



Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2020 – 11:28 pm BST

PDB ID : 1QUF
Title : X-RAY STRUCTURE OF A COMPLEX NADP⁺-FERREDOXIN:NADP⁺ REDUCTASE FROM THE CYANOBACTERIUM ANABAENA PCC 7119 AT 2.25 ANGSTROMS
Authors : Serre, L.; Frey, M.; Vellieux, F.M.D.
Deposited on : 1996-09-07
Resolution : 2.25 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
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) : 2.11

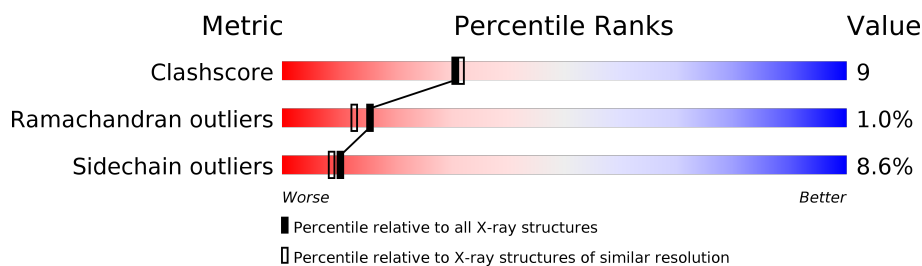
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)

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 $\leq 5\%$.

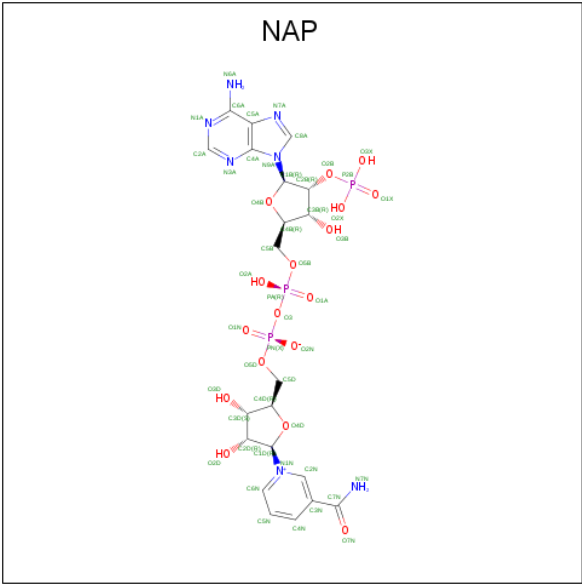
Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	304	

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
2	FAD	A	304	X	-	-	-
3	NAP	A	305	X	-	-	-

(three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			52	21	4	7	17	3		

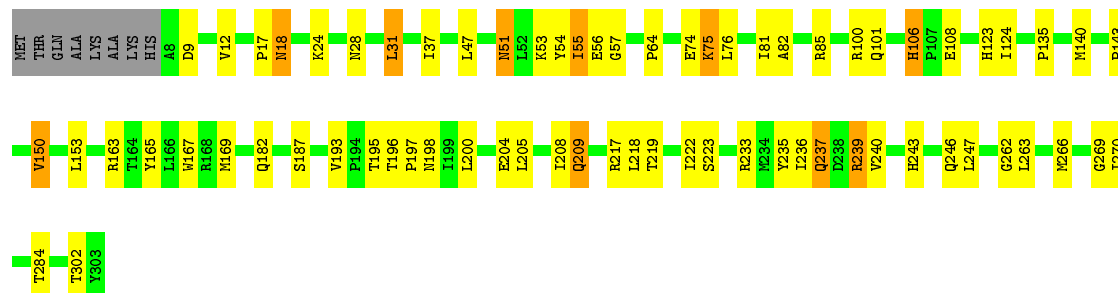
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	439	Total	O	0	0
			439	439		



Note EDS was not executed.

- Chain A: 74% 20% ..



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	85.84Å 85.84Å 97.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.25	Depositor
% Data completeness (in resolution range)	83.0 (15.00-2.25)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.73	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.186 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2874	wwPDB-VP
Average B, all atoms (Å ²)	10.0	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: NAP, FAD

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	0.60	0/2393	0.85	2/3245 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	106	HIS	N-CA-C	7.49	131.24	111.00
1	A	218	LEU	CA-CB-CG	5.21	127.27	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2330	0	2293	42	0
2	A	53	0	30	0	0
3	A	48	4	23	4	0
4	A	439	0	0	5	7
All	All	2870	4	2346	44	7

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 9.

