



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:30 PM UTC

PDB ID : 5YGQ / pdb_00005ygq
Title : Crystal Structure of Ferredoxin NADP⁺ Oxidoreductase from *Rhodopseudomonas palustris*
Authors : Muraki, N.; Seo, D.; Kurisu, G.
Deposited on : 2017-09-25
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

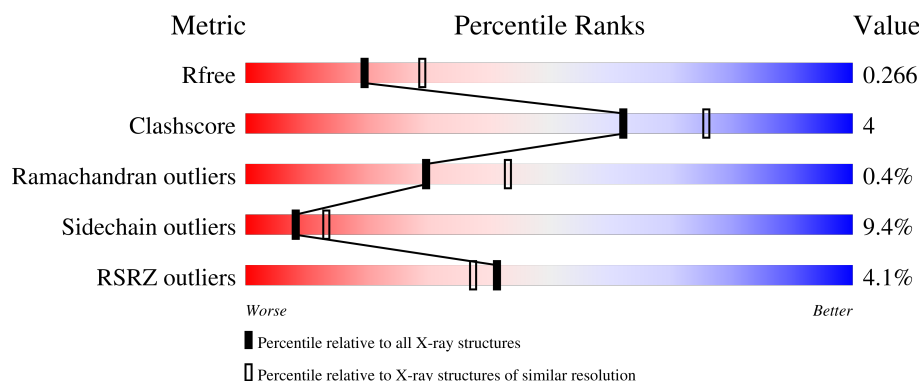
1 Overall quality at a glance

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.

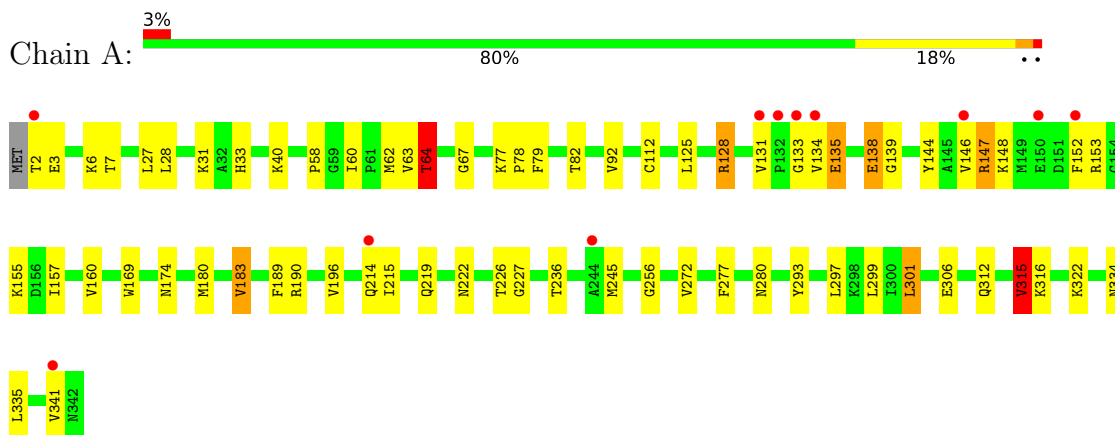
Mol	Chain	Length	Quality of chain
1	A	342	3% 80% 18% ..
1	B	342	5% 83% 14% ...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total 30	O 30	0	0
3	B	21	Total 21	O 21	0	0

