



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:57 PM UTC

PDB ID : 1E1L / pdb_00001e1l
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

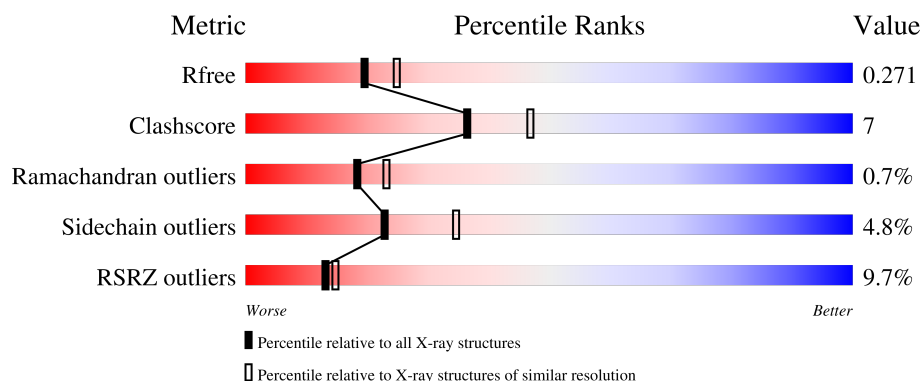
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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	10% 68% 26% • •

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
1	A	455	Total	C	N	O	S	0	0	0
			3505	2215	634	645	11			

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



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

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



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

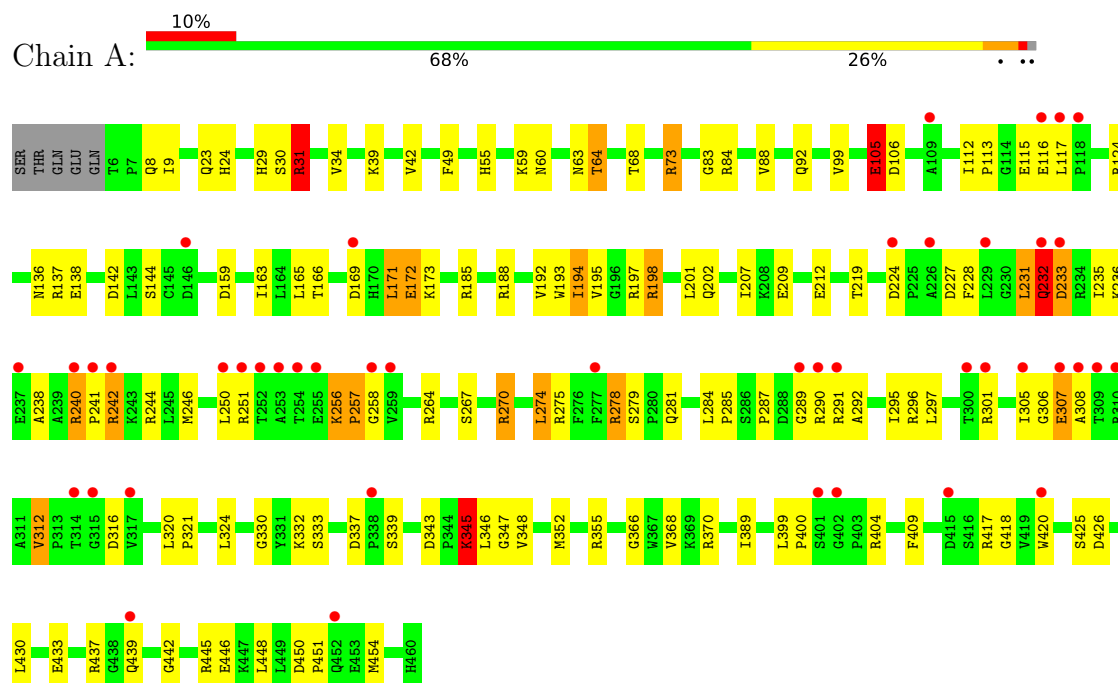
- Molecule 4 is water.

