



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:24 AM UTC

PDB ID : 1QG0 / pdb_00001qg0
Title : WILD-TYPE PEA FNR
Authors : Deng, Z.; Aliverti, A.; Zanetti, G.; Arakaki, A.K.; Ottado, J.; Orellano, E.G.;
Calcaterra, N.B.; Ceccarelli, E.A.; Carrillo, N.; Karplus, P.A.
Deposited on : 1999-04-18
Resolution : 2.50 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

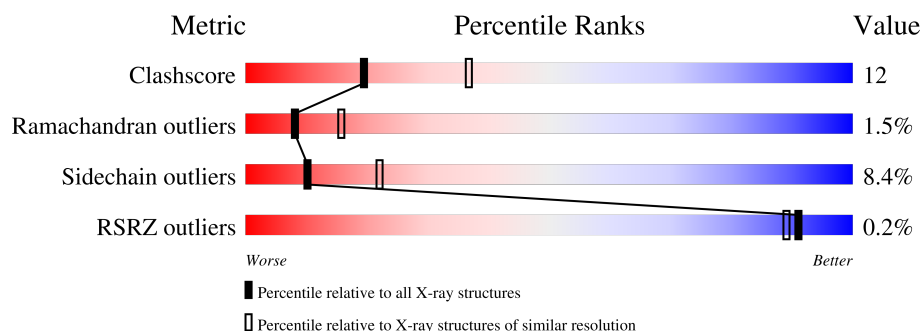
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	308	
1	B	308	

2 Entry composition [i](#)

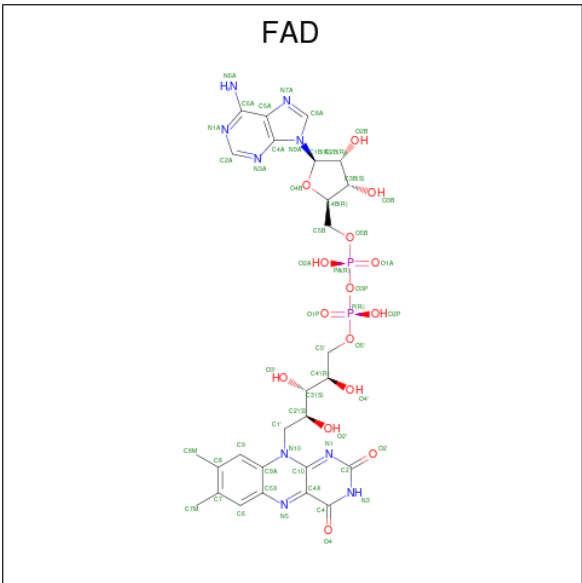
There are 3 unique types of molecules in this entry. The entry contains 5030 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (FERREDOXIN:NADP+ REDUCTASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2357	1510	388	443	16			
1	B	296	Total	C	N	O	S	0	0	0
			2357	1510	388	443	16			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

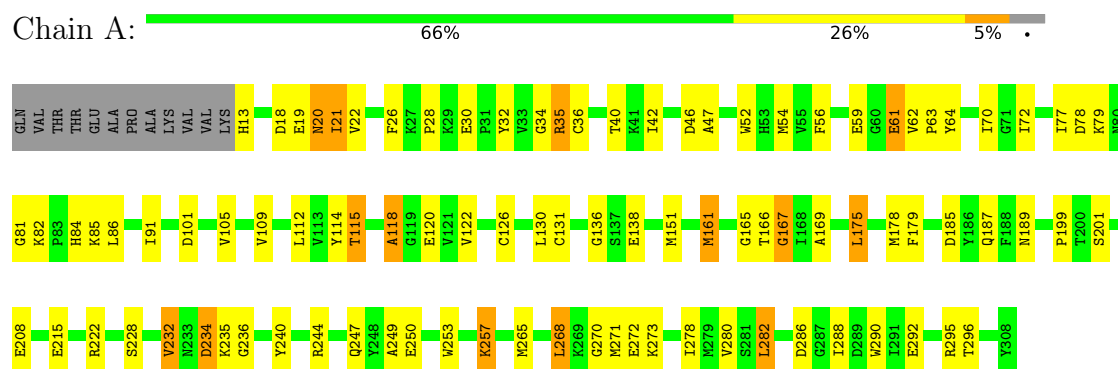
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	143	Total 143	O 143	0	0
3	B	67	Total 67	O 67	0	0