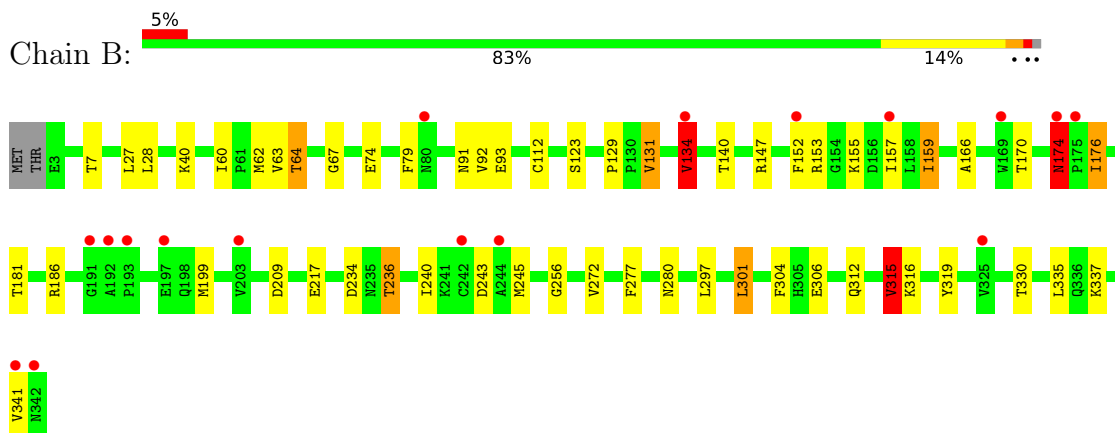
3 Residue-property plots

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: Ferredoxin–NADP reductase



• Molecule 1: Ferredoxin–NADP reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.87Å 81.23Å 122.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.42 – 2.40 36.42 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.4 (36.42-2.40) 94.4 (36.42-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.218 , 0.263 0.220 , 0.266	Depositor DCC
R_{free} test set	1341 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 28.9	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	0.93	EDS
Total number of atoms	5352	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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

5.1 Standard geometry

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	1.24	4/2654 (0.2%)	1.24	15/3603 (0.4%)
1	B	1.19	4/2647 (0.2%)	1.27	12/3593 (0.3%)
All	All	1.22	8/5301 (0.2%)	1.26	27/7196 (0.4%)

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	VAL	CA-C	8.06	1.61	1.52
1	B	174	ASN	CA-C	6.91	1.61	1.52
1	B	341	VAL	CA-C	6.23	1.60	1.52
1	A	341	VAL	CA-C	5.70	1.59	1.52
1	A	334	ASN	CA-C	5.43	1.60	1.52
1	B	209	ASP	CA-CB	5.14	1.60	1.53
1	A	293	TYR	N-CA	-5.11	1.41	1.46
1	B	319	TYR	C-O	-5.01	1.18	1.24

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	PHE	N-CA-C	-11.49	93.42	110.42
1	B	79	PHE	N-CA-C	-10.00	94.52	110.42
1	B	134	VAL	CB-CA-C	-7.64	101.67	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	315	VAL	CB-CA-C	-7.51	102.01	112.14
1	A	315	VAL	N-CA-CB	7.25	120.41	110.54
1	B	315	VAL	N-CA-CB	7.06	120.14	110.54
1	A	138	GLU	N-CA-C	7.01	119.77	111.71
1	B	315	VAL	CB-CA-C	-6.85	102.89	112.14
1	A	135	GLU	N-CA-C	6.80	120.49	109.40
1	A	131	VAL	N-CA-C	6.63	123.20	108.88
1	B	174	ASN	CB-CA-C	6.39	117.17	109.31
1	B	129	PRO	O-C-N	5.84	123.89	121.15
1	A	148	LYS	N-CA-C	-5.67	101.36	110.14
1	B	256	GLY	CA-C-N	5.54	125.21	119.56
1	B	256	GLY	C-N-CA	5.54	125.21	119.56
1	A	125	LEU	CA-C-N	5.44	125.75	119.93
1	A	125	LEU	C-N-CA	5.44	125.75	119.93
1	B	245	MET	CG-SD-CE	5.39	112.76	100.90
1	B	330	THR	N-CA-C	5.27	117.02	111.28
1	A	64	THR	CB-CA-C	5.24	118.99	109.83
1	B	129	PRO	CA-C-O	-5.16	116.65	120.73
1	A	79	PHE	CA-C-N	-5.07	116.80	123.34
1	A	79	PHE	C-N-CA	-5.07	116.80	123.34
1	A	256	GLY	CA-C-N	5.05	126.15	119.84
1	A	256	GLY	C-N-CA	5.05	126.15	119.84
1	A	301	LEU	CA-CB-CG	5.02	133.87	116.30
1	B	301	LEU	CA-CB-CG	5.01	133.84	116.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	VAL	Peptide

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	2601	0	2634	25	0
1	B	2594	0	2627	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	53	0	31	0	0
2	B	53	0	31	0	0
3	A	30	0	0	0	0
3	B	21	0	0	0	0
All	All	5352	0	5323	44	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 4.

