



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 28, 2023 – 07:56 pm GMT

PDB ID : 1E1L
Title : STRUCTURE OF ADRENODOXIN REDUCTASE IN COMPLEX WITH
NADP obtained by cocrystallisation
Authors : Ziegler, G.A.; Schulz, G.E.
Deposited on : 2000-05-09
Resolution : 2.30 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

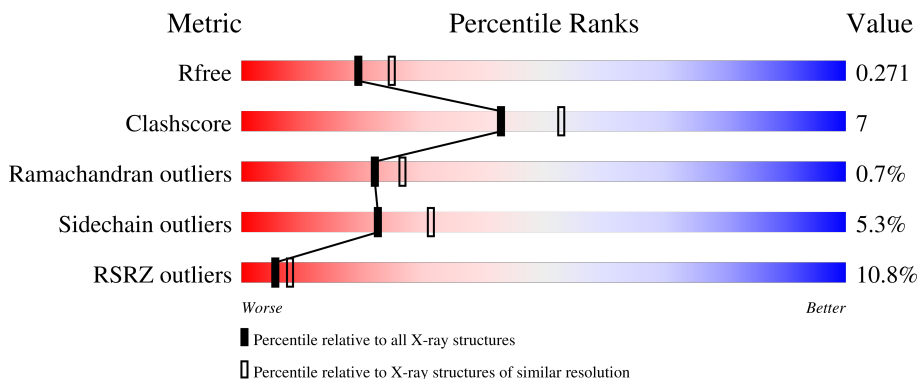
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	

2 Entry composition [i](#)

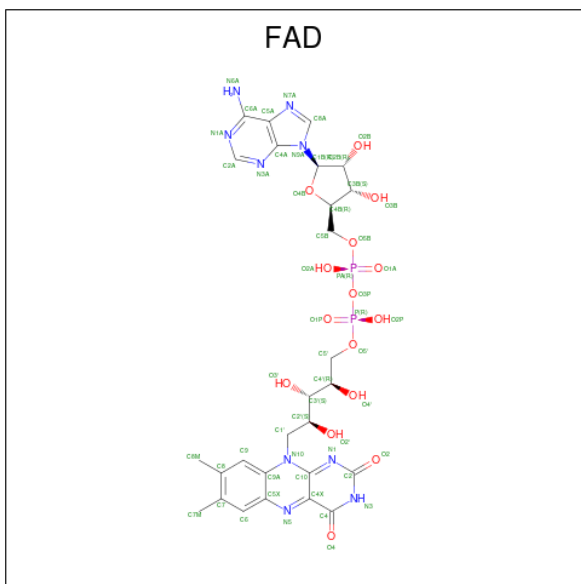
There are 4 unique types of molecules in this entry. The entry contains 3715 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	3505	2215	634	645	11	0	0	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: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	48	21	7	17	3	0	0

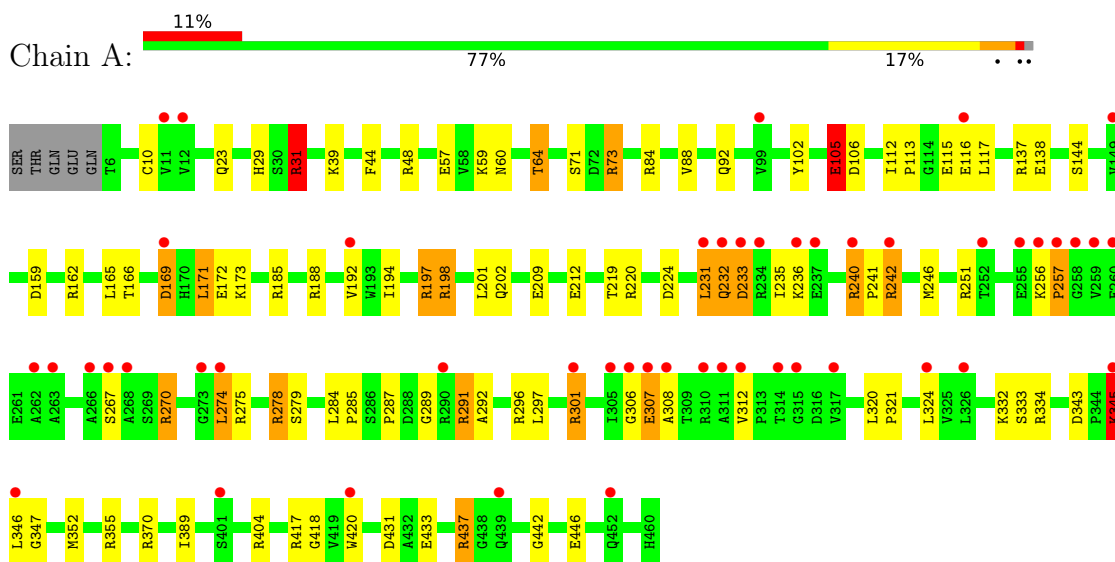
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	109	Total	O	0	0
			109	109		

