



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:35 am BST

PDB ID : 1N2S
Title : CRYSTAL STRUCTURE OF DTDP-6-DEOXY-L-LYXO-4-HEXULOSE
REDUCTASE (RMLD) IN COMPLEX WITH NADH
Authors : Blankenfeldt, W.; Kerr, I.D.; Giraud, M.F.; McMiken, H.J.; Leonard, G.A.;
Whitfield, C.; Messner, P.; Graninger, M.; Naismith, J.H.
Deposited on : 2002-10-24
Resolution : 2.00 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
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) : 2.11

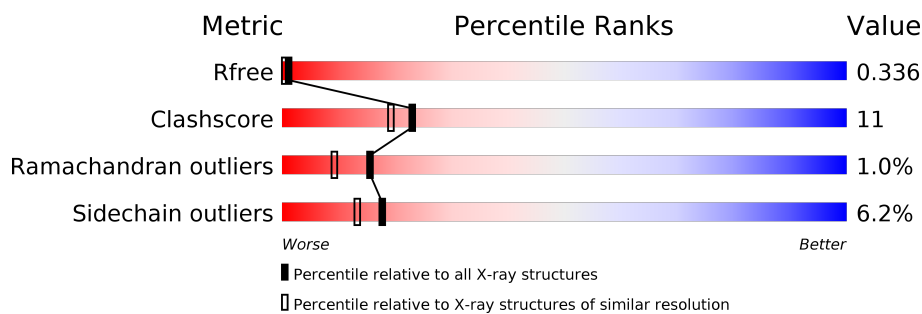
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	299	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2503 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.

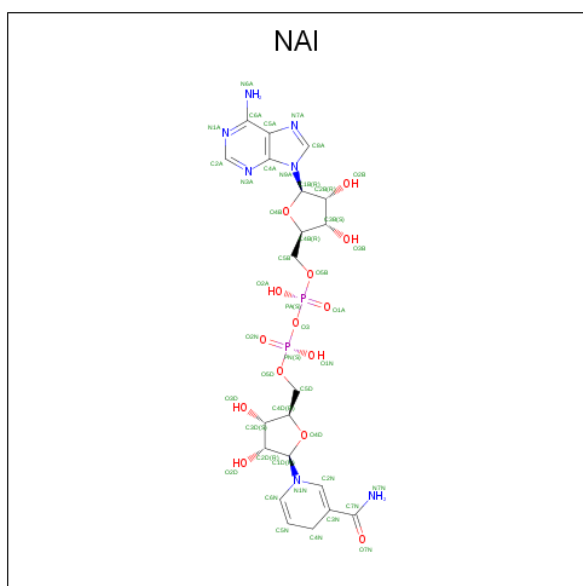
- Molecule 1 is a protein called dTDP-glucose oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	0
			2287	1451	396	433	7			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	1	3		

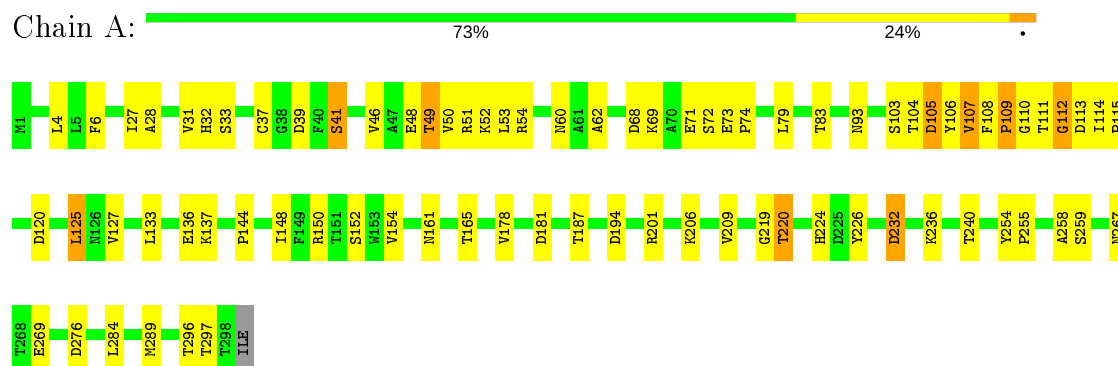
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	163	Total	O	0	0
			163	163		