All (44) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:VAL:HG21	1:A:245:MET:HE2	1.65	0.78
1:A:133:GLY:C	1:A:135:GLU:HG2	2.13	0.73
1:A:160:VAL:HG21	1:A:245:MET:CE	2.23	0.68
1:A:174:ASN:HD22	1:A:180:MET:HE2	1.60	0.66
1:B:159:ILE:HD13	1:B:170:THR:HG23	1.78	0.65
1:B:234:ASP:OD1	1:B:236:THR:HB	1.99	0.62
1:A:135:GLU:O	1:A:138:GLU:HG2	2.01	0.61
1:B:153:ARG:HA	1:B:176:ILE:HG23	1.84	0.59
1:A:183:VAL:HG11	1:A:215:ILE:HD11	1.86	0.57
1:A:128:ARG:HD2	1:A:144:TYR:OH	2.07	0.54
1:B:159:ILE:HD11	1:B:166:ALA:HA	1.90	0.53
1:B:64:THR:HG22	1:B:67:GLY:H	1.73	0.52
1:B:131:VAL:O	1:B:134:VAL:HG22	2.10	0.52
1:A:58:PRO:CB	1:B:304:PHE:CD2	2.94	0.51
1:A:64:THR:HG22	1:A:67:GLY:H	1.76	0.50
1:B:62:MET:HE2	1:B:63:VAL:C	2.36	0.50
1:A:219:GLN:HG2	1:A:227:GLY:C	2.37	0.49
1:A:152:PHE:HA	1:A:155:LYS:HG3	1.96	0.48
1:B:152:PHE:HB3	1:B:157:ILE:HD11	1.96	0.48
1:B:28:LEU:HB3	1:B:315:VAL:HG11	1.97	0.47
1:B:7:THR:O	1:B:112:CYS:HA	2.14	0.47
1:B:159:ILE:HD11	1:B:166:ALA:CA	2.45	0.47
1:A:189:PHE:HB3	1:A:196:VAL:HG22	1.96	0.47
1:A:7:THR:O	1:A:112:CYS:HA	2.15	0.47
1:B:60:ILE:HG21	1:B:63:VAL:HB	1.97	0.46
1:B:159:ILE:HG21	1:B:170:THR:HG22	1.97	0.46
1:A:160:VAL:CG2	1:A:245:MET:HE2	2.42	0.46
1:A:60:ILE:HG21	1:A:63:VAL:HB	1.98	0.45
1:A:146:VAL:HG21	1:A:169:TRP:CH2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:PHE:HB3	1:A:157:ILE:HD11	1.98	0.45
1:A:58:PRO:HB2	1:B:304:PHE:CD2	2.52	0.44
1:A:139:GLY:O	1:A:147:ARG:NH2	2.51	0.44
1:A:146:VAL:HG11	1:A:169:TRP:CZ3	2.52	0.44
1:A:277:PHE:CE1	1:A:306:GLU:HG2	2.53	0.43
1:B:277:PHE:CE1	1:B:306:GLU:HG2	2.54	0.43
1:A:28:LEU:HB3	1:A:315:VAL:HG11	2.00	0.42
1:B:64:THR:CG2	1:B:67:GLY:H	2.32	0.42
1:B:174:ASN:HD22	1:B:174:ASN:HA	1.72	0.42
1:B:155:LYS:HB2	1:B:243:ASP:OD2	2.20	0.42
1:B:181:THR:OG1	1:B:240:ILE:CG2	2.68	0.42
1:A:77:LYS:HB3	1:A:78:PRO:HD3	2.02	0.41
1:A:33:HIS:ND1	1:A:82:THR:HB	2.36	0.40
1:B:181:THR:OG1	1:B:240:ILE:HG21	2.20	0.40
1:A:64:THR:CG2	1:A:67:GLY:H	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	340/342 (99%)	325 (96%)	13 (4%)	2 (1%)	21	32
1	B	339/342 (99%)	329 (97%)	9 (3%)	1 (0%)	36	50
All	All	679/684 (99%)	654 (96%)	22 (3%)	3 (0%)	30	43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	ARG
1	B	280	ASN
1	A	280	ASN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	284/284 (100%)	258 (91%)	26 (9%)	8	14
1	B	283/284 (100%)	256 (90%)	27 (10%)	8	13
All	All	567/568 (100%)	514 (91%)	53 (9%)	8	14