3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: ADRENODOXIN REDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.50Å 62.80Å 85.30Å 90.00° 108.20° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30 28.93 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.7 (15.00-2.30) 91.8 (28.93-2.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.30 (at 2.24Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.219 , 0.279 0.220 , 0.271	Depositor DCC
R_{free} test set	1359 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtrriage
Anisotropy	0.328	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3715	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.14% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, 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	0.86	2/3584 (0.1%)	1.67	71/4871 (1.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	ARG	CD-NE	-5.36	1.37	1.46
1	A	197	ARG	CD-NE	-5.16	1.37	1.46

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	ARG	CD-NE-CZ	23.00	155.80	123.60
1	A	240	ARG	NE-CZ-NH1	13.38	126.99	120.30
1	A	185	ARG	CD-NE-CZ	12.47	141.06	123.60
1	A	275	ARG	NE-CZ-NH2	-12.34	114.13	120.30
1	A	275	ARG	NE-CZ-NH1	11.88	126.24	120.30
1	A	197	ARG	CG-CD-NE	11.84	136.66	111.80
1	A	197	ARG	CD-NE-CZ	11.51	139.71	123.60
1	A	198	ARG	CG-CD-NE	11.26	135.45	111.80
1	A	370	ARG	NE-CZ-NH1	-10.59	115.00	120.30
1	A	307	GLU	CA-C-N	10.47	140.23	117.20
1	A	240	ARG	CD-NE-CZ	10.13	137.78	123.60
1	A	137	ARG	CD-NE-CZ	9.93	137.50	123.60
1	A	185	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	A	162	ARG	NE-CZ-NH1	9.76	125.18	120.30
1	A	220	ARG	NE-CZ-NH1	9.63	125.12	120.30
1	A	48	ARG	NE-CZ-NH1	9.41	125.01	120.30
1	A	251	ARG	NE-CZ-NH2	8.95	124.78	120.30
1	A	370	ARG	CA-CB-CG	8.71	132.55	113.40
1	A	404	ARG	NE-CZ-NH1	8.54	124.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	ARG	NE-CZ-NH1	-8.50	116.05	120.30
1	A	334	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	A	31	ARG	CD-NE-CZ	8.24	135.14	123.60
1	A	162	ARG	NE-CZ-NH2	-8.21	116.20	120.30
1	A	224	ASP	CB-CG-OD1	8.20	125.68	118.30
1	A	291	ARG	NE-CZ-NH1	8.01	124.30	120.30
1	A	307	GLU	CB-CA-C	7.87	126.15	110.40
1	A	197	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	A	370	ARG	NE-CZ-NH2	7.76	124.18	120.30
1	A	137	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	A	270	ARG	CD-NE-CZ	7.70	134.38	123.60
1	A	84	ARG	NE-CZ-NH2	7.54	124.07	120.30
1	A	307	GLU	O-C-N	-7.53	110.66	122.70
1	A	102	TYR	CB-CG-CD2	7.40	125.44	121.00
1	A	301	ARG	NE-CZ-NH1	-7.25	116.67	120.30
1	A	275	ARG	CD-NE-CZ	7.01	133.42	123.60
1	A	185	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	A	31	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	159	ASP	CB-CG-OD1	6.92	124.53	118.30
1	A	106	ASP	CA-CB-CG	6.78	128.31	113.40
1	A	240	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	A	115	GLU	CA-CB-CG	6.50	127.69	113.40
1	A	251	ARG	CG-CD-NE	6.29	125.02	111.80
1	A	404	ARG	CD-NE-CZ	6.24	132.34	123.60
1	A	197	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	A	169	ASP	CB-CG-OD2	-5.93	112.97	118.30
1	A	106	ASP	CB-CG-OD1	5.86	123.57	118.30
1	A	138	GLU	CA-CB-CG	5.86	126.28	113.40
1	A	417	ARG	CD-NE-CZ	5.79	131.71	123.60
1	A	431	ASP	CB-CG-OD2	5.77	123.49	118.30
1	A	278	ARG	CD-NE-CZ	5.75	131.65	123.60
1	A	437	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	A	73	ARG	CD-NE-CZ	-5.71	115.60	123.60
1	A	212	GLU	CA-CB-CG	5.71	125.96	113.40
1	A	169	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	417	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	102	TYR	CB-CG-CD1	-5.65	117.61	121.00
1	A	57	GLU	OE1-CD-OE2	-5.53	116.67	123.30
1	A	345	LYS	CA-CB-CG	5.45	125.39	113.40
1	A	332	LYS	N-CA-CB	5.45	120.41	110.60
1	A	48	ARG	NH1-CZ-NH2	-5.40	113.46	119.40
1	A	23	GLN	CA-CB-CG	5.39	125.26	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	ARG	CA-CB-CG	5.37	125.21	113.40
1	A	446	GLU	N-CA-CB	5.37	120.26	110.60
1	A	417	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	A	159	ASP	CA-CB-CG	5.29	125.03	113.40
1	A	307	GLU	CA-C-O	-5.26	109.06	120.10
1	A	48	ARG	CD-NE-CZ	5.24	130.93	123.60
1	A	105	GLU	O-C-N	-5.22	114.35	122.70
1	A	220	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	296	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	A	44	PHE	CB-CG-CD1	5.06	124.34	120.80