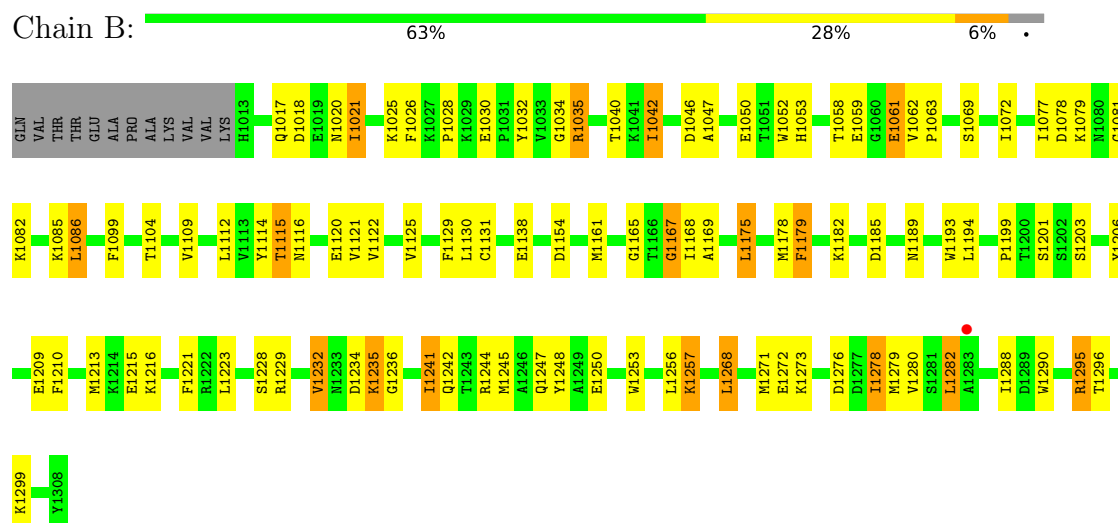
3 Residue-property plots

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: PROTEIN (FERREDOXIN:NADP+ REDUCTASE)



• Molecule 1: PROTEIN (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	73.90Å 94.10Å 140.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50 8.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	83.7 (8.00-2.50) 87.0 (8.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.39Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.218 , 0.273 0.222 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	59.4	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 93.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5030	wwPDB-VP
Average B, all atoms (Å ²)	57.0	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	0.83	2/2410 (0.1%)	1.17	21/3244 (0.6%)
1	B	0.80	1/2410 (0.0%)	1.19	22/3244 (0.7%)
All	All	0.82	3/4820 (0.1%)	1.18	43/6488 (0.7%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	MET	SD-CE	-6.94	1.62	1.79
1	B	1178	MET	SD-CE	-5.19	1.66	1.79
1	A	54	MET	SD-CE	-5.08	1.66	1.79

