



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 07:51 pm GMT

PDB ID : 1QD1
Title : THE CRYSTAL STRUCTURE OF THE FORMIMINOTRANSFERASE DOMAIN OF FORMIMINOTRANSFERASE-CYCLODEAMINASE.
Authors : Kohls, D.; Sulea, T.; Purisima, E.; MacKenzie, R.E.; Vrielink, A.
Deposited on : 1999-07-08
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
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) : recalc28949

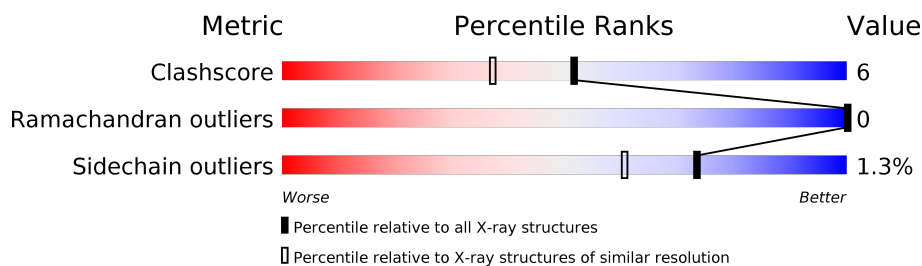
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	325	 84% 14% .
1	B	325	 86% 13%

2 Entry composition [i](#)

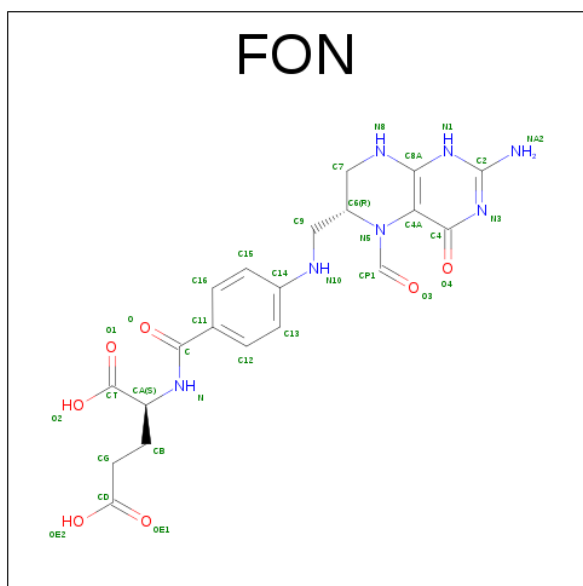
There are 4 unique types of molecules in this entry. The entry contains 6042 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 FORMIMINOTRANSFERASE-CYCLODEAMINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	24	10	0
			2556	1618	452	475	11			
1	B	325	Total	C	N	O	S	31	14	0
			2635	1663	468	493	11			

- Molecule 2 is FOLINIC ACID (three-letter code: FON) (formula: $C_{20}H_{23}N_7O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			34	20	7	7		
2	B	1	Total	C	N	O	0	0
			34	20	7	7		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

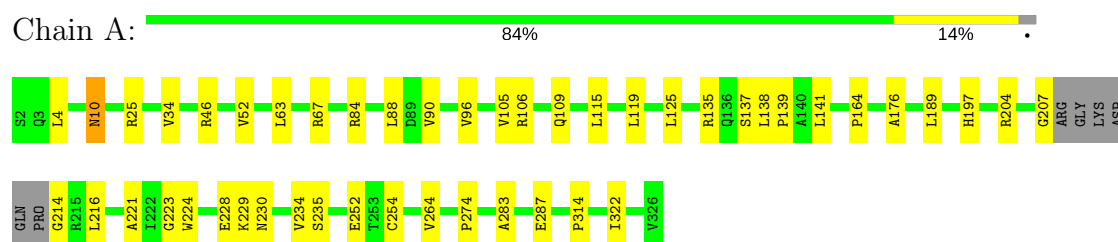
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	365	Total	O	0	0
			365	365		
4	B	406	Total	O	0	0
			406	406		

