 (98%)	118 (100%)	0	100	100
31	DY	111/113 (98%)	111 (100%)	0	100	100
32	Db	70/71 (99%)	70 (100%)	0	100	100
33	UN	98/808 (12%)	98 (100%)	0	100	100
34	JD	133/1140 (12%)	133 (100%)	0	100	100
All	All	3749/7833 (48%)	3736 (100%)	13 (0%)	92	97

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	UB	741	LYS
2	UC	554	ARG
7	CL	174	LEU
7	CL	175	ASP
7	CL	548	ASN
7	CL	943	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	CL	973	ARG
11	JL	164	LEU
11	JL	166	ARG
15	DS	57	ARG
15	DS	71	GLN
19	DA	95	ASN
21	DG	98	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
4	UX	132	HIS
7	CL	855	GLN
11	JL	300	GLN
19	DA	95	ASN
19	DA	232	HIS
20	DE	36	HIS
21	DG	139	ASN
29	DW	24	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
18	D3	1380/1758 (78%)	492 (35%)	34 (2%)
35	D4	21/23 (91%)	7 (33%)	0
36	D5	8/9 (88%)	6 (75%)	1 (12%)
All	All	1409/1790 (78%)	505 (35%)	35 (2%)

All (505) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
18	D3	2	A
18	D3	9	U
18	D3	10	G
18	D3	12	U
18	D3	15	U
18	D3	24	U
18	D3	25	C
18	D3	26	A
18	D3	34	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
18	D3	40	A
18	D3	46	A
18	D3	47	A
18	D3	57	G
18	D3	60	U
18	D3	61	A
18	D3	63	G
18	D3	68	A
18	D3	71	A
18	D3	72	A
18	D3	73	U
18	D3	74	U
18	D3	75	U
18	D3	77	U
18	D3	84	A
18	D3	102	U
18	D3	103	A
18	D3	104	A
18	D3	105	A
18	D3	109	G
18	D3	114	C
18	D3	115	G
18	D3	116	U
18	D3	127	G
18	D3	130	C
18	D3	131	C
18	D3	132	U
18	D3	133	U
18	D3	134	U
18	D3	135	A
18	D3	136	C
18	D3	137	U
18	D3	140	A
18	D3	141	U
18	D3	144	U
18	D3	145	A
18	D3	146	U
18	D3	153	G
18	D3	156	A
18	D3	159	U
18	D3	161	U
18	D3	178	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
18	D3	179	A
18	D3	181	A
18	D3	184	C
18	D3	188	A
18	D3	190	C
18	D3	191	C
18	D3	192	U
18	D3	196	G
18	D3	197	A
18	D3	199	G
18	D3	200	A
18	D3	203	U
18	D3	204	G
18	D3	216	U
18	D3	219	A
18	D3	220	A
18	D3	226	A
18	D3	227	U
18	D3	228	G
18	D3	231	U
18	D3	232	U
18	D3	233	C
18	D3	234	G
18	D3	235	G
18	D3	237	C
18	D3	238	U
18	D3	239	C
18	D3	240	U
18	D3	241	U
18	D3	246	G
18	D3	250	C
18	D3	260	U
18	D3	261	U
18	D3	265	A
18	D3	271	A
18	D3	272	U
18	D3	274	G
18	D3	275	C
18	D3	276	C
18	D3	277	U
18	D3	278	U
18	D3	280	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
18	D3	281	G
18	D3	287	G
18	D3	290	G
18	D3	305	C
18	D3	309	C
18	D3	313	U
18	D3	314	C
18	D3	316	A
18	D3	322	G
18	D3	337	G
18	D3	338	C
18	D3	339	C
18	D3	352	A
18	D3	359	A
18	D3	360	A
18	D3	361	C
18	D3	362	G
18	D3	365	G
18	D3	370	A
18	D3	381	C
18	D3	387	A
18	D3	388	G
18	D3	390	G
18	D3	392	G
18	D3	399	A
18	D3	400	A
18	D3	401	A
18	D3	402	C
18	D3	404	G
18	D3	409	C
18	D3	416	A
18	D3	417	A
18	D3	418	G
18	D3	424	C
18	D3	426	G
18	D3	428	A
18	D3	433	C
18	D3	434	G
18	D3	436	A
18	D3	438	A
18	D3	439	U
18	D3	441	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
18	D3	444	C
18	D3	445	A
18	D3	453	U
18	D3	454	U
18	D3	455	C
18	D3	456	A
18	D3	459	G
18	D3	464	A
18	D3	467	G
18	D3	468	A
18	D3	469	C
18	D3	473	A
18	D3	475	A
18	D3	477	A
18	D3	482	U
18	D3	485	A
18	D3	486	G
18	D3	487	G
18	D3	488	G
18	D3	493	U
18	D3	495	C
18	D3	496	G
18	D3	497	G
18	D3	498	G
18	D3	499	U
18	D3	501	U
18	D3	502	U
18	D3	503	G
18	D3	504	U
18	D3	505	A
18	D3	506	A
18	D3	507	U
18	D3	510	G
18	D3	511	A
18	D3	519	C
18	D3	520	A
18	D3	527	A
18	D3	534	A
18	D3	538	A
18	D3	539	G
18	D3	541	A
18	D3	542	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
18	D3	545	A
18	D3	550	A
18	D3	553	G
18	D3	555	A
18	D3	557	G
18	D3	563	U
18	D3	564	G
18	D3	565	C
18	D3	566	C
18	D3	570	A
18	D3	572	C
18	D3	573	C
18	D3	576	G
18	D3	579	A
18	D3	580	A
18	D3	582	U
18	D3	583	C
18	D3	584	C
18	D3	585	A
18	D3	586	G
18	D3	588	U
18	D3	589	C
18	D3	594	A
18	D3	595	G
18	D3	601	A
18	D3	602	U
18	D3	610	G
18	D3	611	U
18	D3	613	G
18	D3	620	A
18	D3	622	A
18	D3	623	A
18	D3	624	G
18	D3	639	U
18	D3	640	U
18	D3	647	G
18	D3	648	G
18	D3	650	U
18	D3	651	G
18	D3	652	G
18	D3	653	C
18	D3	654	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
18	D3	655	G
