



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 28, 2023 – 07:48 pm GMT

PDB ID : 1E1K
Title : ADRENODOXIN REDUCTASE in complex with NADP⁺ obtained by a soaking experiment
Authors : Ziegler, G.A.; Schulz, G.E.
Deposited on : 2000-05-09
Resolution : 1.95 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

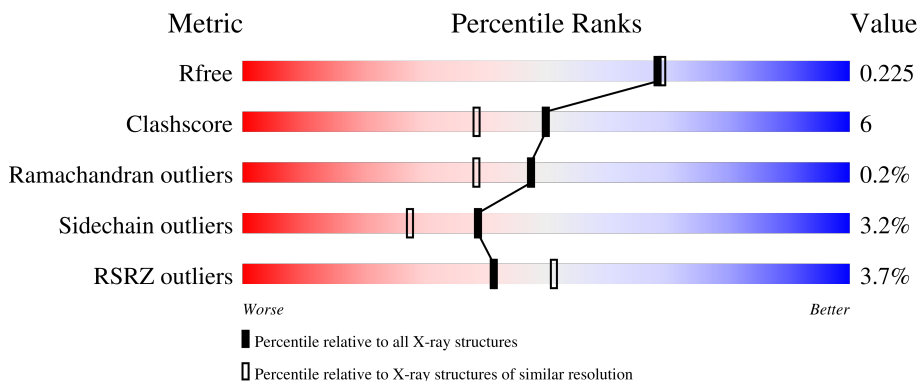
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

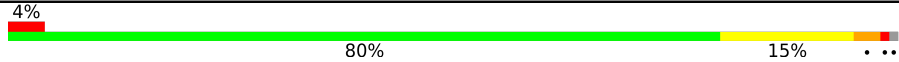
The reported resolution of this entry is 1.95 Å.

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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	460	

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	NAP	A	802	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3959 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 ADRENODOXIN REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	455	3512	2219	637	645	11	0	1	0

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	53	27	9	15	2	0	0

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.90Å 62.40Å 78.20Å 90.00° 106.60° 90.00°	Depositor
Resolution (Å)	20.00 – 1.95 25.78 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.95) 99.8 (25.78-1.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 1.95Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.184 , 0.227 0.184 , 0.225	Depositor DCC
R_{free} test set	2108 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	18.5	Xtrriage
Anisotropy	0.462	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3959	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.65% 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 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	0.63	0/3595	1.53	60/4885 (1.2%)

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	1

There are no bond length outliers.