3 Residue-property plots [i](#)

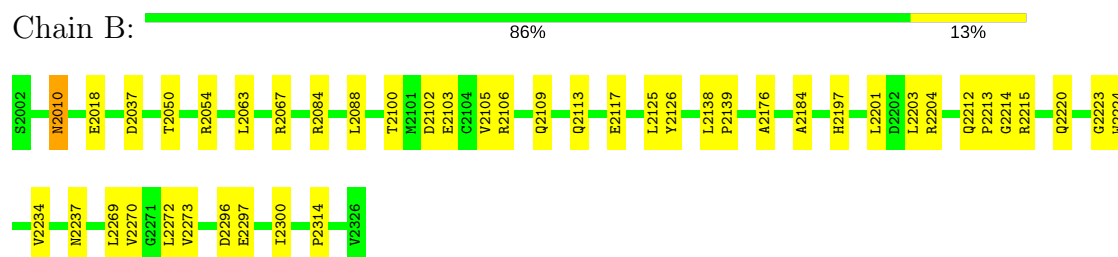
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

Note EDS was not executed.

• Molecule 1: FORMIMINOTRANSFERASE-CYCLODEAMINASE



• Molecule 1: FORMIMINOTRANSFERASE-CYCLODEAMINASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.31Å 103.84Å 122.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.70	Depositor
% Data completeness (in resolution range)	100.0 (50.00-1.70)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.191 , 0.213	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6042	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	A	0.29	0/2604	0.57	2/3533 (0.1%)
1	B	0.29	0/2685	0.58	2/3642 (0.1%)
All	All	0.29	0/5289	0.58	4/7175 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	LEU	N-CA-C	-6.17	94.35	111.00
1	B	2088	LEU	N-CA-C	-5.98	94.84	111.00
1	B	2234	VAL	N-CA-C	-5.53	96.06	111.00
1	A	234	VAL	N-CA-C	-5.28	96.74	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	A	2556	0	2552	36	0
1	B	2635	0	2628	33	0
2	A	34	0	21	1	0
2	B	34	0	21	0	0
3	A	6	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	8	0	0
4	A	365	0	0	5	0
4	B	406	0	0	4	0
All	All	6042	0	5238	67	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 6.