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	3505	0	3535	48	1
2	A	53	0	31	1	0
3	A	48	0	25	2	0
4	A	109	0	0	8	0
All	All	3715	0	3591	49	1

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 7.

All (49) 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:117:LEU:HB3	4:A:2044:HOH:O	1.63	0.98
1:A:345:LYS:HD2	1:A:346:LEU:HG	1.60	0.83
1:A:144:SER:HA	1:A:188:ARG:HG3	1.64	0.79
1:A:165:LEU:HD21	1:A:192:VAL:HG23	1.73	0.70
1:A:301:ARG:HG3	1:A:312:VAL:HG23	1.76	0.67
1:A:343:ASP:OD1	1:A:345:LYS:HG3	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:THR:HG21	4:A:2004:HOH:O	1.95	0.66
1:A:343:ASP:OD2	1:A:345:LYS:NZ	2.29	0.63
1:A:29:HIS:HD2	1:A:31:ARG:H	1.47	0.63
1:A:301:ARG:HG3	1:A:312:VAL:CG2	2.31	0.60
1:A:307:GLU:O	1:A:308:ALA:HB3	2.03	0.58
1:A:116:GLU:HB2	4:A:2043:HOH:O	2.03	0.58
1:A:209:GLU:OE2	3:A:802:NAP:N7N	2.37	0.57
1:A:301:ARG:CD	4:A:2066:HOH:O	2.53	0.56
1:A:301:ARG:HD2	4:A:2066:HOH:O	2.03	0.56
1:A:306:GLY:C	1:A:307:GLU:O	2.43	0.56
1:A:240:ARG:HB3	1:A:241:PRO:HD3	1.87	0.56
1:A:169:ASP:O	1:A:172:GLU:HB2	2.06	0.56
1:A:232:GLN:HA	1:A:232:GLN:OE1	2.06	0.55
1:A:231:LEU:HD11	1:A:246:MET:HB3	1.88	0.55
1:A:88:VAL:HG12	1:A:92:GLN:HE21	1.72	0.55
1:A:198:ARG:HD3	3:A:802:NAP:O2X	2.07	0.54
1:A:112:ILE:HB	1:A:113:PRO:HD2	1.91	0.53
1:A:292:ALA:N	4:A:2044:HOH:O	2.43	0.52
1:A:345:LYS:CD	1:A:346:LEU:HG	2.35	0.49
1:A:59:LYS:HE3	4:A:2057:HOH:O	2.14	0.48
1:A:433:GLU:O	1:A:437:ARG:HG3	2.14	0.47
1:A:284:LEU:HA	1:A:285:PRO:HD3	1.83	0.47
1:A:355:ARG:CZ	1:A:389:ILE:HD11	2.46	0.45
1:A:112:ILE:HB	1:A:113:PRO:CD	2.46	0.45
1:A:333:SER:HB2	1:A:347:GLY:O	2.16	0.45
1:A:301:ARG:HD3	4:A:2066:HOH:O	2.17	0.45
1:A:166:THR:HG21	1:A:171:LEU:HD13	1.99	0.45
1:A:201:LEU:HD22	1:A:242:ARG:NH2	2.33	0.44
1:A:39:LYS:CE	1:A:105:GLU:OE2	2.65	0.44
1:A:320:LEU:HA	1:A:321:PRO:HD3	1.75	0.43
1:A:231:LEU:C	1:A:233:ASP:H	2.21	0.43
1:A:278:ARG:HB3	1:A:297:LEU:HB3	1.99	0.43
1:A:219:THR:HA	1:A:270:ARG:O	2.19	0.43
1:A:73:ARG:HH11	1:A:73:ARG:HD2	1.52	0.43
1:A:301:ARG:CG	1:A:312:VAL:HG23	2.46	0.42
1:A:256:LYS:HA	1:A:257:PRO:HD2	1.85	0.42
1:A:194:ILE:HB	1:A:274:LEU:HD12	2.01	0.41
1:A:232:GLN:OE1	1:A:235:ILE:HD11	2.20	0.41
1:A:173:LYS:HD2	1:A:442:GLY:O	2.21	0.41
1:A:231:LEU:O	1:A:233:ASP:N	2.54	0.40
2:A:801:FAD:H9	2:A:801:FAD:H1'1	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:LEU:C	1:A:233:ASP:N	2.74	0.40
1:A:418:GLY:O	1:A:420:TRP:CZ3	2.74	0.40