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ARG	CD-NE-CZ	15.61	145.46	123.60
1	A	185	ARG	NE-CZ-NH2	-14.60	113.00	120.30
1	A	48	ARG	NE-CZ-NH1	12.39	126.50	120.30
1	A	31	ARG	NE-CZ-NH1	12.16	126.38	120.30
1	A	188	ARG	NE-CZ-NH1	12.03	126.31	120.30
1	A	162	ARG	NE-CZ-NH2	-11.95	114.33	120.30
1	A	278	ARG	NE-CZ-NH2	10.49	125.55	120.30
1	A	264	ARG	NE-CZ-NH2	-10.39	115.10	120.30
1	A	70	ARG	CD-NE-CZ	9.67	137.14	123.60
1	A	445	ARG	NE-CZ-NH2	-9.52	115.54	120.30
1	A	310	ARG	NE-CZ-NH2	-9.37	115.61	120.30
1	A	264	ARG	NE-CZ-NH1	9.32	124.96	120.30
1	A	417	ARG	NE-CZ-NH2	-9.19	115.71	120.30
1	A	188	ARG	CD-NE-CZ	9.03	136.24	123.60
1	A	242	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	A	445	ARG	NE-CZ-NH1	8.59	124.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	A	437	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	A	278	ARG	NH1-CZ-NH2	-8.08	110.52	119.40
1	A	355	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	A	188	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	A	70	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	A	370	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	A	242	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	A	251	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	A	278	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	A	124[A]	ARG	NE-CZ-NH2	7.13	123.86	120.30
1	A	124[B]	ARG	NE-CZ-NH2	7.13	123.86	120.30
1	A	106	ASP	CB-CG-OD1	-6.82	112.17	118.30
1	A	456	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	31	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	A	343	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	A	334	ARG	N-CA-CB	-6.21	99.42	110.60
1	A	185	ARG	NH1-CZ-NH2	6.14	126.16	119.40
1	A	370	ARG	NH1-CZ-NH2	-6.12	112.67	119.40
1	A	171	LEU	CB-CG-CD1	6.10	121.37	111.00
1	A	198	ARG	NE-CZ-NH2	6.08	123.34	120.30
1	A	48	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	A	240	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	A	19	PHE	CB-CG-CD2	5.86	124.90	120.80
1	A	319	ASP	CB-CG-OD1	5.86	123.58	118.30
1	A	106	ASP	CB-CG-OD2	5.85	123.57	118.30
1	A	370	ARG	NE-CZ-NH2	5.83	123.22	120.30
1	A	352	MET	CA-CB-CG	5.76	123.09	113.30
1	A	422	VAL	CA-CB-CG2	-5.76	102.26	110.90
1	A	409	PHE	CB-CG-CD2	5.59	124.71	120.80
1	A	206	THR	CA-CB-CG2	-5.52	104.67	112.40
1	A	256	LYS	CA-CB-CG	5.48	125.45	113.40
1	A	137	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	318	GLU	OE1-CD-OE2	-5.40	116.82	123.30
1	A	137	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	20	TYR	CB-CG-CD2	-5.36	117.79	121.00
1	A	403	PRO	CA-C-N	5.23	128.70	117.20
1	A	19	PHE	CB-CG-CD1	-5.19	117.17	120.80
1	A	211	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	A	110	LEU	CA-CB-CG	5.18	127.21	115.30
1	A	403	PRO	N-CA-C	5.08	125.31	112.10
1	A	57	GLU	CA-CB-CG	5.07	124.56	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	415	ASP	CB-CG-OD2	5.06	122.86	118.30
1	A	171	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	330	GLY	Mainchain