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	3	GLU
1	A	6	LYS
1	A	27	LEU
1	A	31	LYS
1	A	40	LYS
1	A	62	MET
1	A	64	THR
1	A	92	VAL
1	A	128	ARG
1	A	153	ARG
1	A	183	VAL
1	A	190	ARG
1	A	214	GLN
1	A	222	ASN
1	A	226	THR
1	A	236	THR
1	A	272	VAL
1	A	297	LEU
1	A	299	LEU
1	A	301	LEU
1	A	312	GLN
1	A	315	VAL
1	A	316	LYS
1	A	322	LYS
1	A	335	LEU
1	B	27	LEU

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Mol	Chain	Res	Type
1	B	40	LYS
1	B	64	THR
1	B	74	GLU
1	B	91	ASN
1	B	92	VAL
1	B	93	GLU
1	B	123	SER
1	B	131	VAL
1	B	134	VAL
1	B	140	THR
1	B	147	ARG
1	B	159	ILE
1	B	174	ASN
1	B	176	ILE
1	B	186	ARG
1	B	199	MET
1	B	217	GLU
1	B	236	THR
1	B	272	VAL
1	B	297	LEU
1	B	301	LEU
1	B	312	GLN
1	B	315	VAL
1	B	316	LYS
1	B	335	LEU
1	B	337	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	174	ASN
1	A	184	HIS
1	A	194	HIS
1	A	198	GLN
1	A	214	GLN
1	A	268	ASN
1	A	312	GLN
1	B	44	GLN
1	B	66	HIS
1	B	174	ASN
1	B	214	GLN

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Mol	Chain	Res	Type
1	B	219	GLN
1	B	222	ASN
1	B	312	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 oligosaccharides 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	$\# Z > 2$
2	FAD	A	401	-	58,58,58	1.79	9 (15%)	85,89,89	1.70	21 (24%)
2	FAD	B	401	-	58,58,58	1.64	12 (20%)	85,89,89	2.00	28 (32%)

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	401	-	-	8/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	B	401	-	-	5/34/50/50	0/6/6/6

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	FAD	C9A-C5X	6.13	1.51	1.41
2	B	401	FAD	C4-N3	-4.70	1.30	1.38
2	A	401	FAD	P-O3P	4.37	1.64	1.59
2	B	401	FAD	C5A-C4A	4.04	1.46	1.39
2	A	401	FAD	C1'-C2'	-3.95	1.47	1.52
2	A	401	FAD	C8-C7	3.75	1.50	1.40
2	B	401	FAD	C9A-C5X	3.50	1.46	1.41
2	A	401	FAD	PA-O3P	3.45	1.63	1.59
2	B	401	FAD	P-O3P	3.15	1.62	1.59
2	A	401	FAD	C4A-N9A	-3.15	1.31	1.37
2	A	401	FAD	C5A-C4A	3.02	1.44	1.39
2	B	401	FAD	C5'-C4'	2.94	1.55	1.51
2	B	401	FAD	C8-C7	2.81	1.47	1.40
2	B	401	FAD	C2-N3	-2.77	1.32	1.39
2	A	401	FAD	C5X-N5	-2.74	1.34	1.39
2	B	401	FAD	C2-N1	-2.61	1.30	1.36
2	B	401	FAD	C4A-N9A	-2.48	1.32	1.37
2	B	401	FAD	PA-O3P	2.42	1.62	1.59
2	B	401	FAD	C5A-C6A	2.41	1.47	1.41
2	B	401	FAD	C1'-C2'	-2.26	1.49	1.52
2	A	401	FAD	C4-N3	-2.15	1.34	1.38

