



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 10:15 AM UTC

PDB ID : 9ICD / pdb_00009icd
Title : CATALYTIC MECHANISM OF NADP+-DEPENDENT ISOCITRATE DEHYDROGENASE: IMPLICATIONS FROM THE STRUCTURES OF MAGNESIUM-ISOCITRATE AND NADP+ COMPLEXES
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Deposited on : 1991-07-29
Resolution : 2.50 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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

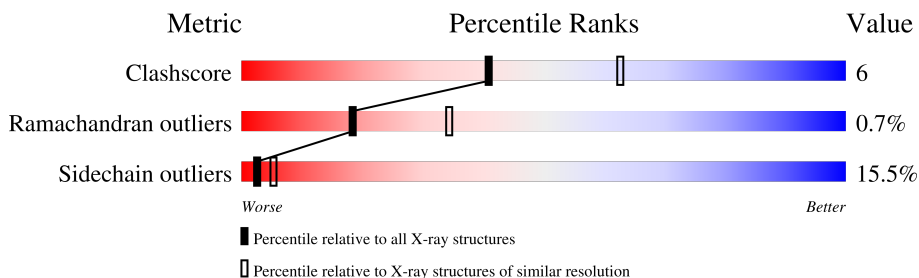
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	416	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3275 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 ISOCITRATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3147	2008	531	590	18			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	101	Total	O	0	0
			101	101		

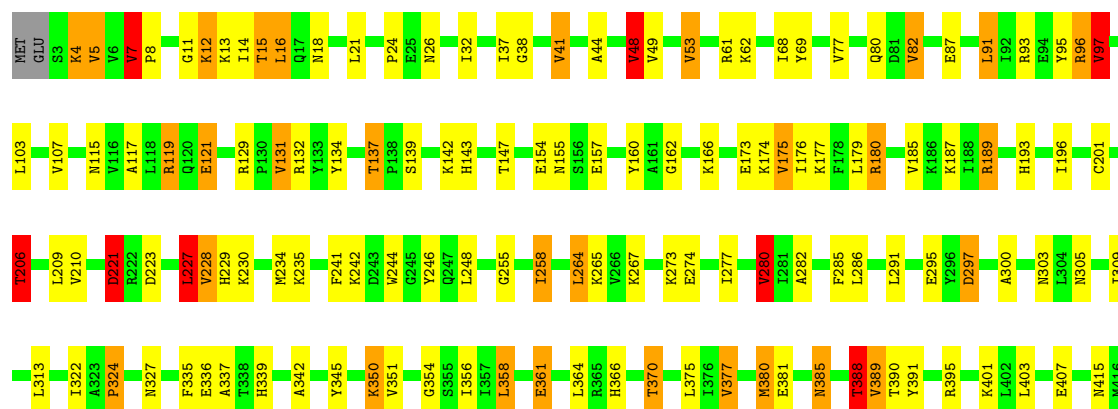
3 Residue-property plots

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: ISOCITRATE DEHYDROGENASE

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.10Å 105.10Å 150.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.181 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3275	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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: NAP

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	1.12	19/3208 (0.6%)	1.81	56/4347 (1.3%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	VAL	CA-CB	7.97	1.64	1.54
1	A	82	VAL	CA-CB	7.69	1.62	1.53
1	A	193	HIS	CD2-NE2	-7.65	1.29	1.37
1	A	280	VAL	CA-CB	6.89	1.64	1.54
1	A	41	VAL	CA-CB	6.60	1.63	1.54
1	A	143	HIS	CD2-NE2	-6.13	1.31	1.37
1	A	229	HIS	CD2-NE2	-5.89	1.31	1.37
1	A	206	THR	CA-CB	5.85	1.62	1.53
1	A	97	VAL	CA-CB	5.78	1.63	1.54
1	A	324	PRO	CA-CB	-5.74	1.46	1.53
1	A	193	HIS	CG-ND1	-5.65	1.32	1.38
1	A	366	HIS	CD2-NE2	-5.63	1.31	1.37
1	A	5	VAL	CA-CB	5.61	1.61	1.54
1	A	339	HIS	CG-ND1	-5.54	1.32	1.38
1	A	48	VAL	CA-CB	5.51	1.61	1.54
1	A	228	VAL	CA-CB	5.50	1.62	1.54
1	A	377	VAL	CA-CB	5.45	1.62	1.54
1	A	7	VAL	CA-CB	5.44	1.61	1.54
1	A	175	VAL	CA-CB	5.16	1.61	1.54