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	3512	0	3544	42	0
2	A	53	0	31	0	0
3	A	48	0	24	3	0
4	A	346	0	0	8	0
All	All	3959	0	3599	42	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 (42) 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:306:GLY:O	1:A:309:THR:HG23	1.85	0.77
1:A:124[A]:ARG:HD2	1:A:331:TYR:HE1	1.50	0.76
1:A:107:HIS:ND1	1:A:124[B]:ARG:NH2	2.36	0.73
1:A:160:VAL:HG11	1:A:326:LEU:HD13	1.71	0.73
1:A:160:VAL:HG11	1:A:326:LEU:CD1	2.19	0.72
1:A:215:GLN:HG2	4:A:2186:HOH:O	1.90	0.70
1:A:29:HIS:HD2	1:A:31:ARG:H	1.41	0.65
1:A:104:ALA:HA	1:A:333:SER:HA	1.80	0.64
1:A:124[B]:ARG:HD3	1:A:331:TYR:HE1	1.64	0.63
1:A:309:THR:C	1:A:310:ARG:HD2	2.19	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:GLU:OE2	3:A:802:NAP:N7N	2.33	0.61
1:A:106:ASP:O	1:A:331:TYR:HD1	1.84	0.60
1:A:124[A]:ARG:HD2	1:A:331:TYR:CE1	2.33	0.59
1:A:77:TYR:CE1	1:A:411:LYS:HE2	2.39	0.57
1:A:229:LEU:HD22	4:A:2192:HOH:O	2.05	0.56
1:A:433:GLU:HG2	1:A:457:LEU:HD13	1.89	0.55
1:A:124[B]:ARG:HD3	1:A:331:TYR:CE1	2.43	0.53
1:A:108:GLN:HE22	1:A:332:LYS:HE3	1.75	0.52
1:A:282:GLN:OE1	4:A:2243:HOH:O	2.19	0.51
1:A:10:CYS:SG	1:A:98:VAL:HG22	2.51	0.51
1:A:404:ARG:HA	4:A:2300:HOH:O	2.10	0.51
1:A:309:THR:HG21	4:A:2251:HOH:O	2.12	0.50
1:A:29:HIS:CD2	1:A:31:ARG:H	2.27	0.48
1:A:309:THR:O	1:A:310:ARG:HD2	2.13	0.48
1:A:373:THR:O	3:A:802:NAP:O3D	2.32	0.47
1:A:396:ALA:HB1	1:A:398:HIS:CE1	2.50	0.47
1:A:375:VAL:HG12	3:A:802:NAP:H2N	1.95	0.47
1:A:215:GLN:NE2	4:A:2184:HOH:O	2.48	0.47
1:A:331:TYR:HD2	4:A:2290:HOH:O	1.98	0.46
1:A:231:LEU:HD23	1:A:250:LEU:HG	1.97	0.46
1:A:259:VAL:HG23	4:A:2214:HOH:O	2.16	0.45
1:A:55:HIS:N	1:A:56:PRO:CD	2.79	0.45
1:A:29:HIS:CD2	1:A:32:ALA:H	2.36	0.43
1:A:211:ARG:HG2	1:A:215:GLN:NE2	2.34	0.42
1:A:110:LEU:O	1:A:111:ASP:HB2	2.19	0.42
1:A:117:LEU:HA	1:A:118:PRO:HD3	1.86	0.41
1:A:19:PHE:HB3	1:A:65:PHE:CD1	2.56	0.41
1:A:229:LEU:O	1:A:229:LEU:HD23	2.20	0.41
1:A:224:ASP:HA	1:A:225:PRO:HD2	1.91	0.40
1:A:240:ARG:HB2	1:A:241:PRO:HD3	2.03	0.40
1:A:194:ILE:HB	1:A:274:LEU:HD12	2.04	0.40
1:A:223:LEU:HD21	1:A:274:LEU:HD22	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	454/460 (99%)	440 (97%)	13 (3%)	1 (0%)	47 38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	404	ARG

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	375/379 (99%)	363 (97%)	12 (3%)	39 27

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ARG
1	A	106	ASP
1	A	110	LEU
1	A	171	LEU
1	A	229	LEU
1	A	233	ASP
1	A	250	LEU
1	A	256	LYS
1	A	274	LEU
1	A	352	MET
1	A	425	SER
1	A	452	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	29	HIS
1	A	108	GLN
1	A	215	GLN
1	A	282	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](#)

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
3	NAP	A	802	-	45,52,52	2.21	9 (20%)	56,80,80	2.29	18 (32%)
2	FAD	A	801	-	53,58,58	1.62	12 (22%)	68,89,89	1.45	10 (14%)

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	NAP	A	802	-	1/1/12/12	6/31/67/67	0/5/5/5
2	FAD	A	801	-	-	2/30/50/50	0/6/6/6