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1061	GLU	N-CA-C	9.32	121.44	111.28
1	B	1228	SER	N-CA-C	8.56	123.47	112.34
1	B	1062	VAL	CA-C-N	7.97	129.81	119.84
1	B	1062	VAL	C-N-CA	7.97	129.81	119.84
1	B	1125	VAL	N-CA-C	7.91	117.97	110.30
1	B	1179	PHE	N-CA-C	7.54	123.41	113.30
1	A	272	GLU	N-CA-C	7.31	119.25	111.28
1	A	62	VAL	CA-C-N	7.13	128.76	119.84
1	A	62	VAL	C-N-CA	7.13	128.76	119.84
1	A	47	ALA	CA-C-N	7.05	128.65	119.84
1	A	47	ALA	C-N-CA	7.05	128.65	119.84
1	A	61	GLU	N-CA-C	7.00	119.94	111.82
1	B	1129	PHE	N-CA-C	-6.87	103.72	111.14
1	A	175	LEU	N-CA-C	6.72	118.60	111.28
1	B	1047	ALA	CA-C-N	6.69	128.20	119.84
1	B	1047	ALA	C-N-CA	6.69	128.20	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	ALA	N-CA-C	6.65	121.90	113.25
1	A	118	ALA	N-CA-C	-6.57	105.25	113.20
1	B	1175	LEU	N-CA-C	6.45	118.31	111.28
1	A	228	SER	N-CA-C	6.29	120.05	112.38
1	B	1042	ILE	N-CA-C	6.27	118.13	112.17
1	B	1241	ILE	N-CA-C	6.27	117.02	110.62
1	A	179	PHE	N-CA-C	6.25	121.67	113.30
1	B	1050	GLU	N-CA-C	6.20	119.04	109.07
1	B	1272	GLU	N-CA-C	6.15	117.98	111.28
1	A	84	HIS	N-CA-C	6.00	118.93	110.23
1	B	1109	VAL	N-CA-C	5.85	116.72	108.36
1	B	1086	LEU	N-CA-C	5.85	117.60	110.41
1	A	167	GLY	N-CA-C	-5.83	108.26	114.67
1	A	109	VAL	N-CA-C	5.68	117.17	108.71
1	B	1169	ALA	N-CA-C	5.66	121.24	113.77
1	B	1121	VAL	CB-CA-C	-5.62	105.16	111.23
1	B	1167	GLY	N-CA-C	-5.39	108.73	114.67
1	A	270	GLY	N-CA-C	5.35	120.34	114.40
1	A	169	ALA	CA-C-N	-5.30	114.20	119.56
1	A	169	ALA	C-N-CA	-5.30	114.20	119.56
1	A	42	ILE	N-CA-C	5.29	117.19	112.17
1	A	85	LYS	N-CA-C	-5.29	103.41	110.55
1	B	1154	ASP	CA-C-N	5.19	126.33	119.84
1	B	1154	ASP	C-N-CA	5.19	126.33	119.84
1	B	1085	LYS	N-CA-C	-5.18	103.55	110.55
1	A	126	CYS	N-CA-C	5.18	116.73	111.14
1	A	240	TYR	N-CA-C	-5.04	103.28	110.59

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	2357	0	2349	51	0
1	B	2357	0	2349	59	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	53	0	31	2	0
2	B	53	0	31	4	0
3	A	143	0	0	6	0
3	B	67	0	0	2	0
All	All	5030	0	4760	111	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 12.