All (1) 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:289:GLY:O	1:A:301:ARG:NH2[2_656]	2.01	0.19

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	453/460 (98%)	425 (94%)	25 (6%)	3 (1%)	22 26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	232	GLN
1	A	257	PRO
1	A	287	PRO

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	374/379 (99%)	354 (95%)	20 (5%)	22 31

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	CYS
1	A	31	ARG
1	A	60	ASN
1	A	64	THR
1	A	71	SER
1	A	105	GLU
1	A	171	LEU
1	A	197	ARG
1	A	202	GLN
1	A	231	LEU
1	A	233	ASP
1	A	236	LYS
1	A	242	ARG
1	A	267	SER
1	A	274	LEU
1	A	279	SER
1	A	291	ARG
1	A	324	LEU
1	A	345	LYS
1	A	352	MET

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

Mol	Chain	Res	Type
1	A	8	GLN
1	A	24	HIS
1	A	29	HIS
1	A	40	GLN
1	A	92	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	2.10	9 (20%)	56,80,80	1.98	20 (35%)
2	FAD	A	801	-	53,58,58	1.75	11 (20%)	68,89,89	1.66	15 (22%)

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	-	-	1/31/67/67	0/5/5/5
2	FAD	A	801	-	-	4/30/50/50	0/6/6/6

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	NAP	P2B-O2B	-7.25	1.45	1.59
3	A	802	NAP	C6N-C5N	5.34	1.50	1.38
3	A	802	NAP	P2B-O2X	5.25	1.75	1.54
2	A	801	FAD	O5'-C5'	4.54	1.62	1.44
2	A	801	FAD	PA-O2A	-3.96	1.36	1.55
3	A	802	NAP	P2B-O3X	-3.95	1.39	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	FAD	C1'-C2'	3.88	1.58	1.52
2	A	801	FAD	O4B-C1B	3.72	1.46	1.41
3	A	802	NAP	C8A-N7A	-3.23	1.28	1.34
2	A	801	FAD	P-O2P	-3.00	1.41	1.55
2	A	801	FAD	C6-C7	-2.97	1.35	1.39
2	A	801	FAD	C5'-C4'	2.88	1.55	1.51
2	A	801	FAD	P-O5'	-2.60	1.48	1.59
2	A	801	FAD	C2-N3	2.55	1.45	1.39
3	A	802	NAP	P2B-O1X	2.45	1.58	1.50
3	A	802	NAP	O4D-C1D	-2.35	1.37	1.41
3	A	802	NAP	C2A-N3A	-2.33	1.28	1.32
2	A	801	FAD	PA-O1A	-2.29	1.42	1.50
2	A	801	FAD	O2B-C2B	-2.13	1.38	1.43
3	A	802	NAP	PA-O2A	-2.10	1.45	1.55