All (44) 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:37:ILE:HG13	4:A:658:HOH:O	1.84	0.77
1:A:153:LEU:HD13	1:A:270:ILE:HD13	1.70	0.72
1:A:165:TYR:O	1:A:169:MET:HG3	1.90	0.71
1:A:237:GLN:HE21	1:A:237:GLN:H	1.40	0.70
1:A:31:LEU:HB3	1:A:200:LEU:HD22	1.76	0.67
1:A:51:ASN:H	1:A:51:ASN:HD22	1.44	0.66
1:A:18:ASN:H	1:A:18:ASN:HD22	1.44	0.66
1:A:223:SER:O	1:A:233:ARG:HD2	1.97	0.63
1:A:75:LYS:HE3	1:A:76:LEU:H	1.65	0.61
1:A:82:ALA:O	1:A:163:ARG:HD3	2.03	0.57
3:A:305:NAP:H3B	4:A:790:HOH:O	2.06	0.56
1:A:196:THR:N	1:A:197:PRO:HD2	2.22	0.54
1:A:55:ILE:HG23	1:A:56:GLU:N	2.23	0.54
1:A:262:GLY:O	1:A:302:THR:HA	2.08	0.53
1:A:243:HIS:HD2	1:A:246:GLN:HE22	1.57	0.52
1:A:18:ASN:H	1:A:18:ASN:ND2	2.08	0.52
1:A:64:PRO:HG2	1:A:74:GLU:HB3	1.91	0.51
1:A:51:ASN:N	1:A:51:ASN:HD22	2.06	0.51
1:A:17:PRO:HG3	1:A:76:LEU:HD23	1.93	0.51
1:A:101:GLN:OE1	1:A:123:HIS:HE1	1.93	0.51
1:A:237:GLN:HG2	1:A:269:GLY:HA3	1.92	0.50
1:A:101:GLN:HB3	3:A:305:NAP:H5N	1.94	0.50
1:A:37:ILE:O	3:A:305:NAP:H52N	2.12	0.49
1:A:54:TYR:CE2	1:A:81:ILE:HG21	2.49	0.47
1:A:193:VAL:O	1:A:222:ILE:HA	2.15	0.47
1:A:17:PRO:HG3	1:A:76:LEU:CD2	2.45	0.47
1:A:64:PRO:HG2	1:A:74:GLU:CB	2.45	0.46
1:A:143:PRO:HG2	4:A:616:HOH:O	2.15	0.46
1:A:54:TYR:CD2	1:A:81:ILE:HD13	2.52	0.45
1:A:150:VAL:O	1:A:187:SER:HA	2.17	0.44
1:A:263:LEU:HB3	4:A:473:HOH:O	2.16	0.44
1:A:233:ARG:HG3	1:A:233:ARG:HH11	1.82	0.44
1:A:28:ASN:ND2	1:A:124:ILE:HG22	2.32	0.43
1:A:236:ILE:O	1:A:240:VAL:HG23	2.20	0.42
1:A:195:THR:OG1	1:A:197:PRO:HG2	2.19	0.42
1:A:235:TYR:HB3	1:A:237:GLN:NE2	2.35	0.42
3:A:305:NAP:H2N	3:A:305:NAP:H71N	1.60	0.42
1:A:57:GLY:HA3	1:A:140:MET:O	2.20	0.41
1:A:53:LYS:O	1:A:135:PRO:HG3	2.21	0.41
1:A:219:THR:HG22	1:A:239:ARG:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209[A]:GLN:NE2	4:A:656:HOH:O	2.54	0.41
1:A:204:GLU:O	1:A:208:ILE:HG13	2.22	0.40
1:A:193:VAL:HG11	1:A:198:ASN:O	2.21	0.40
1:A:233:ARG:HG3	1:A:233:ARG:NH1	2.37	0.40