All (111) 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:B:1253:TRP:HB2	1:B:1282:LEU:HD11	1.52	0.89
1:A:253:TRP:HB2	1:A:282:LEU:HD11	1.53	0.88
1:B:1232:VAL:HG13	1:B:1236:GLY:HA2	1.54	0.88
1:B:1244:ARG:HH11	1:B:1247:GLN:HE22	1.22	0.86
1:A:232:VAL:HG13	1:A:236:GLY:HA2	1.57	0.85
1:B:1035:ARG:HG2	1:B:1035:ARG:HH11	1.42	0.84
1:B:1161:MET:HE1	1:B:1175:LEU:HD21	1.69	0.75
1:B:1035:ARG:HH11	1:B:1035:ARG:CG	2.01	0.73
1:B:1232:VAL:CG1	1:B:1236:GLY:HA2	2.18	0.73
1:A:292:GLU:HB2	3:A:2107:HOH:O	1.89	0.71
1:A:232:VAL:CG1	1:A:236:GLY:HA2	2.21	0.70
1:A:244:ARG:HH11	1:A:247:GLN:HE22	1.41	0.69
1:B:1244:ARG:NH1	1:B:1247:GLN:HE22	1.93	0.67
1:A:118:ALA:O	1:B:1229:ARG:NH1	2.28	0.67
1:B:1244:ARG:HH11	1:B:1247:GLN:NE2	1.90	0.67
1:B:1052:TRP:CD1	1:B:1131:CYS:HG	2.13	0.67
1:A:18:ASP:O	1:A:21:ILE:HG13	1.96	0.65
1:A:161:MET:HE1	1:A:175:LEU:HD21	1.77	0.65
1:A:28:PRO:HB3	1:A:86:LEU:HD23	1.80	0.62
1:B:1182:LYS:HB2	3:B:2106:HOH:O	2.01	0.60
1:B:1028:PRO:HB3	1:B:1086:LEU:HD23	1.85	0.59
1:B:1061:GLU:O	1:B:1063:PRO:HD3	2.02	0.59
1:B:1112:LEU:CD2	2:B:1309:FAD:H52A	2.33	0.58
1:B:1253:TRP:HZ2	1:B:1288:ILE:HD12	1.69	0.58
1:A:61:GLU:O	1:A:63:PRO:HD3	2.05	0.57
1:B:1032:TYR:OH	1:B:1059:GLU:HG2	2.05	0.56
1:B:1116:ASN:HB2	3:B:2083:HOH:O	2.03	0.56
1:B:1268:LEU:O	1:B:1271:MET:HG2	2.05	0.56
1:B:1114:TYR:O	1:B:1122:VAL:N	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1280:VAL:HA	1:B:1290:TRP:HB2	1.87	0.56
1:A:101:ASP:HB2	3:A:2068:HOH:O	2.05	0.55
1:B:1077:ILE:HG23	1:B:1081:GLY:C	2.31	0.55
1:B:1078:ASP:N	1:B:1082:LYS:O	2.36	0.54
1:B:1253:TRP:NE1	1:B:1257:LYS:HE3	2.22	0.54
1:B:1035:ARG:HG2	1:B:1035:ARG:NH1	2.16	0.53
1:A:253:TRP:HZ2	1:A:288:ILE:HD12	1.73	0.53
1:A:52:TRP:CD1	1:A:131:CYS:HG	2.27	0.52
1:A:187:GLN:HB2	3:A:2037:HOH:O	2.08	0.52
1:A:280:VAL:HA	1:A:290:TRP:HB2	1.90	0.52
1:A:114:TYR:O	1:A:122:VAL:N	2.42	0.52
1:A:77:ILE:HG23	1:A:81:GLY:C	2.35	0.51
1:A:115:THR:HA	1:A:120:GLU:O	2.11	0.51
1:B:1018:ASP:O	1:B:1021:ILE:HG13	2.11	0.51
2:B:1309:FAD:H3B	2:B:1309:FAD:H8A	1.91	0.51
1:A:244:ARG:HH11	1:A:247:GLN:NE2	2.09	0.50
1:B:1072:ILE:HG21	1:B:1130:LEU:HD21	1.93	0.49
1:B:1282:LEU:HD22	1:B:1282:LEU:O	2.11	0.49
1:B:1194:LEU:HD23	1:B:1223:LEU:CD1	2.42	0.49
1:A:78:ASP:N	1:A:82:LYS:O	2.36	0.49
1:B:1273:LYS:O	1:B:1276:ASP:HB2	2.12	0.49
1:A:282:LEU:HD22	1:A:282:LEU:O	2.12	0.49
1:A:265:MET:CG	1:A:271:MET:HE2	2.44	0.48
1:A:112:LEU:CD2	2:A:309:FAD:H52A	2.43	0.48
1:A:222:ARG:NH2	3:A:2012:HOH:O	2.43	0.48
1:A:244:ARG:NH1	1:A:247:GLN:HE22	2.11	0.48
1:A:165:GLY:C	1:A:167:GLY:H	2.22	0.47
1:A:22:VAL:HG11	1:A:63:PRO:CG	2.44	0.47
1:B:1179:PHE:CE2	1:B:1221:PHE:HB2	2.49	0.47
1:A:151:MET:CE	1:A:178:MET:HE3	2.44	0.47
1:A:265:MET:HG3	1:A:271:MET:HE2	1.96	0.47
1:A:32:TYR:OH	1:A:59:GLU:HG2	2.15	0.47
1:B:1209:GLU:O	1:B:1213:MET:HG3	2.15	0.47
1:B:1034:GLY:O	1:B:1138:GLU:HA	2.15	0.46
1:A:22:VAL:HG11	1:A:63:PRO:HG3	1.97	0.46
1:B:1025:LYS:HE2	1:B:1026:PHE:CZ	2.51	0.46
1:B:1086:LEU:C	1:B:1086:LEU:HD12	2.40	0.46
1:B:1042:ILE:HD13	1:B:1053:HIS:HB2	1.97	0.46
1:A:72:ILE:HG21	1:A:130:LEU:HD21	1.97	0.46
1:A:151:MET:HE3	1:A:178:MET:HE3	1.97	0.46
1:B:1112:LEU:HD21	2:B:1309:FAD:H52A	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1273:LYS:HA	1:B:1273:LYS:HD2	1.57	0.45
1:A:253:TRP:NE1	1:A:257:LYS:HE3	2.31	0.45
1:B:1165:GLY:C	1:B:1167:GLY:H	2.24	0.45
1:A:253:TRP:CZ2	1:A:288:ILE:HD12	2.50	0.45
1:A:257:LYS:HE2	1:A:286:ASP:OD2	2.16	0.45
1:A:34:GLY:O	1:A:138:GLU:HA	2.16	0.45
1:B:1052:TRP:CD1	1:B:1131:CYS:SG	3.09	0.45
1:A:112:LEU:HD21	2:A:309:FAD:H52A	1.98	0.45
1:B:1201:SER:C	1:B:1203:SER:H	2.24	0.44
1:B:1115:THR:HA	1:B:1120:GLU:O	2.17	0.44
1:A:26:PHE:CD2	1:A:32:TYR:HB2	2.51	0.44
1:A:36:CYS:O	1:A:136:GLY:N	2.40	0.44
1:A:268:LEU:HD13	1:A:268:LEU:N	2.33	0.44
1:B:1099:PHE:CD2	1:B:1104:THR:HG21	2.53	0.43
1:B:1253:TRP:CE3	1:B:1282:LEU:HD13	2.53	0.43
1:A:35:ARG:HG2	3:A:2098:HOH:O	2.17	0.43
1:A:273:LYS:HA	1:A:273:LYS:HD2	1.75	0.43
1:B:1241:ILE:O	1:B:1245:MET:HG3	2.19	0.43
1:A:56:PHE:HB2	1:A:105:VAL:HG12	2.00	0.42
1:A:268:LEU:N	1:A:268:LEU:CD1	2.81	0.42
1:B:1215:GLU:HG3	1:B:1216:LYS:N	2.34	0.42
1:A:35:ARG:CG	3:A:2098:HOH:O	2.68	0.42
1:A:165:GLY:O	1:A:167:GLY:N	2.52	0.42
1:B:1058:THR:O	1:B:1059:GLU:HG2	2.19	0.42
1:A:64:TYR:CD1	1:A:64:TYR:C	2.98	0.42
1:B:1114:TYR:CE1	1:B:1122:VAL:HB	2.55	0.41
1:B:1235:LYS:HD2	1:B:1235:LYS:H	1.85	0.41
1:B:1242:GLN:HB2	1:B:1278:ILE:HG13	2.02	0.41
1:B:1279:MET:HB3	1:B:1290:TRP:CE2	2.55	0.41
1:A:268:LEU:HD13	1:A:268:LEU:H	1.84	0.41
1:B:1194:LEU:HD23	1:B:1223:LEU:HD12	2.02	0.41
1:B:1165:GLY:O	1:B:1167:GLY:N	2.54	0.41
1:B:1206:TYR:HB2	1:B:1210:PHE:CE2	2.56	0.41
1:B:1165:GLY:C	1:B:1167:GLY:N	2.78	0.41
2:B:1309:FAD:H9	2:B:1309:FAD:H1'1	1.87	0.41
1:A:19:GLU:O	1:A:20:ASN:HB2	2.21	0.41
1:B:1256:LEU:HA	1:B:1256:LEU:HD23	1.89	0.40
1:B:1193:TRP:CZ2	1:B:1248:TYR:CD2	3.10	0.40
1:B:1253:TRP:HE1	1:B:1257:LYS:HE3	1.85	0.40
1:B:1295:ARG:HH12	1:B:1299:LYS:NZ	2.19	0.40
1:A:70:ILE:HG23	1:A:91:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	294/308 (96%)	271 (92%)	18 (6%)	5 (2%)	7	13
1	B	294/308 (96%)	272 (92%)	18 (6%)	4 (1%)	9	17
All	All	588/616 (96%)	543 (92%)	36 (6%)	9 (2%)	8	16

