



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 11:07 am GMT

PDB ID : 1ZO1
EMDB ID: : EMD-1248
Title : IF2, IF1, and tRNA fitted to cryo-EM data OF E. COLI 70S initiation complex
Authors : Allen, G.S.; Zavialov, A.; Gursky, R.; Ehrenberg, M.; Frank, J.
Deposited on : 2005-05-12
Resolution : 13.80 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

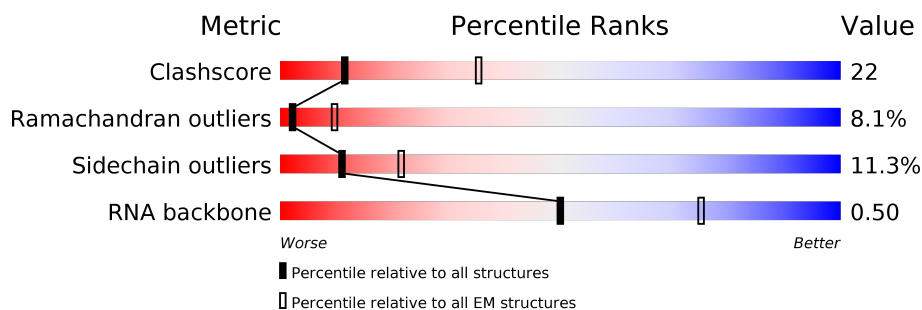
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY




The reported resolution of this entry is 13.80 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	F	76	
2	I	501	
3	W	71	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5992 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called P/I-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	76	Total	C	N	O	P	0	0
			1622	725	293	529	75		

- Molecule 2 is a protein called translation initiation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	501	Total	C	N	O	S	0	0
			3800	2382	667	736	15		

- Molecule 3 is a protein called translation Initiation Factor 1.

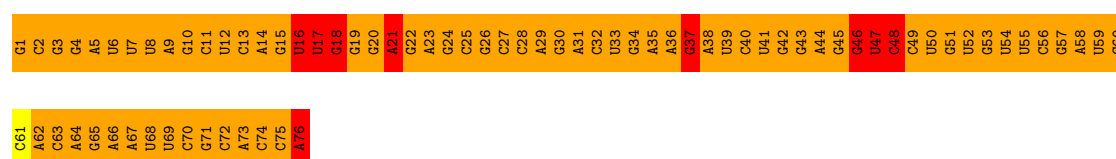
Mol	Chain	Residues	Atoms					AltConf	Trace
3	W	71	Total	C	N	O	S	0	0
			570	362	103	103	2		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

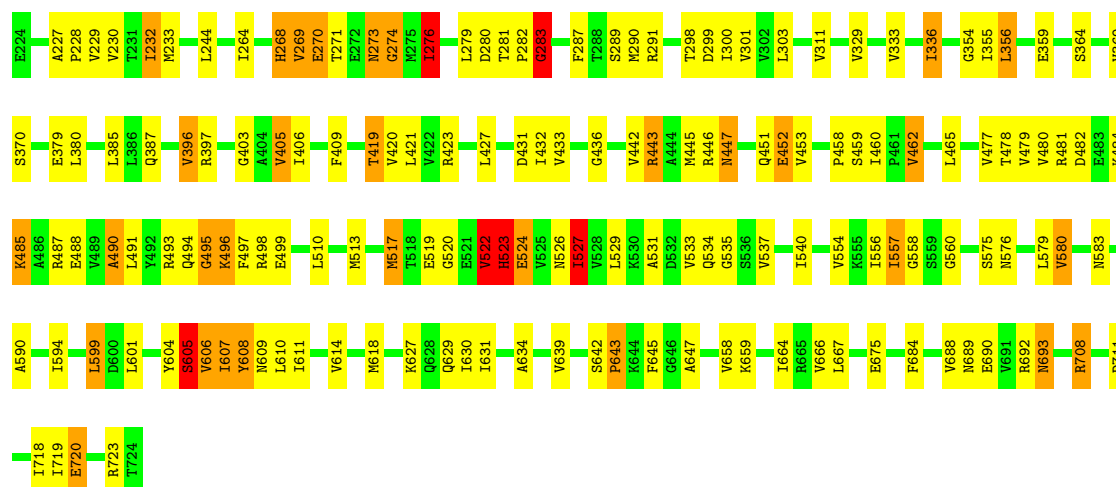
- Molecule 1: P/I-site tRNA

Chain F: 




- Molecule 2: translation initiation factor 2

Chain I: 



- Molecule 3: translation Initiation Factor 1

Chain W: 



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	DEFOCUS GROUPS 0.93-3.93 UM	Depositor
Microscope	TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	-930.00	Depositor
Maximum defocus (nm)	-3930.00	Depositor
Magnification	Not provided	Depositor
Image detector	KODAK SO163 FILM	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	F	5.60	277/1814 (15.3%)	6.11	700/2827 (24.8%)
2	I	0.66	0/3848	0.94	14/5200 (0.3%)
3	W	0.67	0/580	0.79	1/782 (0.1%)
All	All	3.07	277/6242 (4.4%)	3.54	715/8809 (8.1%)

