



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:44 PM UTC

PDB ID : 1E1N / pdb_00001e1n
Title : Structure of adrenodoxin reductase at 2.4 Angstrom in crystal form A'
Authors : Ziegler, G.A.; Schulz, G.E.
Deposited on : 2000-05-09
Resolution : 2.40 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

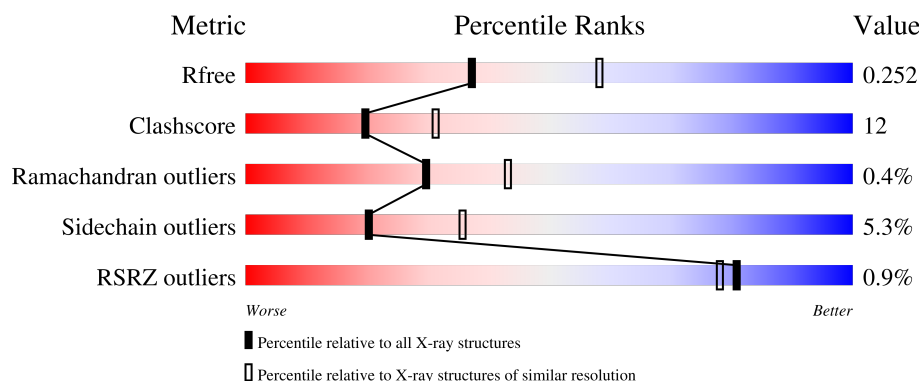
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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.

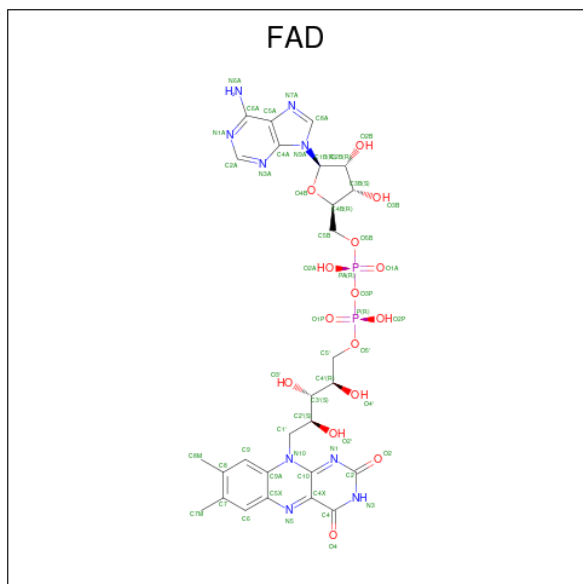
Mol	Chain	Length	Quality of chain
1	A	460	64% 27% 8% ..

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	7	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		

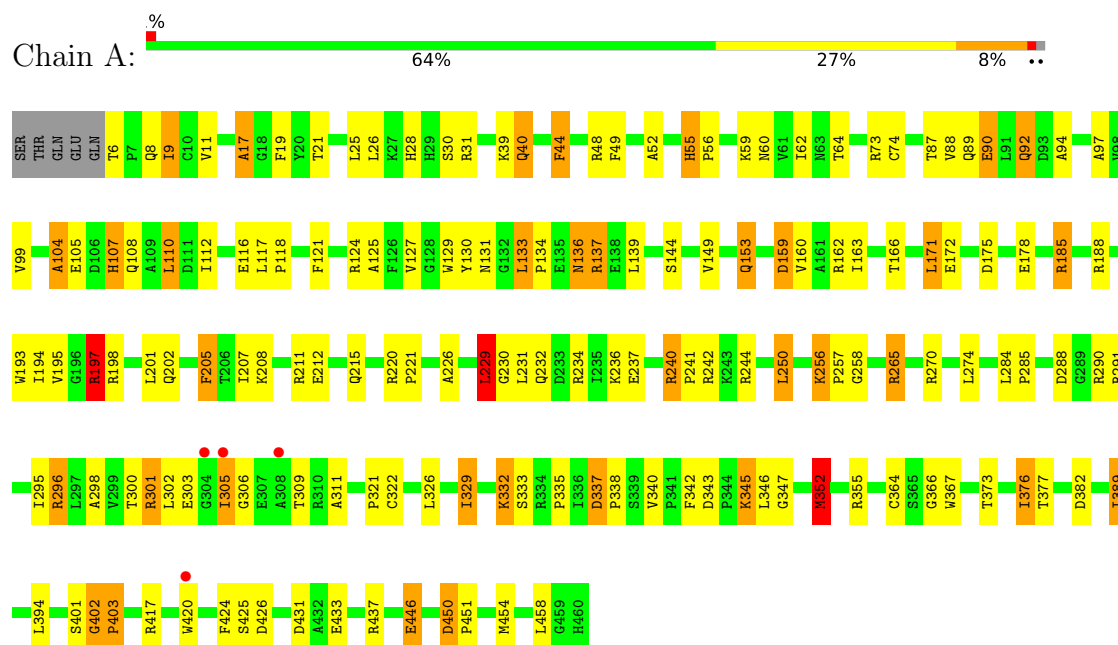
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	119	Total O 119 119	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	57.80Å 62.00Å 83.00Å 90.00° 107.10° 90.00°	Depositor
Resolution (Å)	29.00 – 2.40 29.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	77.6 (29.00-2.40) 77.6 (29.00-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.36Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.201 , 0.265 0.200 , 0.252	Depositor DCC
R_{free} test set	896 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	1.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 32.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3677	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.54% 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