18	D3	656	G
18	D3	658	C
18	D3	677	G
18	D3	679	U
18	D3	681	U
18	D3	687	G
18	D3	694	U
18	D3	696	C
18	D3	697	C
18	D3	698	U
18	D3	699	U
18	D3	700	C
18	D3	702	G
18	D3	703	G
18	D3	705	U
18	D3	706	A
18	D3	707	A
18	D3	708	C
18	D3	709	C
18	D3	710	U
18	D3	712	G
18	D3	715	U
18	D3	717	C
18	D3	718	U
18	D3	719	U
18	D3	720	G
18	D3	721	U
18	D3	722	G
18	D3	725	U
18	D3	726	C
18	D3	727	U
18	D3	728	U
18	D3	729	G
18	D3	730	G
18	D3	731	C
18	D3	732	G
18	D3	734	A
18	D3	735	C
18	D3	736	C
18	D3	737	A
18	D3	738	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
18	D3	740	A
18	D3	741	C
18	D3	742	U
18	D3	743	U
18	D3	745	U
18	D3	749	U
18	D3	765	G
18	D3	766	U
18	D3	767	U
18	D3	771	A
18	D3	772	G
18	D3	774	A
18	D3	775	G
18	D3	778	G
18	D3	780	A
18	D3	781	U
18	D3	782	U
18	D3	783	G
18	D3	784	C
18	D3	789	A
18	D3	793	A
18	D3	794	U
18	D3	795	U
18	D3	800	U
18	D3	810	G
18	D3	811	A
18	D3	812	A
18	D3	813	U
18	D3	814	A
18	D3	815	G
18	D3	816	G
18	D3	818	C
18	D3	819	G
18	D3	820	U
18	D3	821	U
18	D3	822	U
18	D3	823	G
18	D3	824	G
18	D3	826	U
18	D3	827	C
18	D3	829	A
18	D3	830	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
18	D3	831	U
18	D3	832	U
18	D3	833	U
18	D3	834	G
18	D3	838	G
18	D3	839	U
18	D3	841	U
18	D3	844	A
18	D3	845	G
18	D3	848	C
18	D3	850	A
18	D3	851	U
18	D3	852	C
18	D3	854	U
18	D3	861	U
18	D3	862	A
18	D3	863	A
18	D3	873	U
18	D3	881	A
18	D3	886	U
18	D3	898	A
18	D3	904	G
18	D3	913	G
18	D3	914	G
18	D3	915	A
18	D3	928	U
18	D3	932	U
18	D3	933	A
18	D3	934	C
18	D3	935	U
18	D3	940	A
18	D3	942	G
18	D3	944	A
18	D3	945	U
18	D3	960	U
18	D3	966	A
18	D3	990	C
18	D3	992	A
18	D3	993	A
18	D3	999	U
18	D3	1000	C
18	D3	1001	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
18	D3	1002	G
18	D3	1006	C
18	D3	1007	C
18	D3	1010	C
18	D3	1011	G
18	D3	1024	U
18	D3	1026	A
18	D3	1028	C
18	D3	1029	U
18	D3	1030	A
18	D3	1031	U
18	D3	1040	G
18	D3	1052	U
18	D3	1053	G
18	D3	1055	U
18	D3	1057	U
18	D3	1058	U
18	D3	1059	U
18	D3	1060	U
18	D3	1066	C
18	D3	1081	A
18	D3	1086	A
18	D3	1091	A
18	D3	1092	A
18	D3	1096	C
18	D3	1097	U
18	D3	1098	U
18	D3	1099	U
18	D3	1100	G
18	D3	1101	G
18	D3	1109	G
18	D3	1110	G
18	D3	1114	G
18	D3	1115	U
18	D3	1116	A
18	D3	1118	G
18	D3	1119	G
18	D3	1122	G
18	D3	1124	A
18	D3	1129	U
18	D3	1130	A
18	D3	1131	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
18	D3	1149	G
18	D3	1154	G
18	D3	1158	C
18	D3	1159	C
18	D3	1160	A
18	D3	1164	G
18	D3	1167	G
18	D3	1170	G
18	D3	1172	G
18	D3	1177	C
18	D3	1178	G
18	D3	1180	C
18	D3	1181	U
18	D3	1182	U
18	D3	1183	A
18	D3	1460	A
18	D3	1462	G
18	D3	1469	A
18	D3	1471	A
18	D3	1474	G
18	D3	1478	G
18	D3	1480	G
18	D3	1481	C
18	D3	1482	C
18	D3	1486	G
18	D3	1488	G
18	D3	1490	C
18	D3	1492	A
18	D3	1493	A
18	D3	1494	C
18	D3	1496	U
18	D3	1499	G
18	D3	1503	A
18	D3	1507	G
18	D3	1508	U
18	D3	1510	U
18	D3	1512	G
18	D3	1516	A
18	D3	1517	U
18	D3	1520	U
18	D3	1523	G
18	D3	1524	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
18	D3	1532	U
18	D3	1534	G
18	D3	1535	U
18	D3	1536	G
18	D3	1537	C
18	D3	1538	U
18	D3	1539	G
18	D3	1542	G
18	D3	1544	U
18	D3	1546	G
18	D3	1550	A
18	D3	1553	G
18	D3	1557	U
18	D3	1558	U
18	D3	1559	A
18	D3	1561	U
18	D3	1568	C
18	D3	1569	A
18	D3	1573	A
18	D3	1574	G
18	D3	1577	A
18	D3	1578	U
18	D3	1579	U
18	D3	1580	C
18	D3	1582	U
18	D3	1583	A
18	D3	1584	G
18	D3	1590	G
18	D3	1595	U
18	D3	1599	C
18	D3	1600	A
18	D3	1601	G
18	D3	1602	C
18	D3	1607	G
18	D3	1613	U
18	D3	1615	C
18	D3	1619	C
18	D3	1621	U
18	D3	1622	G
18	D3	1626	U
18	D3	1628	U
18	D3	1629	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
18	D3	1630	U
18	D3	1633	A
18	D3	1638	G
18	D3	1639	C
18	D3	1642	G
18	D3	1645	G
18	D3	1649	G
18	D3	1750	A
18	D3	1751	C
18	D3	1777	G
18	D3	1780	G
18	D3	1781	A
18	D3	1782	A
18	D3	1783	C
18	D3	1792	G
18	D3	1794	A
18	D3	1796	C
18	D3	1801	A
18	D3	1802	A
18	D3	1803	G
18	D3	1804	A
35	D4	2	U
35	D4	6	C
35	D4	8	U
35	D4	14	A
35	D4	15	U
35	D4	16	A
35	D4	18	G
36	D5	4	U
36	D5	5	U
36	D5	6	U
36	D5	8	U
36	D5	9	U
36	D5	10	U