All (277) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	39	U	C1'-N1	148.95	3.72	1.48
1	F	55	U	C1'-N1	91.84	2.86	1.48
1	F	75	C	O3'-P	29.95	1.97	1.61
1	F	19	G	N3-C4	13.35	1.44	1.35
1	F	22	G	N3-C4	13.34	1.44	1.35
1	F	20	G	N3-C4	13.29	1.44	1.35
1	F	45	G	N3-C4	13.21	1.44	1.35
1	F	51	G	N3-C4	13.18	1.44	1.35
1	F	18	G	N3-C4	13.18	1.44	1.35
1	F	57	G	N3-C4	13.15	1.44	1.35
1	F	71	G	N3-C4	13.15	1.44	1.35
1	F	26	G	N3-C4	13.11	1.44	1.35
1	F	43	G	N3-C4	13.09	1.44	1.35
1	F	4	G	N3-C4	13.04	1.44	1.35
1	F	30	G	N3-C4	13.02	1.44	1.35
1	F	10	G	N3-C4	13.01	1.44	1.35
1	F	42	G	N3-C4	12.97	1.44	1.35
1	F	24	G	N3-C4	12.96	1.44	1.35
1	F	65	G	N3-C4	12.93	1.44	1.35
1	F	1	G	N3-C4	12.91	1.44	1.35
1	F	46	G	N3-C4	12.87	1.44	1.35
1	F	37	G	N3-C4	12.82	1.44	1.35
1	F	53	G	N3-C4	12.82	1.44	1.35
1	F	34	G	N3-C4	12.80	1.44	1.35
1	F	15	G	N3-C4	12.77	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	3	G	N3-C4	12.56	1.44	1.35
1	F	61	C	C2-N3	11.88	1.45	1.35
1	F	56	C	C2-N3	11.67	1.45	1.35
1	F	32	C	C2-N3	11.58	1.45	1.35
1	F	11	C	C2-N3	11.53	1.45	1.35
1	F	75	C	C2-N3	11.53	1.45	1.35
1	F	74	C	C2-N3	11.48	1.45	1.35
1	F	25	C	C2-N3	11.44	1.45	1.35
1	F	49	C	C2-N3	11.44	1.45	1.35
1	F	48	C	C2-N3	11.41	1.44	1.35
1	F	72	C	C2-N3	11.37	1.44	1.35
1	F	40	C	C2-N3	11.33	1.44	1.35
1	F	27	C	C2-N3	11.32	1.44	1.35
1	F	63	C	C2-N3	11.32	1.44	1.35
1	F	60	C	C2-N3	11.31	1.44	1.35
1	F	2	C	C2-N3	11.25	1.44	1.35
1	F	28	C	C2-N3	11.14	1.44	1.35
1	F	70	C	C2-N3	11.09	1.44	1.35
1	F	13	C	C2-N3	11.07	1.44	1.35
1	F	57	G	N9-C8	-10.69	1.30	1.37
1	F	45	G	N9-C8	-10.42	1.30	1.37
1	F	18	G	N9-C8	-10.32	1.30	1.37
1	F	30	G	N9-C8	-10.31	1.30	1.37
1	F	46	G	N9-C8	-10.28	1.30	1.37
1	F	53	G	N9-C8	-10.18	1.30	1.37
1	F	15	G	N9-C8	-10.15	1.30	1.37
1	F	4	G	N9-C8	-10.14	1.30	1.37
1	F	65	G	N9-C8	-10.12	1.30	1.37
1	F	34	G	N9-C8	-10.11	1.30	1.37
1	F	51	G	N9-C8	-10.10	1.30	1.37
1	F	3	G	N9-C8	-10.10	1.30	1.37
1	F	10	G	N9-C8	-10.08	1.30	1.37
1	F	22	G	N9-C8	-10.04	1.30	1.37
1	F	37	G	N9-C8	-10.04	1.30	1.37
1	F	1	G	N9-C8	-10.01	1.30	1.37
1	F	20	G	N9-C8	-9.98	1.30	1.37
1	F	42	G	N9-C8	-9.94	1.30	1.37
1	F	19	G	N9-C8	-9.93	1.30	1.37
1	F	24	G	N9-C8	-9.79	1.30	1.37
1	F	71	G	N9-C8	-9.73	1.31	1.37
1	F	43	G	N9-C8	-9.72	1.31	1.37
1	F	26	G	N9-C8	-9.54	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	32	C	N3-C4	-9.48	1.27	1.33
1	F	28	C	N3-C4	-9.46	1.27	1.33
1	F	25	C	N3-C4	-9.38	1.27	1.33
1	F	70	C	N3-C4	-9.37	1.27	1.33
1	F	61	C	N3-C4	-9.27	1.27	1.33
1	F	11	C	N3-C4	-9.27	1.27	1.33
1	F	49	C	N3-C4	-9.16	1.27	1.33
1	F	13	C	N3-C4	-9.16	1.27	1.33
1	F	56	C	N3-C4	-9.10	1.27	1.33
1	F	60	C	N3-C4	-9.06	1.27	1.33
1	F	2	C	N3-C4	-9.00	1.27	1.33
1	F	72	C	N3-C4	-8.99	1.27	1.33
1	F	48	C	N3-C4	-8.87	1.27	1.33
1	F	63	C	N3-C4	-8.86	1.27	1.33
1	F	27	C	N3-C4	-8.86	1.27	1.33
1	F	40	C	N3-C4	-8.82	1.27	1.33
1	F	74	C	N3-C4	-8.81	1.27	1.33
1	F	75	C	N3-C4	-8.79	1.27	1.33
1	F	73	A	N7-C5	-8.66	1.34	1.39
1	F	14	A	N9-C8	-8.61	1.30	1.37
1	F	71	G	N9-C4	-8.55	1.31	1.38
1	F	26	G	N9-C4	-8.53	1.31	1.38
1	F	29	A	N9-C8	-8.50	1.30	1.37
1	F	44	A	N9-C8	-8.48	1.30	1.37
1	F	43	G	N9-C4	-8.47	1.31	1.38
1	F	24	G	N9-C4	-8.45	1.31	1.38
1	F	71	G	N7-C5	8.45	1.44	1.39
1	F	19	G	N9-C4	-8.44	1.31	1.38
1	F	51	G	N7-C5	8.43	1.44	1.39
1	F	57	G	N9-C4	-8.43	1.31	1.38
1	F	43	G	N7-C5	8.42	1.44	1.39
1	F	4	G	N9-C4	-8.41	1.31	1.38
1	F	65	G	N9-C4	-8.41	1.31	1.38
1	F	9	A	N7-C5	-8.41	1.34	1.39
1	F	18	G	N9-C4	-8.39	1.31	1.38
1	F	58	A	N9-C8	-8.39	1.31	1.37
1	F	24	G	N7-C5	8.39	1.44	1.39
1	F	31	A	N7-C5	-8.37	1.34	1.39
1	F	64	A	N7-C5	-8.36	1.34	1.39
1	F	10	G	N9-C4	-8.34	1.31	1.38
1	F	14	A	N7-C5	-8.34	1.34	1.39
1	F	9	A	N9-C8	-8.32	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	29	A	N7-C5	-8.31	1.34	1.39
1	F	19	G	N7-C5	8.31	1.44	1.39
1	F	66	A	N9-C8	-8.31	1.31	1.37
1	F	73	A	N9-C8	-8.30	1.31	1.37
1	F	46	G	N9-C4	-8.30	1.31	1.38
1	F	45	G	N7-C5	8.30	1.44	1.39
1	F	22	G	N9-C4	-8.29	1.31	1.38
1	F	42	G	N9-C4	-8.29	1.31	1.38
1	F	20	G	N9-C4	-8.28	1.31	1.38
1	F	1	G	N7-C5	8.28	1.44	1.39
1	F	34	G	N9-C4	-8.26	1.31	1.38
1	F	31	A	N9-C8	-8.26	1.31	1.37
1	F	65	G	N7-C5	8.26	1.44	1.39
1	F	35	A	N7-C5	-8.25	1.34	1.39
1	F	57	G	N7-C5	8.24	1.44	1.39
1	F	22	G	N7-C5	8.22	1.44	1.39
1	F	10	G	N7-C5	8.20	1.44	1.39
1	F	76	A	N9-C8	-8.19	1.31	1.37
1	F	45	G	N9-C4	-8.18	1.31	1.38
1	F	37	G	N7-C5	8.18	1.44	1.39
1	F	21	A	N9-C8	-8.17	1.31	1.37
1	F	51	G	N9-C4	-8.17	1.31	1.38
1	F	20	G	N7-C5	8.16	1.44	1.39
1	F	15	G	N9-C4	-8.16	1.31	1.38
1	F	76	A	N7-C5	-8.14	1.34	1.39
1	F	15	G	N7-C5	8.14	1.44	1.39
1	F	64	A	N9-C8	-8.14	1.31	1.37
1	F	42	G	N7-C5	8.13	1.44	1.39
1	F	58	A	N7-C5	-8.13	1.34	1.39
1	F	67	A	N7-C5	-8.12	1.34	1.39
1	F	53	G	N9-C4	-8.12	1.31	1.38
1	F	23	A	N7-C5	-8.12	1.34	1.39
1	F	1	G	N9-C4	-8.11	1.31	1.38
1	F	36	A	N7-C5	-8.10	1.34	1.39
1	F	38	A	N9-C8	-8.09	1.31	1.37
1	F	37	G	N9-C4	-8.07	1.31	1.38
1	F	3	G	N9-C4	-8.07	1.31	1.38
1	F	38	A	N7-C5	-8.07	1.34	1.39
1	F	18	G	N7-C5	8.06	1.44	1.39
1	F	30	G	N9-C4	-8.06	1.31	1.38
1	F	5	A	N7-C5	-8.05	1.34	1.39
1	F	62	A	N9-C8	-8.05	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	36	A	N9-C8	-8.04	1.31	1.37
1	F	35	A	N9-C8	-8.02	1.31	1.37
1	F	26	G	N7-C5	8.01	1.44	1.39
1	F	46	G	N7-C5	8.01	1.44	1.39
1	F	3	G	N7-C5	7.98	1.44	1.39
1	F	21	A	N7-C5	-7.96	1.34	1.39
1	F	34	G	N7-C5	7.91	1.44	1.39
1	F	23	A	N9-C8	-7.91	1.31	1.37
1	F	62	A	N7-C5	-7.91	1.34	1.39
1	F	5	A	N9-C8	-7.86	1.31	1.37
1	F	53	G	N7-C5	7.85	1.44	1.39
1	F	67	A	N9-C8	-7.81	1.31	1.37
1	F	44	A	N7-C5	-7.79	1.34	1.39
1	F	30	G	N7-C5	7.74	1.43	1.39
1	F	4	G	N7-C5	7.71	1.43	1.39
1	F	66	A	N7-C5	-7.53	1.34	1.39
1	F	22	G	C8-N7	-7.51	1.26	1.30
1	F	1	G	C8-N7	-7.39	1.26	1.30
1	F	71	G	C8-N7	-7.27	1.26	1.30
1	F	37	G	C8-N7	-7.25	1.26	1.30
1	F	42	G	C8-N7	-7.24	1.26	1.30
1	F	4	G	C8-N7	-7.22	1.26	1.30
1	F	24	G	C8-N7	-7.22	1.26	1.30
1	F	43	G	C8-N7	-7.18	1.26	1.30
1	F	18	G	C8-N7	-7.17	1.26	1.30
1	F	26	G	C8-N7	-7.16	1.26	1.30
1	F	65	G	C8-N7	-7.16	1.26	1.30
1	F	30	G	C8-N7	-7.12	1.26	1.30
1	F	20	G	C8-N7	-7.12	1.26	1.30
1	F	15	G	C8-N7	-7.11	1.26	1.30
1	F	45	G	C5-C4	-7.09	1.33	1.38
1	F	37	G	C5-C4	-7.08	1.33	1.38
1	F	65	G	C5-C4	-7.08	1.33	1.38
1	F	46	G	C8-N7	-7.07	1.26	1.30
1	F	3	G	C8-N7	-7.05	1.26	1.30
1	F	18	G	C5-C4	-7.00	1.33	1.38
1	F	19	G	C5-C4	-6.97	1.33	1.38
1	F	51	G	C8-N7	-6.94	1.26	1.30
1	F	45	G	C8-N7	-6.94	1.26	1.30
1	F	10	G	C8-N7	-6.93	1.26	1.30
1	F	20	G	C5-C4	-6.93	1.33	1.38
1	F	22	G	C5-C4	-6.92	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	51	G	C5-C4	-6.91	1.33	1.38
1	F	25	C	C4-C5	6.89	1.48	1.43
1	F	30	G	C5-C4	-6.89	1.33	1.38
1	F	43	G	C5-C4	-6.89	1.33	1.38
1	F	32	C	C4-C5	6.83	1.48	1.43
1	F	34	G	C8-N7	-6.83	1.26	1.30
1	F	19	G	C8-N7	-6.81	1.26	1.30
1	F	11	C	C4-C5	6.79	1.48	1.43
1	F	53	G	C5-C4	-6.78	1.33	1.38
1	F	15	G	C5-C4	-6.77	1.33	1.38
1	F	53	G	C8-N7	-6.76	1.26	1.30
1	F	42	G	C5-C4	-6.74	1.33	1.38
1	F	71	G	C5-C4	-6.74	1.33	1.38
1	F	3	G	C5-C4	-6.69	1.33	1.38
1	F	1	G	C5-C4	-6.68	1.33	1.38
1	F	26	G	C5-C4	-6.67	1.33	1.38
1	F	10	G	C5-C4	-6.65	1.33	1.38
1	F	57	G	C8-N7	-6.63	1.26	1.30
1	F	4	G	C5-C4	-6.61	1.33	1.38
1	F	61	C	C4-C5	6.60	1.48	1.43
1	F	70	C	C4-C5	6.55	1.48	1.43
1	F	75	C	C4-C5	6.55	1.48	1.43
1	F	2	C	C4-C5	6.54	1.48	1.43
1	F	13	C	C4-C5	6.53	1.48	1.43
1	F	74	C	C4-C5	6.51	1.48	1.43
1	F	72	C	C4-C5	6.43	1.48	1.43
1	F	34	G	C5-C4	-6.42	1.33	1.38
1	F	24	G	C5-C4	-6.42	1.33	1.38
1	F	60	C	C4-C5	6.39	1.48	1.43
1	F	49	C	C4-C5	6.38	1.48	1.43
1	F	57	G	C5-C4	-6.35	1.33	1.38
1	F	28	C	C4-C5	6.33	1.48	1.43
1	F	62	A	C8-N7	-6.32	1.27	1.31
1	F	76	A	C8-N7	-6.32	1.27	1.31
1	F	36	A	C8-N7	-6.31	1.27	1.31
1	F	48	C	C4-C5	6.28	1.48	1.43
1	F	58	A	C8-N7	-6.26	1.27	1.31
1	F	56	C	C4-C5	6.17	1.47	1.43
1	F	40	C	C4-C5	6.14	1.47	1.43
1	F	35	A	C8-N7	-6.13	1.27	1.31
1	F	19	G	C2-N3	-6.13	1.27	1.32
1	F	57	G	C2-N3	-6.11	1.27	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	71	G	C2-N3	-6.10	1.27	1.32
1	F	15	G	C2-N3	-6.10	1.27	1.32
1	F	18	G	C2-N3	-6.09	1.27	1.32
1	F	9	A	C8-N7	-6.08	1.27	1.31
1	F	31	A	C8-N7	-6.08	1.27	1.31
1	F	46	G	C5-C4	-6.07	1.34	1.38
1	F	65	G	C2-N3	-6.05	1.27	1.32
1	F	29	A	C8-N7	-6.05	1.27	1.31
1	F	24	G	C2-N3	-6.05	1.27	1.32
1	F	23	A	C8-N7	-6.04	1.27	1.31
1	F	5	A	C8-N7	-6.04	1.27	1.31
1	F	63	C	C4-C5	6.03	1.47	1.43
1	F	64	A	C8-N7	-6.03	1.27	1.31
1	F	10	G	C2-N3	-6.02	1.27	1.32
1	F	44	A	C8-N7	-5.99	1.27	1.31
1	F	73	A	C8-N7	-5.99	1.27	1.31
1	F	21	A	C8-N7	-5.94	1.27	1.31
1	F	27	C	C4-C5	5.92	1.47	1.43
1	F	46	G	C2-N3	-5.91	1.28	1.32
1	F	67	A	C8-N7	-5.91	1.27	1.31
1	F	37	G	C2-N3	-5.89	1.28	1.32
1	F	38	A	C8-N7	-5.89	1.27	1.31
1	F	53	G	C2-N3	-5.86	1.28	1.32
1	F	1	G	C2-N3	-5.85	1.28	1.32
1	F	14	A	C8-N7	-5.84	1.27	1.31
1	F	30	G	C2-N3	-5.82	1.28	1.32
1	F	66	A	C8-N7	-5.81	1.27	1.31
1	F	26	G	C2-N3	-5.80	1.28	1.32
1	F	45	G	C2-N3	-5.80	1.28	1.32
1	F	20	G	C2-N3	-5.74	1.28	1.32
1	F	3	G	C2-N3	-5.71	1.28	1.32
1	F	51	G	C2-N3	-5.68	1.28	1.32
1	F	4	G	C2-N3	-5.66	1.28	1.32
1	F	22	G	C2-N3	-5.63	1.28	1.32
1	F	43	G	C2-N3	-5.59	1.28	1.32
1	F	34	G	C2-N3	-5.48	1.28	1.32
1	F	42	G	C2-N3	-5.47	1.28	1.32
1	F	27	C	N1-C2	-5.11	1.35	1.40
1	F	51	G	C6-N1	-5.11	1.35	1.39
1	F	61	C	N1-C2	-5.04	1.35	1.40
1	F	11	C	N1-C2	-5.04	1.35	1.40
1	F	18	G	C5-C6	5.02	1.47	1.42