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	FAD	O3P-PA-O1A	4.95	125.58	110.70
2	B	401	FAD	O2-C2-N1	-4.91	113.64	121.80
2	B	401	FAD	C4A-N9A-C8A	4.76	110.74	105.74
2	B	401	FAD	O2A-PA-O3P	4.54	119.53	107.27
2	B	401	FAD	N3A-C2A-N1A	-4.46	121.84	128.58
2	B	401	FAD	C4-C4X-N5	4.36	124.22	118.21
2	B	401	FAD	C2B-C3B-C4B	4.22	110.77	102.61
2	A	401	FAD	O2A-PA-O3P	-4.06	96.31	107.27
2	B	401	FAD	N3A-C4A-N9A	3.84	133.69	127.17
2	B	401	FAD	C5A-C4A-N3A	-3.75	121.55	126.72
2	A	401	FAD	C5A-C4A-N3A	-3.68	121.65	126.72
2	B	401	FAD	C4X-C10-N10	3.51	121.50	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	FAD	N3A-C2A-N1A	-3.47	123.33	128.58
2	B	401	FAD	C2A-N3A-C4A	3.41	120.17	111.83
2	B	401	FAD	O3B-C3B-C4B	-3.22	101.83	111.08
2	A	401	FAD	C4'-C3'-C2'	-3.19	108.26	113.57
2	B	401	FAD	C9A-C5X-N5	-3.08	119.19	122.45
2	A	401	FAD	N3A-C4A-N9A	3.00	132.26	127.17
2	A	401	FAD	C2A-N3A-C4A	2.98	119.11	111.83
2	B	401	FAD	N9A-C8A-N7A	-2.92	109.79	113.94
2	A	401	FAD	C4-C4X-N5	2.89	122.20	118.21
2	A	401	FAD	C10-N1-C2	2.83	122.97	116.85
2	A	401	FAD	C4X-C10-N1	-2.78	117.78	124.59
2	B	401	FAD	C4A-N9A-C1B	-2.75	120.19	126.63
2	A	401	FAD	O2-C2-N1	-2.72	117.29	121.80
2	B	401	FAD	C5X-N5-C4X	2.62	122.33	118.09
2	B	401	FAD	C4-N3-C2	-2.59	121.04	125.64
2	A	401	FAD	O2P-P-O1P	2.54	124.25	112.44
2	B	401	FAD	C6A-C5A-N7A	2.52	136.96	132.09
2	B	401	FAD	C10-C4X-N5	-2.52	119.67	124.81
2	B	401	FAD	C7M-C7-C6	2.50	123.98	119.57
2	A	401	FAD	C4X-C10-N10	2.50	120.06	116.48
2	B	401	FAD	C2A-N1A-C6A	2.44	122.73	118.73
2	B	401	FAD	C4X-C10-N1	-2.36	118.79	124.59
2	A	401	FAD	C4A-N9A-C8A	2.33	108.18	105.74
2	B	401	FAD	C4A-C5A-N7A	-2.32	107.93	110.58
2	B	401	FAD	O3P-PA-O1A	-2.32	103.73	110.70
2	A	401	FAD	C2A-N1A-C6A	2.32	122.53	118.73
2	A	401	FAD	C10-C4X-N5	-2.28	120.15	124.81
2	B	401	FAD	C4X-C4-N3	2.24	118.97	113.25
2	A	401	FAD	O2'-C2'-C3'	2.24	114.48	109.25
2	B	401	FAD	C2B-C1B-N9A	2.23	118.84	113.30
2	A	401	FAD	O3P-P-O1P	-2.21	104.04	110.70
2	A	401	FAD	O5'-C5'-C4'	-2.19	103.53	109.36
2	B	401	FAD	C5A-N7A-C8A	2.15	106.82	103.45
2	B	401	FAD	N3-C2-N1	2.14	124.04	119.50
2	A	401	FAD	C5X-N5-C4X	2.11	121.50	118.09
2	A	401	FAD	O3'-C3'-C4'	2.08	113.67	108.93
2	B	401	FAD	C7M-C7-C8	-2.03	116.61	120.76

There are no chirality outliers.