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
18	D3	24	U
18	D3	73	U
18	D3	103	A
18	D3	114	C

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
18	D3	130	C
18	D3	132	U
18	D3	135	A
18	D3	139	C
18	D3	196	G
18	D3	199	G
18	D3	218	A
18	D3	280	U
18	D3	417	A
18	D3	433	C
18	D3	485	A
18	D3	498	G
18	D3	503	G
18	D3	510	G
18	D3	579	A
18	D3	695	U
18	D3	721	U
18	D3	736	C
18	D3	829	A
18	D3	834	G
18	D3	913	G
18	D3	1109	G
18	D3	1115	U
18	D3	1481	C
18	D3	1535	U
18	D3	1568	C
18	D3	1573	A
18	D3	1600	A
18	D3	1800	A
18	D3	1802	A
36	D5	5	U

## 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

Of 41 ligands modelled in this entry, 40 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
38	GTP	CL	2001	39	26,34,34	0.94	1 (3%)	32,54,54	1.50	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
38	GTP	CL	2001	39	-	4/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	CL	2001	GTP	C6-N1	-2.55	1.34	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	CL	2001	GTP	PB-O3B-PG	-4.35	117.91	132.83
38	CL	2001	GTP	C3'-C2'-C1'	3.06	105.58	100.98
38	CL	2001	GTP	PA-O3A-PB	-3.00	122.54	132.83
38	CL	2001	GTP	C5-C6-N1	2.36	118.11	113.95
38	CL	2001	GTP	C8-N7-C5	2.31	107.39	102.99

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
38	CL	2001	GTP	O4'-C4'-C5'-O5'
38	CL	2001	GTP	C3'-C4'-C5'-O5'

*Continued on next page...*

*Continued from previous page...*

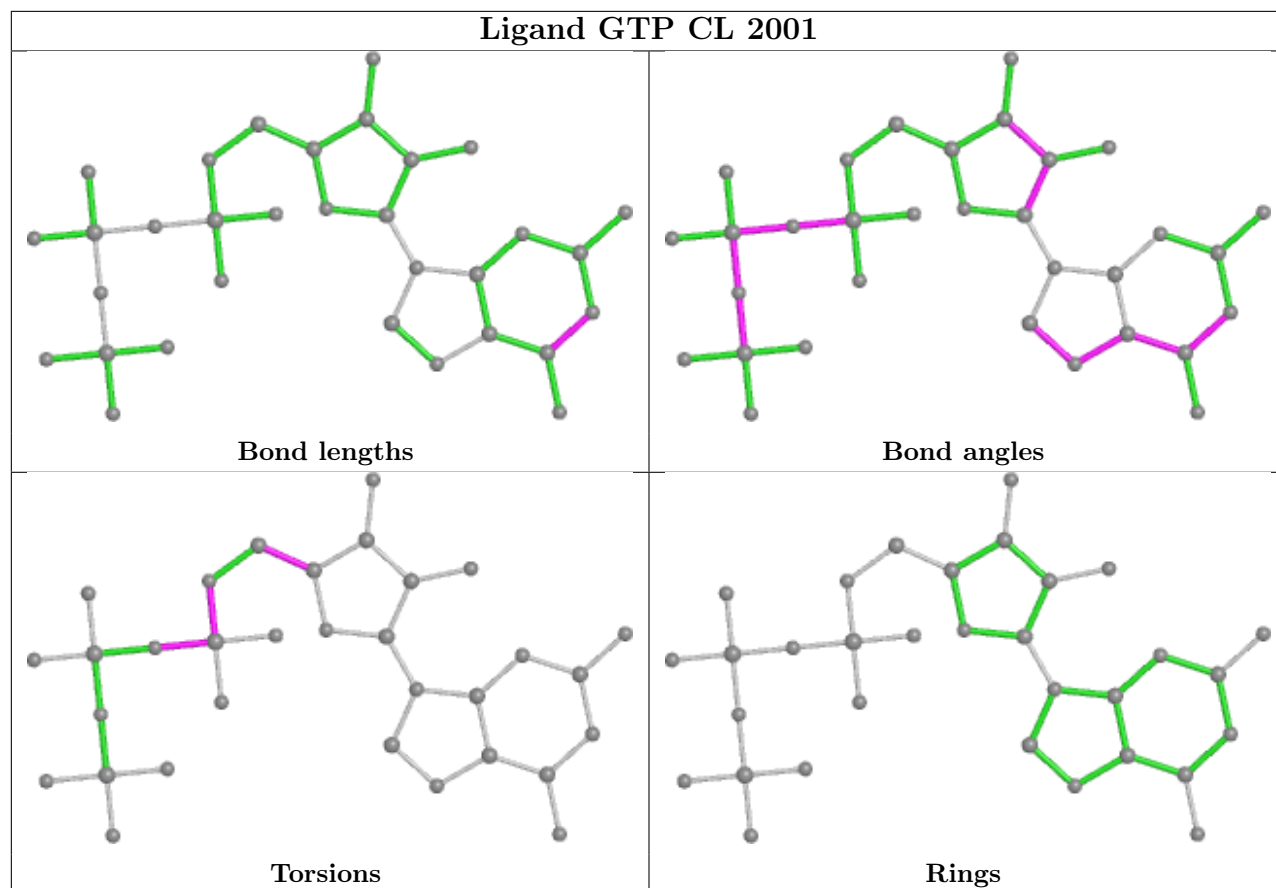
Mol	Chain	Res	Type	Atoms
38	CL	2001	GTP	PB-O3A-PA-O2A
38	CL	2001	GTP	C5'-O5'-PA-O3A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	CL	2001	GTP	1	0

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

There are no chain breaks in this entry.

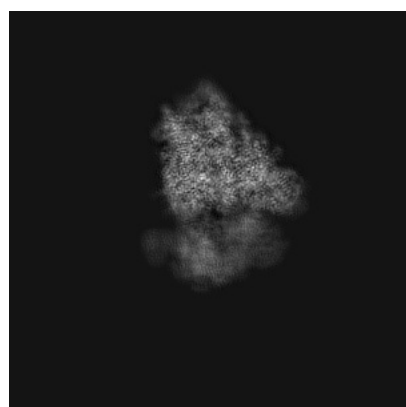
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11363. These allow visual inspection of the internal detail of the map and identification of artifacts.