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	NAP	P2B-O2B	-8.08	1.44	1.59
3	A	802	NAP	C3N-C7N	5.50	1.58	1.50
3	A	802	NAP	P2B-O3X	-4.68	1.36	1.54
3	A	802	NAP	P2B-O2X	4.54	1.72	1.54
3	A	802	NAP	P2B-O1X	4.03	1.63	1.50
2	A	801	FAD	C1'-C2'	3.88	1.58	1.52
2	A	801	FAD	O4B-C1B	3.87	1.46	1.41
2	A	801	FAD	PA-O2A	-3.42	1.39	1.55
2	A	801	FAD	O5'-C5'	3.21	1.57	1.44
2	A	801	FAD	C2A-N3A	3.12	1.37	1.32
3	A	802	NAP	C8A-N7A	-3.06	1.29	1.34
2	A	801	FAD	C5'-C4'	2.83	1.55	1.51
2	A	801	FAD	P-O2P	-2.80	1.42	1.55
3	A	802	NAP	O4D-C1D	-2.64	1.37	1.41
2	A	801	FAD	C6-C7	-2.56	1.35	1.39
3	A	802	NAP	C5N-C4N	2.56	1.44	1.38
2	A	801	FAD	P-O5'	-2.25	1.50	1.59
2	A	801	FAD	O2-C2	-2.12	1.20	1.24
2	A	801	FAD	C5X-N5	-2.11	1.35	1.39
2	A	801	FAD	C4-N3	-2.05	1.35	1.38
3	A	802	NAP	O2B-C2B	-2.00	1.36	1.44

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	NAP	C5N-C4N-C3N	-7.11	111.93	120.34
3	A	802	NAP	C6N-C5N-C4N	6.07	128.26	119.44
3	A	802	NAP	O2X-P2B-O1X	-4.47	93.18	110.68
3	A	802	NAP	O2X-P2B-O2B	4.21	124.83	105.99
2	A	801	FAD	C5'-C4'-C3'	-4.14	104.21	112.20
3	A	802	NAP	O3X-P2B-O2B	4.00	123.93	105.99
3	A	802	NAP	PN-O5D-C5D	3.89	144.51	121.68
3	A	802	NAP	C5N-C6N-N1N	-3.59	115.25	120.40
3	A	802	NAP	O3X-P2B-O2X	-3.56	94.05	107.64
3	A	802	NAP	C4N-C3N-C7N	-3.40	111.95	121.04
3	A	802	NAP	O2B-C2B-C1B	-2.88	99.73	110.10
3	A	802	NAP	C2N-C3N-C7N	2.66	127.19	119.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	FAD	O4-C4-C4X	-2.58	119.75	126.60
3	A	802	NAP	C3D-C2D-C1D	-2.55	97.14	100.98
3	A	802	NAP	O7N-C7N-C3N	2.48	122.61	119.63
3	A	802	NAP	O4B-C4B-C5B	2.47	117.51	109.37
2	A	801	FAD	C9-C9A-N10	2.42	125.11	121.84
3	A	802	NAP	C3N-C2N-N1N	2.40	122.78	120.43
3	A	802	NAP	O5D-C5D-C4D	2.38	117.17	108.99
2	A	801	FAD	C5A-C6A-N1A	-2.35	115.02	120.35
2	A	801	FAD	N6A-C6A-N1A	2.31	123.36	118.57
3	A	802	NAP	C2N-C3N-C4N	2.28	120.85	118.26
2	A	801	FAD	C2A-N1A-C6A	2.27	122.63	118.75
2	A	801	FAD	O3B-C3B-C2B	2.22	119.00	111.82
2	A	801	FAD	C4A-C5A-N7A	2.20	111.69	109.40
2	A	801	FAD	C8M-C8-C9	2.17	123.49	119.49
3	A	802	NAP	C3N-C7N-N7N	-2.11	115.22	117.75
2	A	801	FAD	C10-N1-C2	2.06	121.03	116.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	802	NAP	C4B

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	NAP	C5B-O5B-PA-O3
3	A	802	NAP	O4B-C4B-C5B-O5B
3	A	802	NAP	C5D-O5D-PN-O3
3	A	802	NAP	C5B-O5B-PA-O2A
2	A	801	FAD	O3'-C3'-C4'-C5'
2	A	801	FAD	O4B-C4B-C5B-O5B
3	A	802	NAP	C4B-C5B-O5B-PA
3	A	802	NAP	C5B-O5B-PA-O1A