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

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 15.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.7 (15.00-2.30) 94.7 (15.00-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.30 (at 2.24Å)	Xtriage
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	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3715	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage'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: 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	1.08	6/3584 (0.2%)	1.99	110/4871 (2.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	HIS	CD2-NE2	-6.71	1.30	1.37
1	A	198	ARG	CD-NE	-6.37	1.37	1.46
1	A	197	ARG	CD-NE	-6.13	1.37	1.46
1	A	439	GLN	CD-OE1	5.88	1.34	1.23
1	A	307	GLU	C-O	5.45	1.30	1.24
1	A	232	GLN	CD-OE1	5.31	1.33	1.23

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	ARG	CD-NE-CZ	22.43	155.80	124.40
1	A	106	ASP	CA-CB-CG	15.71	128.31	112.60
1	A	159	ASP	CA-CB-CG	12.43	125.03	112.60
1	A	185	ARG	CD-NE-CZ	11.90	141.06	124.40
1	A	197	ARG	CG-CD-NE	11.21	136.66	112.00
1	A	197	ARG	CD-NE-CZ	10.94	139.71	124.40
1	A	198	ARG	CG-CD-NE	10.66	135.45	112.00
1	A	240	ARG	CD-NE-CZ	9.55	137.78	124.40
1	A	137	ARG	CD-NE-CZ	9.36	137.50	124.40
1	A	370	ARG	CA-CB-CG	9.23	132.55	114.10
1	A	426	ASP	CA-CB-CG	9.16	121.76	112.60
1	A	42	VAL	N-CA-CB	-9.14	105.52	111.83
1	A	307	GLU	O-C-N	-8.97	110.66	122.59
1	A	330	GLY	N-CA-C	8.76	120.28	111.95
1	A	224	ASP	CA-CB-CG	8.59	121.19	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	PHE	CA-CB-CG	8.55	122.35	113.80
1	A	207	ILE	N-CA-C	8.52	118.60	110.42
1	A	307	GLU	CA-C-O	-8.01	109.06	120.51
1	A	337	ASP	CA-CB-CG	7.99	120.59	112.60
1	A	307	GLU	CB-CA-C	7.90	126.15	110.42
1	A	195	VAL	N-CA-C	7.79	120.15	108.23
1	A	31	ARG	CD-NE-CZ	7.67	135.14	124.40
1	A	55	HIS	CA-CB-CG	7.51	121.31	113.80
1	A	194	ILE	CA-C-N	7.40	131.62	122.37
1	A	194	ILE	C-N-CA	7.40	131.62	122.37
1	A	227	ASP	CA-CB-CG	7.37	119.97	112.60
1	A	8	GLN	OE1-CD-NE2	-7.26	115.34	122.60
1	A	316	ASP	CA-CB-CG	7.23	119.83	112.60
1	A	270	ARG	CD-NE-CZ	7.13	134.38	124.40
1	A	115	GLU	CA-CB-CG	6.80	127.69	114.10
1	A	448	LEU	CA-C-O	-6.75	113.00	120.69
1	A	30	SER	N-CA-C	6.59	120.78	112.87
1	A	370	ARG	NE-CZ-NH1	-6.50	115.00	121.50
1	A	425	SER	N-CA-C	-6.45	104.25	111.28
1	A	275	ARG	CD-NE-CZ	6.44	133.42	124.40
1	A	305	ILE	CA-C-N	6.43	131.12	120.25
1	A	305	ILE	C-N-CA	6.43	131.12	120.25
1	A	227	ASP	N-CA-C	-6.35	105.02	112.89
1	A	24	HIS	CB-CG-CD2	-6.32	122.99	131.20
1	A	73	ARG	CD-NE-CZ	-6.28	115.60	124.40
1	A	233	ASP	CA-CB-CG	6.24	118.84	112.60
1	A	251	ARG	NE-CZ-NH2	6.20	124.78	119.20
1	A	207	ILE	CA-C-O	-6.19	114.61	121.17
1	A	193	TRP	CA-C-N	6.17	131.74	123.10
1	A	193	TRP	C-N-CA	6.17	131.74	123.10