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	0.90	2/3584 (0.1%)	1.79	81/4871 (1.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	352	MET	CG-SD	17.94	2.25	1.80
1	A	345	LYS	CD-CE	-9.12	1.25	1.52

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	LYS	CG-CD-CE	12.60	140.29	111.30
1	A	389	ILE	CB-CA-C	-11.18	97.83	111.81
1	A	417	ARG	CD-NE-CZ	10.04	138.45	124.40
1	A	185	ARG	CD-NE-CZ	9.52	137.72	124.40
1	A	337	ASP	CA-CB-CG	9.18	121.78	112.60
1	A	389	ILE	N-CA-CB	8.38	119.75	110.62
1	A	450	ASP	CA-CB-CG	8.36	120.96	112.60
1	A	296	ARG	CD-NE-CZ	7.85	135.39	124.40
1	A	257	PRO	N-CA-C	7.78	128.50	112.47
1	A	431	ASP	CA-CB-CG	7.78	120.38	112.60
1	A	205	PHE	CA-CB-CG	7.78	121.58	113.80
1	A	301	ARG	CA-CB-CG	7.37	128.84	114.10
1	A	39	LYS	CA-CB-CG	7.24	128.57	114.10
1	A	159	ASP	CA-C-O	-7.22	113.24	120.82
1	A	403	PRO	N-CA-CB	-7.20	95.70	103.25
1	A	352	MET	CB-CG-SD	-7.19	91.13	112.70
1	A	28	HIS	CA-CB-CG	-7.19	106.61	113.80
1	A	130	TYR	CA-CB-CG	7.16	126.79	113.90
1	A	244	ARG	CB-CA-C	7.07	121.98	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	LYS	CD-CE-NZ	7.07	134.52	111.90
1	A	8	GLN	CA-C-N	-6.81	112.64	122.45
1	A	8	GLN	C-N-CA	-6.81	112.64	122.45
1	A	90	GLU	CA-C-O	6.76	127.58	120.42
1	A	19	PHE	CA-CB-CG	-6.72	107.08	113.80
1	A	329	ILE	N-CA-C	6.71	123.29	109.34
1	A	240	ARG	CD-NE-CZ	6.64	133.69	124.40
1	A	291	ARG	CD-NE-CZ	6.62	133.67	124.40
1	A	207	ILE	N-CA-C	6.53	118.06	110.62
1	A	30	SER	N-CA-C	6.48	119.17	111.71
1	A	40	GLN	CA-C-O	-6.46	114.62	121.99
1	A	389	ILE	O-C-N	6.46	128.59	121.94
1	A	382	ASP	CA-CB-CG	-6.46	106.14	112.60
1	A	401	SER	N-CA-C	6.38	119.91	110.46
1	A	295	ILE	CA-C-N	6.38	130.90	122.42
1	A	295	ILE	C-N-CA	6.38	130.90	122.42
1	A	195	VAL	N-CA-C	6.38	117.76	108.58
1	A	197	ARG	CD-NE-CZ	6.30	133.22	124.40
1	A	446	GLU	N-CA-CB	6.25	121.00	110.69
1	A	364	CYS	CA-C-O	6.21	127.95	120.99
1	A	55	HIS	CA-CB-CG	6.17	119.97	113.80
1	A	73	ARG	NE-CZ-NH2	6.17	124.75	119.20
1	A	137	ARG	CA-CB-CG	5.96	126.02	114.10
1	A	44	PHE	CA-C-O	5.95	124.06	119.18
1	A	424	PHE	CA-C-N	5.92	128.50	120.38
1	A	424	PHE	C-N-CA	5.92	128.50	120.38
1	A	270	ARG	CD-NE-CZ	5.92	132.69	124.40
1	A	402	GLY	CA-C-N	5.83	127.13	119.84
1	A	402	GLY	C-N-CA	5.83	127.13	119.84
1	A	340	VAL	N-CA-C	5.75	114.21	107.77
1	A	208	LYS	CA-CB-CG	5.71	125.52	114.10
1	A	153	GLN	N-CA-C	5.69	117.73	109.71
1	A	104	ALA	CA-C-N	5.68	127.89	120.28
1	A	104	ALA	C-N-CA	5.68	127.89	120.28
1	A	403	PRO	N-CA-C	5.66	124.13	112.47
1	A	265	ARG	CD-NE-CZ	5.65	132.31	124.40
1	A	425	SER	O-C-N	5.58	128.04	122.12
1	A	90	GLU	CB-CG-CD	5.57	122.07	112.60
1	A	175	ASP	CA-CB-CG	5.56	118.16	112.60
1	A	425	SER	CB-CA-C	-5.55	101.24	110.68
1	A	133	LEU	N-CA-C	-5.50	101.27	109.42
1	A	94	ALA	N-CA-C	5.35	118.97	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	GLN	CA-C-O	-5.33	114.89	120.55
1	A	229	LEU	N-CA-CB	5.30	118.17	109.95
1	A	44	PHE	CA-CB-CG	5.30	119.10	113.80
1	A	105	GLU	N-CA-C	5.28	117.03	111.28
1	A	52	ALA	CA-C-N	5.27	124.89	119.56
1	A	52	ALA	C-N-CA	5.27	124.89	119.56
1	A	343	ASP	CA-C-N	5.24	124.90	119.56
1	A	343	ASP	C-N-CA	5.24	124.90	119.56
1	A	137	ARG	CB-CA-C	5.24	119.58	110.68
1	A	376	ILE	N-CA-C	5.23	115.95	110.62
1	A	450	ASP	CA-C-O	5.20	124.37	119.59
1	A	256	LYS	CA-C-N	5.18	126.31	119.84
1	A	256	LYS	C-N-CA	5.18	126.31	119.84
1	A	136	ASN	CA-CB-CG	5.16	117.76	112.60
1	A	17	ALA	CA-C-O	5.11	126.69	121.07
1	A	212	GLU	CA-CB-CG	5.05	124.20	114.10
1	A	107	HIS	N-CA-C	-5.05	101.64	109.72
1	A	298	ALA	CA-C-O	-5.03	114.95	120.43
1	A	355	ARG	CA-C-O	-5.02	114.81	120.43
1	A	9	ILE	CA-C-O	-5.01	116.06	121.92

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	81	1
2	A	53	0	31	4	0
3	A	119	0	0	16	1
All	All	3677	0	3566	82	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 12.