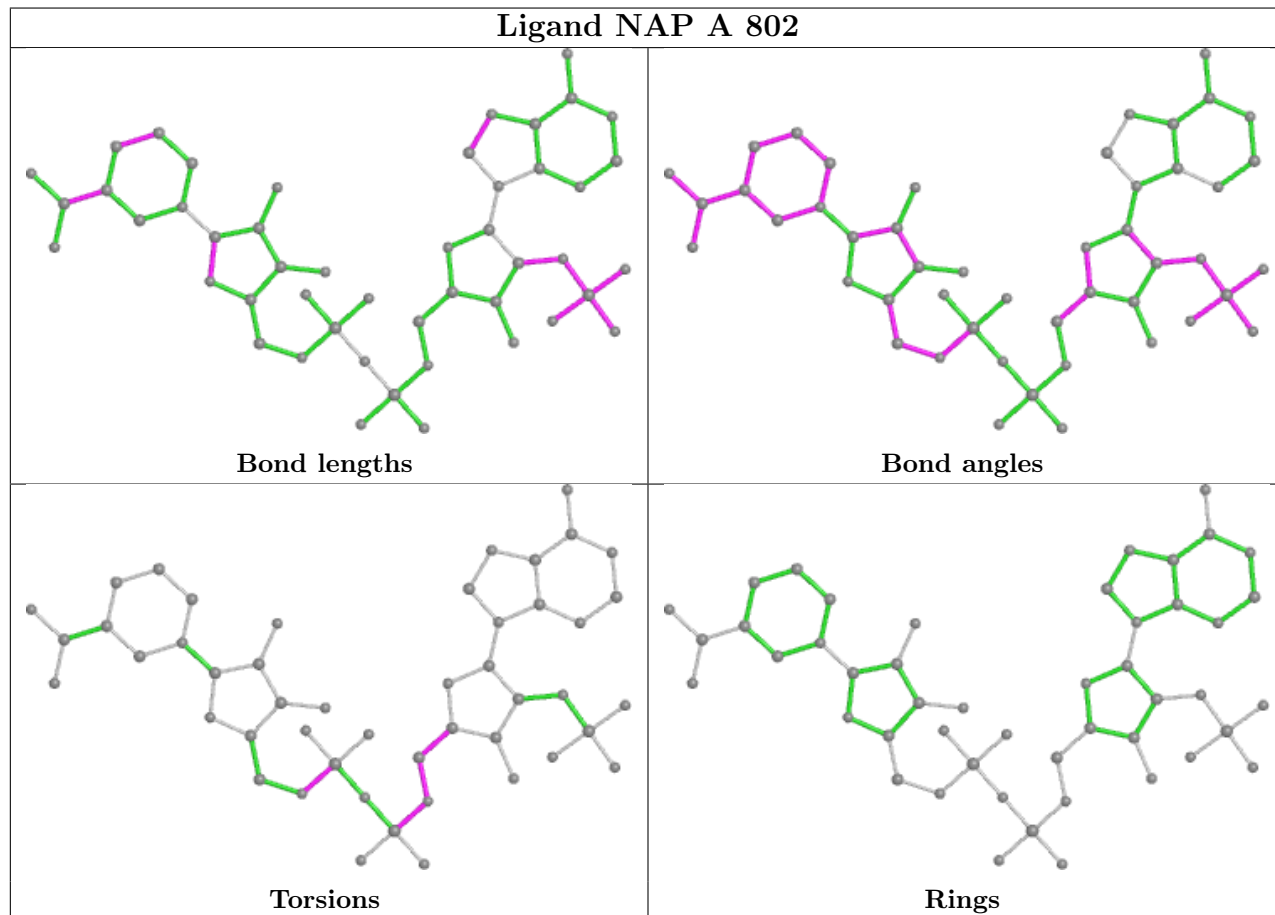
There are no ring outliers.