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	THR
1	A	199	PRO
1	A	20	ASN
1	B	1020	ASN
1	B	1199	PRO
1	A	234	ASP
1	B	1017	GLN
1	B	1234	ASP
1	A	249	ALA

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	257/267 (96%)	234 (91%)	23 (9%)	9	20
1	B	257/267 (96%)	237 (92%)	20 (8%)	11	24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	514/534 (96%)	471 (92%)	43 (8%)	10	22

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	21	ILE
1	A	30	GLU
1	A	35	ARG
1	A	40	THR
1	A	46	ASP
1	A	79	LYS
1	A	115	THR
1	A	185	ASP
1	A	189	ASN
1	A	201	SER
1	A	208	GLU
1	A	215	GLU
1	A	232	VAL
1	A	234	ASP
1	A	235	LYS
1	A	250	GLU
1	A	257	LYS
1	A	268	LEU
1	A	278	ILE
1	A	282	LEU
1	A	295	ARG
1	A	296	THR
1	B	1021	ILE
1	B	1030	GLU
1	B	1035	ARG
1	B	1040	THR
1	B	1046	ASP
1	B	1069	SER
1	B	1079	LYS
1	B	1115	THR
1	B	1168	ILE
1	B	1185	ASP
1	B	1189	ASN
1	B	1232	VAL
1	B	1235	LYS
1	B	1250	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1257	LYS
1	B	1268	LEU
1	B	1278	ILE
1	B	1282	LEU
1	B	1295	ARG
1	B	1296	THR