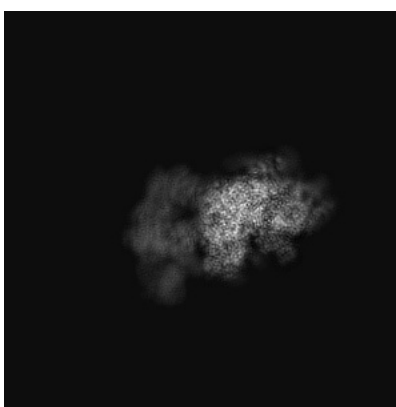
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

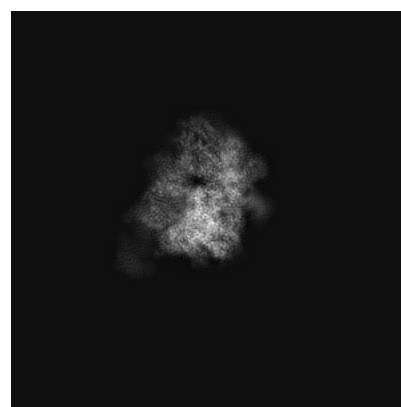
#### 6.1.1 Primary map



X



Y

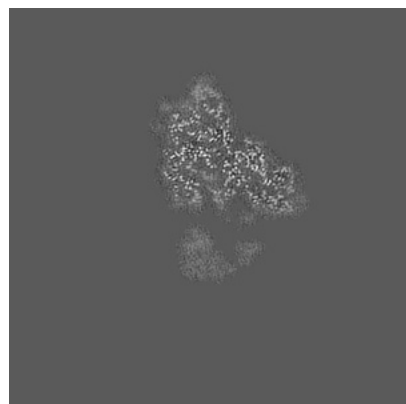


Z

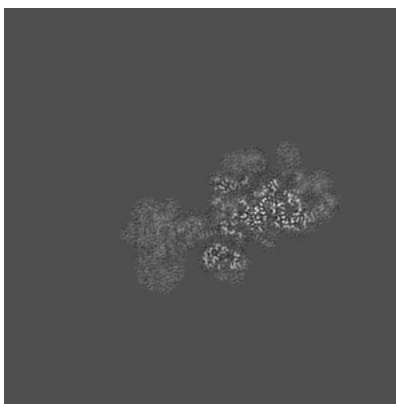
The images above show the map projected in three orthogonal directions.

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

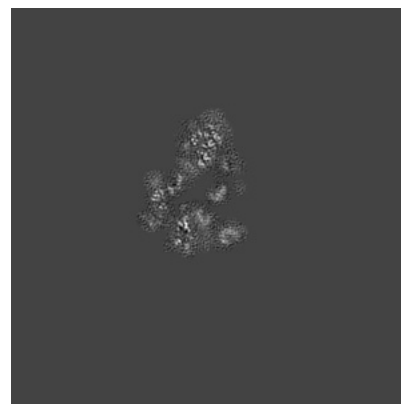
#### 6.2.1 Primary map



X Index: 240



Y Index: 240

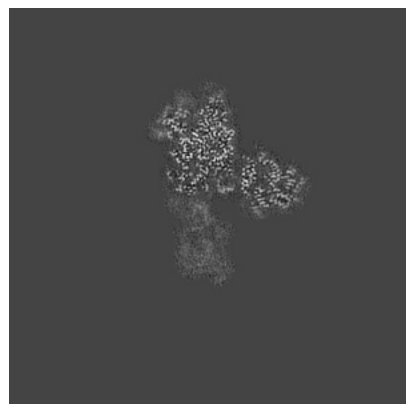


Z Index: 240

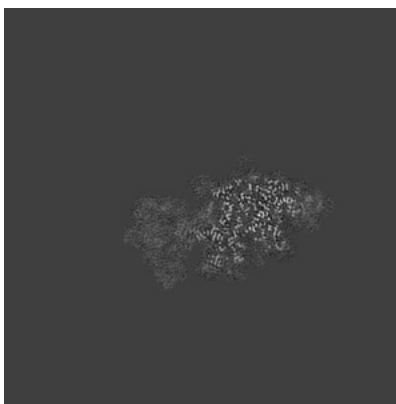
The images above show central slices of the map in three orthogonal directions.

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

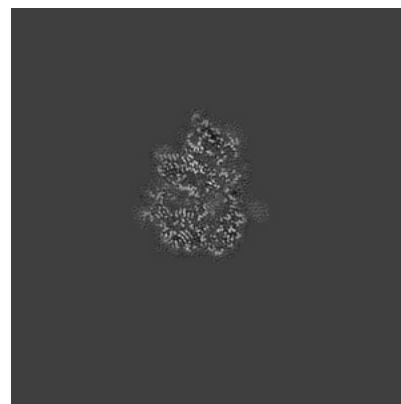
### 6.3.1 Primary map



X Index: 226



Y Index: 219



Z Index: 278

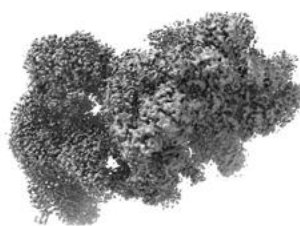
The images above show the largest variance slices of the map in three orthogonal directions.

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

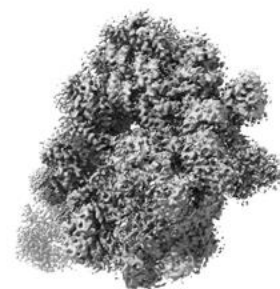
### 6.4.1 Primary map



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.