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	ASP	CA-CB-CG	10.91	123.51	112.60
1	A	389	VAL	N-CA-CB	-8.88	95.93	112.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	ARG	NE-CZ-NH2	8.35	126.72	119.20
1	A	61	ARG	NE-CZ-NH2	7.60	126.04	119.20
1	A	336	GLU	N-CA-C	7.13	120.03	108.76
1	A	390	THR	N-CA-CB	-7.13	99.05	110.46
1	A	388	THR	CA-C-O	7.04	129.77	121.11
1	A	388	THR	N-CA-CB	-6.95	97.63	110.56
1	A	303	ASN	N-CA-C	6.89	119.37	111.11
1	A	274	GLU	CA-CB-CG	-6.82	100.47	114.10
1	A	244	TRP	CG-CD2-CE3	6.61	140.51	133.90
1	A	258	ILE	N-CA-C	-6.52	99.03	108.36
1	A	388	THR	CA-CB-OG1	-6.51	99.83	109.60
1	A	415	ASN	CA-CB-CG	-6.43	106.17	112.60
1	A	223	ASP	N-CA-C	6.36	120.24	112.23
1	A	193	HIS	CB-CG-CD2	-6.33	122.97	131.20
1	A	395	ARG	CB-CA-C	-6.30	99.97	110.68
1	A	361	GLU	CA-CB-CG	6.25	126.60	114.10
1	A	139	SER	O-C-N	-6.24	116.44	121.80
1	A	389	VAL	CB-CA-C	6.14	120.68	110.30
1	A	370	THR	CA-CB-OG1	-6.13	100.40	109.60
1	A	77	VAL	N-CA-C	-6.07	106.98	111.90
1	A	390	THR	CB-CA-C	5.94	120.23	109.83
1	A	131	VAL	CA-C-O	5.92	126.25	120.27
1	A	388	THR	CB-CA-C	5.89	121.42	111.41
1	A	189	ARG	NE-CZ-NH2	5.83	124.45	119.20
1	A	335	PHE	CA-CB-CG	-5.79	108.01	113.80
1	A	337	ALA	N-CA-C	-5.79	100.55	109.76
1	A	129	ARG	NE-CZ-NH1	-5.78	115.72	121.50
1	A	342	ALA	CA-C-N	5.66	125.50	119.28
1	A	342	ALA	C-N-CA	5.66	125.50	119.28
1	A	297	ASP	CA-CB-CG	5.66	118.26	112.60
1	A	69	TYR	N-CA-C	5.62	118.62	109.24
1	A	380	MET	CG-SD-CE	-5.62	88.55	100.90
1	A	96	ARG	NE-CZ-NH2	5.51	124.16	119.20
1	A	132	ARG	CB-CG-CD	-5.47	98.71	111.30
1	A	227	LEU	CA-C-N	-5.44	115.55	123.06
1	A	227	LEU	C-N-CA	-5.44	115.55	123.06
1	A	370	THR	N-CA-CB	-5.39	101.63	110.14
1	A	201	CYS	O-C-N	-5.38	116.02	123.12
1	A	15	THR	CA-CB-OG1	-5.37	101.54	109.60
1	A	244	TRP	CB-CG-CD1	-5.37	118.84	126.90
1	A	166	LYS	CB-CA-C	-5.35	100.83	109.72
1	A	282	ALA	N-CA-C	5.28	117.78	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	LYS	N-CA-C	5.24	117.07	111.36
1	A	174	LYS	CA-C-O	-5.24	115.31	120.70
1	A	142	LYS	CB-CA-C	-5.19	102.03	110.85
1	A	147	THR	CA-CB-OG1	-5.18	101.82	109.60
1	A	391	TYR	N-CA-C	5.17	117.58	111.33
1	A	273	LYS	N-CA-C	5.14	117.32	110.53
1	A	180	ARG	NE-CZ-NH1	-5.14	116.36	121.50
1	A	370	THR	CA-CB-CG2	5.13	119.22	110.50
1	A	137	THR	N-CA-C	-5.08	103.67	110.07
1	A	277	ILE	N-CA-C	-5.03	100.50	107.80
1	A	196	ILE	O-C-N	-5.02	117.77	123.20
1	A	230	LYS	CG-CD-CE	-5.01	99.78	111.30