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. 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: dTDP-glucose oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	47.44Å 71.57Å 82.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.70 – 2.00 54.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (81.70-2.00) 99.7 (54.00-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.199 , 0.253 0.308 , 0.336	Depositor DCC
R_{free} test set	996 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	2503	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.14% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, NAI, MG

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	0.95	2/2338 (0.1%)	1.02	9/3187 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	ALA	CA-CB	5.61	1.64	1.52
1	A	201	ARG	NE-CZ	-5.39	1.26	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	A	120	ASP	CB-CG-OD2	7.86	125.38	118.30
1	A	105	ASP	CB-CG-OD2	7.05	124.65	118.30
1	A	276	ASP	CB-CG-OD2	6.97	124.57	118.30
1	A	232	ASP	CB-CG-OD2	6.41	124.07	118.30
1	A	68	ASP	CB-CG-OD2	6.25	123.93	118.30
1	A	201	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	A	194	ASP	CB-CG-OD1	5.26	123.04	118.30
1	A	181	ASP	CB-CG-OD2	5.18	122.96	118.30

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	A	2287	0	2278	53	0
2	A	1	0	0	0	0
3	A	44	0	26	0	0
4	A	8	0	12	0	0
5	A	163	0	0	4	0
All	All	2503	0	2316	53	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.

All (53) 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:52:LYS:HB2	5:A:1032:HOH:O	1.77	0.84
1:A:133:LEU:HG	1:A:137:LYS:HZ2	1.47	0.77
1:A:103:SER:HB3	1:A:150:ARG:HG2	1.72	0.72
1:A:46:VAL:HA	1:A:49:THR:OG1	1.93	0.69
1:A:136:GLU:OE1	1:A:150:ARG:NH2	2.25	0.69
1:A:31:VAL:HG23	1:A:32:HIS:CD2	2.32	0.64
1:A:52:LYS:CB	5:A:1032:HOH:O	2.40	0.64
1:A:136:GLU:HB2	1:A:148:ILE:HD13	1.81	0.63
1:A:161:ASN:O	1:A:165:THR:HG23	2.00	0.61
1:A:109:PRO:HA	1:A:125:LEU:HG	1.82	0.60
1:A:267:ASN:OD1	1:A:269:GLU:HG2	2.02	0.59
1:A:27:ILE:CD1	1:A:53:LEU:HD22	2.32	0.59
1:A:105:ASP:C	1:A:107:VAL:H	2.04	0.58
1:A:110:GLY:O	1:A:111:THR:OG1	2.20	0.58
1:A:37:CYS:O	1:A:49:THR:HG21	2.06	0.56
1:A:54:ARG:HH11	1:A:54:ARG:HG3	1.71	0.55
1:A:111:THR:O	1:A:112:GLY:O	2.25	0.55
1:A:46:VAL:O	1:A:50:VAL:HG23	2.06	0.55
1:A:71:GLU:CG	1:A:258:ALA:HB2	2.38	0.53
1:A:27:ILE:HD13	1:A:53:LEU:HD22	1.89	0.53
1:A:54:ARG:HB2	5:A:1008:HOH:O	2.10	0.52
1:A:71:GLU:OE2	1:A:127:VAL:HG23	2.11	0.51
1:A:108:PHE:HB3	1:A:109:PRO:HD2	1.93	0.50
1:A:54:ARG:NH1	1:A:54:ARG:HG3	2.26	0.50
1:A:39:ASP:OD1	1:A:41:SER:HB2	2.12	0.49
1:A:71:GLU:HG2	1:A:258:ALA:HB2	1.94	0.49
1:A:73:GLU:O	1:A:73:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ASP:OD1	1:A:232:ASP:C	2.52	0.47
1:A:178:VAL:HG13	1:A:224:HIS:HB2	1.97	0.47
1:A:93:ASN:ND2	1:A:144:PRO:HD2	2.29	0.47
1:A:107:VAL:HG22	1:A:133:LEU:HD13	1.96	0.46
1:A:114:ILE:HA	1:A:115:PRO:HD3	1.81	0.46
1:A:112:GLY:O	1:A:113:ASP:HB2	2.16	0.46
1:A:254:TYR:HA	1:A:255:PRO:HD3	1.78	0.46
1:A:206:LYS:NZ	5:A:939:HOH:O	2.48	0.45
1:A:105:ASP:C	1:A:107:VAL:N	2.70	0.45
1:A:32:HIS:O	1:A:33:SER:C	2.55	0.45
1:A:53:LEU:O	1:A:54:ARG:HB2	2.17	0.44
1:A:105:ASP:O	1:A:107:VAL:N	2.50	0.44
1:A:107:VAL:CG2	1:A:133:LEU:HD13	2.48	0.44
1:A:154:VAL:HA	1:A:187:THR:O	2.18	0.43
1:A:114:ILE:O	1:A:114:ILE:HG22	2.18	0.43
1:A:4:LEU:HD21	1:A:6:PHE:CZ	2.55	0.42
1:A:60:ASN:ND2	1:A:62:ALA:H	2.16	0.42
1:A:69:LYS:HD2	1:A:69:LYS:HA	1.86	0.42
1:A:73:GLU:N	1:A:74:PRO:HD3	2.35	0.42
1:A:48:GLU:HA	1:A:51:ARG:CZ	2.50	0.41
1:A:206:LYS:O	1:A:209:VAL:HG22	2.21	0.41
1:A:31:VAL:HG23	1:A:32:HIS:CG	2.56	0.41
1:A:133:LEU:HG	1:A:137:LYS:NZ	2.28	0.40
1:A:232:ASP:OD1	1:A:236:LYS:HD2	2.21	0.40
1:A:79:LEU:HA	1:A:83:THR:HB	2.04	0.40
1:A:219:GLY:C	1:A:220:THR:HG22	2.41	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	296/299 (99%)	285 (96%)	8 (3%)	3 (1%)	15 9