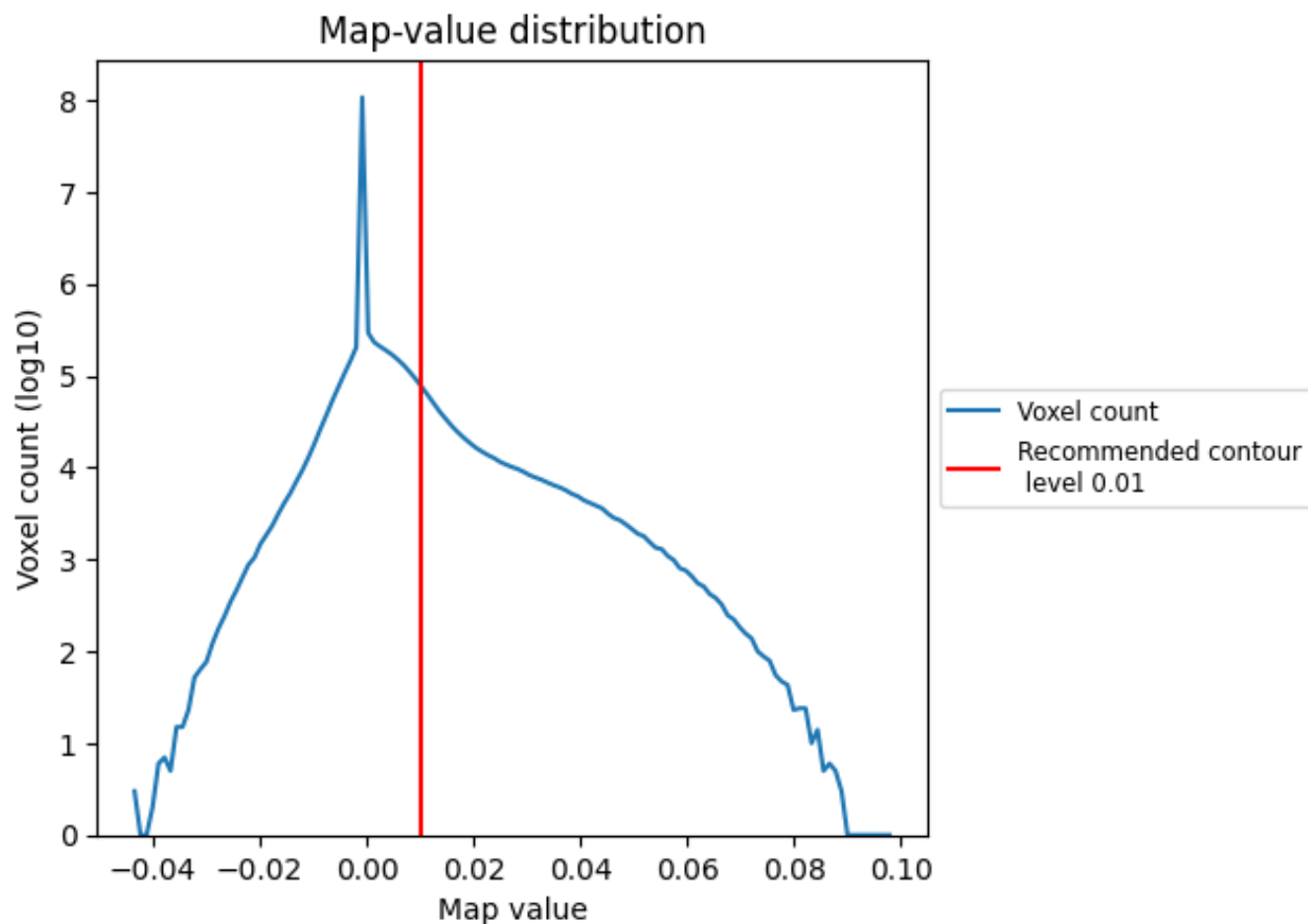
## 6.5 Mask visualisation

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.

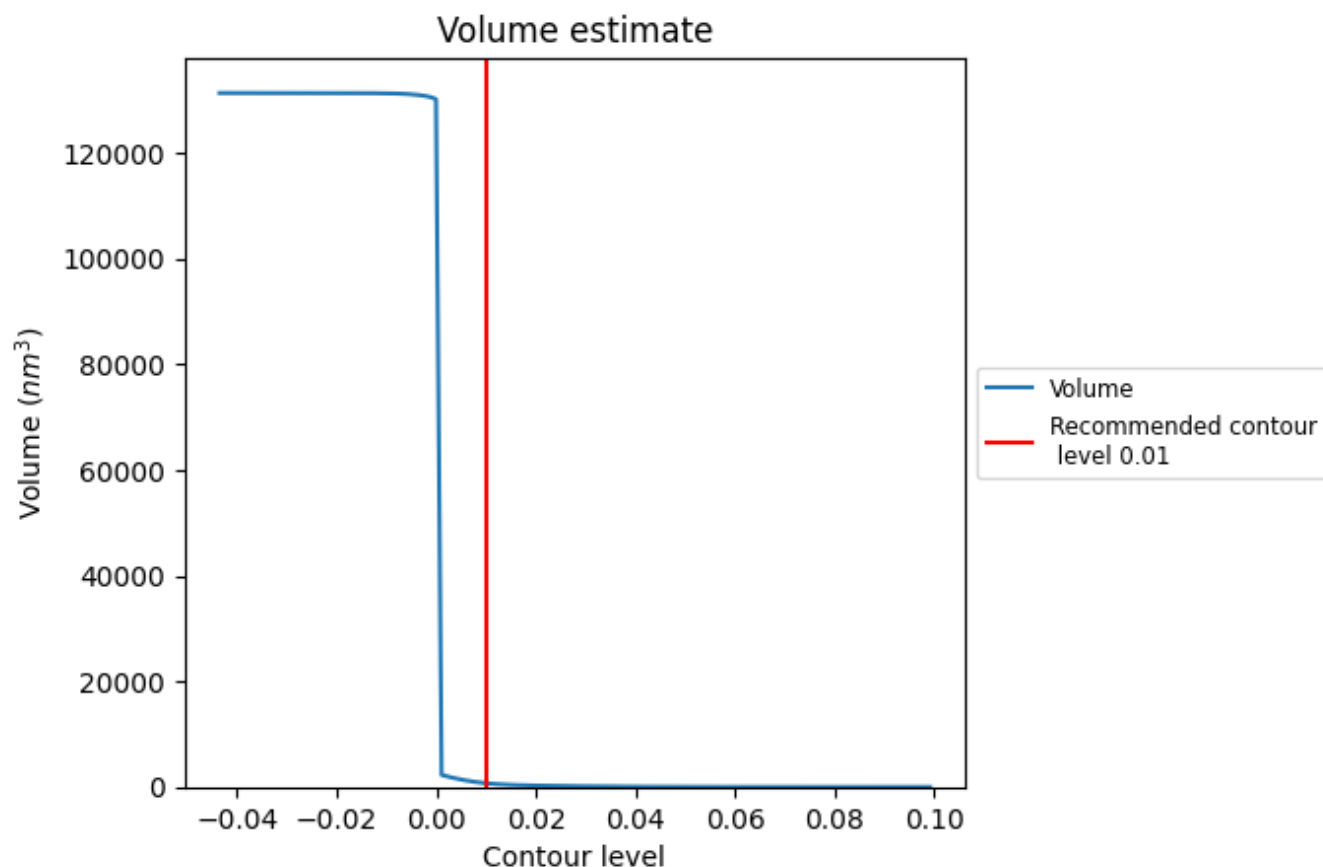
### 7.1 Map-value distribution [i](#)



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.