1	A	430	LEU	O-C-N	6.14	128.63	122.12
1	A	138	GLU	CA-CB-CG	6.09	126.28	114.10
1	A	446	GLU	N-CA-CB	6.08	120.26	110.65
1	A	366	GLY	N-CA-C	6.04	122.72	112.22
1	A	238	ALA	N-CA-C	6.03	118.55	110.35
1	A	63	ASN	CA-CB-CG	5.97	118.57	112.60
1	A	450	ASP	CA-CB-CG	5.96	118.56	112.60
1	A	290	ARG	N-CA-C	5.95	119.64	112.38
1	A	212	GLU	CA-CB-CG	5.93	125.96	114.10
1	A	251	ARG	CG-CD-NE	5.92	125.02	112.00
1	A	24	HIS	CB-CG-ND1	5.88	131.52	122.70
1	A	339	SER	N-CA-C	-5.77	105.73	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	409	PHE	CA-CB-CG	5.77	119.57	113.80
1	A	307	GLU	CB-CG-CD	5.75	122.38	112.60
1	A	264	ARG	N-CA-C	-5.69	104.99	111.14
1	A	404	ARG	CD-NE-CZ	5.67	132.34	124.40
1	A	345	LYS	CA-CB-CG	5.64	125.39	114.10
1	A	275	ARG	NE-CZ-NH2	-5.63	114.13	119.20
1	A	142	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	256	LYS	CA-C-N	5.61	126.86	119.84
1	A	256	LYS	C-N-CA	5.61	126.86	119.84
1	A	23	GLN	CA-CB-CG	5.58	125.26	114.10
1	A	296	ARG	CA-CB-CG	5.56	125.21	114.10
1	A	233	ASP	N-CA-C	-5.55	106.56	113.55
1	A	370	ARG	NE-CZ-NH2	5.54	124.18	119.20
1	A	34	VAL	CA-C-O	-5.51	114.70	120.27
1	A	281	GLN	OE1-CD-NE2	-5.50	117.10	122.60
1	A	240	ARG	NE-CZ-NH1	5.49	126.99	121.50
1	A	68	THR	CA-C-N	5.48	128.63	120.31
1	A	68	THR	C-N-CA	5.48	128.63	120.31
1	A	251	ARG	NE-CZ-NH1	-5.45	116.05	121.50
1	A	9	ILE	CA-C-N	-5.42	113.43	122.21
1	A	9	ILE	C-N-CA	-5.42	113.43	122.21
1	A	244	ARG	CB-CA-C	5.42	119.39	110.88
1	A	84	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	A	307	GLU	N-CA-C	-5.38	99.34	110.80
1	A	368	VAL	O-C-N	-5.38	115.01	122.05
1	A	84	ARG	N-CA-CB	5.35	119.53	110.49
1	A	83	GLY	N-CA-C	-5.33	107.99	114.92
1	A	163	ILE	CB-CG1-CD1	5.33	124.99	113.80
1	A	332	LYS	N-CA-CB	5.32	120.41	110.99
1	A	8	GLN	CB-CG-CD	5.29	121.60	112.60
1	A	195	VAL	CB-CA-C	-5.27	104.58	110.96
1	A	425	SER	CB-CA-C	-5.23	102.10	110.79
1	A	417	ARG	CD-NE-CZ	5.22	131.71	124.40
1	A	258	GLY	N-CA-C	-5.20	103.62	110.74
1	A	278	ARG	CD-NE-CZ	5.18	131.65	124.40
1	A	228	PHE	N-CA-C	5.15	118.69	112.93
1	A	244	ARG	CA-CB-CG	5.13	124.36	114.10
1	A	8	GLN	CG-CD-NE2	5.13	124.09	116.40
1	A	172	GLU	N-CA-C	5.11	119.74	111.37
1	A	448	LEU	O-C-N	5.11	129.01	123.04
1	A	99	VAL	N-CA-C	5.10	114.92	107.37
1	A	198	ARG	CA-C-O	-5.10	115.02	119.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	ARG	CA-CB-CG	5.09	124.28	114.10
1	A	224	ASP	CA-C-N	5.08	124.69	119.05
1	A	224	ASP	C-N-CA	5.08	124.69	119.05
1	A	136	ASN	CA-CB-CG	5.05	117.65	112.60
1	A	250	LEU	CB-CA-C	5.05	118.88	110.90
1	A	105	GLU	N-CA-C	5.04	119.14	113.15
1	A	445	ARG	CA-C-O	-5.04	115.56	121.10
1	A	124	ARG	CD-NE-CZ	-5.03	117.36	124.40
1	A	105	GLU	O-C-N	-5.01	114.35	122.42
1	A	312	VAL	CA-C-N	5.01	125.40	119.99
1	A	312	VAL	C-N-CA	5.01	125.40	119.99

