



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 25, 2024 – 10:36 PM EDT

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

<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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

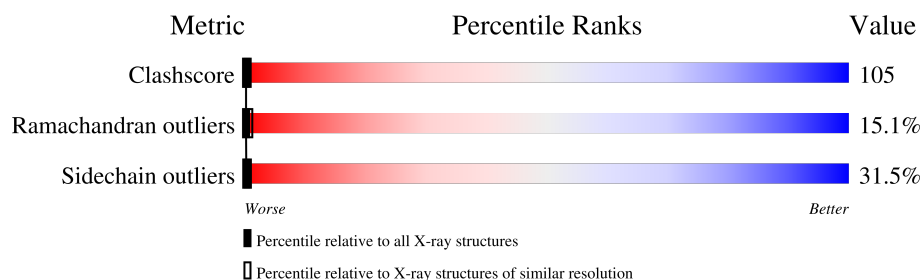
1 Overall quality at a glance

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	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	374	<div> <div style="width: 5%; background-color: green;"></div> <div style="width: 37%; background-color: yellow;"></div> <div style="width: 41%; background-color: orange;"></div> <div style="width: 18%; background-color: red;"></div> </div> <div>5% 37% 41% 18%</div>

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.

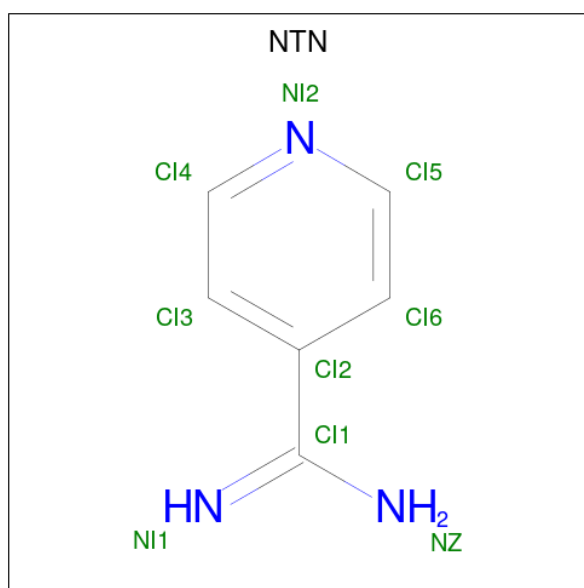
- Molecule 1 is a protein called ISONICOTINIMIDYLATED LIVER ALCOHOL DEHYDROGENASE.

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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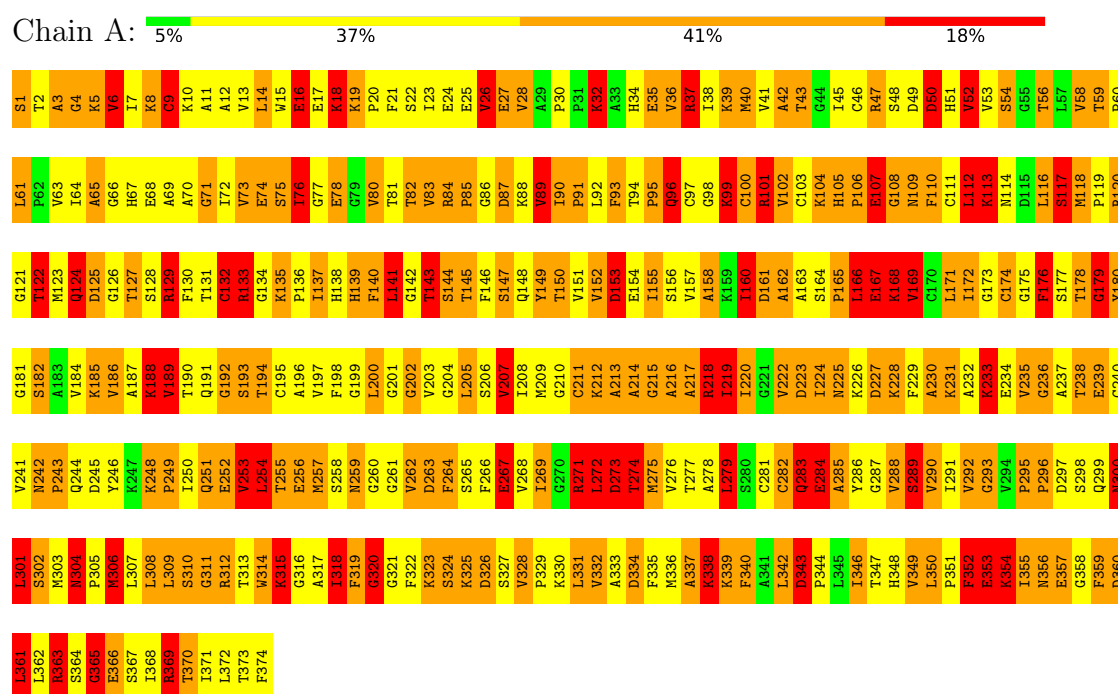
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			8	6	2		
3	A	1	Total	C	N	0	0
			8	6	2		
3	A	1	Total	C	N	0	0
			8	6	2		
3	A	1	Total	C	N	0	0
			8	6	2		
3	A	1	Total	C	N	0	0
			8	6	2		
3	A	1	Total	C	N	0	0
			8	6	2		
3	A	1	Total	C	N	0	0
			8	6	2		
3	A	1	Total	C	N	0	0
			8	6	2		
3	A	1	Total	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, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