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	13	HIS
1	A	17	GLN
1	A	247	GLN
1	A	302	GLN
1	B	1017	GLN
1	B	1247	GLN
1	B	1302	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	B	1309	-	58,58,58	1.35	9 (15%)	85,89,89	0.95	4 (4%)
2	FAD	A	309	-	58,58,58	1.43	7 (12%)	85,89,89	0.92	3 (3%)

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	B	1309	-	-	3/34/50/50	0/6/6/6
2	FAD	A	309	-	-	1/34/50/50	0/6/6/6

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	309	FAD	P-O3P	-5.62	1.53	1.59
2	A	309	FAD	PA-O3P	-3.25	1.56	1.59
2	B	1309	FAD	P-O3P	-3.19	1.56	1.59
2	A	309	FAD	C4X-N5	3.12	1.37	1.30
2	B	1309	FAD	P-O2P	-2.88	1.42	1.55
2	B	1309	FAD	PA-O5B	-2.81	1.48	1.59
2	B	1309	FAD	C4X-N5	2.58	1.36	1.30
2	A	309	FAD	O5'-C5'	2.52	1.54	1.44
2	B	1309	FAD	C5'-C4'	2.49	1.55	1.51
2	B	1309	FAD	C4'-C3'	-2.27	1.49	1.53
2	B	1309	FAD	C10-N1	2.27	1.37	1.33
2	A	309	FAD	PA-O2A	-2.12	1.45	1.55
2	A	309	FAD	P-O2P	-2.09	1.45	1.55
2	B	1309	FAD	C1B-N9A	-2.08	1.40	1.46
2	A	309	FAD	P-O1P	-2.06	1.43	1.50
2	B	1309	FAD	C2B-C3B	-2.06	1.47	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	309	FAD	C5A-N7A-C8A	2.78	107.82	103.45
2	B	1309	FAD	C4A-C5A-N7A	-2.75	107.44	110.58
2	B	1309	FAD	C5A-N7A-C8A	2.72	107.72	103.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	309	FAD	C4A-C5A-N7A	-2.44	107.79	110.58
2	B	1309	FAD	C2B-C1B-N9A	-2.39	107.37	113.30
2	A	309	FAD	C4-N3-C2	-2.23	121.69	125.64
2	B	1309	FAD	C4-N3-C2	-2.04	122.03	125.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