All (82) 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:234:ARG:HB3	3:A:2064:HOH:O	1.77	0.85
1:A:59:LYS:HE2	3:A:2116:HOH:O	1.80	0.80
1:A:345:LYS:HG3	1:A:346:LEU:HD23	1.68	0.76
1:A:178:GLU:HG3	3:A:2112:HOH:O	1.88	0.74
1:A:108:GLN:HG2	1:A:332:LYS:HZ2	1.53	0.72
1:A:258:GLY:HA3	3:A:2069:HOH:O	1.90	0.71
1:A:284:LEU:HD21	1:A:296:ARG:HB2	1.79	0.64
1:A:87:THR:OG1	1:A:90:GLU:HG3	1.99	0.62
1:A:144:SER:HA	1:A:188:ARG:HG3	1.79	0.62
1:A:88:VAL:O	1:A:92:GLN:HG3	1.99	0.62
1:A:166:THR:HG21	1:A:171:LEU:HD13	1.80	0.61
1:A:9:ILE:HG23	1:A:97:ALA:HB3	1.82	0.61
1:A:198:ARG:NH1	1:A:202:GLN:HG2	2.17	0.59
1:A:232:GLN:HB2	1:A:250:LEU:HD11	1.85	0.59
1:A:159:ASP:HA	1:A:162:ARG:HH12	1.69	0.58
1:A:300:THR:HB	1:A:311:ALA:HB1	1.83	0.58
1:A:134:PRO:HA	3:A:2040:HOH:O	2.04	0.57
1:A:160:VAL:HG21	1:A:326:LEU:HD13	1.87	0.57
1:A:107:HIS:HB3	3:A:2035:HOH:O	2.05	0.57
1:A:221:PRO:HD3	3:A:2072:HOH:O	2.03	0.57
1:A:402:GLY:HA2	3:A:2099:HOH:O	2.06	0.56
1:A:116:GLU:HG2	1:A:117:LEU:N	2.20	0.55
1:A:211:ARG:HG3	1:A:215:GLN:HE21	1.71	0.55
1:A:302:LEU:HD22	1:A:309:THR:HB	1.88	0.55
1:A:433:GLU:O	1:A:437:ARG:HG2	2.07	0.55
1:A:159:ASP:HA	1:A:162:ARG:NH1	2.22	0.54
1:A:226:ALA:HA	1:A:229:LEU:HD22	1.88	0.54
1:A:127:VAL:O	1:A:131:ASN:HB2	2.10	0.52
1:A:121:PHE:CD2	1:A:139:LEU:HD11	2.45	0.52
1:A:205:PHE:HZ	1:A:274:LEU:HD21	1.75	0.52
1:A:17:ALA:HB2	1:A:366:GLY:HA3	1.92	0.51
1:A:451:PRO:HA	1:A:454:MET:HE3	1.91	0.51
1:A:153:GLN:HG2	1:A:194:ILE:HG22	1.93	0.51
1:A:220:ARG:HD3	1:A:265:ARG:O	2.11	0.51
1:A:197:ARG:HH11	1:A:197:ARG:HG3	1.76	0.50
1:A:301:ARG:NH1	1:A:303:GLU:OE2	2.45	0.49
1:A:337:ASP:CG	1:A:338:PRO:HD2	2.38	0.49
1:A:376:ILE:HG13	2:A:801:FAD:N1	2.28	0.48
1:A:367:TRP:CZ2	2:A:801:FAD:H3'	2.49	0.48
1:A:129:TRP:HB2	1:A:139:LEU:HD23	1.95	0.48
1:A:237:GLU:HB3	3:A:2063:HOH:O	2.14	0.47