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	NAP	O3X-P2B-O2X	-4.60	90.04	107.64
2	A	801	FAD	C5A-C6A-N6A	4.34	126.94	120.35
3	A	802	NAP	O2X-P2B-O2B	4.22	124.91	105.99
3	A	802	NAP	O2X-P2B-O1X	-4.12	94.54	110.68
3	A	802	NAP	PN-O5D-C5D	3.65	143.07	121.68
3	A	802	NAP	C4N-C3N-C7N	-3.28	112.27	121.04
2	A	801	FAD	C10-N1-C2	3.15	123.20	116.90
2	A	801	FAD	O4-C4-C4X	-3.14	118.27	126.60
2	A	801	FAD	O4B-C1B-C2B	-3.13	102.36	106.93
2	A	801	FAD	C4-N3-C2	-3.12	119.87	125.64
2	A	801	FAD	C3B-C2B-C1B	-2.97	96.50	100.98
2	A	801	FAD	O4'-C4'-C3'	2.96	116.31	109.10
3	A	802	NAP	O5D-C5D-C4D	2.93	119.06	108.99
3	A	802	NAP	O3X-P2B-O2B	2.87	118.84	105.99
3	A	802	NAP	O2N-PN-O5D	2.85	120.97	107.75
2	A	801	FAD	O3'-C3'-C2'	-2.80	102.04	108.81
3	A	802	NAP	C2N-C3N-C4N	2.71	121.33	118.26
2	A	801	FAD	C4X-C10-N1	-2.70	118.46	124.73
3	A	802	NAP	C3N-C2N-N1N	2.68	123.05	120.43
3	A	802	NAP	C5N-C6N-N1N	-2.67	116.58	120.40
3	A	802	NAP	O2B-C2B-C1B	-2.63	100.64	110.10
3	A	802	NAP	C5N-C4N-C3N	-2.53	117.34	120.34
2	A	801	FAD	N3A-C2A-N1A	-2.43	124.87	128.68
2	A	801	FAD	O2-C2-N3	-2.43	113.92	118.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	NAP	O5B-C5B-C4B	2.43	117.36	108.99
2	A	801	FAD	C5A-C6A-N1A	-2.42	114.86	120.35
3	A	802	NAP	C2N-C3N-C7N	2.38	126.39	119.46
3	A	802	NAP	C3D-C2D-C1D	-2.32	97.49	100.98
3	A	802	NAP	O5B-PA-O1A	2.31	118.08	109.07
3	A	802	NAP	O4B-C4B-C5B	2.18	116.53	109.37
2	A	801	FAD	C2A-N1A-C6A	2.17	122.47	118.75
3	A	802	NAP	O5D-PN-O1N	2.12	117.37	109.07
3	A	802	NAP	O2N-PN-O1N	-2.09	101.90	112.24
2	A	801	FAD	O2-C2-N1	2.07	125.26	121.83
2	A	801	FAD	C4X-C4-N3	2.00	118.27	113.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

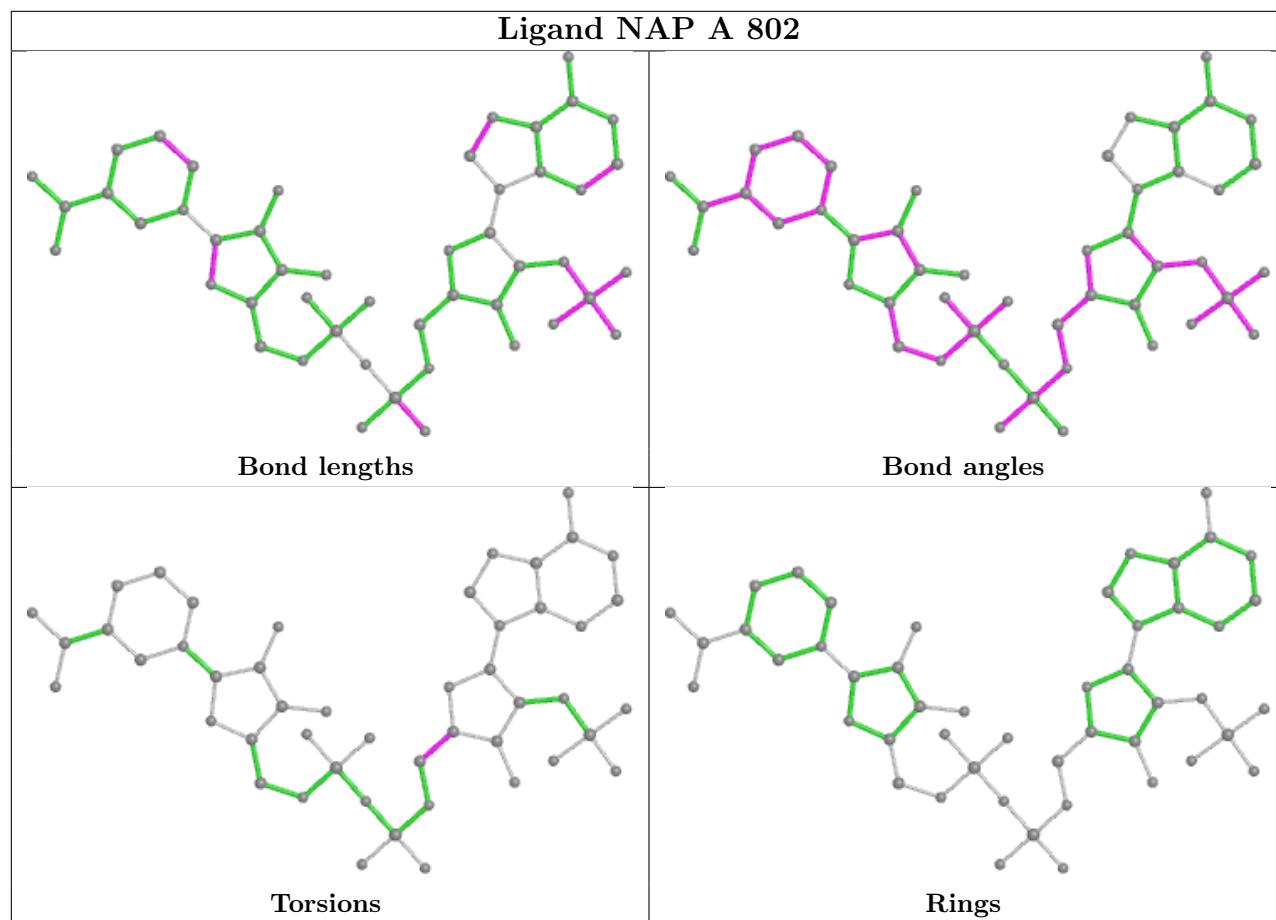
Mol	Chain	Res	Type	Atoms
2	A	801	FAD	O3'-C3'-C4'-C5'
2	A	801	FAD	O3'-C3'-C4'-O4'
2	A	801	FAD	PA-O3P-P-O5'
3	A	802	NAP	O4B-C4B-C5B-O5B
2	A	801	FAD	O4B-C4B-C5B-O5B

