



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:58 PM GMT

PDB ID : 7ADH
Title : THREE-DIMENSIONAL STRUCTURE OF ISONICOTINIMIDYLATED
LIVER ALCOHOL DEHYDROGENASE
Authors : Plapp, B.; Eklund, H.
Deposited on : 1984-01-16
Resolution : 3.20 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
<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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

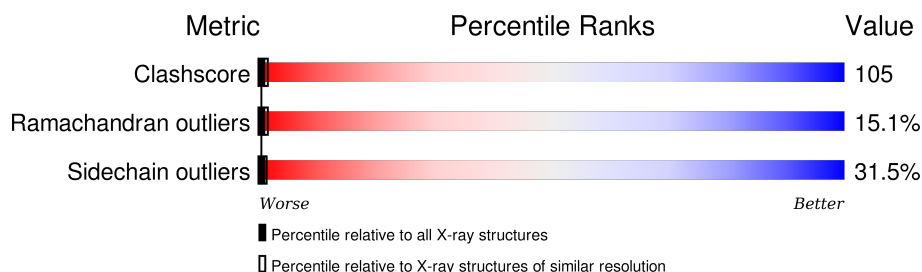
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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	374	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NTN	A	377	-	-	X	-
3	NTN	A	378	-	-	X	-
3	NTN	A	379	-	-	X	-
3	NTN	A	382	-	-	X	-
3	NTN	A	383	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NTN	A	385	-	-	X	-
3	NTN	A	386	-	-	X	-
3	NTN	A	390	-	-	X	-
3	NTN	A	391	-	-	X	-
3	NTN	A	397	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2970 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.

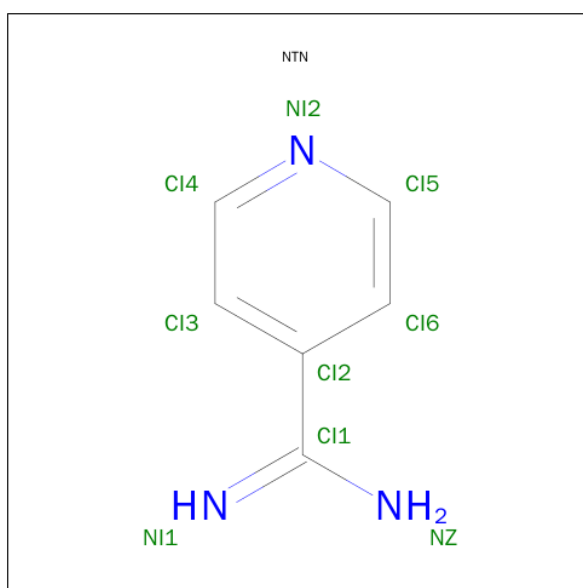
- Molecule 1 is a protein called ISONICOTINIMIDYLATED LIVER ALCOHOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	32	0	0
			2784	1769	472	520	23			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is ISONICOTINAMIDINE (three-letter code: NTN) (formula: C₆H₇N₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			8	6	2		
3	A	1	Total	C	N	0	0
			8	6	2		