1:A:321:PRO:O	1:A:322:CYS:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ALA:HB1	1:A:136:ASN:ND2	2.29	0.47
1:A:44:PHE:CE2	1:A:62:ILE:HG23	2.49	0.47
1:A:201:LEU:O	1:A:242:ARG:NH2	2.48	0.47
1:A:333:SER:HB2	1:A:347:GLY:O	2.16	0.46
1:A:26:LEU:HD11	1:A:74:CYS:HB2	1.98	0.46
1:A:124:ARG:HH12	1:A:367:TRP:HZ3	1.64	0.45
1:A:240:ARG:HB3	1:A:241:PRO:HD3	1.98	0.45
1:A:241:PRO:HB2	3:A:2065:HOH:O	2.16	0.45
1:A:450:ASP:HA	1:A:451:PRO:HD3	1.79	0.45
1:A:108:GLN:HG2	1:A:332:LYS:NZ	2.29	0.45
1:A:48:ARG:HB2	3:A:2051:HOH:O	2.17	0.45
1:A:256:LYS:HG2	3:A:2068:HOH:O	2.17	0.44
2:A:801:FAD:HM83	2:A:801:FAD:HM71	1.73	0.44
1:A:178:GLU:HB2	1:A:446:GLU:OE1	2.18	0.44
1:A:17:ALA:HB3	3:A:2004:HOH:O	2.16	0.43
1:A:230:GLY:O	1:A:234:ARG:HG3	2.18	0.43
1:A:335:PRO:HG3	1:A:342:PHE:CD2	2.53	0.43
1:A:426:ASP:HB3	1:A:458:LEU:HD11	2.00	0.43
1:A:394:LEU:C	1:A:394:LEU:HD23	2.43	0.43
1:A:172:GLU:OE1	1:A:185:ARG:NH2	2.51	0.43
1:A:110:LEU:HB3	1:A:112:ILE:HG12	2.00	0.43
1:A:11:VAL:HG12	1:A:99:VAL:HB	2.01	0.43
1:A:376:ILE:HG13	2:A:801:FAD:C2	2.49	0.43
1:A:104:ALA:HA	1:A:333:SER:HA	2.00	0.42
1:A:305:ILE:HG22	1:A:306:GLY:N	2.34	0.42
1:A:40:GLN:NE2	1:A:40:GLN:HA	2.34	0.42
1:A:117:LEU:HA	1:A:118:PRO:HD3	1.93	0.42
1:A:197:ARG:HH11	1:A:197:ARG:CG	2.33	0.42
1:A:21:THR:O	1:A:25:LEU:HG	2.19	0.42
1:A:124:ARG:NH1	1:A:367:TRP:HZ3	2.17	0.42
1:A:284:LEU:HA	1:A:285:PRO:HD3	1.85	0.42
1:A:49:PHE:CE1	1:A:133:LEU:HA	2.55	0.41
1:A:89:GLN:HB2	3:A:2082:HOH:O	2.20	0.41
1:A:197:ARG:CZ	3:A:2058:HOH:O	2.67	0.41
1:A:337:ASP:OD1	1:A:338:PRO:HD2	2.21	0.41
1:A:55:HIS:N	1:A:56:PRO:CD	2.83	0.41
1:A:149:VAL:HG22	1:A:193:TRP:HB2	2.03	0.41
1:A:194:ILE:HB	1:A:274:LEU:HD12	2.03	0.40
1:A:288:ASP:OD2	1:A:290:ARG:HG3	2.20	0.40
1:A:242:ARG:HB2	3:A:2065:HOH:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:MET:CE	3:A:2103:HOH:O[2_545]	1.34	0.86