All (715) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	55	U	C6-N1-C1'	-83.91	3.73	121.20
1	F	39	U	C6-N1-C1'	-73.66	18.07	121.20
1	F	55	U	C5-C6-N1	-50.74	97.33	122.70
1	F	55	U	C6-N1-C2	28.91	138.35	121.00
1	F	10	G	C4-C5-N7	-24.56	100.98	110.80
1	F	22	G	C4-C5-N7	-24.41	101.04	110.80
1	F	20	G	C4-C5-N7	-24.40	101.04	110.80
1	F	46	G	C4-C5-N7	-24.39	101.04	110.80
1	F	18	G	C4-C5-N7	-24.34	101.06	110.80
1	F	24	G	C4-C5-N7	-24.30	101.08	110.80
1	F	45	G	C4-C5-N7	-24.29	101.08	110.80
1	F	19	G	C4-C5-N7	-24.21	101.11	110.80
1	F	42	G	C4-C5-N7	-24.17	101.13	110.80
1	F	51	G	C4-C5-N7	-24.15	101.14	110.80
1	F	57	G	C4-C5-N7	-24.14	101.14	110.80
1	F	37	G	C4-C5-N7	-24.09	101.16	110.80
1	F	43	G	C4-C5-N7	-24.06	101.18	110.80
1	F	71	G	C4-C5-N7	-24.05	101.18	110.80
1	F	26	G	C4-C5-N7	-23.96	101.22	110.80
1	F	15	G	C4-C5-N7	-23.92	101.23	110.80
1	F	1	G	C4-C5-N7	-23.90	101.24	110.80
1	F	34	G	C4-C5-N7	-23.86	101.25	110.80
1	F	3	G	C4-C5-N7	-23.85	101.26	110.80
1	F	65	G	C4-C5-N7	-23.84	101.27	110.80
1	F	4	G	C4-C5-N7	-23.83	101.27	110.80
1	F	53	G	C4-C5-N7	-23.74	101.31	110.80
1	F	30	G	C4-C5-N7	-23.53	101.39	110.80
1	F	55	U	C4-C5-C6	23.16	133.59	119.70
1	F	39	U	O4'-C1'-N1	-21.01	91.39	108.20
1	F	55	U	C2-N3-C4	-20.09	114.95	127.00
1	F	46	G	N3-C4-C5	-19.69	118.75	128.60
1	F	34	G	N3-C4-C5	-19.42	118.89	128.60
1	F	43	G	N3-C4-C5	-19.30	118.95	128.60
1	F	24	G	N3-C4-C5	-19.15	119.02	128.60
1	F	10	G	N3-C4-C5	-19.14	119.03	128.60
1	F	26	G	N3-C4-C5	-19.10	119.05	128.60
1	F	51	G	N3-C4-C5	-19.07	119.06	128.60
1	F	57	G	N3-C4-C5	-19.06	119.07	128.60
1	F	18	G	N3-C4-C5	-19.05	119.07	128.60
1	F	30	G	N3-C4-C5	-19.04	119.08	128.60
1	F	65	G	N3-C4-C5	-19.01	119.09	128.60
1	F	22	G	N3-C4-C5	-19.01	119.10	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1	G	N3-C4-C5	-18.99	119.10	128.60
1	F	42	G	N3-C4-C5	-18.94	119.13	128.60
1	F	71	G	N3-C4-C5	-18.88	119.16	128.60
1	F	20	G	N3-C4-C5	-18.73	119.23	128.60
1	F	4	G	N3-C4-C5	-18.70	119.25	128.60
1	F	45	G	N3-C4-C5	-18.66	119.27	128.60
1	F	3	G	N3-C4-C5	-18.56	119.32	128.60
1	F	53	G	N3-C4-C5	-18.39	119.40	128.60
1	F	37	G	N3-C4-C5	-18.37	119.42	128.60
1	F	15	G	N3-C4-C5	-18.33	119.43	128.60
1	F	19	G	N3-C4-C5	-18.09	119.56	128.60
1	F	57	G	C2-N3-C4	17.08	120.44	111.90
1	F	34	G	C2-N3-C4	16.92	120.36	111.90
1	F	43	G	C2-N3-C4	16.91	120.36	111.90
1	F	46	G	C2-N3-C4	16.87	120.34	111.90
1	F	24	G	C2-N3-C4	16.83	120.31	111.90
1	F	10	G	C2-N3-C4	16.82	120.31	111.90
1	F	65	G	C2-N3-C4	16.73	120.27	111.90
1	F	15	G	C2-N3-C4	16.71	120.25	111.90
1	F	30	G	C2-N3-C4	16.69	120.24	111.90
1	F	71	G	C2-N3-C4	16.62	120.21	111.90
1	F	26	G	C2-N3-C4	16.62	120.21	111.90
1	F	45	G	C2-N3-C4	16.58	120.19	111.90
1	F	22	G	C2-N3-C4	16.57	120.19	111.90
1	F	3	G	C2-N3-C4	16.57	120.18	111.90
1	F	18	G	C2-N3-C4	16.55	120.18	111.90
1	F	1	G	C2-N3-C4	16.54	120.17	111.90
1	F	42	G	C2-N3-C4	16.54	120.17	111.90
1	F	37	G	C2-N3-C4	16.52	120.16	111.90
1	F	20	G	C2-N3-C4	16.44	120.12	111.90
1	F	53	G	C2-N3-C4	16.43	120.11	111.90
1	F	4	G	C2-N3-C4	16.38	120.09	111.90
1	F	51	G	C2-N3-C4	16.36	120.08	111.90
1	F	19	G	C2-N3-C4	16.13	119.97	111.90
1	F	20	G	N9-C4-C5	15.57	111.63	105.40
1	F	10	G	N9-C4-C5	15.46	111.58	105.40
1	F	45	G	N9-C4-C5	15.41	111.56	105.40
1	F	22	G	N9-C4-C5	15.39	111.56	105.40
1	F	18	G	N9-C4-C5	15.37	111.55	105.40
1	F	19	G	N9-C4-C5	15.26	111.50	105.40
1	F	51	G	N9-C4-C5	15.19	111.48	105.40
1	F	43	G	N9-C4-C5	15.17	111.47	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	26	G	N9-C4-C5	15.13	111.45	105.40
1	F	24	G	N9-C4-C5	15.10	111.44	105.40
1	F	37	G	N9-C4-C5	15.04	111.42	105.40
1	F	42	G	N9-C4-C5	15.01	111.41	105.40
1	F	64	A	C2-N3-C4	15.00	118.10	110.60
1	F	65	G	N9-C4-C5	14.98	111.39	105.40
1	F	71	G	N9-C4-C5	14.94	111.37	105.40
1	F	38	A	C2-N3-C4	14.92	118.06	110.60
1	F	46	G	N9-C4-C5	14.87	111.35	105.40
1	F	76	A	C2-N3-C4	14.84	118.02	110.60
1	F	15	G	N9-C4-C5	14.81	111.33	105.40
1	F	5	A	C2-N3-C4	14.76	117.98	110.60
1	F	1	G	N9-C4-C5	14.73	111.29	105.40
1	F	67	A	C2-N3-C4	14.71	117.95	110.60
1	F	44	A	C2-N3-C4	14.70	117.95	110.60
1	F	57	G	N9-C4-C5	14.66	111.26	105.40
1	F	14	A	C2-N3-C4	14.64	117.92	110.60
1	F	58	A	C2-N3-C4	14.63	117.92	110.60
1	F	73	A	C2-N3-C4	14.60	117.90	110.60
1	F	34	G	N9-C4-C5	14.55	111.22	105.40
1	F	4	G	N9-C4-C5	14.55	111.22	105.40
1	F	53	G	N9-C4-C5	14.54	111.22	105.40
1	F	23	A	C2-N3-C4	14.54	117.87	110.60
1	F	3	G	N9-C4-C5	14.53	111.21	105.40
1	F	29	A	C2-N3-C4	14.53	117.86	110.60
1	F	66	A	C2-N3-C4	14.52	117.86	110.60
1	F	35	A	C2-N3-C4	14.50	117.85	110.60
1	F	9	A	C2-N3-C4	14.44	117.82	110.60
1	F	36	A	C2-N3-C4	14.44	117.82	110.60
1	F	31	A	C2-N3-C4	14.43	117.81	110.60
1	F	30	G	N9-C4-C5	14.36	111.14	105.40
1	F	62	A	C2-N3-C4	14.26	117.73	110.60
1	F	21	A	C2-N3-C4	14.13	117.66	110.60
1	F	55	U	C2-N1-C1'	14.10	134.62	117.70
1	F	34	G	C5-C6-O6	-13.90	120.26	128.60
1	F	67	A	N1-C2-N3	-13.79	122.41	129.30
1	F	5	A	N1-C2-N3	-13.67	122.47	129.30
1	F	30	G	C5-C6-O6	-13.64	120.41	128.60
1	F	15	G	C6-C5-N7	13.63	138.58	130.40
1	F	19	G	C6-C5-N7	13.61	138.57	130.40
1	F	37	G	C6-C5-N7	13.60	138.56	130.40
1	F	36	A	N1-C2-N3	-13.58	122.51	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	66	A	N1-C2-N3	-13.57	122.51	129.30
1	F	20	G	C6-C5-N7	13.52	138.51	130.40
1	F	38	A	N1-C2-N3	-13.45	122.58	129.30
1	F	45	G	C6-C5-N7	13.45	138.47	130.40
1	F	14	A	N1-C2-N3	-13.44	122.58	129.30
1	F	29	A	N1-C2-N3	-13.43	122.58	129.30
1	F	64	A	N1-C2-N3	-13.43	122.59	129.30
1	F	10	G	C6-C5-N7	13.39	138.43	130.40
1	F	65	G	C5-C6-O6	-13.37	120.58	128.60
1	F	51	G	C5-C6-O6	-13.35	120.59	128.60
1	F	23	A	N1-C2-N3	-13.33	122.63	129.30
1	F	18	G	C6-C5-N7	13.29	138.38	130.40
1	F	22	G	C6-C5-N7	13.30	138.38	130.40
1	F	22	G	C5-C6-O6	-13.28	120.64	128.60
1	F	71	G	C6-C5-N7	13.28	138.37	130.40
1	F	57	G	C6-C5-N7	13.26	138.36	130.40
1	F	21	A	N1-C2-N3	-13.24	122.68	129.30
1	F	53	G	C6-C5-N7	13.23	138.34	130.40
1	F	3	G	C6-C5-N7	13.22	138.33	130.40
1	F	43	G	C5-C6-O6	-13.21	120.67	128.60
1	F	62	A	N1-C2-N3	-13.20	122.70	129.30
1	F	58	A	N1-C2-N3	-13.17	122.71	129.30
1	F	31	A	N1-C2-N3	-13.17	122.72	129.30
1	F	71	G	C5-C6-O6	-13.16	120.70	128.60
1	F	1	G	C5-C6-O6	-13.16	120.70	128.60
1	F	42	G	C6-C5-N7	13.16	138.30	130.40
1	F	9	A	N1-C2-N3	-13.15	122.72	129.30
1	F	76	A	N1-C2-N3	-13.14	122.73	129.30
1	F	73	A	N1-C2-N3	-13.11	122.74	129.30
1	F	4	G	C5-C6-O6	-13.10	120.74	128.60
1	F	3	G	C5-C6-O6	-13.10	120.74	128.60
1	F	24	G	C6-C5-N7	13.10	138.26	130.40
1	F	42	G	C5-C6-O6	-13.09	120.75	128.60
1	F	46	G	C6-C5-N7	13.02	138.21	130.40
1	F	1	G	C6-C5-N7	13.01	138.21	130.40
1	F	26	G	C5-C6-O6	-13.01	120.80	128.60
1	F	51	G	C6-C5-N7	13.00	138.20	130.40
1	F	4	G	C6-C5-N7	13.00	138.20	130.40
1	F	37	G	C5-C6-O6	-13.00	120.80	128.60
1	F	53	G	C5-C6-O6	-12.97	120.82	128.60
1	F	44	A	N1-C2-N3	-12.96	122.82	129.30
1	F	43	G	C6-C5-N7	12.91	138.15	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	65	G	C6-C5-N7	12.91	138.14	130.40
1	F	46	G	C5-C6-O6	-12.90	120.86	128.60
1	F	34	G	C6-C5-N7	12.89	138.13	130.40
1	F	35	A	N1-C2-N3	-12.88	122.86	129.30
1	F	15	G	C5-C6-O6	-12.87	120.88	128.60
1	F	26	G	C6-C5-N7	12.85	138.11	130.40
1	F	10	G	C5-C6-O6	-12.78	120.93	128.60
1	F	30	G	C6-C5-N7	12.78	138.06	130.40