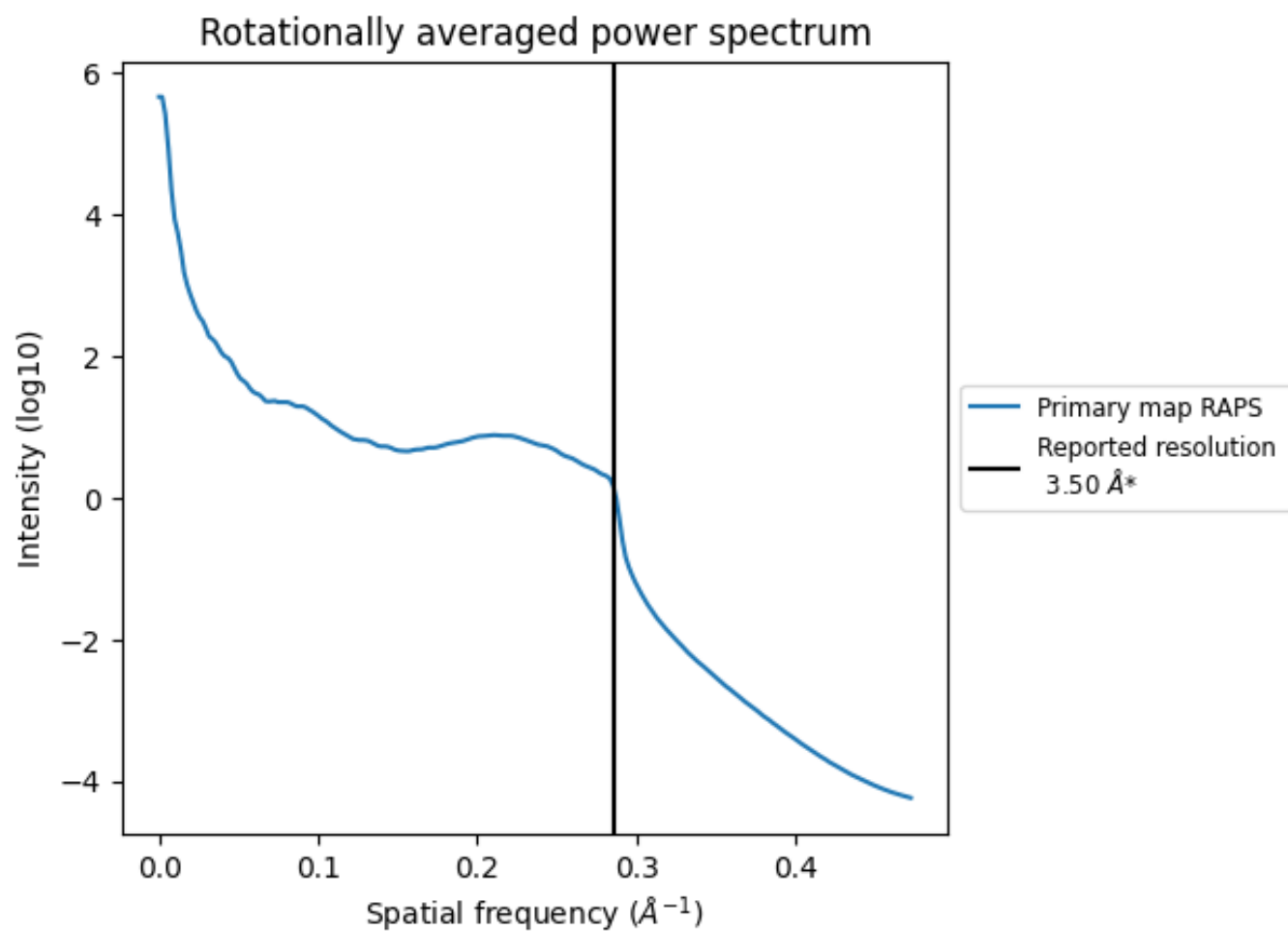
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 707  $\text{nm}^3$ ; this corresponds to an approximate mass of 638 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 ⓘ