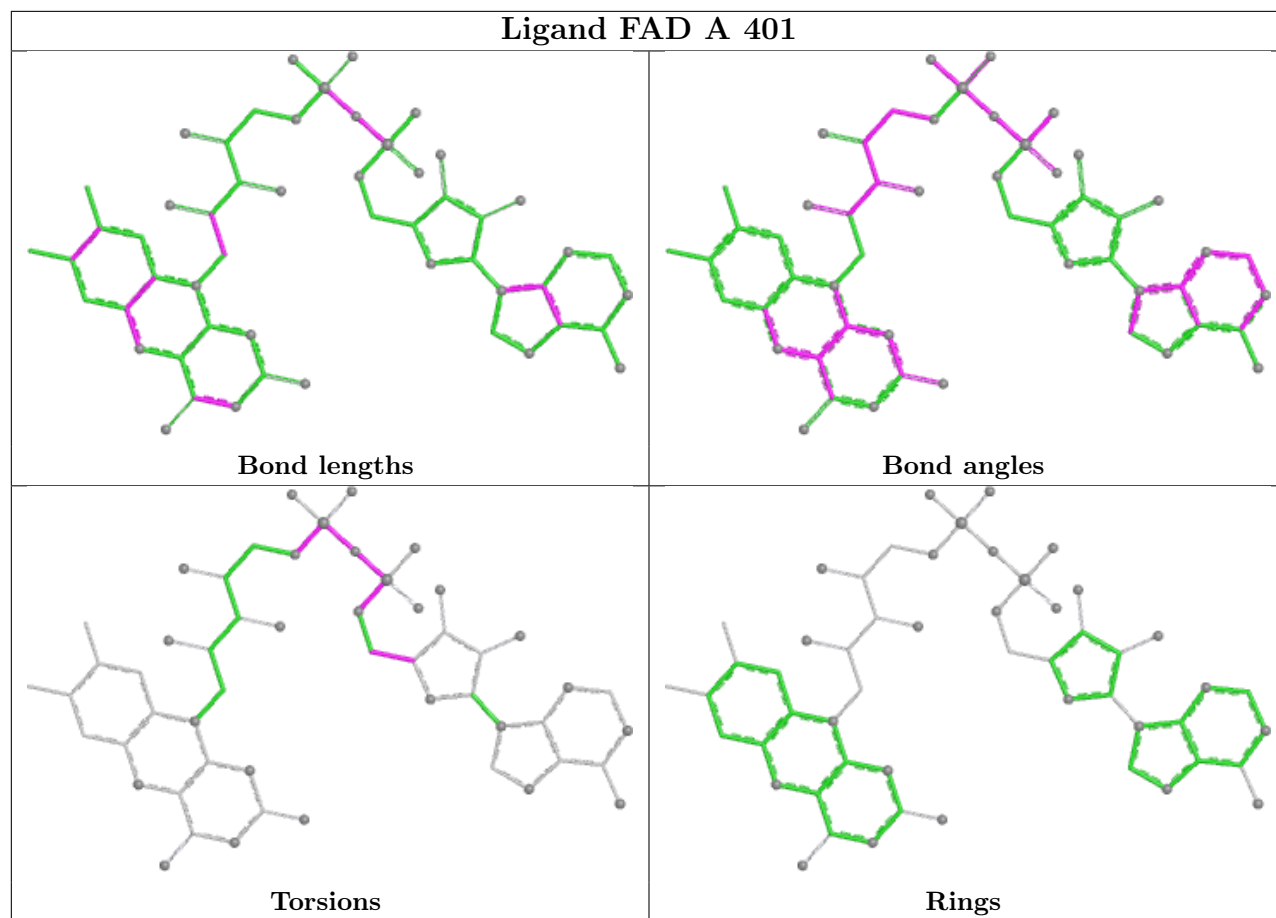
All (13) torsion outliers are listed below:

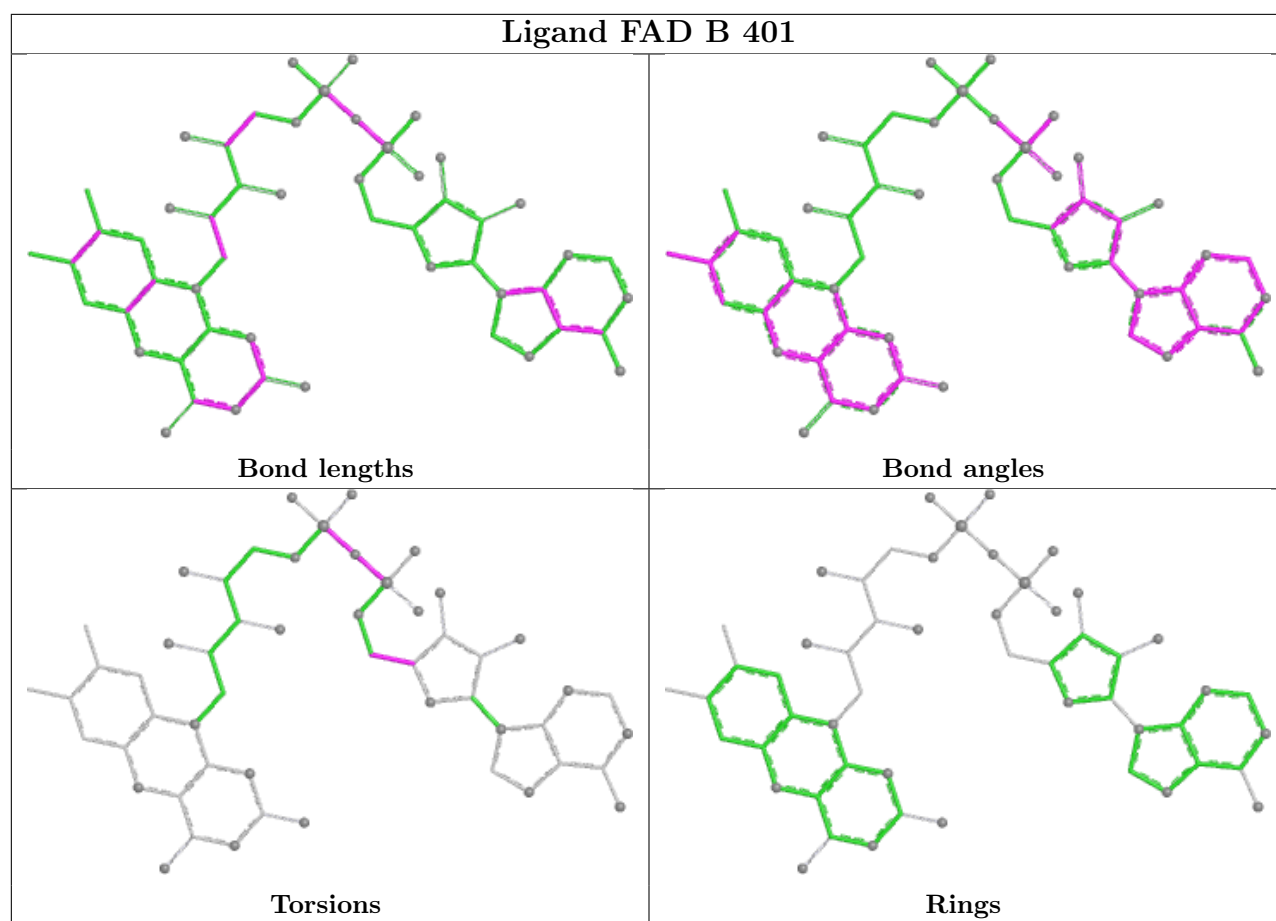
Mol	Chain	Res	Type	Atoms
2	A	401	FAD	C5B-O5B-PA-O2A
2	A	401	FAD	C5'-O5'-P-O1P
2	A	401	FAD	C3B-C4B-C5B-O5B
2	A	401	FAD	O4B-C4B-C5B-O5B
2	A	401	FAD	PA-O3P-P-O5'
2	B	401	FAD	PA-O3P-P-O5'
2	A	401	FAD	C5'-O5'-P-O3P
2	A	401	FAD	PA-O3P-P-O1P
2	B	401	FAD	P-O3P-PA-O2A
2	B	401	FAD	P-O3P-PA-O1A
2	A	401	FAD	P-O3P-PA-O2A
2	B	401	FAD	PA-O3P-P-O2P
2	B	401	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

No monomer is involved in short contacts.