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	51	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	52	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 (52) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ASP:OD1	1:A:345:LYS:HG3	1.93	0.67
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	0.65
1:A:451:PRO:HA	1:A:454:MET:HE3	1.79	0.63
1:A:29:HIS:HD2	1:A:31:ARG:H	1.47	0.63
1:A:306:GLY:C	1:A:307:GLU:O	2.43	0.61
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: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:231:LEU:C	1:A:233:ASP:H	2.21	0.48
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:231:LEU:C	1:A:233:ASP:N	2.74	0.44
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ASP:C	1:A:235:ILE:H	2.29	0.41
1:A:399:LEU:O	1:A:400:PRO:C	2.64	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
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%)	18 23

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%)	356 (95%)	18 (5%)	23	35

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ARG
1	A	60	ASN
1	A	64	THR
1	A	105	GLU
1	A	171	LEU
1	A	202	GLN
1	A	231	LEU
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	295	ILE
1	A	324	LEU
1	A	345	LYS
1	A	348	VAL
1	A	352	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	28	HIS
1	A	29	HIS
1	A	33	HIS
1	A	40	GLN
1	A	92	GLN
1	A	136	ASN
1	A	186	GLN
1	A	215	GLN
1	A	282	GLN

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 oligosaccharides 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	801	-	58,58,58	2.14	13 (22%)	85,89,89	1.48	13 (15%)
3	NAP	A	802	-	50,52,52	2.23	10 (20%)	71,80,80	2.06	21 (29%)

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	801	-	-	5/34/50/50	0/6/6/6
3	NAP	A	802	-	-	0/35/67/67	0/5/5/5

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	FAD	P-O3P	-9.72	1.49	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	NAP	P2B-O2B	-7.94	1.45	1.59
3	A	802	NAP	C6N-C5N	5.70	1.50	1.38
3	A	802	NAP	P2B-O2X	5.46	1.75	1.54
3	A	802	NAP	PA-O3	4.79	1.64	1.59
2	A	801	FAD	O5'-C5'	4.66	1.62	1.44
3	A	802	NAP	P2B-O3X	-4.09	1.39	1.54
2	A	801	FAD	PA-O2A	-4.01	1.36	1.55
2	A	801	FAD	C1'-C2'	3.93	1.58	1.52
2	A	801	FAD	C6-C7	-3.22	1.35	1.39
3	A	802	NAP	C2A-N3A	-3.17	1.28	1.33
2	A	801	FAD	P-O2P	-3.04	1.41	1.55
2	A	801	FAD	C5'-C4'	2.98	1.55	1.51
2	A	801	FAD	C2-N3	2.72	1.45	1.39
2	A	801	FAD	P-O5'	-2.71	1.48	1.59
3	A	802	NAP	P2B-O1X	2.57	1.58	1.50
2	A	801	FAD	C5A-C6A	2.37	1.47	1.41
3	A	802	NAP	O4D-C1D	-2.35	1.37	1.40
2	A	801	FAD	PA-O1A	-2.31	1.42	1.50
3	A	802	NAP	PA-O2A	-2.13	1.45	1.55
2	A	801	FAD	C2A-N1A	2.07	1.37	1.33
3	A	802	NAP	C3B-C2B	-2.05	1.48	1.53
2	A	801	FAD	O2B-C2B	-2.02	1.38	1.43