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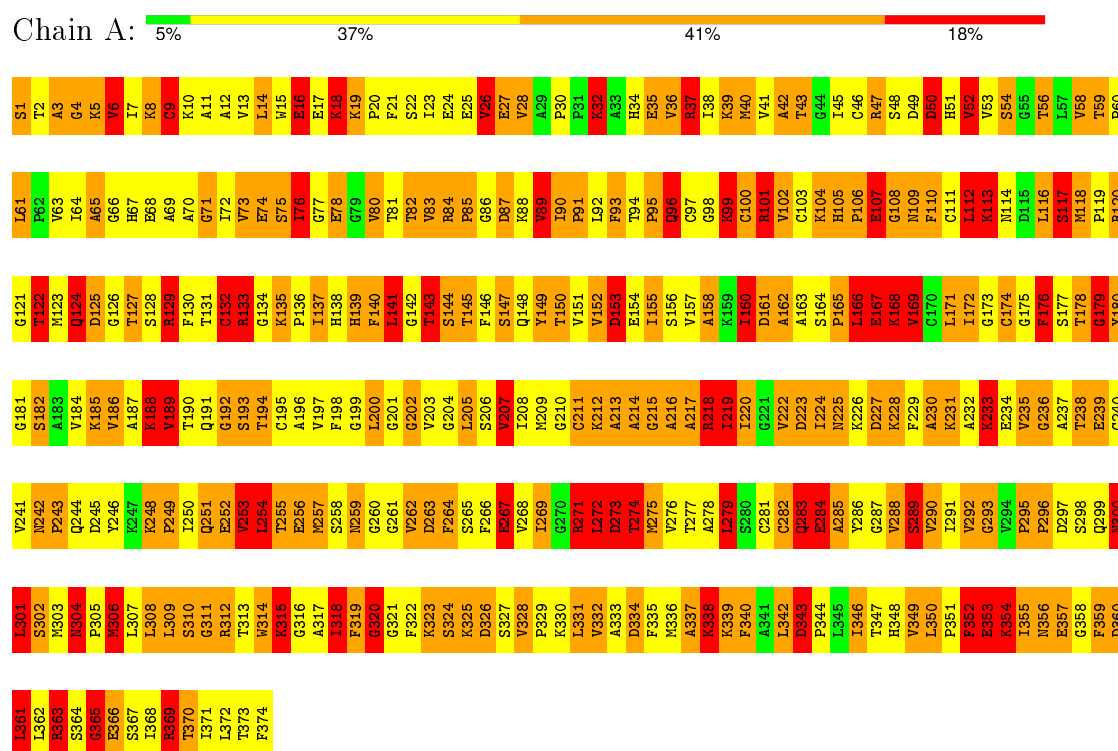
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			8	6	2		
3	A	1	Total	C	N	0	0
			8	6	2		
3	A	1	Total	C	N	0	0
			8	6	2		
3	A	1	Total	C	N	0	0
			8	6	2		
3	A	1	Total	C	N	0	0
			8	6	2		
3	A	1	Total	C	N	0	0
			8	6	2		
3	A	1	Total	C	N	0	0
			8	6	2		
3	A	1	Total	C	N	0	0
			8	6	2		
3	A	1	Total	C	N	0	0
			8	6	2		
3	A	1	Total	C	N	0	0
			8	6	2		
3	A	1	Total	C	N	0	0
			8	6	2		
3	A	1	Total	C	N	0	0
			8	6	2		
3	A	1	Total	C	N	0	0
			8	6	2		
3	A	1	Total	C	N	0	0
			8	6	2		
3	A	1	Total	C	N	0	0
			8	6	2		
3	A	1	Total	C	N	0	0
			8	6	2		
3	A	1	Total	C	N	0	0
			8	6	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 errors 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: ISONICOTINIMIDYLATED LIVER ALCOHOL DEHYDROGENASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	177.80Å 61.20Å 56.50Å 90.00° 104.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CORELS	Depositor
R, R_{free}	0.290 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2970	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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: ZN, NTN

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	1.68	20/2836 (0.7%)	2.78	264/3834 (6.9%)

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	A	0	4

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	GLN	CA-CB	-23.87	1.01	1.53
1	A	96	GLN	N-CA	11.88	1.70	1.46
1	A	364	SER	CB-OG	8.78	1.53	1.42
1	A	35	GLU	CG-CD	-6.34	1.42	1.51
1	A	192	GLY	N-CA	6.29	1.55	1.46

The worst 5 of 264 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	ARG	NE-CZ-NH2	-21.26	109.67	120.30
1	A	120	ARG	NE-CZ-NH2	-17.88	111.36	120.30
1	A	363	ARG	NE-CZ-NH2	-14.40	113.10	120.30
1	A	117	SER	N-CA-CB	13.27	130.41	110.50
1	A	239	GLU	OE1-CD-OE2	13.20	139.14	123.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	ARG	Sidechain
1	A	271	ARG	Sidechain
1	A	363	ARG	Sidechain
1	A	37	ARG	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	A	2784	0	2788	603	730
2	A	2	0	0	0	1
3	A	184	0	92	9	145
All	All	2970	0	2880	604	734

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 105.