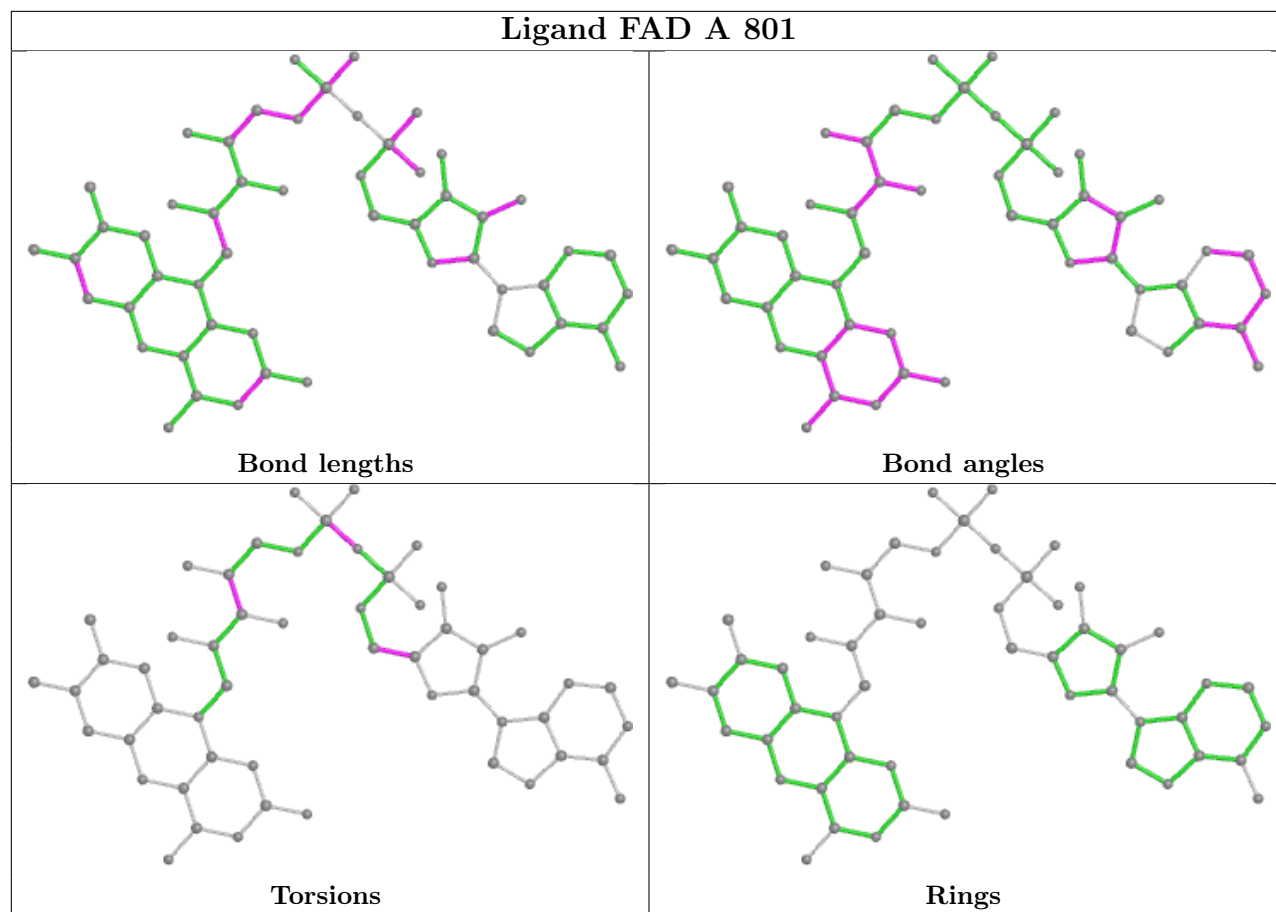
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	NAP	2	0
2	A	801	FAD	1	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