All (67) 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:B:2197:HIS:HD2	1:B:2223:GLY:H	1.20	0.90
1:B:2037:ASP:HB3	1:B:2050[B]:THR:HG22	1.66	0.77
1:A:197:HIS:HD2	1:A:223:GLY:H	1.33	0.74
1:B:2269[B]:LEU:HD13	1:B:2273[B]:VAL:HG21	1.69	0.74
1:A:283:ALA:O	1:A:287:GLU:HG3	1.87	0.73
1:A:204:ARG:O	1:A:214:GLY:HA3	1.90	0.72
1:B:2037:ASP:HB3	1:B:2050[B]:THR:CG2	2.22	0.68
1:A:216:LEU:HD21	1:A:252:GLU:HG3	1.74	0.68
1:B:2113:GLN:O	1:B:2117:GLU:HG3	1.96	0.66
1:B:2204:ARG:O	1:B:2214:GLY:HA3	1.96	0.65
1:B:2237:ASN:ND2	4:B:909:HOH:O	2.30	0.65
1:A:314:PRO:HG3	1:B:2314:PRO:HG3	1.78	0.64
1:A:221:ALA:HA	3:A:480:GOL:O1	1.97	0.63
1:A:230:ASN:HD22	1:B:2297:GLU:CD	2.09	0.56
1:B:2102[A]:ASP:O	1:B:2106[A]:ARG:HG3	2.05	0.56
1:B:2100:THR:OG1	1:B:2103[B]:GLU:HG3	2.06	0.55
1:A:90[B]:VAL:HG21	1:A:138:LEU:HD21	1.90	0.54
1:A:204:ARG:HG3	1:A:207:GLY:H	1.72	0.54
1:A:137:SER:OG	1:A:139:PRO:HD2	2.08	0.53
1:B:2138:LEU:HB3	1:B:2139:PRO:HD3	1.90	0.52
1:B:2184:ALA:HB3	1:B:2270:VAL:HB	1.89	0.52
1:B:2197:HIS:O	1:B:2201:LEU:HD13	2.10	0.52
1:B:2220:GLN:HB2	1:B:2237:ASN:HB2	1.92	0.51
1:A:228:GLU:HG2	1:A:229:LYS:HG2	1.93	0.51
1:A:164:PRO:HG2	4:A:1087:HOH:O	2.11	0.49
1:B:2197:HIS:CD2	1:B:2223:GLY:H	2.12	0.49
1:A:235:SER:O	3:A:480:GOL:O1	2.31	0.49
1:A:46:ARG:HD3	2:A:330:FON:C13	2.43	0.49
1:B:2050[B]:THR:HG23	1:B:2050[B]:THR:O	2.13	0.49
1:B:2050[A]:THR:HG21	1:B:2272:LEU:HD12	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ARG:HD2	4:A:989:HOH:O	2.12	0.48
1:B:2010:ASN:N	1:B:2010:ASN:HD22	2.12	0.48
1:A:115:LEU:HD11	1:A:119:LEU:HD12	1.95	0.48
1:A:138:LEU:HB3	1:A:139:PRO:HD3	1.94	0.48
1:A:189:LEU:CD2	1:A:264:VAL:HG22	2.43	0.48
1:B:2063:LEU:O	1:B:2067:ARG:HG3	2.14	0.47
1:B:2103[A]:GLU:HA	1:B:2106[A]:ARG:HD2	1.95	0.47
1:B:2113:GLN:HG2	1:B:2117:GLU:OE2	2.15	0.47
1:A:254[B]:CYS:SG	4:A:1272:HOH:O	2.56	0.46
1:B:2203:LEU:HD23	1:B:2215:ARG:HD3	1.96	0.46
1:A:4[A]:LEU:HD23	1:A:96:VAL:HG11	1.97	0.46
1:A:115:LEU:CD1	1:A:119:LEU:HD12	2.46	0.46
1:B:2212:GLN:N	1:B:2213:PRO:HD3	2.31	0.45
1:A:197:HIS:CD2	1:A:223:GLY:H	2.23	0.45
1:B:2197:HIS:HE1	4:B:925:HOH:O	1.99	0.45
1:A:63:LEU:O	1:A:67:ARG:HG3	2.17	0.44
1:B:2054:ARG:HH11	1:B:2054:ARG:HG2	1.83	0.44
1:B:2125:LEU:HA	1:B:2176:ALA:O	2.18	0.44
1:A:4[A]:LEU:HD11	1:A:52:VAL:HB	2.00	0.44
1:B:2050[B]:THR:HG21	1:B:2272:LEU:HG	1.98	0.44
1:A:105:VAL:O	1:A:109:GLN:HG3	2.19	0.43
1:A:10:ASN:N	1:A:10:ASN:HD22	2.16	0.43
1:B:2018:GLU:HG3	4:B:1015:HOH:O	2.18	0.43
1:A:204:ARG:HG3	1:A:207:GLY:N	2.32	0.43
1:A:274:PRO:HG3	1:A:322:ILE:HD12	2.02	0.42
1:A:138:LEU:N	1:A:139:PRO:CD	2.82	0.42
1:A:25[B]:ARG:NH1	1:A:25[B]:ARG:HB2	2.35	0.42
1:B:2138:LEU:HD23	4:B:1131:HOH:O	2.19	0.41
1:A:106:ARG:HD2	4:A:1091:HOH:O	2.20	0.41
1:A:125:LEU:HA	1:A:176:ALA:O	2.20	0.41
1:B:2197:HIS:CE1	1:B:2201:LEU:HD11	2.55	0.41
1:B:2296:ASP:O	1:B:2300[B]:ILE:HG12	2.21	0.41
1:A:189:LEU:HD21	1:A:264:VAL:HG22	2.02	0.41
1:A:135:ARG:HG2	1:A:141:LEU:HD21	2.03	0.41
1:A:254[A]:CYS:HB3	4:A:1272:HOH:O	2.20	0.40
1:A:34[A]:VAL:HG13	1:A:52:VAL:HG22	2.03	0.40
1:B:2105:VAL:O	1:B:2109:GLN:HG3	2.20	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 X-ray entries followed by that with respect to entries of similar resolution.

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	A	325/325 (100%)	317 (98%)	8 (2%)	0	100	100
1	B	337/325 (104%)	327 (97%)	10 (3%)	0	100	100
All	All	662/650 (102%)	644 (97%)	18 (3%)	0	100	100

There are no Ramachandran outliers to report.

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 X-ray entries followed by that with respect to entries of similar resolution.