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%)	428 (94%)	23 (5%)	2 (0%)	30	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	403	PRO
1	A	329	ILE

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%)	20	36

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

Mol	Chain	Res	Type
1	A	6	THR
1	A	31	ARG

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Mol	Chain	Res	Type
1	A	60	ASN
1	A	64	THR
1	A	110	LEU
1	A	137	ARG
1	A	163	ILE
1	A	171	LEU
1	A	197	ARG
1	A	229	LEU
1	A	231	LEU
1	A	236	LYS
1	A	250	LEU
1	A	305	ILE
1	A	332	LYS
1	A	352	MET
1	A	373	THR
1	A	377	THR
1	A	389	ILE
1	A	420	TRP

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	28	HIS
1	A	40	GLN
1	A	136	ASN
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

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	FAD	A	801	-	58,58,58	2.26	10 (17%)	85,89,89	1.47	15 (17%)

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	-	-	11/34/50/50	0/6/6/6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	FAD	P-O3P	-11.37	1.47	1.59
2	A	801	FAD	C1'-C2'	4.98	1.59	1.52
2	A	801	FAD	O5'-C5'	4.26	1.60	1.44
2	A	801	FAD	PA-O2A	-3.95	1.37	1.55
2	A	801	FAD	P-O2P	-3.48	1.39	1.55
2	A	801	FAD	C6-C7	-3.11	1.35	1.39
2	A	801	FAD	C5'-C4'	3.02	1.55	1.51
2	A	801	FAD	O2-C2	-2.40	1.19	1.24
2	A	801	FAD	C5A-C6A	2.15	1.47	1.41
2	A	801	FAD	O4B-C1B	2.05	1.46	1.42

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	FAD	O4'-C4'-C3'	3.49	117.42	109.25
2	A	801	FAD	O2'-C2'-C3'	3.26	116.88	109.25
2	A	801	FAD	O3'-C3'-C2'	-3.13	101.81	108.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	FAD	O4-C4-C4X	-2.76	119.25	126.53
2	A	801	FAD	O4B-C1B-C2B	-2.74	100.75	106.62
2	A	801	FAD	O2A-PA-O1A	2.74	125.17	112.44
2	A	801	FAD	C4B-O4B-C1B	-2.54	103.85	109.47
2	A	801	FAD	O2A-PA-O3P	2.38	113.71	107.27
2	A	801	FAD	O4-C4-N3	2.29	124.42	120.11
2	A	801	FAD	O3'-C3'-C4'	-2.23	103.87	108.93
2	A	801	FAD	O5'-P-O1P	-2.21	100.18	108.94
2	A	801	FAD	O5B-PA-O1A	-2.18	100.29	108.94
2	A	801	FAD	C7M-C7-C8	-2.15	116.37	120.76
2	A	801	FAD	C5'-C4'-C3'	-2.07	108.32	112.22
2	A	801	FAD	C7M-C7-C6	2.05	123.19	119.57