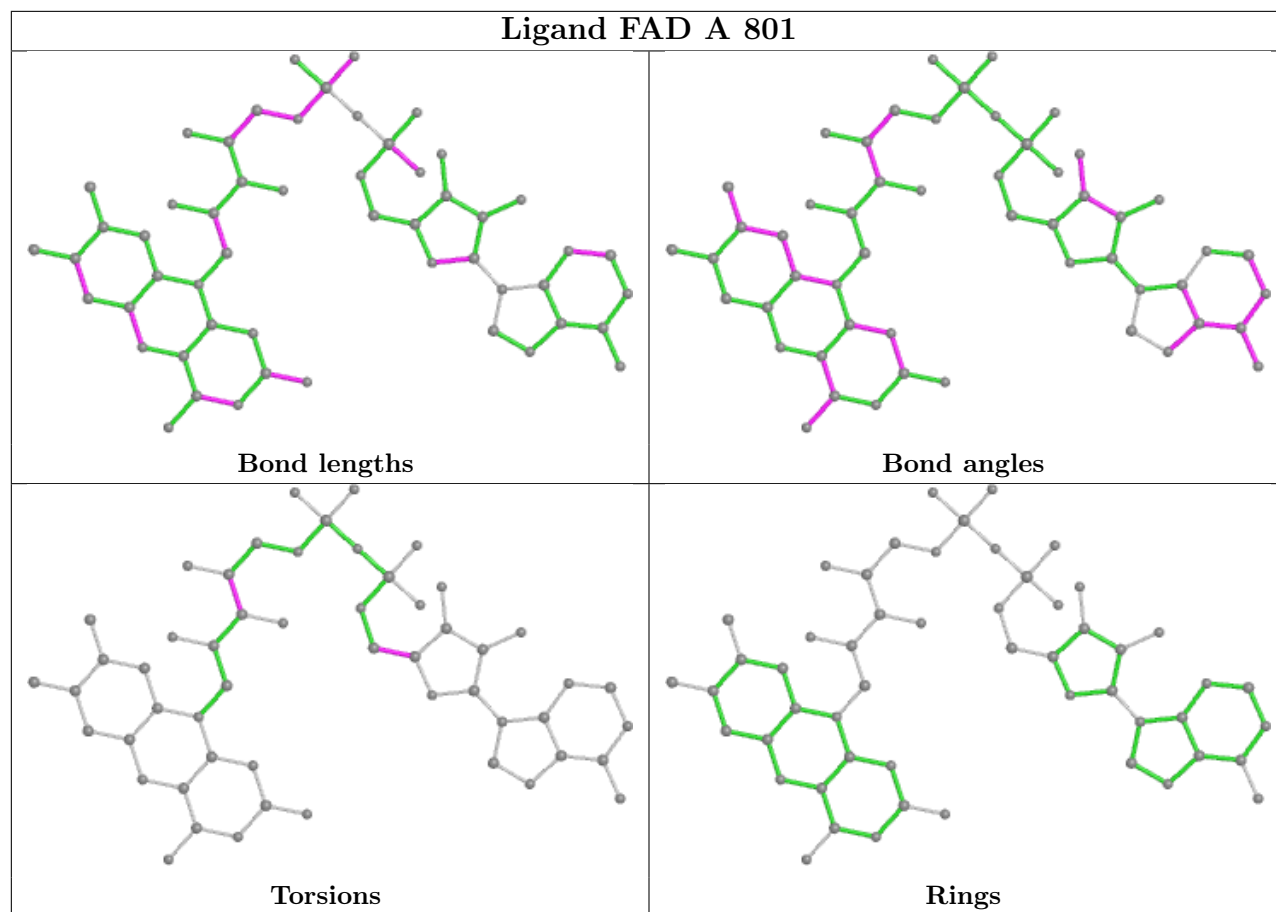
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	NAP	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	455/460 (98%)	0.01	17 (3%) 41 51	13, 23, 44, 69	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	401	SER	7.2
1	A	331	TYR	4.4
1	A	403	PRO	4.4
1	A	345	LYS	3.9
1	A	346	LEU	3.8
1	A	402	GLY	3.3
1	A	398	HIS	3.3
1	A	99	VAL	2.8
1	A	236	LYS	2.6
1	A	399	LEU	2.5
1	A	400	PRO	2.5
1	A	305	ILE	2.4
1	A	237	GLU	2.4
1	A	10	CYS	2.4
1	A	310	ARG	2.4
1	A	31	ARG	2.2
1	A	12	VAL	2.2