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	A	271/266 (102%)	268 (99%)	3 (1%)	78	68
1	B	280/266 (105%)	276 (99%)	4 (1%)	71	58
All	All	551/532 (104%)	544 (99%)	7 (1%)	73	60

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	84	ARG
1	A	224	TRP
1	B	2010	ASN
1	B	2084	ARG
1	B	2126	TYR
1	B	2224	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	HIS
1	A	290	ASN
1	B	2155	GLN
1	B	2197	HIS
1	B	2220	GLN
1	B	2237	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 ⓘ

4 ligands are modelled in this entry.

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	$\# Z > 2$
2	FON	A	330	-	24,36,36	3.12	12 (50%)	29,50,50	2.37	11 (37%)
3	GOL	A	480	-	5,5,5	0.49	0	5,5,5	0.60	0
2	FON	B	2330	-	24,36,36	3.03	11 (45%)	29,50,50	2.44	9 (31%)
3	GOL	B	2480	-	5,5,5	0.74	0	5,5,5	0.55	0

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
2	FON	A	330	-	-	0/18/37/37	0/2/3/3
3	GOL	A	480	-	-	0/4/4/4	0/0/0/0
2	FON	B	2330	-	-	0/18/37/37	0/2/3/3
3	GOL	B	2480	-	-	0/4/4/4	0/0/0/0

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2330	FON	C2-N3	-7.04	1.22	1.35
2	A	330	FON	C2-N3	-6.75	1.23	1.35
2	B	2330	FON	CB-CA	-4.40	1.47	1.53
2	A	330	FON	CB-CA	-4.16	1.47	1.53
2	B	2330	FON	C13-C12	2.25	1.42	1.38
2	A	330	FON	C-N	2.29	1.39	1.34
2	B	2330	FON	C16-C11	2.31	1.43	1.39
2	B	2330	FON	C14-N10	2.36	1.45	1.38
2	A	330	FON	C14-N10	2.72	1.46	1.38
2	B	2330	FON	C15-C14	2.85	1.44	1.39
2	B	2330	FON	O3-CP1	2.91	1.44	1.23
2	A	330	FON	C12-C11	3.13	1.44	1.39
2	A	330	FON	O3-CP1	3.18	1.46	1.23
2	A	330	FON	C15-C14	3.23	1.44	1.39
2	A	330	FON	C16-C15	3.54	1.45	1.38
2	A	330	FON	C16-C11	3.57	1.45	1.39
2	B	2330	FON	C12-C11	3.85	1.45	1.39
2	B	2330	FON	C4-N3	3.93	1.40	1.33
2	A	330	FON	C4-N3	3.96	1.40	1.33
2	A	330	FON	O4-C4	5.71	1.38	1.24
2	B	2330	FON	O4-C4	5.72	1.38	1.24
2	B	2330	FON	C2-NA2	6.38	1.47	1.34
2	A	330	FON	C2-NA2	6.48	1.47	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	330	FON	NA2-C2-N3	-4.47	110.10	117.24
2	B	2330	FON	NA2-C2-N3	-4.37	110.25	117.24
2	B	2330	FON	C12-C13-C14	-3.94	115.68	120.30
2	A	330	FON	C13-C14-N10	-3.80	113.38	121.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	330	FON	C4A-C4-N3	-3.53	117.83	123.37
2	B	2330	FON	C4A-C4-N3	-3.51	117.87	123.37
2	A	330	FON	C12-C13-C14	-2.80	117.02	120.30
2	B	2330	FON	CB-CA-N	-2.69	106.14	110.22
2	B	2330	FON	C13-C14-N10	-2.54	115.92	121.03
2	A	330	FON	CB-CA-CT	-2.03	109.33	112.28
2	A	330	FON	C15-C16-C11	-2.01	118.54	120.79
2	B	2330	FON	C15-C14-C13	2.13	122.02	119.04
2	A	330	FON	C13-C12-C11	2.27	123.33	120.79
2	A	330	FON	C11-C-N	2.45	121.50	116.97
2	A	330	FON	C9-N10-C14	2.63	128.46	121.52
2	B	2330	FON	C11-C-N	2.92	122.36	116.97
2	A	330	FON	C4-C4A-C8A	5.11	118.50	114.43
2	A	330	FON	N3-C2-N1	5.41	134.21	125.45
2	B	2330	FON	N3-C2-N1	5.70	134.68	125.45
2	B	2330	FON	C4-C4A-C8A	6.58	119.67	114.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	330	FON	1	0
3	A	480	GOL	2	0

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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.