1	F	45	G	C5-C6-O6	-12.65	121.01	128.60
1	F	19	G	C5-C6-O6	-12.64	121.02	128.60
1	F	20	G	C5-C6-O6	-12.62	121.03	128.60
1	F	57	G	C5-C6-O6	-12.60	121.04	128.60
1	F	24	G	C5-C6-O6	-12.58	121.06	128.60
1	F	14	A	C5-N7-C8	12.46	110.13	103.90
1	F	67	A	C5-N7-C8	12.42	110.11	103.90
1	F	31	A	C5-N7-C8	12.41	110.11	103.90
1	F	58	A	C5-N7-C8	12.41	110.11	103.90
1	F	73	A	C5-N7-C8	12.34	110.07	103.90
1	F	18	G	C5-C6-O6	-12.34	121.20	128.60
1	F	76	A	C5-N7-C8	12.32	110.06	103.90
1	F	21	A	C5-N7-C8	12.29	110.05	103.90
1	F	62	A	C5-N7-C8	12.25	110.03	103.90
1	F	5	A	C5-N7-C8	12.23	110.02	103.90
1	F	9	A	C5-N7-C8	12.23	110.01	103.90
1	F	64	A	C5-N7-C8	12.19	109.99	103.90
1	F	29	A	C5-N7-C8	12.16	109.98	103.90
1	F	75	C	P-O3'-C3'	-12.16	105.11	119.70
1	F	35	A	C5-N7-C8	12.12	109.96	103.90
1	F	36	A	C5-N7-C8	12.12	109.96	103.90
1	F	23	A	C5-N7-C8	12.04	109.92	103.90
1	F	38	A	C5-N7-C8	11.94	109.87	103.90
1	F	44	A	C5-N7-C8	11.88	109.84	103.90
1	F	66	A	C5-N7-C8	11.55	109.67	103.90
2	I	524	GLU	N-CA-C	11.38	141.73	111.00
1	F	11	C	N3-C4-C5	-11.26	117.39	121.90
1	F	50	U	C5-C4-O4	-11.24	119.16	125.90
1	F	39	U	C2-N1-C1'	-11.12	104.36	117.70
1	F	23	A	C4-C5-C6	11.12	122.56	117.00
1	F	75	C	N3-C4-C5	-11.10	117.46	121.90
1	F	48	C	N3-C4-C5	-11.09	117.46	121.90
1	F	17	U	C5-C4-O4	-11.09	119.25	125.90
1	F	25	C	N3-C4-C5	-11.06	117.48	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	69	U	C5-C4-O4	-11.06	119.27	125.90
1	F	72	C	N3-C4-C5	-11.04	117.48	121.90
1	F	32	C	N3-C4-C5	-11.03	117.49	121.90
1	F	41	U	C5-C4-O4	-10.93	119.34	125.90
1	F	54	U	C5-C4-O4	-10.91	119.36	125.90
1	F	14	A	C4-C5-N7	-10.90	105.25	110.70
1	F	13	C	N3-C4-C5	-10.89	117.55	121.90
1	F	74	C	N3-C4-C5	-10.88	117.55	121.90
1	F	12	U	C5-C4-O4	-10.87	119.38	125.90
1	F	59	U	C5-C4-O4	-10.86	119.38	125.90
1	F	35	A	C4-C5-C6	10.85	122.43	117.00
1	F	44	A	C4-C5-C6	10.84	122.42	117.00
1	F	38	A	C4-C5-C6	10.84	122.42	117.00
1	F	56	C	N3-C4-C5	-10.84	117.56	121.90
1	F	66	A	C4-C5-C6	10.84	122.42	117.00
1	F	58	A	C4-C5-N7	-10.82	105.29	110.70
1	F	60	C	N3-C4-C5	-10.80	117.58	121.90
1	F	70	C	N3-C4-C5	-10.81	117.58	121.90
1	F	52	U	C5-C4-O4	-10.79	119.43	125.90
1	F	64	A	C4-C5-C6	10.79	122.39	117.00
1	F	49	C	N3-C4-C5	-10.75	117.60	121.90
1	F	68	U	C5-C4-O4	-10.75	119.45	125.90
1	F	76	A	C4-C5-N7	-10.75	105.33	110.70
1	F	44	A	C4-C5-N7	-10.73	105.33	110.70
1	F	7	U	C5-C4-O4	-10.72	119.47	125.90
1	F	47	U	C5-C4-O4	-10.71	119.47	125.90
1	F	62	A	C4-C5-C6	10.68	122.34	117.00
1	F	16	U	C5-C4-O4	-10.67	119.50	125.90
1	F	6	U	C5-C4-O4	-10.66	119.50	125.90
1	F	5	A	C4-C5-N7	-10.65	105.37	110.70
1	F	5	A	C4-C5-C6	10.63	122.32	117.00
1	F	21	A	C4-C5-N7	-10.63	105.38	110.70
1	F	67	A	C4-C5-N7	-10.63	105.38	110.70
1	F	36	A	C4-C5-N7	-10.63	105.39	110.70
1	F	2	C	N3-C4-C5	-10.62	117.65	121.90
1	F	33	U	C5-C4-O4	-10.60	119.54	125.90
1	F	62	A	C4-C5-N7	-10.60	105.40	110.70
1	F	28	C	N3-C4-C5	-10.58	117.67	121.90
1	F	63	C	N3-C4-C5	-10.58	117.67	121.90
1	F	67	A	C4-C5-C6	10.57	122.29	117.00
1	F	23	A	C4-C5-N7	-10.57	105.41	110.70
1	F	10	G	C5-N7-C8	10.57	109.58	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	73	A	C4-C5-C6	10.56	122.28	117.00
1	F	73	A	C4-C5-N7	-10.56	105.42	110.70
1	F	8	U	C5-C4-O4	-10.52	119.59	125.90
1	F	37	G	C5-N7-C8	10.52	109.56	104.30
1	F	58	A	C4-C5-C6	10.51	122.25	117.00
1	F	21	A	C4-C5-C6	10.51	122.25	117.00
1	F	42	G	C5-N7-C8	10.50	109.55	104.30
1	F	31	A	C4-C5-N7	-10.50	105.45	110.70
1	F	3	G	C5-N7-C8	10.48	109.54	104.30
1	F	64	A	C4-C5-N7	-10.48	105.46	110.70
1	F	9	A	C4-C5-N7	-10.46	105.47	110.70
1	F	46	G	C5-N7-C8	10.46	109.53	104.30
1	F	19	G	C5-N7-C8	10.46	109.53	104.30
1	F	20	G	C5-N7-C8	10.46	109.53	104.30
1	F	22	G	C5-N7-C8	10.45	109.53	104.30
1	F	38	A	C4-C5-N7	-10.44	105.48	110.70
1	F	35	A	C4-C5-N7	-10.43	105.48	110.70
1	F	53	G	C5-N7-C8	10.42	109.51	104.30
1	F	24	G	C5-N7-C8	10.41	109.51	104.30
1	F	4	G	C5-N7-C8	10.39	109.49	104.30
1	F	34	G	C5-N7-C8	10.37	109.49	104.30
1	F	26	G	C5-N7-C8	10.36	109.48	104.30
1	F	27	C	N3-C4-C5	-10.37	117.75	121.90
1	F	29	A	C4-C5-N7	-10.36	105.52	110.70
1	F	76	A	C4-C5-C6	10.36	122.18	117.00
1	F	18	G	C5-N7-C8	10.34	109.47	104.30
1	F	55	U	C5-C4-O4	-10.33	119.70	125.90
1	F	71	G	C5-N7-C8	10.33	109.46	104.30
1	F	61	C	N3-C4-C5	-10.32	117.77	121.90
1	F	29	A	C4-C5-C6	10.31	122.16	117.00
1	F	44	A	N3-C4-C5	-10.31	119.58	126.80
1	F	40	C	N3-C4-C5	-10.30	117.78	121.90
1	F	43	G	C5-N7-C8	10.28	109.44	104.30
1	F	51	G	C5-N7-C8	10.27	109.44	104.30
1	F	14	A	C4-C5-C6	10.26	122.13	117.00
1	F	36	A	C4-C5-C6	10.26	122.13	117.00
1	F	64	A	N3-C4-C5	-10.26	119.62	126.80
1	F	9	A	C4-C5-C6	10.26	122.13	117.00
1	F	66	A	C4-C5-N7	-10.26	105.57	110.70
1	F	30	G	C5-N7-C8	10.24	109.42	104.30
1	F	15	G	C5-N7-C8	10.24	109.42	104.30
1	F	1	G	C5-N7-C8	10.24	109.42	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	45	G	C5-N7-C8	10.23	109.41	104.30
1	F	35	A	N3-C4-C5	-10.17	119.68	126.80
1	F	23	A	N3-C4-C5	-10.13	119.71	126.80
1	F	57	G	C5-N7-C8	10.10	109.35	104.30
1	F	76	A	N3-C4-C5	-10.10	119.73	126.80
1	F	31	A	C4-C5-C6	10.06	122.03	117.00
1	F	38	A	N3-C4-C5	-10.06	119.76	126.80
1	F	65	G	C5-N7-C8	10.05	109.33	104.30
1	F	58	A	N3-C4-C5	-10.03	119.78	126.80
1	F	39	U	C5-C4-O4	-9.94	119.94	125.90
1	F	14	A	N3-C4-C5	-9.93	119.85	126.80
1	F	73	A	N3-C4-C5	-9.93	119.85	126.80
1	F	5	A	N3-C4-C5	-9.89	119.87	126.80
1	F	66	A	N3-C4-C5	-9.82	119.93	126.80
1	F	29	A	N3-C4-C5	-9.80	119.94	126.80
1	F	62	A	N3-C4-C5	-9.77	119.96	126.80
1	F	36	A	N3-C4-C5	-9.76	119.97	126.80
1	F	67	A	N3-C4-C5	-9.76	119.97	126.80
1	F	31	A	N3-C4-C5	-9.73	119.99	126.80
1	F	9	A	N3-C4-C5	-9.72	119.99	126.80
1	F	21	A	N3-C4-C5	-9.64	120.05	126.80
1	F	47	U	O4'-C1'-N1	9.40	115.72	108.20
1	F	16	U	C2-N3-C4	-8.93	121.64	127.00
1	F	8	U	C2-N3-C4	-8.80	121.72	127.00
1	F	39	U	C2-N3-C4	-8.71	121.77	127.00
1	F	54	U	C2-N3-C4	-8.71	121.77	127.00
1	F	59	U	C2-N3-C4	-8.68	121.80	127.00
1	F	6	U	C2-N3-C4	-8.64	121.81	127.00
1	F	52	U	C2-N3-C4	-8.58	121.85	127.00
1	F	17	U	C2-N3-C4	-8.52	121.89	127.00
1	F	44	A	N3-C4-N9	8.50	134.20	127.40
1	F	64	A	N3-C4-N9	8.48	134.18	127.40
1	F	50	U	C2-N3-C4	-8.46	121.92	127.00
1	F	47	U	C2-N3-C4	-8.44	121.94	127.00
1	F	69	U	C2-N3-C4	-8.37	121.98	127.00
2	I	495	GLY	N-CA-C	8.34	133.95	113.10
1	F	29	A	N3-C4-N9	8.31	134.05	127.40
1	F	41	U	C2-N3-C4	-8.31	122.01	127.00
1	F	68	U	C2-N3-C4	-8.31	122.01	127.00
1	F	76	A	N3-C4-N9	8.24	133.99	127.40
1	F	35	A	N3-C4-N9	8.23	133.99	127.40
1	F	38	A	N3-C4-N9	8.22	133.97	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	75	C	OP1-P-O3'	8.22	123.28	105.20
1	F	31	A	N3-C4-N9	8.20	133.96	127.40
1	F	58	A	N3-C4-N9	8.18	133.95	127.40
1	F	7	U	C2-N3-C4	-8.18	122.09	127.00
1	F	14	A	N3-C4-N9	8.17	133.94	127.40
1	F	33	U	C2-N3-C4	-8.12	122.13	127.00
1	F	23	A	N3-C4-N9	8.11	133.89	127.40
1	F	73	A	N3-C4-N9	8.11	133.89	127.40
1	F	12	U	C2-N3-C4	-8.08	122.15	127.00
1	F	36	A	N3-C4-N9	8.07	133.86	127.40
1	F	9	A	N3-C4-N9	8.05	133.84	127.40
1	F	62	A	N3-C4-N9	8.02	133.81	127.40
1	F	5	A	N3-C4-N9	7.91	133.73	127.40
1	F	21	A	N3-C4-N9	7.90	133.72	127.40
1	F	66	A	N3-C4-N9	7.87	133.70	127.40
1	F	67	A	N3-C4-N9	7.83	133.66	127.40
1	F	34	G	C5-C6-N1	7.78	115.39	111.50
1	F	19	G	N7-C8-N9	-7.52	109.34	113.10