The worst 5 of 604 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:A:96:GLN:N	1:A:96:GLN:CA	1.70	1.55
1:A:45:ILE:HD12	1:A:359:PHE:CE1	1.69	1.27
1:A:15:TRP:O	1:A:16:GLU:HG3	1.45	1.16
1:A:5:LYS:O	1:A:6:VAL:O	1.62	1.14
1:A:14:LEU:HB2	1:A:21:PHE:HE2	1.08	1.13

The worst 5 of 734 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:CYS:C	1:A:325:LYS:N[2_556]	0.24	1.96
1:A:9:CYS:C	1:A:10:LYS:N[2_555]	0.30	1.90
1:A:34:HIS:CB	1:A:188:LYS:NZ[2_556]	0.31	1.89
1:A:24:GLU:CG	3:A:379:NTN:CI5[2_555]	0.38	1.82
1:A:123:MET:O	1:A:316:GLY:N[2_556]	0.38	1.82

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
1	A	372/374 (100%)	247 (66%)	69 (18%)	56 (15%)	0 1

5 of 56 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	8	LYS
1	A	9	CYS
1	A	16	GLU
1	A	32	LYS

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
1	A	308/308 (100%)	211 (68%)	97 (32%)	0 1

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	VAL
1	A	207	VAL
1	A	343	ASP
1	A	174	CYS
1	A	185	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	ASN
1	A	304	ASN
1	A	251	GLN
1	A	124	GLN
1	A	244	GLN

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 ⓘ

Of 25 ligands modelled in this entry, 2 are monoatomic - leaving 23 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	$\# Z > 2$
3	NTN	A	377	1	7,8,9	1.46	2 (28%)	9,9,11	1.25	2 (22%)
3	NTN	A	378	1	7,8,9	2.70	5 (71%)	9,9,11	2.03	2 (22%)
3	NTN	A	379	1	7,8,9	1.49	2 (28%)	9,9,11	1.32	2 (22%)
3	NTN	A	380	1	7,8,9	1.33	2 (28%)	9,9,11	1.32	1 (11%)
3	NTN	A	381	1	7,8,9	1.61	3 (42%)	9,9,11	2.35	4 (44%)
3	NTN	A	382	1	7,8,9	1.28	2 (28%)	9,9,11	1.32	2 (22%)
3	NTN	A	383	1	7,8,9	1.48	2 (28%)	9,9,11	3.39	5 (55%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NTN	A	384	1	7,8,9	1.40	2 (28%)	9,9,11	1.29	2 (22%)
3	NTN	A	385	1	7,8,9	1.38	2 (28%)	9,9,11	2.97	4 (44%)
3	NTN	A	386	1	7,8,9	1.34	2 (28%)	9,9,11	2.65	5 (55%)
3	NTN	A	387	1	7,8,9	1.43	2 (28%)	9,9,11	2.41	3 (33%)
3	NTN	A	388	1	7,8,9	1.58	3 (42%)	9,9,11	1.61	3 (33%)
3	NTN	A	389	1	7,8,9	2.13	4 (57%)	9,9,11	1.29	1 (11%)
3	NTN	A	390	1	7,8,9	1.33	2 (28%)	9,9,11	2.23	3 (33%)
3	NTN	A	391	1	7,8,9	2.20	3 (42%)	9,9,11	2.02	2 (22%)
3	NTN	A	392	1	7,8,9	1.44	1 (14%)	9,9,11	4.48	5 (55%)
3	NTN	A	393	1	7,8,9	1.56	2 (28%)	9,9,11	1.28	2 (22%)
3	NTN	A	394	1	7,8,9	1.29	2 (28%)	9,9,11	1.88	3 (33%)
3	NTN	A	395	1	7,8,9	2.36	4 (57%)	9,9,11	1.33	1 (11%)
3	NTN	A	396	1	7,8,9	1.22	2 (28%)	9,9,11	1.87	3 (33%)
3	NTN	A	397	1	7,8,9	1.26	2 (28%)	9,9,11	1.49	2 (22%)
3	NTN	A	398	1	7,8,9	1.42	2 (28%)	9,9,11	2.00	3 (33%)
3	NTN	A	399	1	7,8,9	1.20	2 (28%)	9,9,11	1.57	2 (22%)