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 is therefore 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

5.1 Standard geometry

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 0

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

Mol	Chain	Res	Type
1	A	222	VAL
1	A	273	ASP
1	A	228	LYS
1	A	253	VAL
1	A	284	GLU

Sometimes 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	283	GLN
1	A	304	ASN
1	A	191	GLN
1	A	242	ASN
1	A	244	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	391	1	7,8,9	2.06	3 (42%)	7,9,11	1.78	2 (28%)
3	NTN	A	397	1	7,8,9	1.27	2 (28%)	7,9,11	1.63	2 (28%)
3	NTN	A	381	1	7,8,9	1.59	3 (42%)	7,9,11	2.02	3 (42%)
3	NTN	A	394	1	7,8,9	1.31	2 (28%)	7,9,11	1.78	2 (28%)
3	NTN	A	396	1	7,8,9	1.23	2 (28%)	7,9,11	1.83	3 (42%)
3	NTN	A	399	1	7,8,9	1.22	2 (28%)	7,9,11	1.65	2 (28%)
3	NTN	A	388	1	7,8,9	1.54	2 (28%)	7,9,11	1.54	2 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NTN	A	378	1	7,8,9	2.53	5 (71%)	7,9,11	1.83	2 (28%)
3	NTN	A	385	1	7,8,9	1.40	3 (42%)	7,9,11	2.45	2 (28%)
3	NTN	A	398	1	7,8,9	1.40	2 (28%)	7,9,11	2.02	3 (42%)
3	NTN	A	384	1	7,8,9	1.38	2 (28%)	7,9,11	1.40	2 (28%)
3	NTN	A	386	1	7,8,9	1.35	2 (28%)	7,9,11	2.19	4 (57%)
3	NTN	A	389	1	7,8,9	2.02	4 (57%)	7,9,11	1.36	1 (14%)
3	NTN	A	383	1	7,8,9	1.45	1 (14%)	7,9,11	2.89	3 (42%)
3	NTN	A	393	1	7,8,9	1.52	2 (28%)	7,9,11	1.40	2 (28%)
3	NTN	A	380	1	7,8,9	1.33	2 (28%)	7,9,11	1.45	1 (14%)
3	NTN	A	395	1	7,8,9	2.24	4 (57%)	7,9,11	1.39	1 (14%)
3	NTN	A	377	1	7,8,9	1.44	2 (28%)	7,9,11	1.38	2 (28%)
3	NTN	A	387	1	7,8,9	1.42	2 (28%)	7,9,11	2.03	3 (42%)
3	NTN	A	379	1	7,8,9	1.46	2 (28%)	7,9,11	1.40	2 (28%)
3	NTN	A	382	1	7,8,9	1.28	2 (28%)	7,9,11	1.46	2 (28%)
3	NTN	A	392	1	7,8,9	1.41	1 (14%)	7,9,11	3.68	4 (57%)
3	NTN	A	390	1	7,8,9	1.33	2 (28%)	7,9,11	2.00	2 (28%)

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	391	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	381	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	396	1	–	0/2/2/4	0/1/1/1
3	NTN	A	399	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	378	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	398	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	386	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	383	1	–	0/2/2/4	0/1/1/1
3	NTN	A	393	1	–	0/2/2/4	0/1/1/1
3	NTN	A	380	1	–	0/2/2/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NTN	A	395	1	-	0/2/2/4	0/1/1/1
3	NTN	A	377	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	379	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	392	1	-	0/2/2/4	0/1/1/1
3	NTN	A	390	1	-	0/2/2/4	0/1/1/1

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	378	NTN	CI2-CI1	4.43	1.56	1.47
3	A	395	NTN	CI2-CI1	3.53	1.54	1.47
3	A	391	NTN	CI2-CI1	3.41	1.54	1.47
3	A	389	NTN	CI2-CI1	3.13	1.53	1.47
3	A	395	NTN	CI3-CI4	2.71	1.44	1.38

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	392	NTN	CI2-CI1-NI1	8.40	138.53	121.66
3	A	383	NTN	CI2-CI1-NI1	5.94	133.57	121.66
3	A	385	NTN	CI2-CI1-NI1	4.97	131.63	121.66
3	A	386	NTN	CI2-CI1-NI1	-4.02	113.59	121.66
3	A	381	NTN	CI2-CI1-NI1	3.78	129.25	121.66

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	391	NTN	1	33
3	A	397	NTN	0	8
3	A	381	NTN	3	0
3	A	399	NTN	2	0
3	A	378	NTN	0	20
3	A	385	NTN	0	13
3	A	386	NTN	0	14
3	A	389	NTN	2	0
3	A	383	NTN	1	18

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	377	NTN	0	10
3	A	387	NTN	1	0
3	A	379	NTN	0	16
3	A	382	NTN	0	13
3	A	390	NTN	0	4

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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.