1	F	30	G	N1-C6-O6	7.51	124.40	119.90
1	F	71	G	C5-C6-N1	7.49	115.25	111.50
1	F	29	A	N1-C6-N6	7.48	123.09	118.60
1	F	43	G	C5-C6-N1	7.47	115.23	111.50
1	F	20	G	C5-C6-N1	7.43	115.22	111.50
1	F	49	C	N3-C4-N4	7.43	123.20	118.00
1	F	34	G	N1-C6-O6	7.42	124.35	119.90
1	F	35	A	N1-C6-N6	7.42	123.05	118.60
1	F	51	G	C5-C6-N1	7.42	115.21	111.50
1	F	37	G	C5-C6-N1	7.41	115.21	111.50
1	F	53	G	N7-C8-N9	-7.41	109.39	113.10
1	F	8	U	N1-C2-N3	7.39	119.33	114.90
1	F	25	C	N3-C4-N4	7.39	123.17	118.00
1	F	65	G	N1-C6-O6	7.36	124.32	119.90
1	F	30	G	C5-C6-N1	7.36	115.18	111.50
1	F	53	G	C5-C6-N1	7.36	115.18	111.50
1	F	45	G	C5-C6-N1	7.35	115.17	111.50
1	F	23	A	N1-C6-N6	7.33	123.00	118.60
1	F	3	G	N1-C6-O6	7.32	124.29	119.90
1	F	32	C	N3-C4-N4	7.30	123.11	118.00
1	F	71	G	N7-C8-N9	-7.29	109.45	113.10
1	F	3	G	N7-C8-N9	-7.28	109.46	113.10
1	F	22	G	C5-C6-N1	7.26	115.13	111.50
1	F	1	G	N1-C6-O6	7.26	124.25	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	31	A	N1-C6-N6	7.26	122.95	118.60
1	F	34	G	N7-C8-N9	-7.24	109.48	113.10
1	F	15	G	C5-C6-N1	7.24	115.12	111.50
1	F	37	G	N7-C8-N9	-7.23	109.48	113.10
2	I	520	GLY	N-CA-C	7.23	131.17	113.10
1	F	22	G	N1-C6-O6	7.22	124.23	119.90
1	F	57	G	C5-C6-N1	7.21	115.11	111.50
1	F	43	G	N7-C8-N9	-7.21	109.50	113.10
1	F	65	G	C5-C6-N1	7.21	115.11	111.50
1	F	28	C	N3-C4-N4	7.20	123.04	118.00
1	F	46	G	C5-C6-N1	7.20	115.10	111.50
1	F	26	G	N1-C6-O6	7.20	124.22	119.90
1	F	42	G	N7-C8-N9	-7.20	109.50	113.10
1	F	4	G	C5-C6-N1	7.19	115.10	111.50
1	F	10	G	N7-C8-N9	-7.19	109.50	113.10
1	F	26	G	N7-C8-N9	-7.19	109.51	113.10
1	F	4	G	N7-C8-N9	-7.18	109.51	113.10
1	F	9	A	OP1-P-OP2	-7.17	108.84	119.60
1	F	64	A	N1-C6-N6	7.17	122.91	118.60
1	F	51	G	N1-C6-O6	7.17	124.20	119.90
1	F	61	C	N3-C4-N4	7.16	123.01	118.00
1	F	11	C	N3-C4-N4	7.16	123.01	118.00
1	F	19	G	C5-C6-N1	7.15	115.07	111.50
1	F	42	G	N1-C6-O6	7.15	124.19	119.90
1	F	5	A	N1-C6-N6	7.14	122.88	118.60
1	F	70	C	N3-C4-N4	7.14	123.00	118.00
1	F	73	A	N1-C6-N6	7.14	122.88	118.60
1	F	18	G	OP1-P-OP2	-7.13	108.90	119.60
1	F	21	A	N1-C6-N6	7.13	122.88	118.60
1	F	42	G	C5-C6-N1	7.13	115.06	111.50
1	F	13	C	N3-C4-N4	7.12	122.98	118.00
1	F	16	U	N1-C2-N3	7.11	119.17	114.90
1	F	4	G	N1-C6-O6	7.11	124.17	119.90
1	F	39	U	N1-C2-N3	7.10	119.16	114.90
1	F	44	A	N1-C6-N6	7.10	122.86	118.60
1	F	30	G	N7-C8-N9	-7.08	109.56	113.10
1	F	1	G	C5-C6-N1	7.08	115.04	111.50
1	F	24	G	N7-C8-N9	-7.08	109.56	113.10
1	F	51	G	N7-C8-N9	-7.07	109.56	113.10
2	I	599	LEU	CA-CB-CG	7.06	131.54	115.30
1	F	2	C	N3-C4-N4	7.05	122.94	118.00
1	F	24	G	C5-C6-N1	7.05	115.03	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	58	A	OP1-P-OP2	-7.05	109.03	119.60
1	F	38	A	N1-C6-N6	7.04	122.83	118.60
1	F	57	G	N7-C8-N9	-7.04	109.58	113.10
1	F	27	C	N3-C4-N4	7.04	122.93	118.00
1	F	20	G	N7-C8-N9	-7.04	109.58	113.10
1	F	75	C	N3-C4-N4	7.04	122.93	118.00
1	F	72	C	N3-C4-N4	7.03	122.92	118.00
1	F	62	A	N1-C6-N6	7.03	122.82	118.60
1	F	65	G	N7-C8-N9	-7.02	109.59	113.10
1	F	45	G	OP1-P-OP2	-7.02	109.08	119.60
1	F	18	G	N7-C8-N9	-7.02	109.59	113.10
1	F	40	C	N3-C4-N4	7.01	122.90	118.00
1	F	10	G	N1-C6-O6	6.99	124.09	119.90
1	F	48	C	OP1-P-OP2	-6.99	109.12	119.60
1	F	15	G	N7-C8-N9	-6.99	109.61	113.10
1	F	43	G	N1-C6-O6	6.99	124.09	119.90
1	F	26	G	C5-C6-N1	6.97	114.99	111.50
1	F	68	U	OP1-P-OP2	-6.96	109.16	119.60
1	F	36	A	OP1-P-OP2	-6.96	109.16	119.60
1	F	10	G	C5-C6-N1	6.95	114.98	111.50
1	F	45	G	N7-C8-N9	-6.95	109.62	113.10
1	F	27	C	OP1-P-OP2	-6.95	109.18	119.60
1	F	3	G	C5-C6-N1	6.94	114.97	111.50
1	F	18	G	C5-C6-N1	6.94	114.97	111.50
1	F	8	U	OP1-P-OP2	-6.94	109.20	119.60
1	F	39	U	OP1-P-OP2	-6.93	109.20	119.60
1	F	71	G	N1-C6-O6	6.92	124.05	119.90
1	F	19	G	OP1-P-OP2	-6.92	109.22	119.60
1	F	55	U	OP1-P-OP2	-6.92	109.22	119.60
1	F	73	A	OP1-P-OP2	-6.91	109.23	119.60
1	F	22	G	N7-C8-N9	-6.91	109.64	113.10
1	F	46	G	N1-C6-O6	6.90	124.04	119.90
1	F	4	G	OP1-P-OP2	-6.90	109.25	119.60
1	F	21	A	OP1-P-OP2	-6.89	109.26	119.60
1	F	48	C	N3-C4-N4	6.88	122.82	118.00
1	F	16	U	OP1-P-OP2	-6.88	109.28	119.60
1	F	51	G	OP1-P-OP2	-6.88	109.28	119.60
1	F	67	A	OP1-P-OP2	-6.88	109.28	119.60
1	F	46	G	N7-C8-N9	-6.88	109.66	113.10
1	F	40	C	OP1-P-OP2	-6.87	109.30	119.60
1	F	50	U	OP1-P-OP2	-6.87	109.30	119.60
1	F	56	C	N3-C4-N4	6.86	122.80	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	74	C	OP1-P-OP2	-6.86	109.31	119.60
1	F	62	A	OP1-P-OP2	-6.86	109.31	119.60
1	F	24	G	OP1-P-OP2	-6.86	109.31	119.60
1	F	25	C	OP1-P-OP2	-6.86	109.31	119.60
1	F	63	C	N3-C4-N4	6.86	122.80	118.00
1	F	12	U	OP1-P-OP2	-6.86	109.32	119.60
1	F	74	C	N3-C4-N4	6.86	122.80	118.00
1	F	67	A	N1-C6-N6	6.85	122.71	118.60
1	F	1	G	N7-C8-N9	-6.85	109.67	113.10
1	F	35	A	OP1-P-OP2	-6.85	109.33	119.60
1	F	48	C	C4-C5-C6	6.84	120.82	117.40
1	F	37	G	OP1-P-OP2	-6.84	109.34	119.60
1	F	66	A	N1-C6-N6	6.84	122.70	118.60
1	F	53	G	N1-C6-O6	6.84	124.00	119.90
1	F	41	U	OP1-P-OP2	-6.84	109.35	119.60
1	F	54	U	OP1-P-OP2	-6.83	109.35	119.60
1	F	31	A	OP1-P-OP2	-6.83	109.35	119.60
1	F	2	C	OP1-P-OP2	-6.83	109.36	119.60
1	F	33	U	OP1-P-OP2	-6.83	109.36	119.60
1	F	47	U	OP1-P-OP2	-6.83	109.36	119.60
1	F	57	G	OP1-P-OP2	-6.83	109.36	119.60
1	F	15	G	N1-C6-O6	6.82	123.99	119.90
1	F	37	G	N1-C6-O6	6.82	123.99	119.90
1	F	5	A	OP1-P-OP2	-6.82	109.37	119.60
1	F	7	U	OP1-P-OP2	-6.82	109.37	119.60
1	F	38	A	OP1-P-OP2	-6.82	109.38	119.60
1	F	43	G	OP1-P-OP2	-6.81	109.38	119.60
1	F	53	G	OP1-P-OP2	-6.81	109.39	119.60
1	F	70	C	OP1-P-OP2	-6.81	109.39	119.60
1	F	60	C	N3-C4-N4	6.81	122.77	118.00
1	F	44	A	OP1-P-OP2	-6.80	109.39	119.60
1	F	75	C	OP1-P-OP2	-6.80	109.40	119.60
1	F	26	G	OP1-P-OP2	-6.80	109.40	119.60
1	F	76	A	OP1-P-OP2	-6.80	109.40	119.60
1	F	72	C	OP1-P-OP2	-6.80	109.41	119.60
1	F	6	U	OP1-P-OP2	-6.79	109.41	119.60
1	F	58	A	N1-C6-N6	6.79	122.68	118.60
1	F	42	G	OP1-P-OP2	-6.79	109.42	119.60
1	F	36	A	N1-C6-N6	6.79	122.67	118.60
1	F	69	U	OP1-P-OP2	-6.78	109.43	119.60
1	F	52	U	OP1-P-OP2	-6.78	109.43	119.60
1	F	66	A	OP1-P-OP2	-6.78	109.43	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	32	C	OP1-P-OP2	-6.78	109.43	119.60
1	F	20	G	OP1-P-OP2	-6.77	109.44	119.60
1	F	29	A	OP1-P-OP2	-6.77	109.45	119.60
1	F	76	A	N1-C6-N6	6.76	122.66	118.60
1	F	14	A	OP1-P-OP2	-6.75	109.47	119.60
1	F	63	C	OP1-P-OP2	-6.75	109.47	119.60
1	F	71	G	OP1-P-OP2	-6.75	109.47	119.60
1	F	59	U	N1-C2-N3	6.74	118.94	114.90
1	F	60	C	OP1-P-OP2	-6.74	109.49	119.60
1	F	68	U	N1-C2-N3	6.74	118.94	114.90
1	F	9	A	N1-C6-N6	6.74	122.64	118.60
1	F	3	G	OP1-P-OP2	-6.74	109.50	119.60
1	F	23	A	OP1-P-OP2	-6.74	109.50	119.60
1	F	34	G	OP1-P-OP2	-6.73	109.50	119.60
1	F	11	C	OP1-P-OP2	-6.72	109.52	119.60
1	F	28	C	OP1-P-OP2	-6.72	109.52	119.60
1	F	65	G	OP1-P-OP2	-6.72	109.52	119.60
1	F	49	C	OP1-P-OP2	-6.72	109.52	119.60
1	F	30	G	OP1-P-OP2	-6.71	109.53	119.60
1	F	46	G	OP1-P-OP2	-6.71	109.53	119.60
1	F	24	G	N1-C6-O6	6.70	123.92	119.90
1	F	64	A	OP1-P-OP2	-6.70	109.56	119.60
1	F	56	C	OP1-P-OP2	-6.69	109.56	119.60
1	F	15	G	OP1-P-OP2	-6.69	109.56	119.60
1	F	61	C	OP1-P-OP2	-6.69	109.56	119.60
1	F	47	U	N1-C2-N3	6.68	118.91	114.90
1	F	59	U	OP1-P-OP2	-6.68	109.58	119.60
1	F	19	G	N1-C6-O6	6.68	123.91	119.90
1	F	22	G	OP1-P-OP2	-6.66	109.60	119.60
1	F	60	C	C4-C5-C6	6.66	120.73	117.40