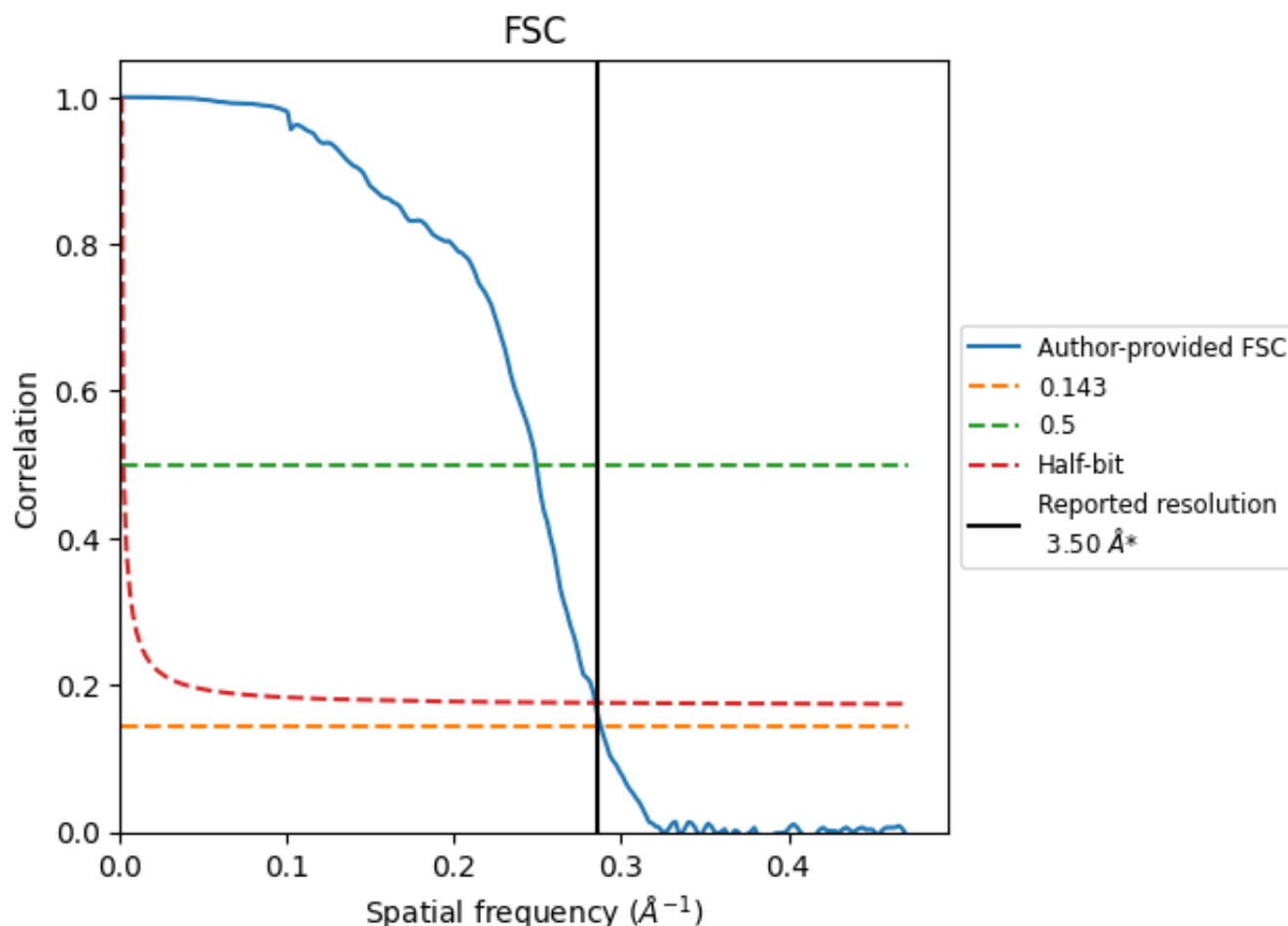


\*Reported resolution corresponds to spatial frequency of 0.286 Å<sup>-1</sup>

## 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 0.286 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

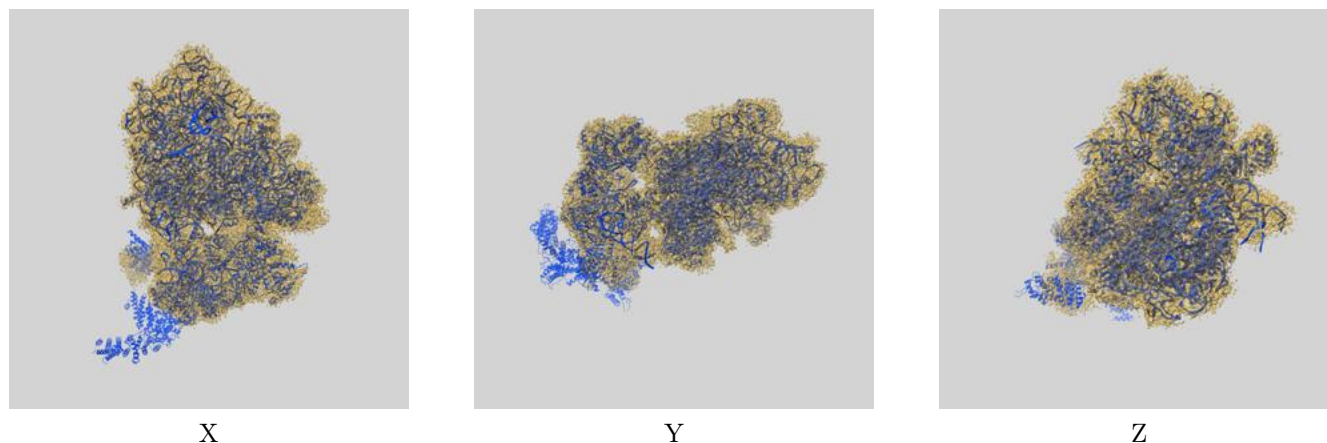
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.47	4.01	3.52
Unmasked-calculated*	-	-	-

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

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

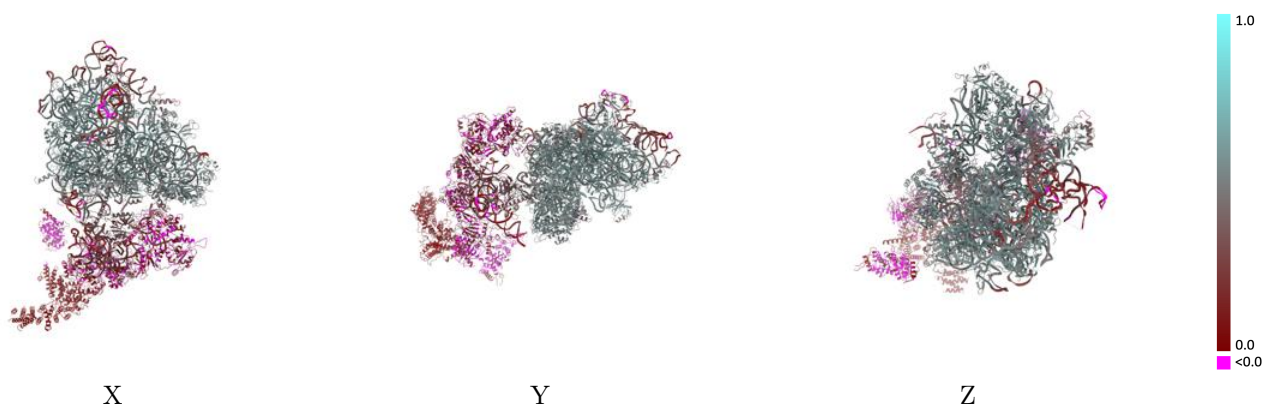
This section contains information regarding the fit between EMDB map EMD-11363 and PDB model 6ZQG. Per-residue inclusion information can be found in section 3 on page 12.