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	FAD	O3'-C3'-C4'-O4'
2	A	801	FAD	O3'-C3'-C4'-C5'
2	A	801	FAD	O4B-C4B-C5B-O5B
2	A	801	FAD	C3B-C4B-C5B-O5B
2	A	801	FAD	C2'-C3'-C4'-O4'
2	A	801	FAD	PA-O3P-P-O5'
2	A	801	FAD	C5B-O5B-PA-O1A
2	A	801	FAD	C5B-O5B-PA-O2A
2	A	801	FAD	C5B-O5B-PA-O3P
2	A	801	FAD	P-O3P-PA-O2A
2	A	801	FAD	C2'-C3'-C4'-C5'

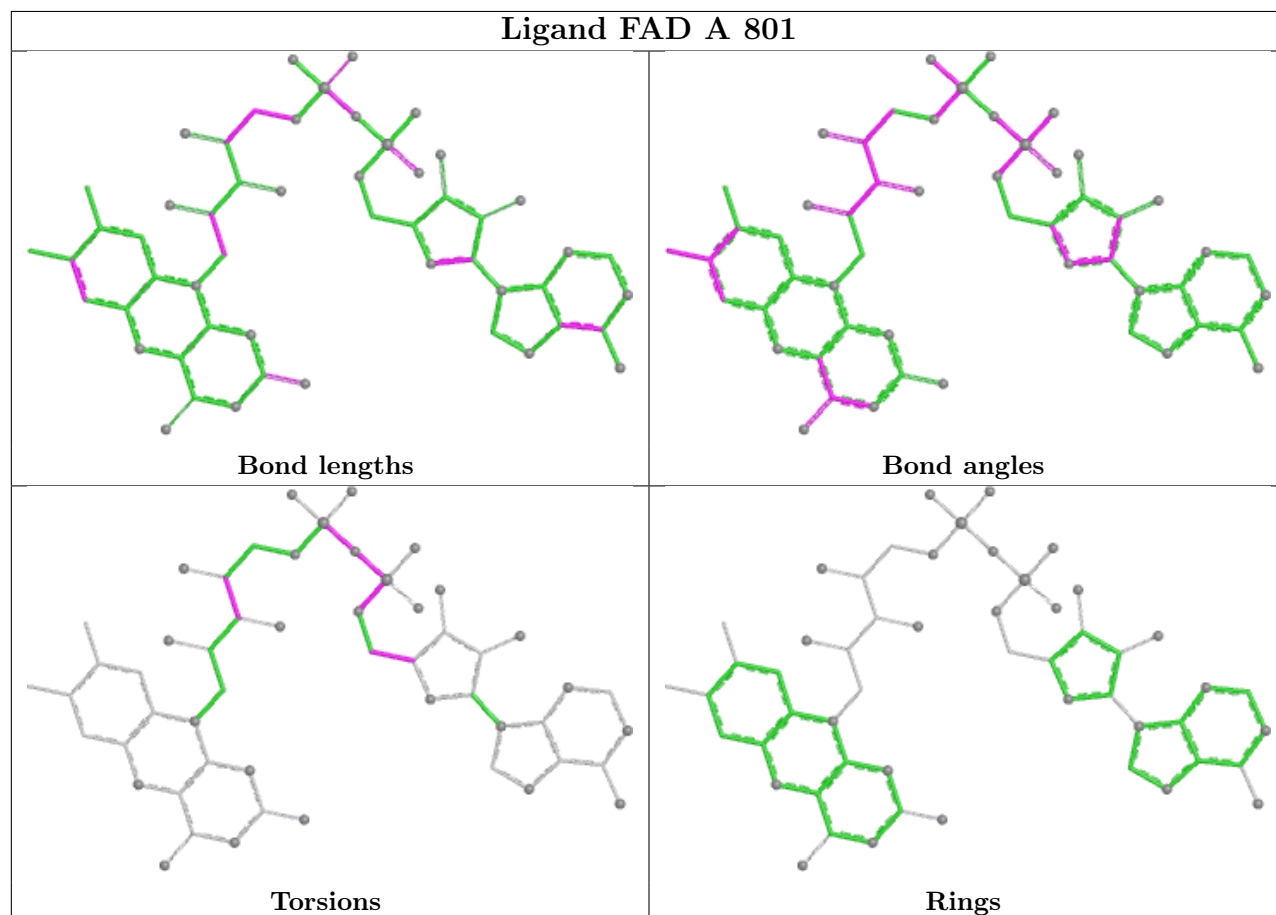
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	FAD	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 [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%)	-0.14	4 (0%) 81 78	15, 40, 73, 104	3 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	420	TRP	3.6
1	A	308	ALA	2.8
1	A	305	ILE	2.7
1	A	304	GLY	2.5