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%)	0.47	49 (10%) 5 8	29, 57, 90, 90	1 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	259	VAL	7.0
1	A	237	GLU	4.9
1	A	233	ASP	4.3
1	A	310	ARG	4.3
1	A	232	GLN	4.2
1	A	258	GLY	4.2
1	A	260	GLU	4.0
1	A	263	ALA	4.0
1	A	256	LYS	3.9
1	A	420	TRP	3.8
1	A	257	PRO	3.8
1	A	346	LEU	3.6
1	A	401	SER	3.6
1	A	307	GLU	3.5
1	A	312	VAL	3.4
1	A	236	LYS	3.4
1	A	255	GLU	3.3
1	A	169	ASP	3.1
1	A	266	ALA	2.9
1	A	305	ILE	2.8
1	A	99	VAL	2.7
1	A	317	VAL	2.7
1	A	240	ARG	2.7
1	A	267	SER	2.7
1	A	262	ALA	2.7
1	A	308	ALA	2.6
1	A	452	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	439	GLN	2.5
1	A	315	GLY	2.4
1	A	116	GLU	2.4
1	A	306	GLY	2.4
1	A	11	VAL	2.4
1	A	314	THR	2.4
1	A	326	LEU	2.4
1	A	311	ALA	2.3
1	A	149	VAL	2.3
1	A	234	ARG	2.3
1	A	345	LYS	2.2
1	A	242	ARG	2.2
1	A	274	LEU	2.2
1	A	290	ARG	2.2
1	A	12	VAL	2.2
1	A	273	GLY	2.2
1	A	252	THR	2.1
1	A	268	ALA	2.1
1	A	231	LEU	2.1
1	A	324	LEU	2.1
1	A	192	VAL	2.0
1	A	301	ARG	2.0

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.

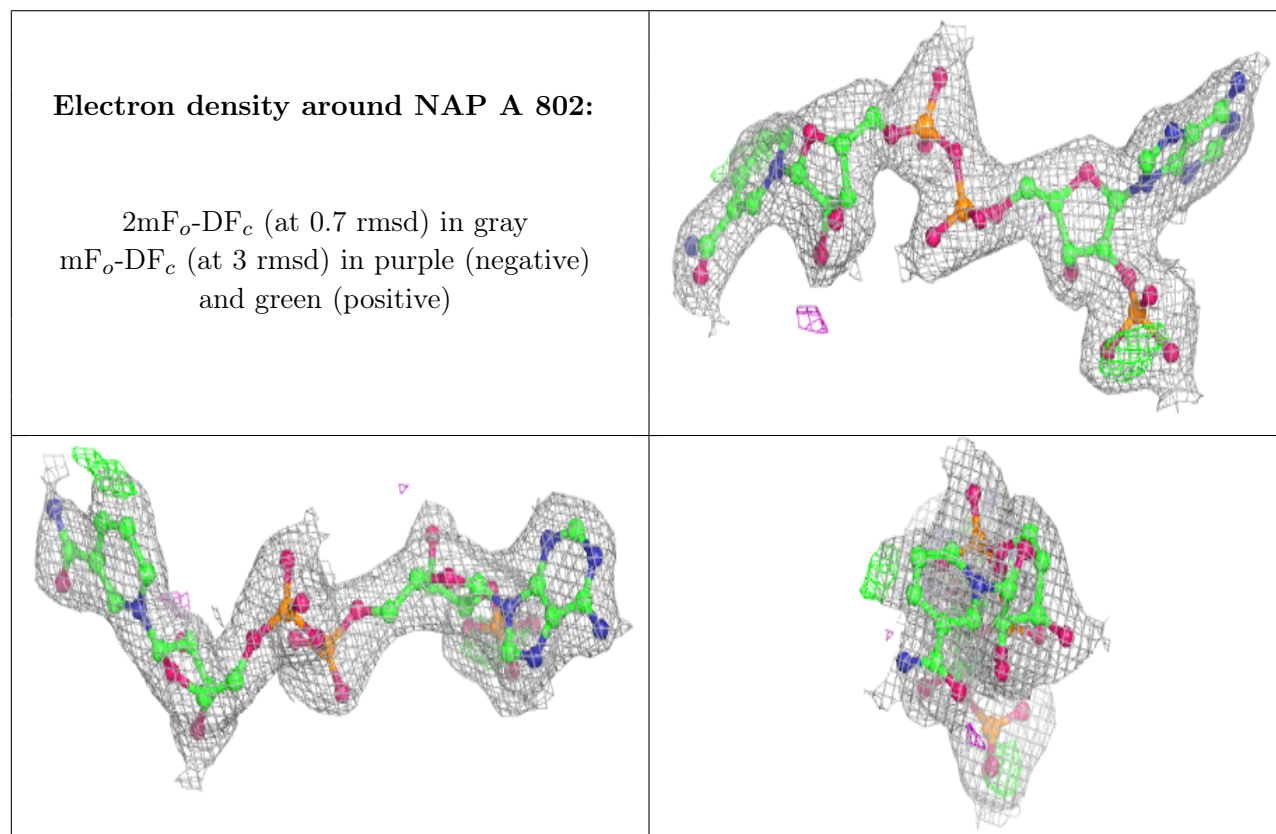
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAP	A	802	48/48	0.93	0.15	52,66,74,77	0