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

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

6.3 Carbohydrates [i](#)

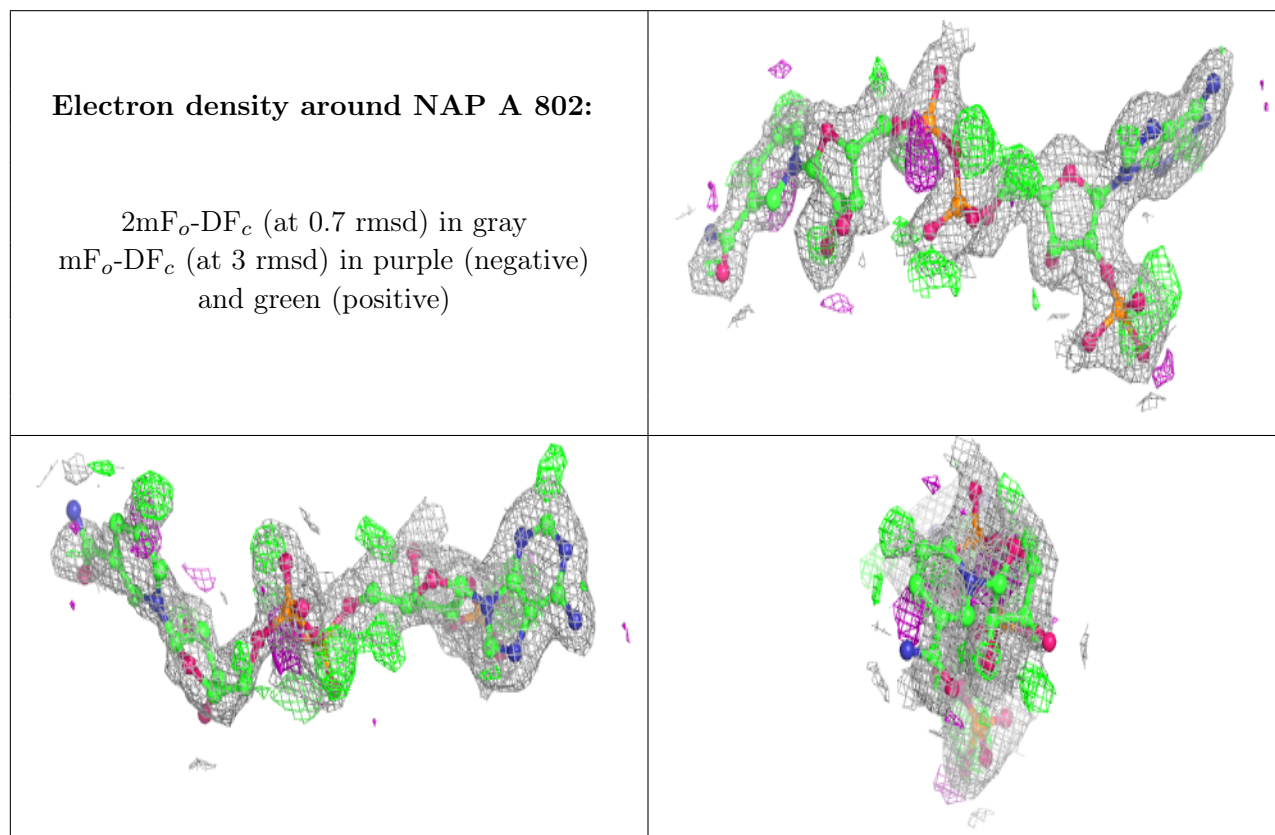
There are no monosaccharides in this entry.