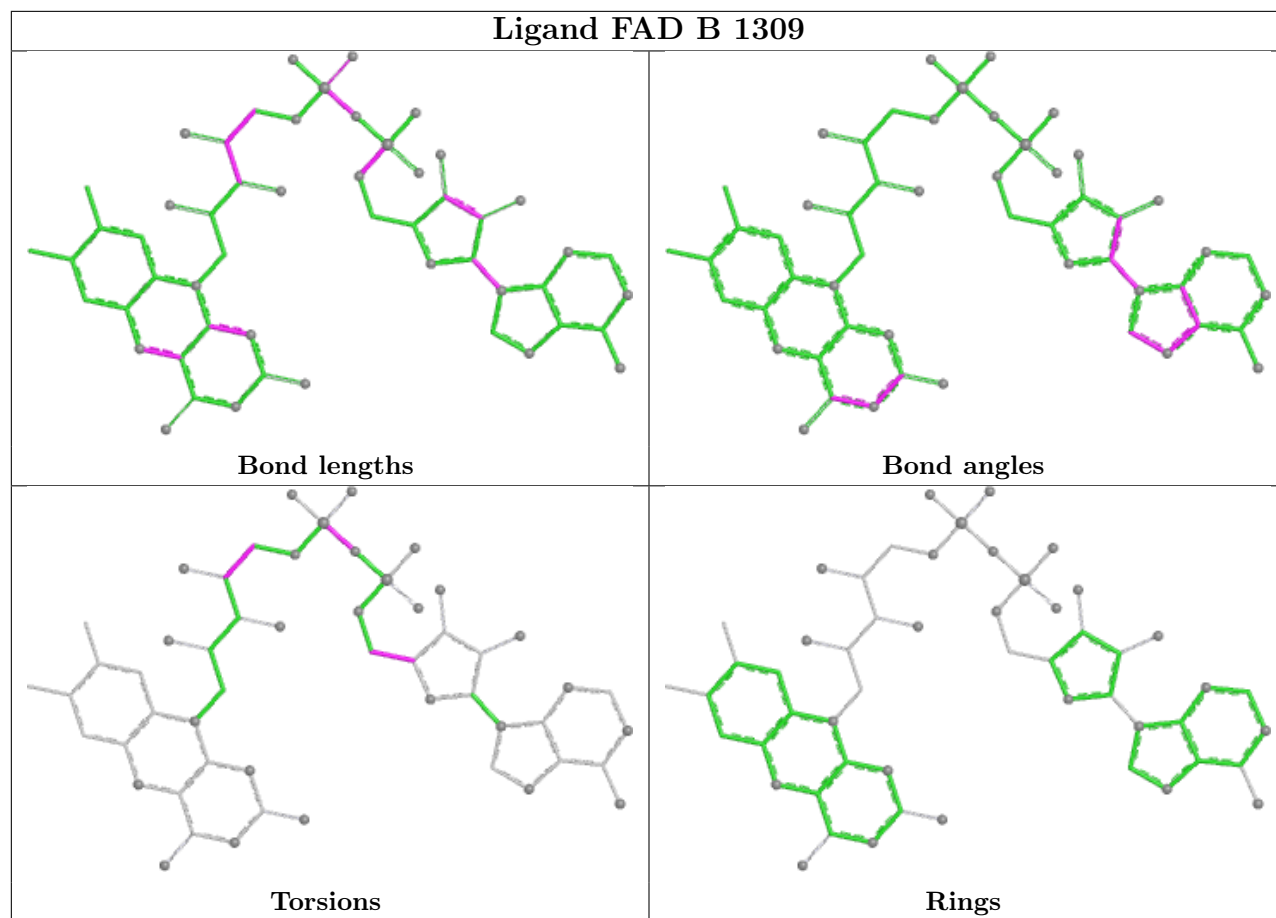
Mol	Chain	Res	Type	Atoms
2	A	309	FAD	C3'-C4'-C5'-O5'
2	B	1309	FAD	C3'-C4'-C5'-O5'
2	B	1309	FAD	C3B-C4B-C5B-O5B
2	B	1309	FAD	PA-O3P-P-O2P