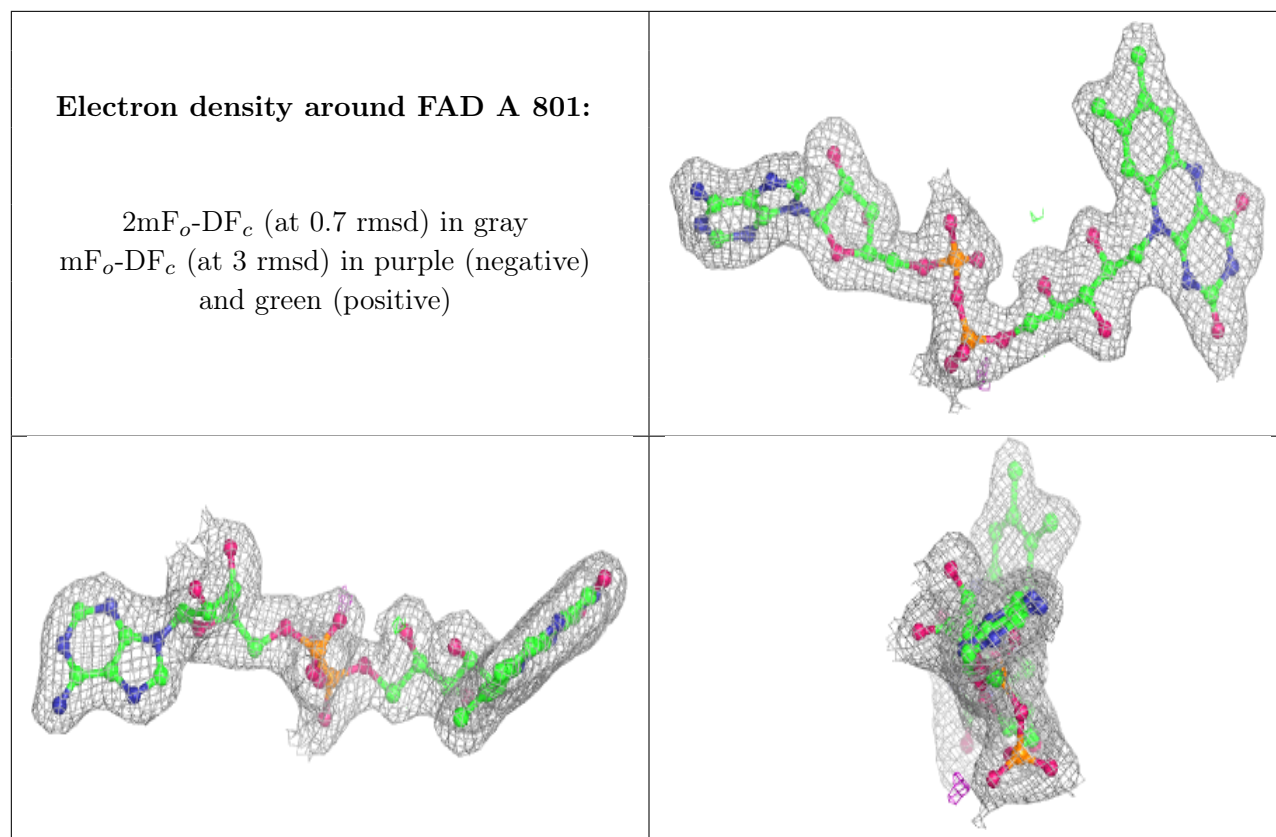
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FAD	A	801	53/53	0.96	0.15	28,35,43,46	0

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.