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	GLY
1	A	106	TYR
1	A	109	PRO

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	240/241 (100%)	225 (94%)	15 (6%)	18 13

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	SER
1	A	49	THR
1	A	72	SER
1	A	104	THR
1	A	107	VAL
1	A	125	LEU
1	A	152	SER
1	A	220	THR
1	A	226	TYR
1	A	240	THR
1	A	259	SER
1	A	284	LEU
1	A	289	MET
1	A	296	THR
1	A	297	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	60	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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$
4	TRS	A	601	-	7,7,7	0.38	0	9,9,9	0.32	0
3	NAI	A	901	-	42,48,48	1.53	8 (19%)	47,73,73	1.71	12 (25%)

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	TRS	A	601	-	-	5/9/9/9	-
3	NAI	A	901	-	-	8/25/72/72	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	NAI	C2A-N3A	4.37	1.39	1.32
3	A	901	NAI	O3D-C3D	-2.89	1.36	1.43
3	A	901	NAI	C2D-C3D	-2.49	1.46	1.53
3	A	901	NAI	C2B-C1B	-2.49	1.50	1.53
3	A	901	NAI	C7N-C3N	-2.36	1.43	1.48
3	A	901	NAI	PA-O2A	-2.17	1.45	1.55
3	A	901	NAI	O5D-C5D	-2.15	1.36	1.44
3	A	901	NAI	C6A-C5A	-2.02	1.35	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	NAI	N3A-C2A-N1A	-4.25	122.03	128.68
3	A	901	NAI	O4D-C4D-C3D	3.73	112.50	105.11
3	A	901	NAI	O2D-C2D-C1D	3.12	120.45	110.02
3	A	901	NAI	C4D-O4D-C1D	-2.95	102.96	109.47
3	A	901	NAI	O7N-C7N-N7N	2.58	128.91	122.88
3	A	901	NAI	O1N-PN-O2N	2.51	124.64	112.24
3	A	901	NAI	C5A-C6A-N6A	2.51	124.16	120.35
3	A	901	NAI	O4B-C4B-C3B	2.50	110.05	105.11
3	A	901	NAI	C3N-C7N-N7N	-2.49	113.25	117.67
3	A	901	NAI	C2B-C3B-C4B	-2.47	97.84	102.64
3	A	901	NAI	O3D-C3D-C4D	-2.34	104.27	111.05
3	A	901	NAI	PN-O3-PA	-2.09	125.65	132.83