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	3147	0	3142	41	0
2	A	27	0	11	0	0
3	A	101	0	0	3	0
All	All	3275	0	3153	41	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 (41) 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:401:LYS:HE3	1:A:403:LEU:HD11	1.62	0.82
1:A:322:ILE:HG22	1:A:354:GLY:HA3	1.74	0.69
1:A:134:TYR:O	1:A:137:THR:HG23	1.96	0.64
1:A:16:LEU:HD23	1:A:96:ARG:HD2	1.79	0.63
1:A:345:TYR:CD2	1:A:350:LYS:HD2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:PRO:HB3	1:A:358:LEU:HB3	1.83	0.60
1:A:206:THR:HB	1:A:241:PHE:CD2	2.37	0.59
1:A:117:ALA:O	1:A:121:GLU:HB2	2.02	0.59
1:A:162:GLY:HA2	3:A:490:HOH:O	2.02	0.59
1:A:280:VAL:HG22	1:A:285:PHE:HB2	1.87	0.55
1:A:305:ASN:O	1:A:309:ILE:HG12	2.07	0.54
1:A:26:ASN:HA	1:A:62:LYS:O	2.09	0.52
1:A:115:ASN:O	1:A:119:ARG:HG3	2.10	0.51
1:A:246:TYR:HD1	1:A:264:LEU:HD22	1.76	0.51
1:A:154:GLU:HA	1:A:209:LEU:HD13	1.93	0.50
1:A:14:ILE:HD12	1:A:97:VAL:HG13	1.94	0.50
1:A:388:THR:HG21	3:A:463:HOH:O	2.12	0.49
1:A:37:ILE:HB	1:A:351:VAL:HG21	1.95	0.49
1:A:44:ALA:O	1:A:48:VAL:HG13	2.13	0.48
1:A:11:GLY:HA2	1:A:26:ASN:O	2.14	0.47
1:A:87:GLU:O	1:A:91:LEU:HD22	2.16	0.46
1:A:176:ILE:O	1:A:180:ARG:HG3	2.16	0.46
1:A:206:THR:O	1:A:210:VAL:HG23	2.17	0.45
1:A:258:ILE:HD11	1:A:265:LYS:HG3	2.00	0.44
1:A:26:ASN:HB3	3:A:466:HOH:O	2.18	0.44
1:A:206:THR:HB	1:A:241:PHE:HD2	1.82	0.44
1:A:12:LYS:HB3	1:A:24:PRO:HG3	2.00	0.43
1:A:32:ILE:HG13	1:A:68:ILE:HG13	2.01	0.43
1:A:255:GLY:HA2	1:A:265:LYS:O	2.19	0.43
1:A:119:ARG:HD2	1:A:155:ASN:ND2	2.34	0.43
1:A:13:LYS:HG2	1:A:95:TYR:CE1	2.54	0.42
1:A:4:LYS:HB2	1:A:4:LYS:NZ	2.34	0.42
1:A:381:GLU:O	1:A:385:ASN:HB2	2.20	0.41
1:A:119:ARG:HD3	1:A:327:ASN:OD1	2.20	0.41
1:A:49:VAL:O	1:A:53:VAL:HG13	2.20	0.41
1:A:179:LEU:O	1:A:185:VAL:HG13	2.20	0.41
1:A:16:LEU:HD22	1:A:21:LEU:HD23	2.01	0.41
1:A:7:VAL:HA	1:A:8:PRO:HD3	1.90	0.41
1:A:403:LEU:HB3	1:A:407:GLU:HB2	2.03	0.41
1:A:38:GLY:HA2	1:A:41:VAL:HG22	2.02	0.40
1:A:227:LEU:HD12	1:A:300:ALA:HB3	2.03	0.40

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	
1	A	412/416 (99%)	395 (96%)	14 (3%)	3 (1%)	18	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	221	ASP
1	A	297	ASP

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	323/338 (96%)	273 (84%)	50 (16%)	2	5

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	5	VAL
1	A	7	VAL
1	A	12	LYS
1	A	15	THR
1	A	16	LEU
1	A	48	VAL
1	A	53	VAL

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Mol	Chain	Res	Type
1	A	80	GLN
1	A	82	VAL
1	A	91	LEU
1	A	93	ARG
1	A	97	VAL
1	A	103	LEU
1	A	107	VAL
1	A	121	GLU
1	A	131	VAL
1	A	157	GLU
1	A	160	TYR
1	A	173	GLU
1	A	175	VAL
1	A	177	LYS
1	A	187	LYS
1	A	189	ARG
1	A	206	THR
1	A	221	ASP
1	A	227	LEU
1	A	228	VAL
1	A	234	MET
1	A	242	LYS
1	A	248	LEU
1	A	264	LEU
1	A	267	LYS
1	A	280	VAL
1	A	286	LEU
1	A	291	LEU
1	A	295	GLU
1	A	313	LEU
1	A	350	LYS
1	A	356	ILE
1	A	358	LEU
1	A	361	GLU
1	A	364	LEU
1	A	370	THR
1	A	375	LEU
1	A	377	VAL
1	A	380	MET
1	A	385	ASN
1	A	388	THR
1	A	389	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	80	GLN
1	A	120	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	NAP	A	417	-	29,29,52	1.36	5 (17%)	44,45,80	1.35	6 (13%)

