



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 10, 2022 – 08:07 PM EST

PDB ID : 1NH3
Title : Human Topoisomerase I Ara-C Complex
Authors : Chrencik, J.E.; Burgin, A.B.; Pommier, Y.; Stewart, L.; Redinbo, M.R.
Deposited on : 2002-12-18
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

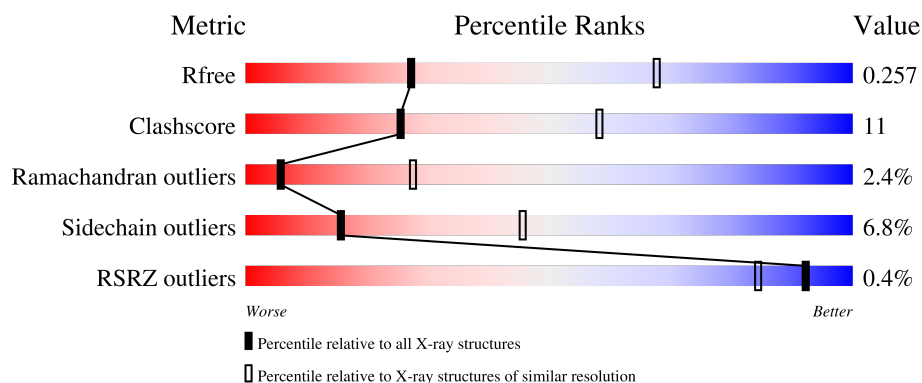
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	B	10	<div> <div>30%</div> <div>50%</div> <div>20%</div> </div>
2	C	12	<div> <div>25%</div> <div>58%</div> <div>17%</div> </div>
3	D	22	<div> <div>23%</div> <div>68%</div> <div>9%</div> </div>
4	A	563	<div> <div>72%</div> <div>10%</div> <div>16%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4394 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 DNA chain called 5'-D(*AP*AP*AP*AP*AP*GP*AP*CP*UP*(UBB))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	10	Total	C	N	O	P	0	0	0
			201	97	42	53	9			

- Molecule 2 is a DNA chain called 5'-D(*(GNG)P*GP*AP*AP*AP*AP*AP*UP*UP*UP*UP*P*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	12	Total	C	N	O	P	0	0	0
			242	116	45	70	11			

- Molecule 3 is DNA/RNA hybrid called 5'-D(*AP*AP*AP*AP*AP*TP*UP*UP*UP*UP*CP*(CAR)P*AP*AP*GP*UP*CP*UP*UP*UP*UP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	22	Total	C	N	O	P	0	0	0
			435	208	71	135	21			

- Molecule 4 is a protein called DNA topoisomerase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	471	Total	C	N	O	P	S	0	0
			3483	2227	612	625	1	18		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	699	MET	-	initiating methionine	UNP P11387
A	723	PTR	TYR	modified residue	UNP P11387

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total 2	O 2	0	0
5	C	5	Total 5	O 5	0	0
5	D	5	Total 5	O 5	0	0
5	A	21	Total 21	O 21	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	72.97Å 72.97Å 186.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.29 – 3.10 44.29 – 3.00	Depositor EDS
% Data completeness (in resolution range)	74.6 (44.29-3.10) 81.1 (44.29-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.235 , 0.311 0.255 , 0.257	Depositor DCC
R_{free} test set	857 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	1.403	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 90.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l 0.062 for h,-h-k,-l 0.038 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4394	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: GNG, PTR, CAR, UBB

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	B	0.61	0/207	0.86	0/317
2	C	0.58	0/250	0.82	0/382
3	D	0.57	0/463	0.76	0/706
4	A	0.69	0/3558	1.03	12/4798 (0.3%)
All	All	0.67	0/4478	0.99	12/6203 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	C	0	1
3	D	0	1
4	A	0	3
All	All	0	6

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	557	ASN	N-CA-CB	-25.02	65.56	110.60
4	A	556	GLU	O-C-N	-24.66	83.24	122.70
4	A	556	GLU	CA-C-N	19.44	159.97	117.20
4	A	555	MET	O-C-N	-14.85	98.94	122.70
4	A	555	MET	C-N-CA	14.73	158.52	121.70

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	555	MET	Mainchain
4	A	556	GLU	Mainchain
1	B	8	DC	Sidechain
2	C	18	DU	Sidechain
3	D	115	DG	Sidechain

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	B	201	0	109	11	0
2	C	242	0	131	17	0
3	D	435	0	237	36	0
4	A	3483	0	3180	35	0
5	A	21	0	0	0	0
5	B	2	0	0	0	0
5	C	5	0	0	1	0
5	D	5	0	0	2	0
All	All	4394	0	3657	84	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 11.