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	TRS	C1-C-C3-O3
4	A	601	TRS	C2-C-C3-O3
4	A	601	TRS	N-C-C3-O3
3	A	901	NAI	C5D-O5D-PN-O1N
3	A	901	NAI	C5D-O5D-PN-O3
4	A	601	TRS	C2-C-C1-O1
4	A	601	TRS	N-C-C1-O1
3	A	901	NAI	O4D-C1D-N1N-C6N
3	A	901	NAI	PN-O3-PA-O1A
3	A	901	NAI	PN-O3-PA-O2A
3	A	901	NAI	C5D-O5D-PN-O2N
3	A	901	NAI	O4B-C4B-C5B-O5B

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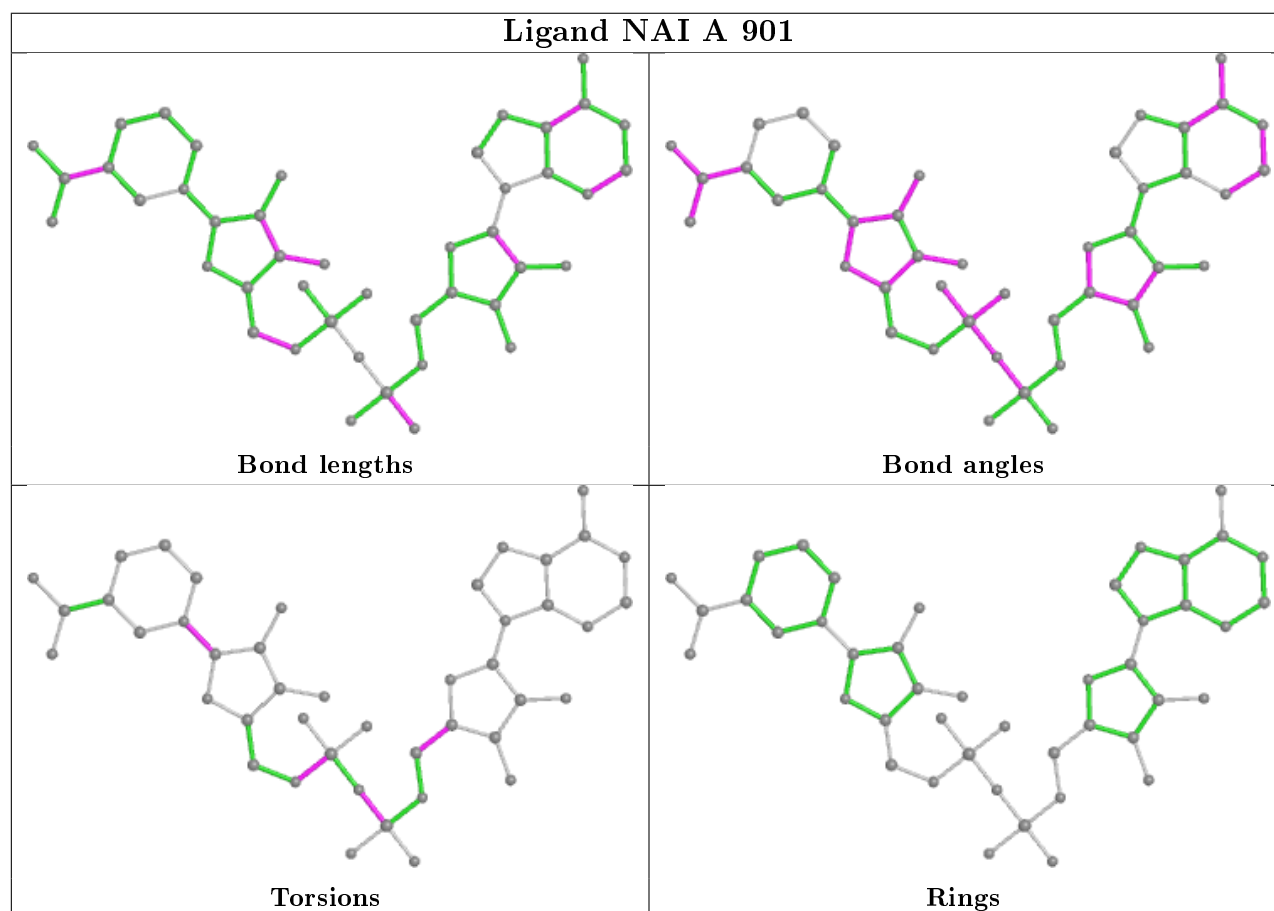
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Mol	Chain	Res	Type	Atoms
3	A	901	NAI	C2D-C1D-N1N-C6N