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



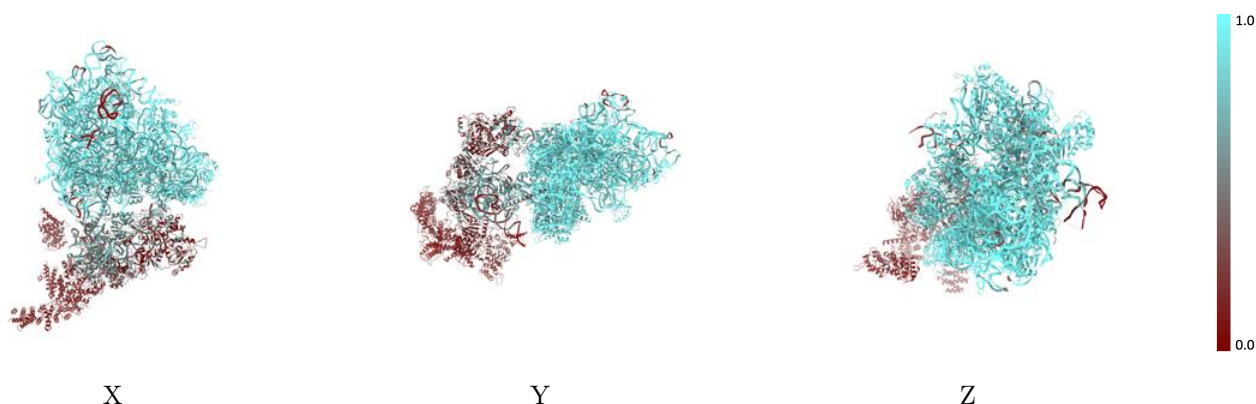
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



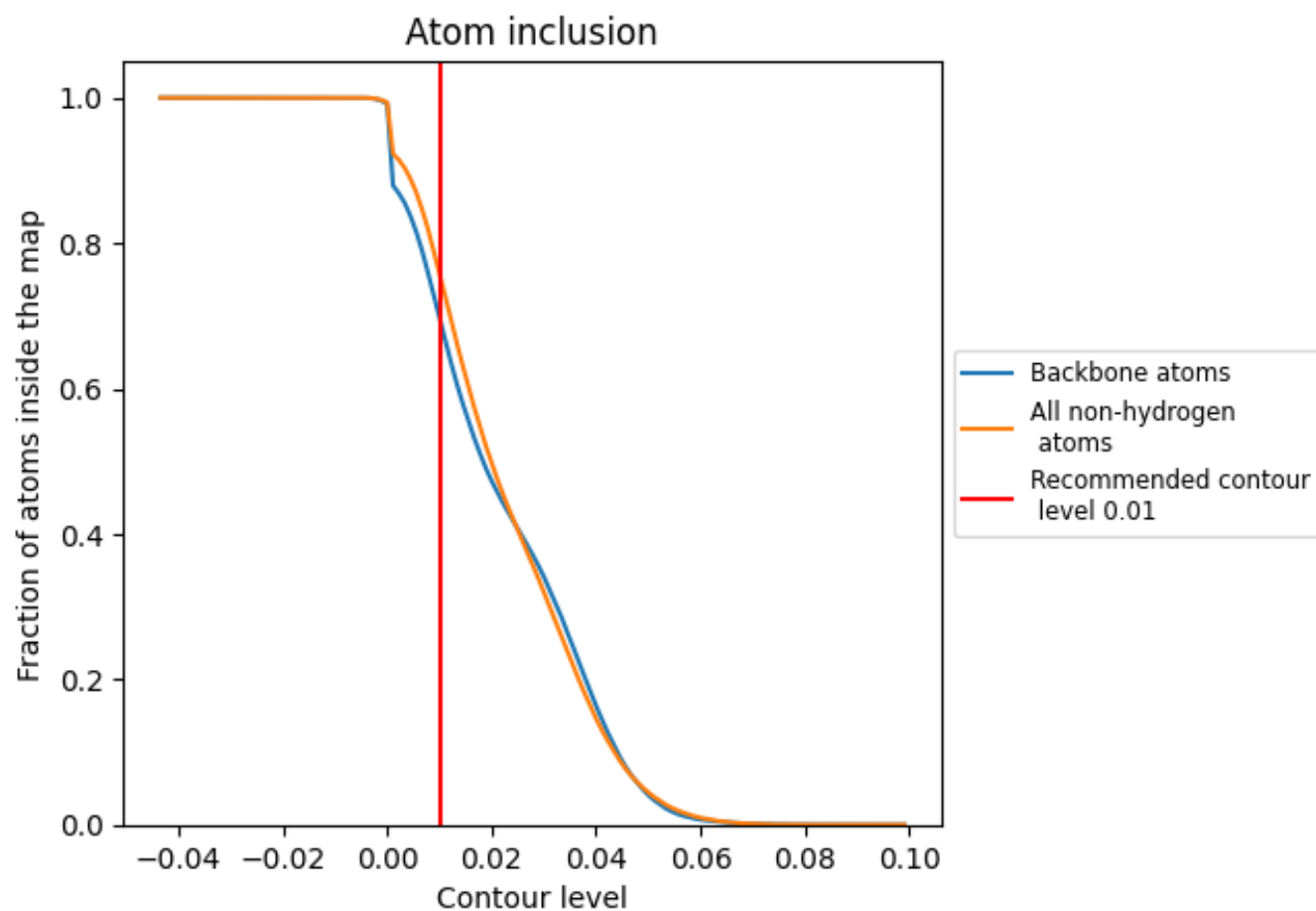
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ



At the recommended contour level, 70% of all backbone atoms, 76% 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	 0.7580	 0.4050
CJ	 0.6030	 0.3060
CK	 0.7461	 0.4080
CL	 0.9182	 0.5250
CM	 0.9408	 0.5440
D3	 0.8655	 0.4250
D4	 0.9798	 0.4900
D5	 0.3833	 0.2000
DA	 0.9428	 0.5380
DE	 0.9618	 0.5680
DF	 0.4186	 0.1550
DG	 0.9428	 0.5120
DH	 0.9132	 0.4860
DI	 0.9575	 0.5480
DJ	 0.9438	 0.5550
DL	 0.9314	 0.5520
DN	 0.9567	 0.5520
DO	 0.9594	 0.5380
DQ	 0.3506	 0.1660
DS	 0.3247	 0.1450
DT	 0.4186	 0.1510
DW	 0.9679	 0.5730
DX	 0.9035	 0.5490
DY	 0.9440	 0.5520
DZ	 0.2620	 0.1620
Db	 0.9301	 0.5260
Dc	 0.3161	 0.1410
JD	 0.4491	 0.2300
JF	 0.0738	 0.0360
JG	 0.1515	 0.1140
JH	 0.0456	 -0.0270
JJ	 0.9158	 0.5250
JL	 0.9143	 0.5300
UB	 0.0757	 0.0720
UC	 0.9129	 0.5480



*Continued on next page...*



*Continued from previous page...*

Chain	Atom inclusion	Q-score
UN	 0.8739	 0.5350
US	 0.0000	 -0.0000
UX	 0.9100	 0.5380