1	F	50	U	N1-C2-N3	6.63	118.88	114.90
1	F	52	U	N1-C2-N3	6.63	118.88	114.90
1	F	6	U	N1-C2-N3	6.61	118.87	114.90
1	F	57	G	N1-C6-O6	6.59	123.86	119.90
2	I	605	SER	N-CA-C	6.58	128.76	111.00
1	F	14	A	N1-C6-N6	6.56	122.53	118.60
1	F	18	G	N1-C6-O6	6.55	123.83	119.90
1	F	17	U	OP1-P-OP2	-6.54	109.80	119.60
1	F	45	G	N1-C6-O6	6.52	123.81	119.90
1	F	33	U	N1-C2-N3	6.51	118.80	114.90
1	F	46	G	N3-C4-N9	6.50	129.90	126.00
1	F	34	G	N3-C4-N9	6.48	129.89	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	10	G	OP1-P-OP2	-6.48	109.89	119.60
1	F	17	U	N1-C2-N3	6.46	118.78	114.90
1	F	20	G	N1-C6-O6	6.43	123.76	119.90
1	F	69	U	N1-C2-N3	6.43	118.76	114.90
1	F	13	C	OP1-P-OP2	-6.39	110.02	119.60
1	F	54	U	N1-C2-N3	6.37	118.72	114.90
1	F	72	C	C4-C5-C6	6.34	120.57	117.40
1	F	21	A	O4'-C1'-N9	6.32	113.25	108.20
1	F	74	C	C4-C5-C6	6.32	120.56	117.40
1	F	41	U	N1-C2-N3	6.31	118.69	114.90
1	F	74	C	N3-C2-O2	-6.29	117.50	121.90
1	F	30	G	N3-C4-N9	6.29	129.78	126.00
1	F	32	C	C4-C5-C6	6.29	120.55	117.40
1	F	7	U	N1-C2-N3	6.28	118.67	114.90
1	F	75	C	N3-C2-O2	-6.28	117.51	121.90
1	F	12	U	N1-C2-N3	6.26	118.66	114.90
1	F	46	G	O4'-C1'-N9	6.21	113.16	108.20
1	F	61	C	N3-C2-O2	-6.20	117.56	121.90
1	F	27	C	N3-C2-O2	-6.17	117.58	121.90
1	F	27	C	N1-C2-O2	6.17	122.60	118.90
1	F	56	C	C4-C5-C6	6.16	120.48	117.40
1	F	13	C	C4-C5-C6	6.14	120.47	117.40
2	I	465	LEU	CA-CB-CG	6.14	129.43	115.30
1	F	25	C	C4-C5-C6	6.13	120.46	117.40
1	F	11	C	C4-C5-C6	6.12	120.46	117.40
1	F	54	U	N3-C4-C5	6.11	118.27	114.60
1	F	57	G	N3-C4-N9	6.11	129.67	126.00
1	F	63	C	C4-C5-C6	6.11	120.45	117.40
1	F	75	C	N1-C2-O2	6.09	122.56	118.90
1	F	67	A	N7-C8-N9	-6.09	110.75	113.80
1	F	70	C	C4-C5-C6	6.09	120.45	117.40
1	F	2	C	C4-C5-C6	6.08	120.44	117.40
1	F	69	U	N3-C4-C5	6.06	118.24	114.60
1	F	73	A	N7-C8-N9	-6.06	110.77	113.80
1	F	40	C	N3-C2-O2	-6.05	117.66	121.90
1	F	74	C	N1-C2-O2	6.04	122.53	118.90
1	F	21	A	N7-C8-N9	-6.03	110.78	113.80
1	F	1	G	N3-C4-N9	6.01	129.60	126.00
1	F	16	U	N3-C4-C5	6.00	118.20	114.60
1	F	61	C	N1-C2-O2	6.00	122.50	118.90
1	F	31	A	N7-C8-N9	-5.99	110.81	113.80
1	F	43	G	N3-C4-N9	5.97	129.58	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	8	U	N1-C1'-C2'	-5.97	105.44	112.00
1	F	11	C	N3-C2-O2	-5.94	117.74	121.90
1	F	14	A	N7-C8-N9	-5.94	110.83	113.80
1	F	63	C	N1-C2-O2	5.94	122.47	118.90
1	F	50	U	N3-C4-C5	5.94	118.16	114.60
1	F	38	A	N7-C8-N9	-5.93	110.83	113.80
1	F	6	U	N3-C4-C5	5.93	118.16	114.60
1	F	32	C	N3-C2-O2	-5.92	117.75	121.90
1	F	35	A	N7-C8-N9	-5.91	110.84	113.80
1	F	24	G	N3-C4-N9	5.89	129.53	126.00
1	F	59	U	N3-C4-C5	5.89	118.14	114.60
1	F	4	G	N3-C4-N9	5.89	129.53	126.00
1	F	27	C	C4-C5-C6	5.88	120.34	117.40
1	F	13	C	N3-C2-O2	-5.88	117.78	121.90
1	F	25	C	N1-C2-O2	5.88	122.43	118.90
1	F	60	C	N3-C2-O2	-5.87	117.79	121.90
1	F	58	A	N7-C8-N9	-5.87	110.86	113.80
1	F	55	U	N1-C2-N3	5.86	118.42	114.90
1	F	63	C	N3-C2-O2	-5.86	117.80	121.90
1	F	7	U	N3-C4-C5	5.86	118.11	114.60
1	F	65	G	N3-C4-N9	5.85	129.51	126.00
1	F	5	A	N7-C8-N9	-5.85	110.88	113.80
1	F	17	U	N3-C4-C5	5.85	118.11	114.60
1	F	49	C	N1-C2-O2	5.85	122.41	118.90
1	F	49	C	N3-C2-O2	-5.85	117.81	121.90
1	F	56	C	N3-C2-O2	-5.85	117.81	121.90
1	F	52	U	N3-C4-C5	5.85	118.11	114.60
1	F	64	A	N7-C8-N9	-5.83	110.88	113.80
1	F	26	G	N3-C4-N9	5.83	129.50	126.00
1	F	40	C	C4-C5-C6	5.83	120.31	117.40
1	F	47	U	N3-C4-C5	5.83	118.09	114.60
1	F	40	C	N1-C2-O2	5.82	122.39	118.90
1	F	49	C	C4-C5-C6	5.81	120.30	117.40
1	F	32	C	N1-C2-O2	5.79	122.38	118.90
1	F	56	C	N1-C2-O2	5.79	122.37	118.90
1	F	28	C	C4-C5-C6	5.78	120.29	117.40
1	F	3	G	N3-C4-N9	5.78	129.47	126.00
1	F	13	C	N1-C2-O2	5.78	122.37	118.90
1	F	11	C	N1-C2-O2	5.78	122.36	118.90
1	F	42	G	N3-C4-N9	5.78	129.47	126.00
1	F	25	C	N3-C2-O2	-5.77	117.86	121.90
1	F	71	G	N3-C4-N9	5.77	129.46	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	283	GLY	N-CA-C	5.77	127.52	113.10
1	F	51	G	N3-C4-N9	5.76	129.46	126.00
1	F	18	G	O4'-C1'-N9	5.76	112.81	108.20
1	F	41	U	N3-C4-C5	5.76	118.06	114.60
1	F	70	C	N3-C2-O2	-5.75	117.87	121.90
1	F	60	C	N1-C2-O2	5.75	122.35	118.90
1	F	33	U	N3-C4-C5	5.73	118.04	114.60
1	F	2	C	N3-C2-O2	-5.73	117.89	121.90
1	F	9	A	N7-C8-N9	-5.73	110.94	113.80
1	F	29	A	N7-C8-N9	-5.72	110.94	113.80
1	F	72	C	N3-C2-O2	-5.72	117.90	121.90
1	F	75	C	C4-C5-C6	5.72	120.26	117.40
1	F	61	C	C4-C5-C6	5.71	120.25	117.40
1	F	12	U	N3-C4-C5	5.70	118.02	114.60
2	I	522	VAL	N-CA-C	-5.68	95.66	111.00
1	F	68	U	N3-C4-C5	5.67	118.00	114.60
1	F	57	G	C8-N9-C4	5.66	108.66	106.40
1	F	36	A	N7-C8-N9	-5.66	110.97	113.80
1	F	62	A	N7-C8-N9	-5.65	110.97	113.80
1	F	10	G	N3-C4-N9	5.65	129.39	126.00
1	F	8	U	N3-C4-C5	5.63	117.98	114.60
1	F	18	G	N3-C4-N9	5.63	129.38	126.00
1	F	53	G	N3-C4-N9	5.63	129.38	126.00
1	F	44	A	N7-C8-N9	-5.62	110.99	113.80
1	F	5	A	C6-N1-C2	5.62	121.97	118.60
1	F	76	A	N7-C8-N9	-5.62	110.99	113.80
1	F	36	A	C6-N1-C2	5.62	121.97	118.60
1	F	23	A	N7-C8-N9	-5.61	111.00	113.80
1	F	70	C	N1-C2-O2	5.61	122.27	118.90
1	F	39	U	N3-C4-C5	5.58	117.95	114.60
1	F	22	G	N3-C4-N9	5.58	129.35	126.00
1	F	76	A	O4'-C1'-N9	5.53	112.62	108.20
1	F	15	G	N9-C1'-C2'	-5.51	105.94	112.00
1	F	68	U	C5'-C4'-C3'	-5.49	107.21	116.00
2	I	268	HIS	N-CA-C	5.48	125.80	111.00
1	F	28	C	N3-C2-O2	-5.48	118.06	121.90
1	F	45	G	N9-C1'-C2'	-5.48	105.97	112.00
1	F	72	C	N1-C2-O2	5.47	122.18	118.90
1	F	28	C	N1-C2-O2	5.46	122.18	118.90
1	F	21	A	C6-N1-C2	5.44	121.86	118.60
1	F	53	G	C8-N9-C4	5.43	108.57	106.40
1	F	66	A	C6-N1-C2	5.43	121.86	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	67	A	C6-N1-C2	5.43	121.86	118.60
1	F	64	A	C6-N1-C2	5.42	121.85	118.60
1	F	29	A	C6-N1-C2	5.41	121.85	118.60
1	F	2	C	N1-C2-O2	5.40	122.14	118.90
1	F	15	G	N3-C4-N9	5.40	129.24	126.00
1	F	21	A	C1'-O4'-C4'	-5.40	105.58	109.90
1	F	34	G	C8-N9-C4	5.40	108.56	106.40
1	F	38	A	C6-N1-C2	5.39	121.83	118.60
1	F	66	A	N7-C8-N9	-5.39	111.10	113.80
2	I	560	GLY	N-CA-C	-5.37	99.67	113.10
2	I	523	HIS	N-CA-C	5.36	125.47	111.00
2	I	356	LEU	CA-CB-CG	5.35	127.60	115.30
1	F	48	C	N3-C2-O2	-5.34	118.16	121.90
1	F	23	A	C6-N1-C2	5.32	121.79	118.60
1	F	3	G	C8-N9-C4	5.30	108.52	106.40
1	F	71	G	C8-N9-C4	5.30	108.52	106.40
1	F	45	G	N3-C4-N9	5.28	129.17	126.00
1	F	37	G	N3-C4-N9	5.28	129.17	126.00
1	F	19	G	C8-N9-C4	5.28	108.51	106.40
1	F	4	G	C8-N9-C4	5.27	108.51	106.40
1	F	14	A	C6-N1-C2	5.24	121.74	118.60
1	F	20	G	N3-C4-N9	5.23	129.14	126.00
2	I	510	LEU	CA-CB-CG	5.23	127.33	115.30
1	F	30	G	C8-N9-C4	5.22	108.49	106.40
1	F	31	A	C6-N1-C2	5.20	121.72	118.60
1	F	2	C	C5'-C4'-C3'	-5.20	107.68	116.00
1	F	9	A	C6-N1-C2	5.11	121.67	118.60
2	I	523	HIS	C-N-CA	5.09	134.43	121.70
1	F	59	U	C5'-C4'-C3'	-5.08	107.88	116.00
3	W	34	ALA	N-CA-C	5.07	124.68	111.00
1	F	55	U	N3-C4-O4	5.07	122.95	119.40
1	F	65	G	C8-N9-C4	5.06	108.42	106.40
1	F	62	A	C6-N1-C2	5.06	121.64	118.60
1	F	46	G	C8-N9-C4	5.05	108.42	106.40
1	F	43	G	C8-N9-C4	5.04	108.42	106.40
1	F	16	U	O4'-C1'-N1	5.03	112.23	108.20
1	F	24	G	C8-N9-C4	5.03	108.41	106.40
1	F	48	C	N1-C2-O2	5.03	121.92	118.90
1	F	73	A	C6-N1-C2	5.02	121.61	118.60
1	F	15	G	C8-N9-C4	5.02	108.41	106.40
1	F	58	A	C6-N1-C2	5.01	121.60	118.60
1	F	76	A	C6-N1-C2	5.01	121.60	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	42	G	C8-N9-C4	5.00	108.40	106.40