All (7) 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)
4:A:614:HOH:O	4:A:816:HOH:O[3_665]	0.81	1.39
4:A:629:HOH:O	4:A:810:HOH:O[3_665]	1.32	0.88
4:A:639:HOH:O	4:A:649:HOH:O[3_665]	1.44	0.76
4:A:605:HOH:O	4:A:810:HOH:O[3_665]	1.78	0.42
4:A:549:HOH:O	4:A:705:HOH:O[5_555]	2.05	0.15
4:A:540:HOH:O	4:A:824:HOH:O[4_654]	2.08	0.12
4:A:666:HOH:O	4:A:825:HOH:O[2_654]	2.13	0.07

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	296/304 (97%)	282 (95%)	11 (4%)	3 (1%)	15 13

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	HIS
1	A	9	ASP
1	A	108	GLU

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	246 / 256 (96%)	224 (91%)	22 (9%)	9 8

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	18	ASN
1	A	24	LYS
1	A	31	LEU
1	A	47	LEU
1	A	51	ASN
1	A	55	ILE
1	A	75	LYS
1	A	85	ARG
1	A	100	ARG
1	A	150	VAL
1	A	167	TRP
1	A	182	GLN
1	A	205	LEU
1	A	209[A]	GLN
1	A	209[B]	GLN
1	A	217	ARG
1	A	237	GLN
1	A	239	ARG
1	A	247	LEU
1	A	266	MET
1	A	284	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	51	ASN
1	A	123	HIS

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Mol	Chain	Res	Type
1	A	182	GLN
1	A	237	GLN
1	A	243	HIS
1	A	299	HIS

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 ⓘ

2 ligands 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	$\# Z > 2$
2	FAD	A	304	-	51,58,58	1.47	6 (11%)	60,89,89	2.24	9 (15%)
3	NAP	A	305	-	45,52,52	2.67	10 (22%)	56,80,80	6.80	21 (37%)

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	FAD	A	304	-	1/1/9/9	2/30/50/50	0/6/6/6
3	NAP	A	305	-	1/1/12/12	10/31/67/67	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	305	NAP	P2B-O2B	-10.25	1.39	1.59
3	A	305	NAP	C2N-N1N	6.95	1.43	1.35
3	A	305	NAP	O4D-C1D	6.88	1.50	1.41
2	A	304	FAD	C4-C4X	5.45	1.50	1.41
3	A	305	NAP	C2D-C1D	-5.06	1.46	1.53
3	A	305	NAP	C3N-C7N	4.28	1.57	1.50
2	A	304	FAD	C1'-N10	4.12	1.52	1.48
3	A	305	NAP	P2B-O2X	-3.82	1.40	1.54
2	A	304	FAD	C4X-C10	3.67	1.42	1.38
3	A	305	NAP	C3B-C2B	2.97	1.59	1.52
3	A	305	NAP	P2B-O3X	-2.86	1.43	1.54
3	A	305	NAP	C4A-N3A	-2.71	1.31	1.35
2	A	304	FAD	C8A-N7A	-2.68	1.29	1.34
3	A	305	NAP	C5A-N7A	-2.61	1.30	1.39
2	A	304	FAD	C4-N3	2.25	1.37	1.33
2	A	304	FAD	C5X-N5	-2.11	1.31	1.35

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	305	NAP	C1B-N9A-C4A	26.26	172.78	126.64
3	A	305	NAP	C2N-N1N-C1D	24.97	174.74	119.14
3	A	305	NAP	C6N-N1N-C2N	-24.57	99.57	121.97
3	A	305	NAP	C3N-C2N-N1N	16.15	136.21	120.43
2	A	304	FAD	C4-N3-C2	12.61	125.79	115.14
3	A	305	NAP	C5N-C6N-N1N	8.48	132.56	120.40
2	A	304	FAD	C4X-C4-N3	-6.27	114.85	123.43
3	A	305	NAP	N3A-C2A-N1A	-5.84	119.55	128.68
3	A	305	NAP	O4D-C1D-C2D	-5.78	98.48	106.93
3	A	305	NAP	C4A-C5A-N7A	-5.74	103.42	109.40
3	A	305	NAP	O5B-C5B-C4B	5.70	128.62	108.99
3	A	305	NAP	C5N-C4N-C3N	-5.57	113.75	120.34
2	A	304	FAD	C1'-N10-C9A	4.72	122.00	118.29
3	A	305	NAP	O5B-PA-O1A	-4.61	91.07	109.07
3	A	305	NAP	C3D-C2D-C1D	4.44	107.67	100.98
3	A	305	NAP	O4D-C4D-C5D	4.25	123.36	109.37
3	A	305	NAP	O3B-C3B-C2B	4.07	122.71	111.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	305	NAP	C5A-C6A-N6A	3.68	125.94	120.35
2	A	304	FAD	C4X-N5-C5X	3.43	120.19	116.77
3	A	305	NAP	O4D-C4D-C3D	-3.23	98.72	105.11
3	A	305	NAP	C4N-C3N-C7N	2.91	128.84	121.04
2	A	304	FAD	O4B-C1B-C2B	2.87	111.13	106.93
3	A	305	NAP	C2D-C3D-C4D	2.77	108.02	102.64
3	A	305	NAP	C2B-C3B-C4B	2.55	107.54	101.99
3	A	305	NAP	C2N-C3N-C7N	-2.39	112.53	119.46
3	A	305	NAP	O5D-C5D-C4D	2.38	117.17	108.99
2	A	304	FAD	C4-C4X-C10	-2.31	118.42	119.95
2	A	304	FAD	C3B-C2B-C1B	-2.27	97.56	100.98
2	A	304	FAD	C9A-N10-C10	-2.26	118.95	121.91
2	A	304	FAD	C4-C4X-N5	2.15	121.06	118.60