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	NAP	O4B-C1B-N9A	6.59	120.75	108.09
3	A	802	NAP	P2B-O2B-C2B	-5.47	108.82	123.43
3	A	802	NAP	O2X-P2B-O2B	4.89	124.91	105.85
3	A	802	NAP	O3X-P2B-O2X	-4.74	90.04	107.80
3	A	802	NAP	O2X-P2B-O1X	-4.18	94.54	110.83
3	A	802	NAP	PN-O5D-C5D	3.79	143.07	121.35
3	A	802	NAP	O3X-P2B-O2B	3.33	118.84	105.85
2	A	801	FAD	C4-N3-C2	-3.25	119.87	125.64
3	A	802	NAP	C4N-C3N-C7N	-3.23	112.27	121.06
2	A	801	FAD	O4-C4-C4X	-3.13	118.27	126.53
3	A	802	NAP	C5N-C4N-C3N	-3.07	117.34	120.36
2	A	801	FAD	O3'-C3'-C2'	-3.03	102.04	108.93
2	A	801	FAD	O4'-C4'-C3'	3.02	116.31	109.25
3	A	802	NAP	O2N-PN-O5D	2.96	120.97	107.57
3	A	802	NAP	O5D-C5D-C4D	2.96	119.06	108.99
2	A	801	FAD	C10-N1-C2	2.93	123.20	116.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	NAP	C5N-C6N-N1N	-2.79	116.58	120.38
3	A	802	NAP	O2B-C2B-C1B	-2.68	100.64	110.05
3	A	802	NAP	C2N-C3N-C4N	2.64	121.33	118.26
2	A	801	FAD	C3B-C2B-C1B	-2.62	96.50	101.46
2	A	801	FAD	O2A-PA-O3P	2.51	114.05	107.27
2	A	801	FAD	C4X-C10-N1	-2.50	118.46	124.59
3	A	802	NAP	O5B-C5B-C4B	2.46	117.36	108.99
2	A	801	FAD	N3A-C2A-N1A	-2.45	124.87	128.58
2	A	801	FAD	O2-C2-N3	-2.43	113.92	118.58
3	A	802	NAP	C2N-C3N-C7N	2.40	126.39	119.46
3	A	802	NAP	O5B-PA-O1A	2.31	118.08	108.94
2	A	801	FAD	O2P-P-O3P	-2.29	101.09	107.27
2	A	801	FAD	C2A-N1A-C6A	2.27	122.47	118.73
3	A	802	NAP	O2N-PN-O1N	-2.27	101.90	112.44
3	A	802	NAP	O4B-C4B-C5B	2.25	116.53	109.33
3	A	802	NAP	O5D-PN-O1N	2.13	117.37	108.94
2	A	801	FAD	O2-C2-N1	2.09	125.26	121.80
3	A	802	NAP	O2A-PA-O3	2.02	112.74	107.27

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'
2	A	801	FAD	C2B-C1B-N9A-C8A
2	A	801	FAD	C2'-C3'-C4'-O4'