There are no chirality outliers.

There are no planarity outliers.

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	F	1622	0	821	149	0
2	I	3800	0	3868	101	0
3	W	570	0	599	1	0
All	All	5992	0	5288	248	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 22.

All (248) 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:F:75:C:O3'	1:F:76:A:P	1.97	1.23
1:F:36:A:H2'	1:F:37:G:H5''	1.15	1.09
1:F:74:C:H2'	1:F:75:C:C6	1.95	1.01
1:F:18:G:N2	1:F:57:G:H2'	1.78	0.99
2:I:432:ILE:HD12	2:I:445:MET:HG2	1.48	0.94
1:F:36:A:C2'	1:F:37:G:H5''	1.97	0.94
2:I:522:VAL:HG13	2:I:523:HIS:H	1.35	0.91
1:F:20:G:H21	1:F:22:G:H5'	1.35	0.90
1:F:20:G:H2'	1:F:21:A:H5''	1.54	0.87
1:F:32:C:H2'	1:F:33:U:C6	2.12	0.84
1:F:68:U:H2'	1:F:69:U:H6	1.44	0.82
2:I:405:VAL:HG12	2:I:406:ILE:H	1.43	0.82
2:I:405:VAL:O	2:I:406:ILE:HD12	1.81	0.81
1:F:63:C:H2'	1:F:64:A:H8	1.46	0.80
1:F:66:A:H2'	1:F:67:A:H8	1.46	0.80
1:F:47:U:H5''	1:F:47:U:C6	2.17	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:74:C:H2'	1:F:75:C:H6	1.47	0.78
1:F:20:G:N2	1:F:22:G:H5'	1.98	0.78
2:I:406:ILE:HD13	2:I:420:VAL:HA	1.65	0.77
1:F:14:A:H2'	1:F:15:G:H8	1.49	0.77
1:F:75:C:C3'	1:F:76:A:P	2.72	0.76
1:F:20:G:C2'	1:F:21:A:H5''	2.16	0.75
2:I:336:ILE:HD13	2:I:336:ILE:O	1.87	0.74
1:F:44:A:H2'	1:F:45:G:H8	1.53	0.73
1:F:75:C:H1'	2:I:708:ARG:HH11	1.53	0.72
1:F:16:U:H3	1:F:60:C:H1'	1.53	0.72
1:F:6:U:H2'	1:F:7:U:C6	2.25	0.72
1:F:32:C:H2'	1:F:33:U:H6	1.51	0.71
1:F:28:C:H2'	1:F:29:A:H8	1.56	0.69
1:F:44:A:H2'	1:F:45:G:C8	2.28	0.69
1:F:68:U:H2'	1:F:69:U:C6	2.27	0.69
2:I:522:VAL:HG13	2:I:523:HIS:N	2.05	0.69
1:F:14:A:H2'	1:F:15:G:C8	2.29	0.68
1:F:9:A:H61	1:F:22:G:H2'	1.59	0.68
1:F:34:G:H2'	1:F:35:A:O4'	1.94	0.68
1:F:6:U:H2'	1:F:7:U:H6	1.58	0.67
1:F:33:U:H3	1:F:35:A:H3'	1.59	0.67
1:F:37:G:H2'	1:F:38:A:H8	1.58	0.67
1:F:74:C:H2'	1:F:75:C:C5	2.29	0.67
2:I:406:ILE:HD13	2:I:420:VAL:CA	2.24	0.66
1:F:63:C:H2'	1:F:64:A:C8	2.30	0.66
2:I:406:ILE:HD11	2:I:421:LEU:HB2	1.76	0.66
1:F:47:U:N3	1:F:50:U:H5''	2.12	0.65
2:I:405:VAL:HG11	2:I:487:ARG:NH2	2.12	0.65
2:I:403:GLY:HA2	2:I:423:ARG:HE	1.62	0.65
2:I:405:VAL:C	2:I:406:ILE:HD12	2.17	0.65
2:I:443:ARG:H	2:I:443:ARG:HE	1.43	0.64
1:F:31:A:O2'	1:F:32:C:H5'	1.97	0.64
2:I:443:ARG:H	2:I:443:ARG:NE	1.96	0.63
2:I:718:ILE:HD12	2:I:718:ILE:H	1.64	0.63
1:F:10:G:H2'	1:F:11:C:C6	2.33	0.63
2:I:405:VAL:HG12	2:I:406:ILE:N	2.12	0.62
1:F:8:U:H5'	1:F:49:C:OP2	1.99	0.62
2:I:301:VAL:HB	2:I:329:VAL:HG12	1.82	0.62
1:F:16:U:N3	1:F:60:C:H1'	2.13	0.62
1:F:66:A:H2'	1:F:67:A:C8	2.33	0.62
1:F:25:C:O2'	1:F:26:G:H5'	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:39:U:H2'	1:F:40:C:C6	2.36	0.61
2:I:419:THR:HB	2:I:478:THR:HG22	1.82	0.61
1:F:72:C:H2'	1:F:73:A:H8	1.64	0.61
2:I:607:ILE:CD1	2:I:608:TYR:H	2.14	0.60
1:F:37:G:H2'	1:F:38:A:C8	2.35	0.60
1:F:54:U:O2'	1:F:55:U:H5'	2.01	0.60
1:F:10:G:O2'	1:F:11:C:H5'	2.02	0.60
1:F:68:U:H6	1:F:68:U:O5'	1.85	0.60
2:I:446:ARG:HH21	2:I:479:VAL:HG22	1.67	0.60
1:F:1:G:O2'	1:F:2:C:H5'	2.01	0.59
1:F:47:U:H5''	1:F:47:U:H6	1.67	0.59
2:I:269:VAL:HG13	2:I:273:ASN:HB3	1.83	0.59
1:F:8:U:H5'	1:F:49:C:P	2.42	0.59
1:F:19:G:H5''	1:F:60:C:H42	1.67	0.59
1:F:23:A:H2'	1:F:24:G:C8	2.37	0.59
2:I:575:SER:OG	2:I:611:ILE:HD12	2.03	0.59
1:F:3:G:H2'	1:F:4:G:H8	1.67	0.59
1:F:18:G:H1'	1:F:57:G:N2	2.17	0.58
1:F:75:C:H1'	2:I:708:ARG:NH1	2.19	0.58
1:F:76:A:H4'	2:I:711:ASP:OD1	2.03	0.58
1:F:33:U:N3	1:F:35:A:H3'	2.18	0.58
1:F:8:U:H4'	1:F:48:C:H4'	1.84	0.58
2:I:533:VAL:HG12	2:I:535:GLY:H	1.67	0.58
2:I:299:ASP:HB2	2:I:300:ILE:HD12	1.86	0.58
1:F:30:G:O2'	1:F:31:A:H5'	2.04	0.57
1:F:53:G:O2'	1:F:54:U:H5'	2.04	0.57
1:F:26:G:H2'	1:F:27:C:C6	2.38	0.57
1:F:56:C:O2'	1:F:57:G:H5'	2.04	0.57
1:F:64:A:H2'	1:F:65:G:H8	1.69	0.57
2:I:232:ILE:HD13	2:I:244:LEU:HD23	1.86	0.57
1:F:62:A:H2'	1:F:63:C:C6	2.39	0.57
1:F:11:C:H2'	1:F:12:U:C6	2.40	0.57
1:F:71:G:O2'	1:F:72:C:H5'	2.05	0.57
2:I:311:VAL:HG13	2:I:355:ILE:CD1	2.35	0.56
1:F:20:G:C3'	1:F:21:A:H5''	2.35	0.56
2:I:406:ILE:HG13	2:I:533:VAL:HG13	1.87	0.56
1:F:23:A:H2'	1:F:24:G:H8	1.70	0.56
1:F:40:C:O2'	1:F:41:U:H5'	2.06	0.56
1:F:43:G:H2'	1:F:44:A:C8	2.40	0.56
1:F:67:A:O2'	1:F:68:U:H5'	2.06	0.56
2:I:311:VAL:HG13	2:I:355:ILE:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:666:VAL:HG12	2:I:667:LEU:H	1.71	0.55
1:F:41:U:H2'	1:F:42:G:H8	1.72	0.55
2:I:485:LYS:H	2:I:485:LYS:HD3	1.71	0.55
2:I:433:VAL:HG11	2:I:493:ARG:HH21	1.71	0.55
2:I:300:ILE:N	2:I:300:ILE:HD12	2.22	0.54
1:F:51:G:H2'	1:F:52:U:C6	2.42	0.54
2:I:527:ILE:HG22	2:I:607:ILE:HG23	1.90	0.54
2:I:405:VAL:HG11	2:I:487:ARG:HH21	1.72	0.54
2:I:659:LYS:HG2	2:I:690:GLU:HG2	1.89	0.54
2:I:487:ARG:HE	2:I:491:LEU:HD21	1.73	0.54
1:F:29:A:O2'	1:F:30:G:H5'	2.08	0.53
1:F:18:G:H22	1:F:57:G:H2'	1.71	0.53
1:F:39:U:H2'	1:F:40:C:H6	1.73	0.53
1:F:27:C:H2'	1:F:28:C:C6	2.44	0.53
2:I:419:THR:HA	2:I:478:THR:HA	1.91	0.53
1:F:2:C:H2'	1:F:3:G:C8	2.44	0.52
1:F:49:C:H2'	1:F:50:U:H6	1.74	0.52
1:F:47:U:C6	1:F:47:U:C5'	2.91	0.52
2:I:405:VAL:CG1	2:I:406:ILE:H	2.19	0.52
2:I:664:ILE:HG22	2:I:675:GLU:HB3	1.90	0.52
2:I:590:ALA:O	2:I:594:ILE:HG12	2.10	0.52
1:F:35:A:O2'	1:F:36:A:H5'	2.09	0.52
1:F:75:C:C2'	1:F:76:A:P	2.97	0.52
2:I:276:ILE:HD13	2:I:276:ILE:C	2.30	0.52
1:F:52:U:O2'	1:F:53:G:H5'	2.10	0.52
1:F:18:G:H1'	1:F:57:G:C2	2.45	0.52
1:F:38:A:O2'	1:F:39:U:H5'	2.09	0.52
1:F:47:U:H3	1:F:50:U:H5''	1.74	0.51
1:F:55:U:O4	1:F:57:G:H3'	2.10	0.51
1:F:73:A:O2'	1:F:74:C:H5'	2.10	0.51
2:I:406:ILE:CD1	2:I:421:LEU:N	2.74	0.51
2:I:406:ILE:HD13	2:I:420:VAL:C	2.31	0.51
2:I:718:ILE:HD12	2:I:718:ILE:N	2.24	0.51
1:F:14:A:C2	1:F:15:G:H1'	2.46	0.51
1:F:19:G:N2	1:F:57:G:H1'	2.25	0.51
2:I:575:SER:HA	2:I:610:LEU:HB3	1.92	0.50
2:I:513:MET:O	2:I:517:MET:HB2	2.11	0.50
1:F:24:G:O2'	1:F:25:C:H5'	2.11	0.50
3:W:33:LEU:HD23	3:W:63:THR:HG22	1.94	0.50
1:F:10:G:H2'	1:F:11:C:H6	1.77	0.50
2:I:436:GLY:H	2:I:491:LEU:HD13	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:58:A:H4'	1:F:59:U:OP1	2.12	0.49
2:I:634:ALA:HB1	2:I:658:VAL:HG22	1.93	0.49
1:F:58:A:H1'	1:F:60:C:OP2	2.11	0.49
1:F:18:G:H21	1:F:57:G:H2'	1.73	0.49
2:I:336:ILE:HG22	2:I:370:SER:HB2	1.94	0.49
2:I:229:VAL:HB	2:I:298:THR:HA	1.95	0.48
2:I:264:ILE:HD12	2:I:264:ILE:N	2.28	0.48
1:F:37:G:O2'	1:F:38:A:H5'	2.13	0.48
1:F:47:U:C5'	1:F:47:U:H6	2.25	0.48
1:F:64:A:O2'	1:F:65:G:H5'	2.14	0.48
2:I:289:SER:C	2:I:291:ARG:H	2.17	0.48
1:F:20:G:H2'	1:F:21:A:C5'	2.35	0.48
2:I:692:ARG:HG2	2:I:693:ASN:H	1.78	0.48
1:F:3:G:C6	1:F:71:G:C6	3.02	0.48
1:F:33:U:H2'	1:F:35:A:OP2	2.14	0.47
2:I:271:THR:HG23	2:I:385:LEU:HD11	1.97	0.47
2:I:453:VAL:HG13	2:I:477:VAL:HG21	1.97	0.47
1:F:35:A:C4	1:F:36:A:C8	3.02	0.47
2:I:396:VAL:HG13	2:I:397:ARG:H	1.79	0.47
1:F:9:A:N6	1:F:22:G:H2'	2.26	0.47
1:F:44:A:H2'	1:F:45:G:O4'	2.14	0.47
2:I:447:ASN:HD22	2:I:480:VAL:HG12	1.80	0.47
1:F:4:G:C6	1:F:70:C:N3	2.83	0.47
1:F:17:U:O3'	1:F:18:G:H3'	2.15	0.47
1:F:4:G:H1	1:F:69:U:H3	1.62	0.47
2:I:279:LEU:HD13	2:I:290:MET:SD	2.54	0.47
2:I:329:VAL:HG23	2:I:364:SER:OG	2.15	0.47
2:I:432:ILE:HD12	2:I:445:MET:CG	2.32	0.46
2:I:488:GLU:O	2:I:491:LEU:HD23	2.15	0.46
1:F:18:G:P	1:F:18:G:H3'	2.55	0.46
1:F:5:A:H2'	1:F:6:U:C6	2.50	0.46
2:I:594:ILE:HG21	2:I:601:LEU:HD22	1.96	0.46
1:F:26:G:H2'	1:F:27:C:H6	1.80	0.46
2:I:406:ILE:HD11	2:I:421:LEU:N	2.30	0.46
2:I:228:PRO:O	2:I:230:VAL:HG23	2.15	0.46
1:F:51:G:C6	1:F:64:A:C6	3.04	0.46
2:I:232:ILE:HD13	2:I:244:LEU:CD2	2.45	0.46
2:I:607:ILE:HD13	2:I:608:TYR:H	1.79	0.46
1:F:65:G:O2'	1:F:66:A:H5'	2.16	0.45
1:F:67:A:H2'	1:F:68:U:C6	2.50	0.45
2:I:283:GLY:HA3	2:I:540:ILE:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:38:A:H2'	1:F:39:U:H6	1.81	0.45
2:I:369:VAL:HG21	2:I:380:LEU:HD22	1.99	0.45
2:I:405:VAL:O	2:I:534:GLN:HB2	2.16	0.45
1:F:72:C:O2'	1:F:73:A:H5'	2.16	0.45
2:I:269:VAL:HG13	2:I:274:GLY:H	1.81	0.45
2:I:481:ARG:HB2	2:I:484:LYS:HE2	1.99	0.45
1:F:20:G:H3'	1:F:21:A:H5''	1.98	0.45
1:F:5:A:O2'	1:F:6:U:H5'	2.18	0.44
2:I:557:ILE:HG13	2:I:558:GLY:H	1.82	0.44
2:I:580:VAL:HG23	2:I:605:SER:OG	2.17	0.44
2:I:490:ALA:H	2:I:534:GLN:NE2	2.15	0.44
1:F:13:C:O2'	1:F:14:A:H5'	2.17	0.44
2:I:607:ILE:CD1	2:I:608:TYR:N	2.80	0.44
1:F:4:G:C2	1:F:5:A:C4	3.05	0.44
1:F:62:A:O2'	1:F:63:C:H5'	2.18	0.44
2:I:432:ILE:CD1	2:I:445:MET:HG2	2.33	0.44
2:I:227:ALA:HA	2:I:228:PRO:HD3	1.88	0.44
1:F:36:A:H2'	1:F:37:G:C5'	2.11	0.44
1:F:35:A:H2'	1:F:36:A:H8	1.83	0.43
1:F:18:G:C6	1:F:58:A:C5	3.06	0.43
2:I:458:PRO:O	2:I:460:ILE:N	2.50	0.43
1:F:2:C:H2'	1:F:3:G:H8	1.81	0.43
1:F:14:A:O2'	1:F:15:G:H5'	2.17	0.43
1:F:29:A:C6	1:F:42:G:C6	3.06	0.43
1:F:41:U:H2'	1:F:42:G:C8	2.51	0.43
2:I:396:VAL:HG13	2:I:397:ARG:N	2.33	0.43
2:I:421:LEU:HD13	2:I:533:VAL:HG11	2.01	0.43
2:I:533:VAL:O	2:I:537:VAL:HG23	2.19	0.43
1:F:33:U:C6	1:F:35:A:OP2	2.71	0.43
2:I:409:PHE:HE2	2:I:419:THR:HG22	1.83	0.43
2:I:522:VAL:CG1	2:I:523:HIS:N	2.75	0.43
2:I:268:HIS:HB3	2:I:269:VAL:H	1.64	0.43
1:F:14:A:H2'	1:F:15:G:O4'	2.19	0.42
1:F:57:G:O2'	1:F:58:A:H5'	2.18	0.42
1:F:68:U:O2'	1:F:69:U:H5'	2.19	0.42
2:I:432:ILE:HD11	2:I:445:MET:CE	2.49	0.42
2:I:642:SER:HA	2:I:643:PRO:HD2	1.80	0.42
1:F:8:U:H2'	1:F:46:G:N2	2.35	0.42
1:F:49:C:O2'	1:F:50:U:H5'	2.19	0.42
2:I:531:ALA:HB3	2:I:537:VAL:HG22	2.02	0.42
1:F:51:G:C5	1:F:52:U:C4	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:55:U:H2'	1:F:56:C:H3'	2.02	0.42
1:F:19:G:H5''	1:F:60:C:N4	2.33	0.42
1:F:30:G:C6	1:F:31:A:C5	3.07	0.42
2:I:420:VAL:HG11	2:I:493:ARG:NH1	2.35	0.42
2:I:484:LYS:HB2	2:I:487:ARG:HH11	1.85	0.41
1:F:33:U:C2	1:F:35:A:H3'	2.55	0.41
2:I:299:ASP:CB	2:I:300:ILE:HD12	2.50	0.41
2:I:442:VAL:HG13	2:I:443:ARG:HH21	1.85	0.41
1:F:11:C:H2'	1:F:12:U:H6	1.84	0.41
1:F:18:G:H4'	1:F:19:G:OP1	2.20	0.41
2:I:403:GLY:HA2	2:I:423:ARG:NE	2.31	0.41
2:I:527:ILE:C	2:I:527:ILE:HD12	2.41	0.41
1:F:42:G:H2'	1:F:43:G:H8	1.86	0.41
1:F:51:G:O2'	1:F:52:U:H5'	2.21	0.41
1:F:11:C:H6	1:F:11:C:O5'	2.04	0.41
1:F:25:C:H2'	1:F:26:G:O4'	2.21	0.41
1:F:42:G:O2'	1:F:43:G:H5'	2.21	0.41
2:I:270:GLU:HB3	2:I:271:THR:H	1.67	0.40
1:F:14:A:C4	1:F:15:G:C8	3.09	0.40
1:F:39:U:O2'	1:F:40:C:H5'	2.20	0.40
1:F:18:G:OP1	1:F:18:G:H2'	2.21	0.40
2:I:233:MET:HE2	2:I:301:VAL:HG11	2.03	0.40
2:I:452:GLU:HG2	2:I:453:VAL:N	2.36	0.40
2:I:692:ARG:HG2	2:I:693:ASN:N	2.37	0.40
1:F:8:U:O2	1:F:21:A:H2	2.04	0.40
1:F:32:C:O2'	1:F:33:U:H5'	2.20	0.40
2:I:369:VAL:HG12	2:I:370:SER:N	2.37	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	
2	I	499/501 (100%)	399 (80%)	60 (12%)	40 (8%)	1	17
3	W	69/71 (97%)	57 (83%)	6 (9%)	6 (9%)	1	15
All	All	568/572 (99%)	456 (80%)	66 (12%)	46 (8%)	2	16