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
3	NTN	A	377	1	-	0/2/2/4	0/1/1/1
3	NTN	A	378	1	-	0/2/2/4	0/1/1/1
3	NTN	A	379	1	-	0/2/2/4	0/1/1/1
3	NTN	A	380	1	-	0/2/2/4	0/1/1/1
3	NTN	A	381	1	-	0/2/2/4	0/1/1/1
3	NTN	A	382	1	-	0/2/2/4	0/1/1/1
3	NTN	A	383	1	-	0/2/2/4	0/1/1/1
3	NTN	A	384	1	-	0/2/2/4	0/1/1/1
3	NTN	A	385	1	-	0/2/2/4	0/1/1/1
3	NTN	A	386	1	-	0/2/2/4	0/1/1/1
3	NTN	A	387	1	-	0/2/2/4	0/1/1/1
3	NTN	A	388	1	-	0/2/2/4	0/1/1/1
3	NTN	A	389	1	-	0/2/2/4	0/1/1/1
3	NTN	A	390	1	-	0/2/2/4	0/1/1/1
3	NTN	A	391	1	-	0/2/2/4	0/1/1/1
3	NTN	A	392	1	-	0/2/2/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NTN	A	393	1	-	0/2/2/4	0/1/1/1
3	NTN	A	394	1	-	0/2/2/4	0/1/1/1
3	NTN	A	395	1	-	0/2/2/4	0/1/1/1
3	NTN	A	396	1	-	0/2/2/4	0/1/1/1
3	NTN	A	397	1	-	0/2/2/4	0/1/1/1
3	NTN	A	398	1	-	0/2/2/4	0/1/1/1
3	NTN	A	399	1	-	0/2/2/4	0/1/1/1

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	383	NTN	CI2-CI1	-2.08	1.43	1.47
3	A	390	NTN	CI5-NI2	2.02	1.39	1.33
3	A	385	NTN	CI3-CI4	2.06	1.42	1.38
3	A	398	NTN	CI5-NI2	2.07	1.40	1.33
3	A	381	NTN	CI5-NI2	2.07	1.40	1.33

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	386	NTN	CI2-CI1-NI1	-6.31	113.59	122.25
3	A	387	NTN	CI2-CI1-NI1	-5.77	114.32	122.25
3	A	391	NTN	CI2-CI1-NI1	-4.80	115.65	122.25
3	A	378	NTN	CI2-CI1-NI1	-4.70	115.80	122.25
3	A	392	NTN	CI6-CI2-CI1	-3.54	113.66	120.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 154 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	377	NTN	0	10
3	A	378	NTN	0	20
3	A	379	NTN	0	16
3	A	381	NTN	3	0
3	A	382	NTN	0	13
3	A	383	NTN	1	18
3	A	385	NTN	0	13
3	A	386	NTN	0	14
3	A	387	NTN	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	389	NTN	2	0
3	A	390	NTN	0	4
3	A	391	NTN	1	33
3	A	397	NTN	0	8
3	A	399	NTN	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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.