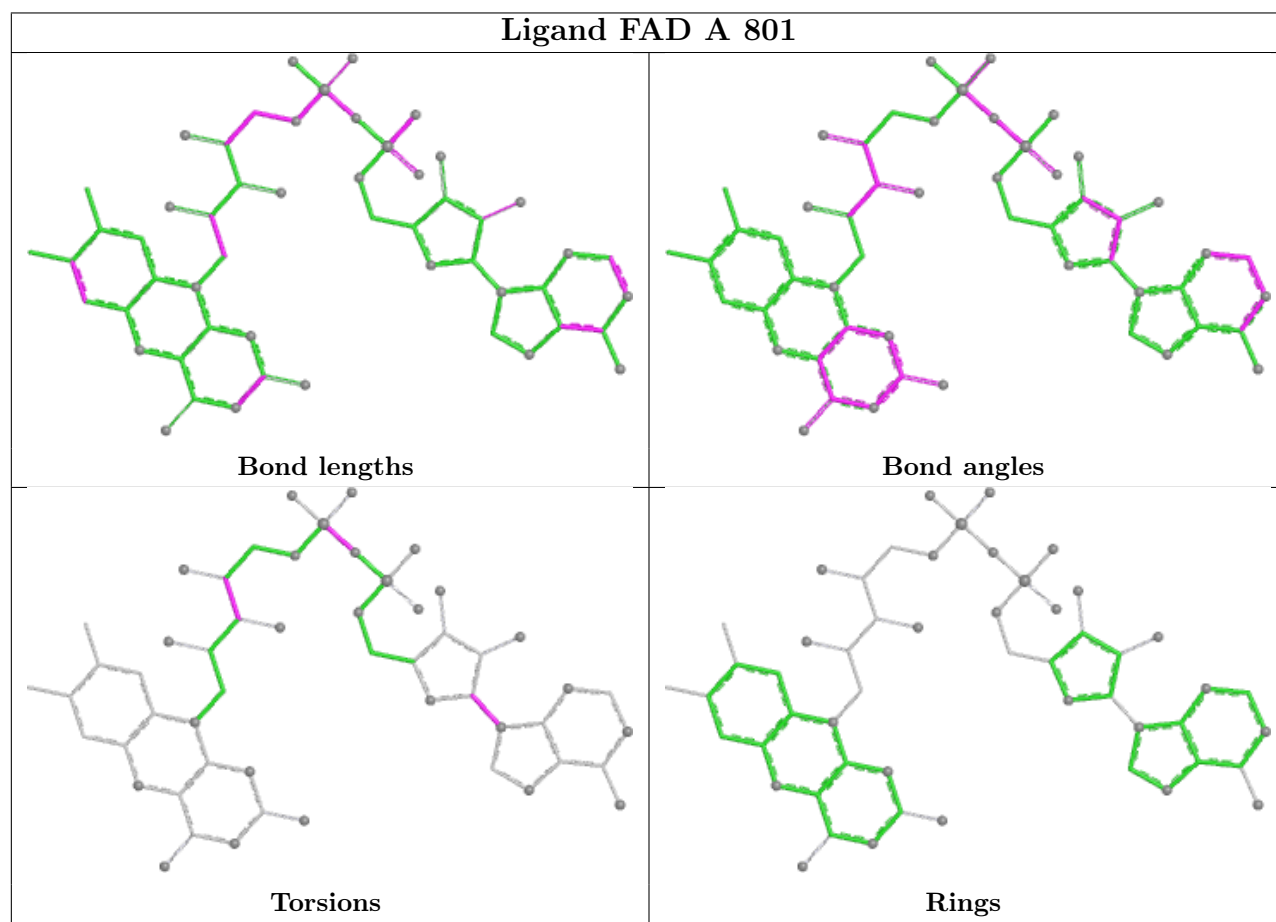
There are no ring outliers.