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	270	GLU
2	I	283	GLY
2	I	287	PHE
2	I	396	VAL
2	I	459	SER
2	I	490	ALA
2	I	495	GLY
2	I	522	VAL
2	I	524	GLU
2	I	583	ASN
2	I	606	VAL
2	I	645	PHE
2	I	720	GLU
3	W	24	VAL
3	W	45	ILE
2	I	462	VAL
2	I	523	HIS
2	I	527	ILE
2	I	557	ILE
2	I	607	ILE
2	I	608	TYR
3	W	2	LYS
3	W	34	ALA
2	I	273	ASN
2	I	482	ASP
2	I	496	LYS
2	I	526	ASN
2	I	609	ASN
2	I	630	ILE
2	I	684	PHE
2	I	693	ASN
2	I	627	LYS
2	I	643	PRO
2	I	647	ALA
3	W	44	TYR

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Mol	Chain	Res	Type
2	I	447	ASN
2	I	605	SER
2	I	274	GLY
2	I	280	ASP
2	I	276	ILE
2	I	281	THR
2	I	719	ILE
3	W	30	PRO
2	I	631	ILE
2	I	354	GLY
2	I	405	VAL

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	
2	I	406/406 (100%)	361 (89%)	45 (11%)	7	29
3	W	62/62 (100%)	54 (87%)	8 (13%)	5	25
All	All	468/468 (100%)	415 (89%)	53 (11%)	11	29

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	232	ILE
2	I	269	VAL
2	I	276	ILE
2	I	282	PRO
2	I	303	LEU
2	I	333	VAL
2	I	336	ILE
2	I	356	LEU
2	I	359	GLU
2	I	379	GLU
2	I	387	GLN
2	I	419	THR

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Mol	Chain	Res	Type
2	I	427	LEU
2	I	431	ASP
2	I	443	ARG
2	I	451	GLN
2	I	452	GLU
2	I	462	VAL
2	I	485	LYS
2	I	494	GLN
2	I	496	LYS
2	I	497	PHE
2	I	498	ARG
2	I	499	GLU
2	I	517	MET
2	I	519	GLU
2	I	527	ILE
2	I	529	LEU
2	I	554	VAL
2	I	556	ILE
2	I	576	ASN
2	I	579	LEU
2	I	580	VAL
2	I	599	LEU
2	I	604	TYR
2	I	606	VAL
2	I	614	VAL
2	I	618	MET
2	I	629	GLN
2	I	639	VAL
2	I	688	VAL
2	I	689	ASN
2	I	708	ARG
2	I	720	GLU
2	I	723	ARG
3	W	5	ASP
3	W	31	GLU
3	W	32	ILE
3	W	42	MET
3	W	52	ARG
3	W	63	THR
3	W	68	VAL
3	W	71	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
2	I	334	ASN
2	I	365	GLN
2	I	447	ASN
2	I	534	GLN
2	I	689	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	F	75/76 (98%)	9 (12%)	0

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	F	16	U
1	F	17	U
1	F	18	G
1	F	21	A
1	F	37	G
1	F	46	G
1	F	47	U
1	F	48	C
1	F	76	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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.