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	NAP	A	417	-	-	3/15/31/67	0/3/3/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	417	NAP	PA-O3	3.16	1.66	1.54
2	A	417	NAP	PA-O5B	3.11	1.70	1.60
2	A	417	NAP	P2B-O2B	3.00	1.64	1.59
2	A	417	NAP	P2B-O3X	2.17	1.62	1.54
2	A	417	NAP	C8A-N9A	2.05	1.41	1.37

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	417	NAP	O5B-C5B-C4B	3.63	121.37	108.99
2	A	417	NAP	O2B-C2B-C1B	-3.55	97.56	110.05
2	A	417	NAP	C3B-C2B-C1B	-3.34	96.42	102.81
2	A	417	NAP	O2X-P2B-O1X	2.63	121.07	110.83
2	A	417	NAP	O4B-C4B-C5B	2.56	117.54	109.33
2	A	417	NAP	O4B-C1B-N9A	2.33	112.56	108.09

There are no chirality outliers.

All (3) torsion outliers are listed below:

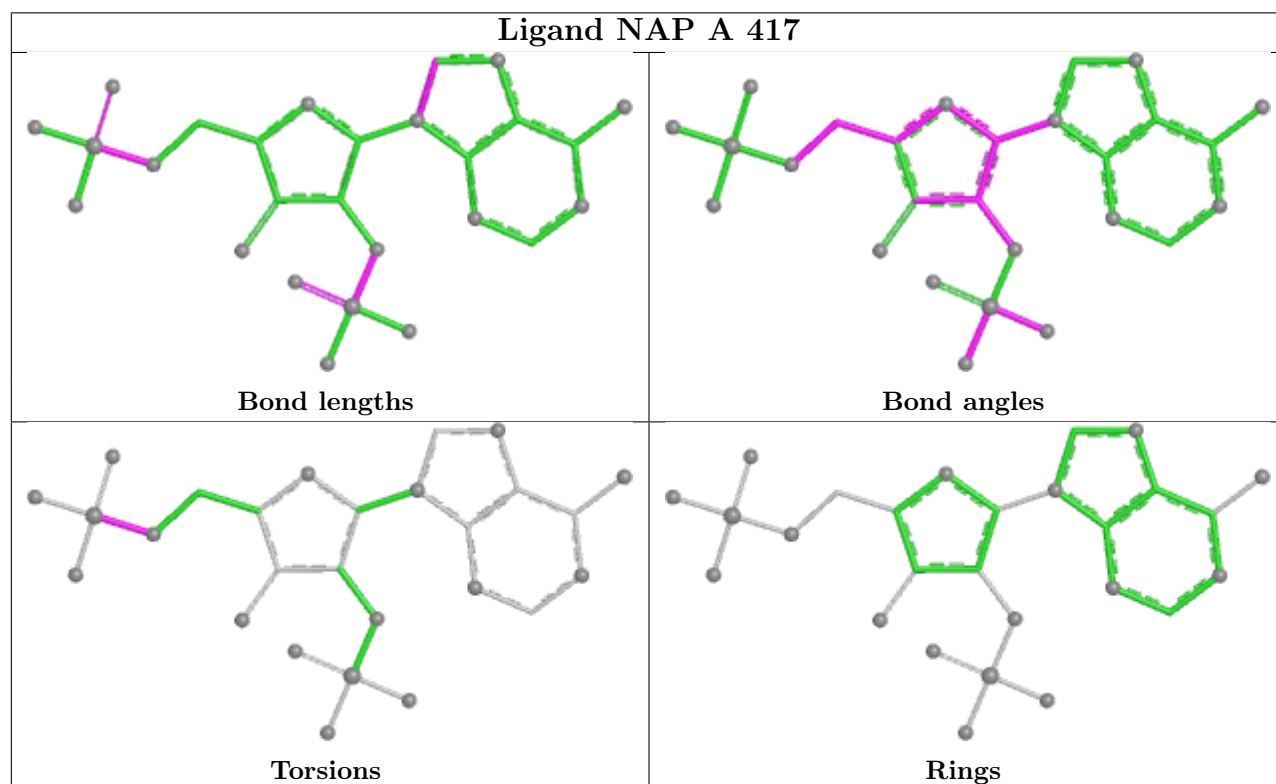
Mol	Chain	Res	Type	Atoms
2	A	417	NAP	C5B-O5B-PA-O1A
2	A	417	NAP	C5B-O5B-PA-O2A
2	A	417	NAP	C5B-O5B-PA-O3

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

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.