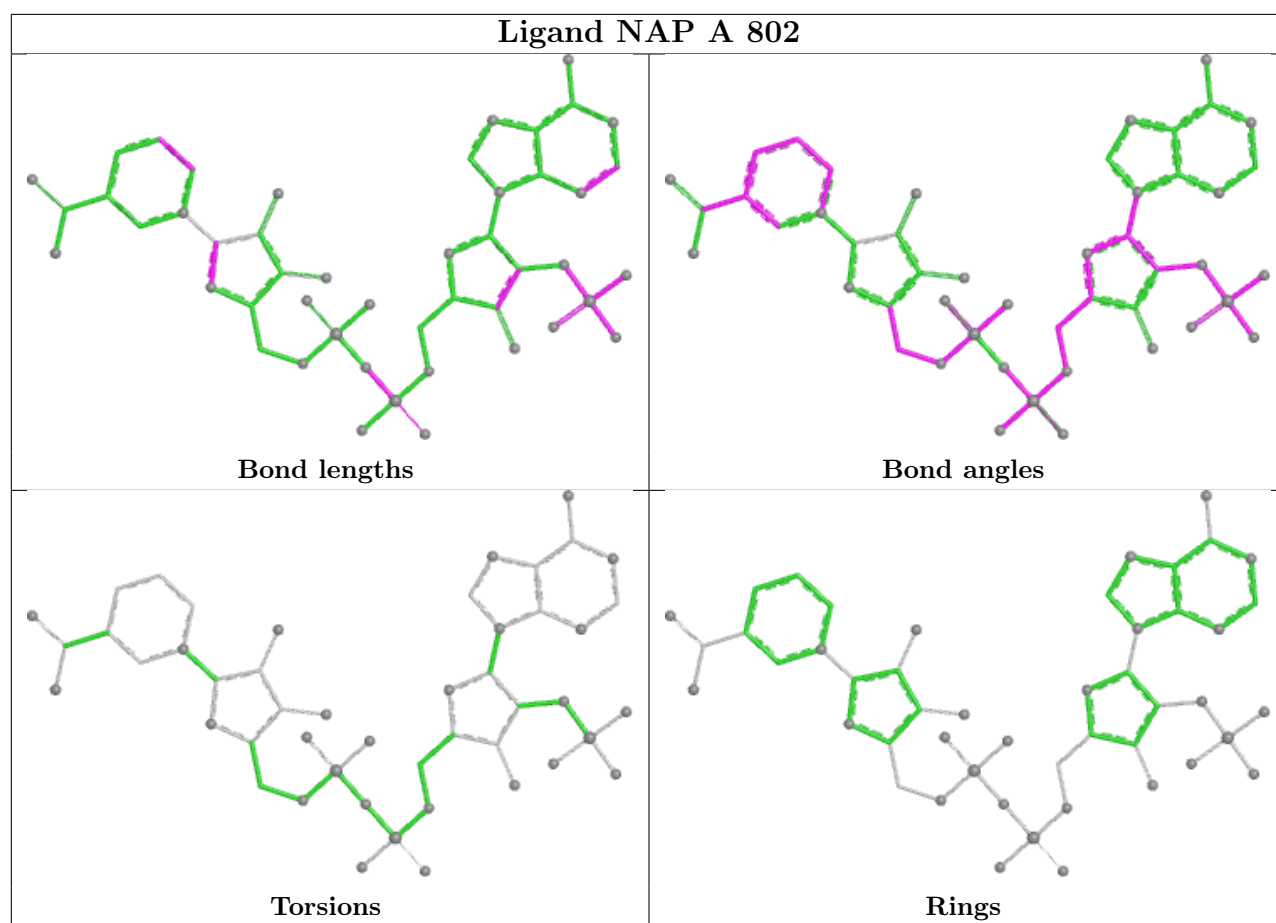
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	FAD	1	0
3	A	802	NAP	2	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%)	0.44	44 (9%) 13 15	29, 57, 90, 90	1 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	169	ASP	4.6
1	A	301	ARG	4.1
1	A	317	VAL	4.1
1	A	420	TRP	3.9
1	A	237	GLU	3.4
1	A	232	GLN	3.2
1	A	255	GLU	3.1
1	A	309	THR	3.1
1	A	402	GLY	3.0
1	A	242	ARG	3.0
1	A	315	GLY	2.9
1	A	277	PHE	2.9
1	A	439	GLN	2.8
1	A	259	VAL	2.8
1	A	229	LEU	2.8
1	A	240	ARG	2.8
1	A	310	ARG	2.7
1	A	226	ALA	2.7
1	A	116	GLU	2.7
1	A	291	ARG	2.7
1	A	452	GLN	2.6
1	A	308	ALA	2.5
1	A	109	ALA	2.5
1	A	314	THR	2.5
1	A	290	ARG	2.5
1	A	250	LEU	2.5
1	A	289	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	252	THR	2.4
1	A	305	ILE	2.4
1	A	307	GLU	2.4
1	A	401	SER	2.4
1	A	415	ASP	2.3
1	A	117	LEU	2.2
1	A	233	ASP	2.2
1	A	254	THR	2.2
1	A	253	ALA	2.2
1	A	224	ASP	2.2
1	A	258	GLY	2.1
1	A	146	ASP	2.1
1	A	300	THR	2.1
1	A	251	ARG	2.1
1	A	118	PRO	2.0
1	A	241	PRO	2.0
1	A	338	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