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

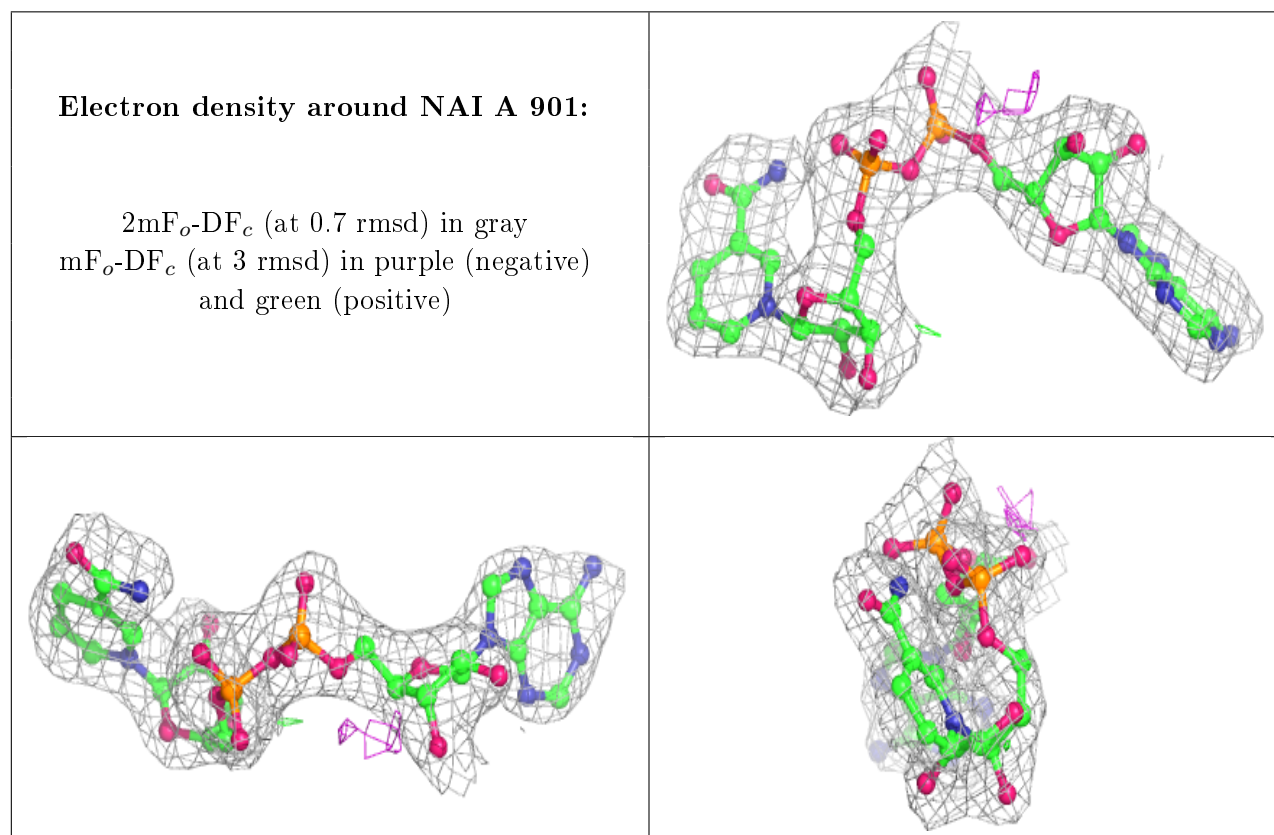
6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.