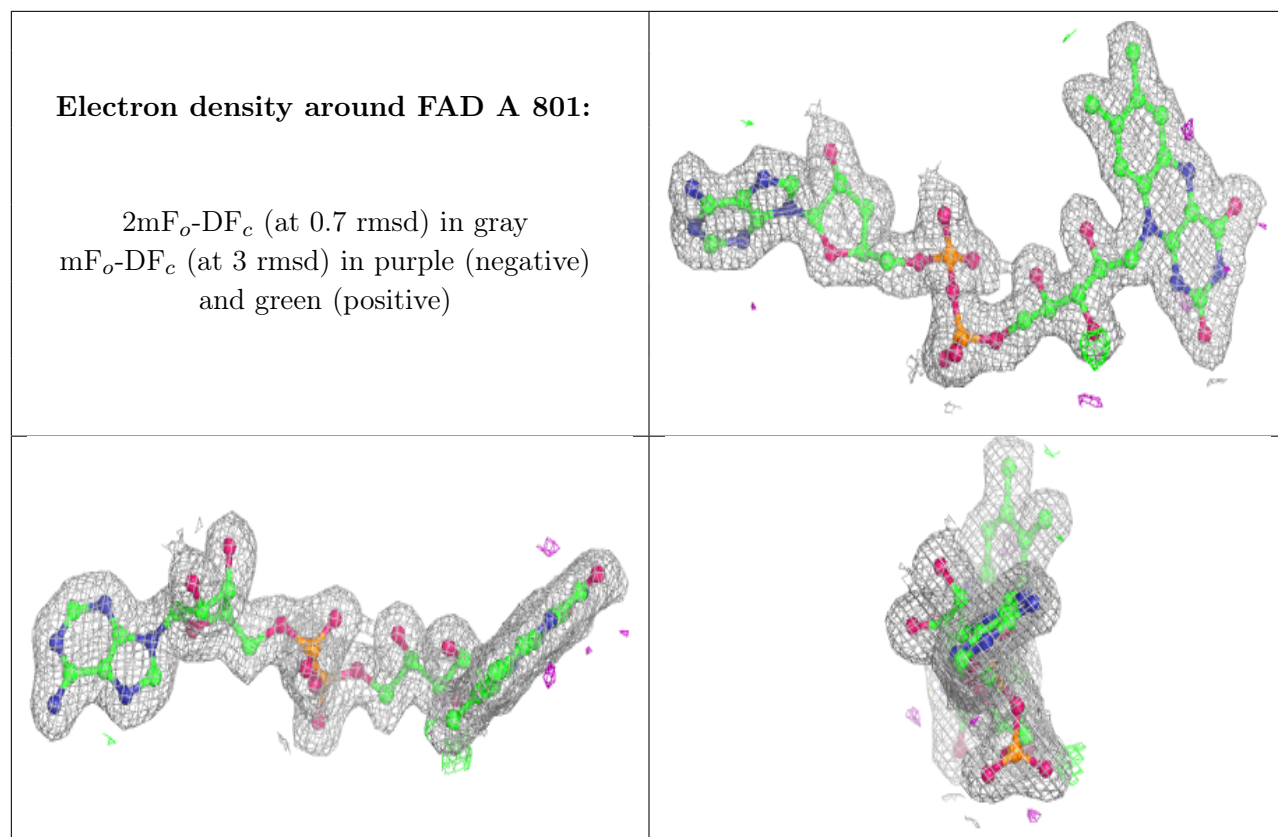
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAP	A	802	48/48	0.87	0.18	25,42,64,66	0
2	FAD	A	801	53/53	0.97	0.09	13,17,22,25	0

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 [i](#)

There are no such residues in this entry.