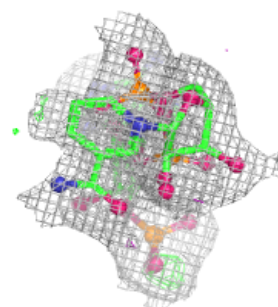
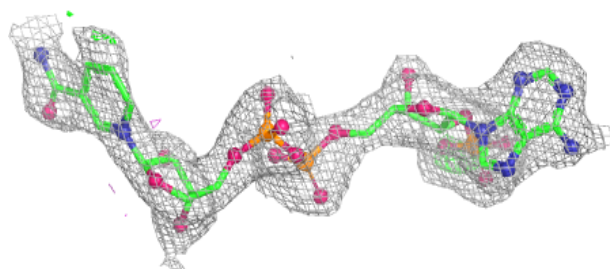
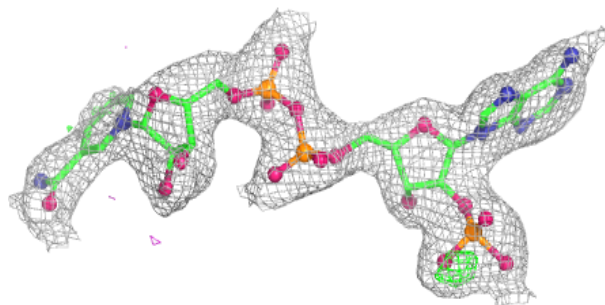
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAP	A	802	48/48	0.95	0.11	52,66,74,77	0
2	FAD	A	801	53/53	0.98	0.05	28,35,43,46	0

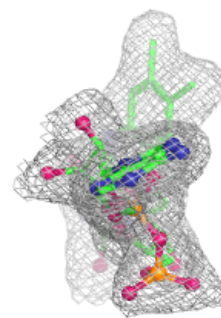
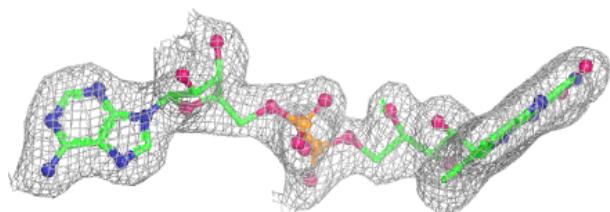
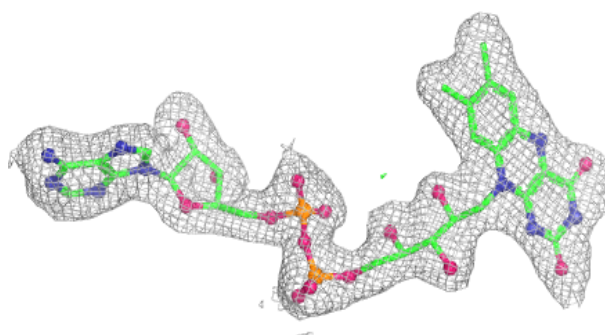
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP A 802:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around FAD A 801:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.