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	304	FAD	C1B
3	A	305	NAP	C1B

All (12) torsion outliers are listed below:

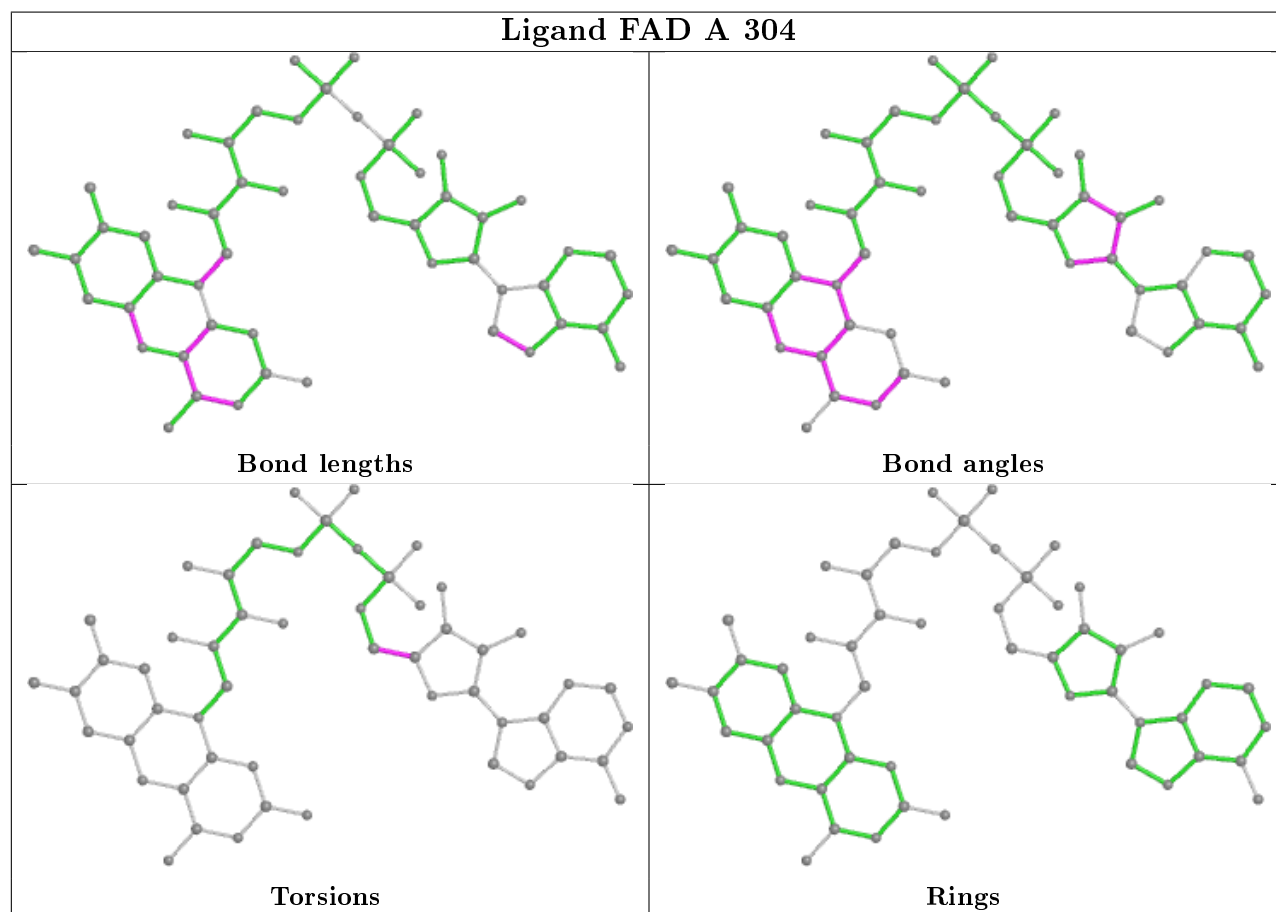
Mol	Chain	Res	Type	Atoms
2	A	304	FAD	O4B-C4B-C5B-O5B
3	A	305	NAP	C5D-O5D-PN-O1N
3	A	305	NAP	O4D-C1D-N1N-C6N
3	A	305	NAP	C2D-C1D-N1N-C2N
3	A	305	NAP	C2D-C1D-N1N-C6N
3	A	305	NAP	O4B-C4B-C5B-O5B
3	A	305	NAP	C3B-C4B-C5B-O5B
2	A	304	FAD	C3B-C4B-C5B-O5B
3	A	305	NAP	C5D-O5D-PN-O3
3	A	305	NAP	C4B-C5B-O5B-PA
3	A	305	NAP	C3D-C4D-C5D-O5D
3	A	305	NAP	C5B-O5B-PA-O1A