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.

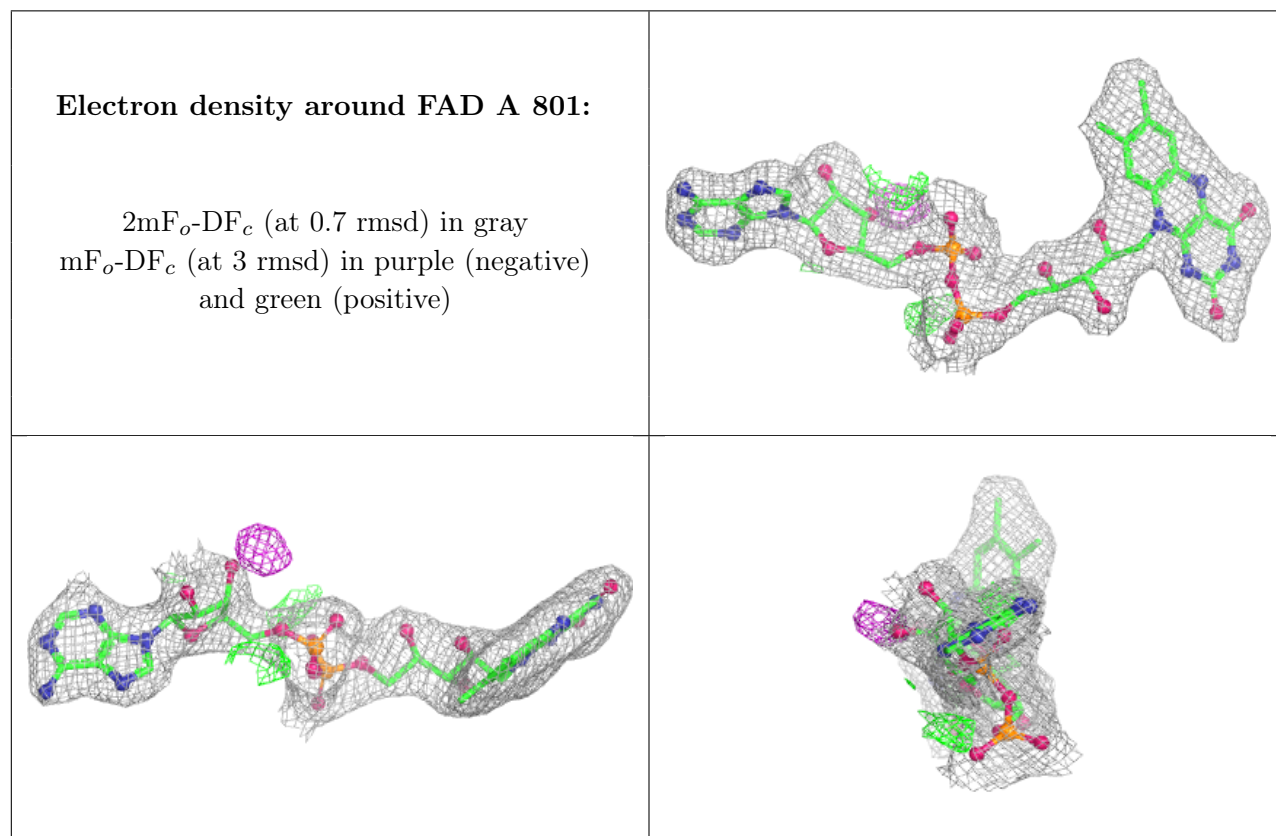
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
2	FAD	A	801	53/53	0.97	0.06	16,26,30,32	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 ⓘ

There are no such residues in this entry.