The worst 5 of 84 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)
3:D:110:DU:H2'	3:D:111:DC:H5''	1.22	1.18
2:C:17:DA:H2''	2:C:18:DU:H5''	1.30	1.11
3:D:110:DU:H2'	3:D:111:DC:C5'	1.93	0.97
3:D:101:DA:H2''	3:D:102:DA:OP2	1.69	0.93
3:D:110:DU:C2'	3:D:111:DC:H5''	2.04	0.86

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	
4	A	466/563 (83%)	402 (86%)	53 (11%)	11 (2%)	6	27

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	612	ILE
4	A	397	PRO
4	A	470	MET
4	A	240	PHE
4	A	345	ASN

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	
4	A	325/506 (64%)	303 (93%)	22 (7%)	16	45

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	491	ASN
4	A	555	MET
4	A	553	LEU
4	A	570	THR
4	A	391	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such

sidechains are listed below:

Mol	Chain	Res	Type
4	A	491	ASN
4	A	578	GLN
4	A	722	ASN
4	A	408	ASN
4	A	385	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
4	PTR	A	723	4,1	15,16,17	1.14	0	19,22,24	0.86	0
2	GNG	C	11	2,3	16,21,21	1.17	3 (18%)	19,31,31	1.45	3 (15%)
3	CAR	D	112	2,3	18,21,22	0.61	0	26,30,33	0.79	1 (3%)
1	UBB	B	10	4,1,3	16,19,20	0.39	0	20,26,29	0.73	1 (5%)

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
4	PTR	A	723	4,1	-	1/10/11/13	0/1/1/1
2	GNG	C	11	2,3	-	0/2/18/18	0/3/3/3
3	CAR	D	112	2,3	-	3/7/25/26	0/2/2/2
1	UBB	B	10	4,1,3	-	1/7/18/19	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	11	GNG	C5-C6	-2.78	1.42	1.47
2	C	11	GNG	C8-N7	-2.39	1.31	1.35
2	C	11	GNG	C2-N1	2.08	1.38	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	11	GNG	C5-C6-N1	-4.40	111.70	117.85
1	B	10	UBB	C2'-C1'-N1	2.59	117.31	112.40
2	C	11	GNG	C6-N1-C2	2.45	124.92	118.93
3	D	112	CAR	C2'-C1'-N1	2.34	119.84	113.22
2	C	11	GNG	N2-C2-N1	-2.08	115.69	119.73

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	723	PTR	O-C-CA-CB
3	D	112	CAR	C4'-C5'-O5'-P
3	D	112	CAR	O4'-C4'-C5'-O5'
1	B	10	UBB	O4'-C1'-N1-C6
3	D	112	CAR	C3'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	723	PTR	2	0
2	C	11	GNG	1	0
3	D	112	CAR	3	0
1	B	10	UBB	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	B	8/10 (80%)	-0.49	0	100 100	17, 37, 64, 71	0
2	C	7/12 (58%)	-0.45	0	100 100	36, 45, 73, 91	0
3	D	12/22 (54%)	-0.13	0	100 100	24, 54, 88, 122	0
4	A	470/563 (83%)	-0.41	2 (0%)	92 84	9, 68, 138, 199	0
All	All	497/607 (81%)	-0.40	2 (0%)	92 84	9, 66, 138, 199	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	293	ILE	4.5
4	A	759	ALA	2.9

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PTR	A	723	16/17	0.89	0.33	105,106,108,108	0
3	CAR	D	112	20/21	0.91	0.18	25,46,55,55	0
2	GNG	C	11	19/19	0.94	0.21	26,38,70,74	0
1	UBB	B	10	18/19	0.96	0.18	14,23,34,36	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.