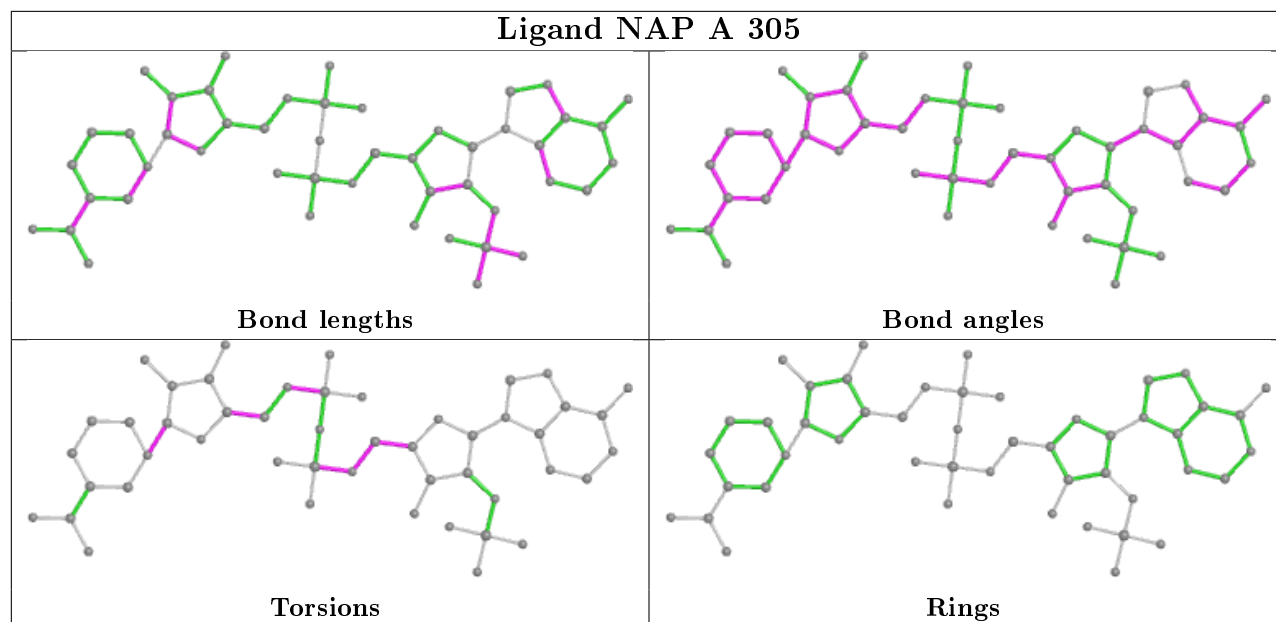
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	305	NAP	4	0

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.