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	341/342 (99%)	0.15	11 (3%) 50 46	18, 41, 81, 115	1 (0%)
1	B	340/342 (99%)	0.38	17 (5%) 34 30	24, 49, 83, 142	1 (0%)
All	All	681/684 (99%)	0.26	28 (4%) 41 37	18, 46, 83, 142	2 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	133	GLY	5.4
1	B	152	PHE	4.8
1	B	192	ALA	4.6
1	A	134	VAL	4.4
1	A	132	PRO	4.1
1	A	244	ALA	4.1
1	B	341	VAL	4.1
1	B	193	PRO	4.0
1	B	244	ALA	3.6
1	A	2	THR	3.4
1	B	175	PRO	2.9
1	A	131	VAL	2.9
1	B	134	VAL	2.8
1	B	191	GLY	2.7
1	A	152	PHE	2.6
1	B	174	ASN	2.5
1	A	150	GLU	2.4
1	A	146	VAL	2.4
1	B	157	ILE	2.3
1	B	242	CYS	2.3
1	B	80[A]	ASN	2.3
1	A	214	GLN	2.3
1	B	203	VAL	2.1
1	B	325	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	341	VAL	2.1
1	B	342	ASN	2.1
1	B	197	GLU	2.0
1	B	169	TRP	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](#)

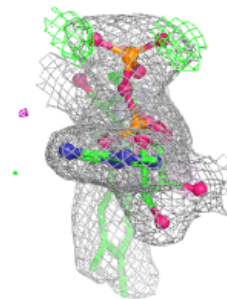
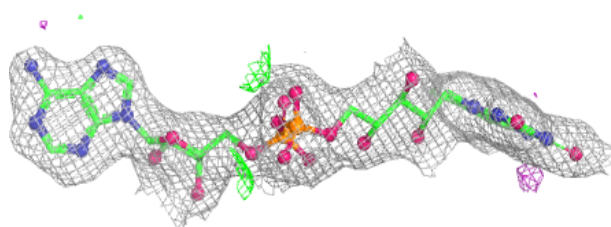
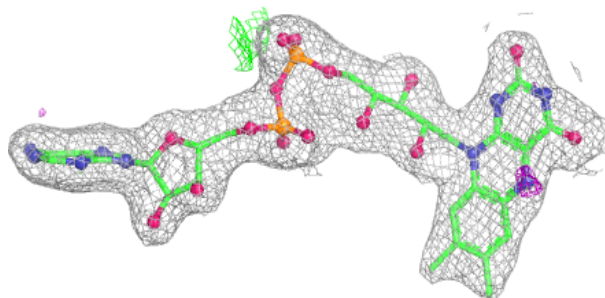
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	FAD	A	401	53/53	0.97	0.06	25,31,37,41	0
2	FAD	B	401	53/53	0.97	0.06	27,31,35,38	0

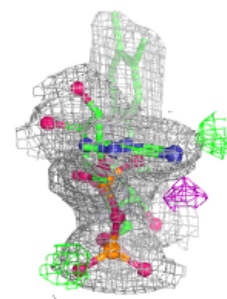
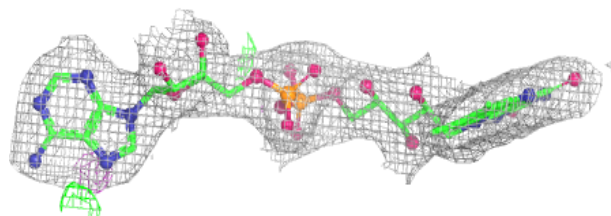
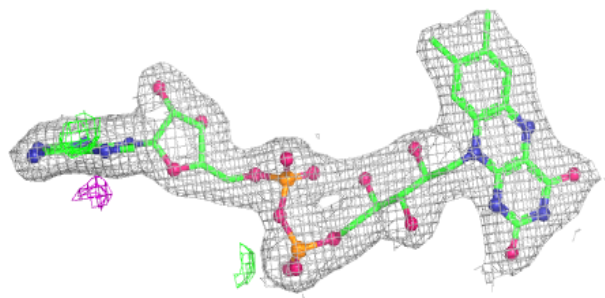
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD A 401:

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

**Electron density around FAD B 401:**

$2mF_o-DF_c$ (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.