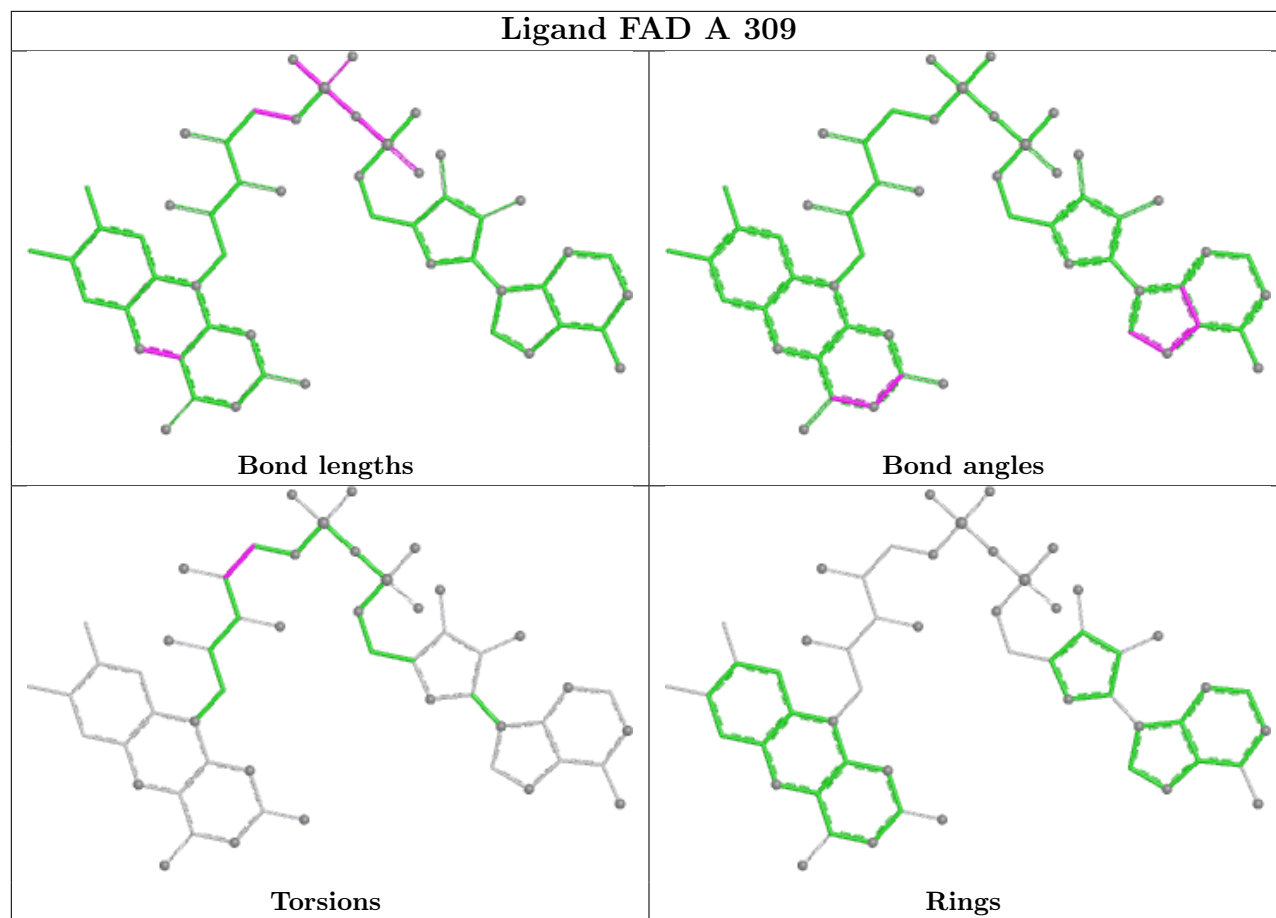
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1309	FAD	4	0
2	A	309	FAD	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 [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	296/308 (96%)	-0.65	0	100 100	30, 49, 86, 99	0
1	B	296/308 (96%)	-0.49	1 (0%)	90 87	32, 57, 89, 100	0
All	All	592/616 (96%)	-0.57	1 (0%)	91 89	30, 53, 88, 100	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1283	ALA	2.4

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.

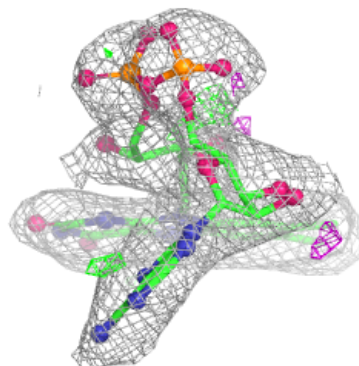
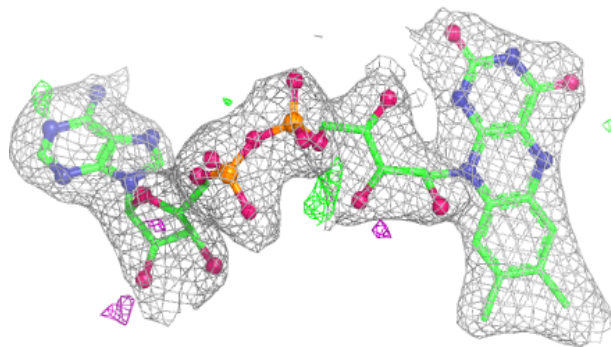
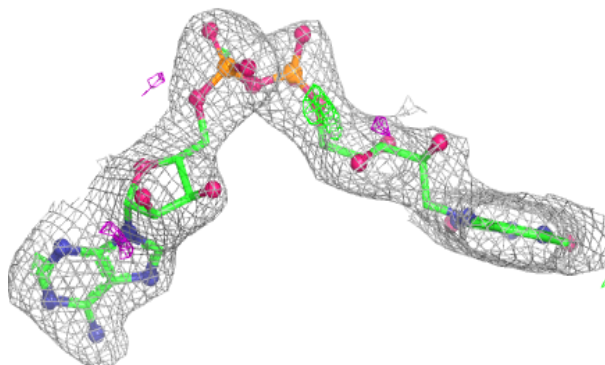
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
2	FAD	B	1309	53/53	0.94	0.06	29,44,72,78	0
2	FAD	A	309	53/53	0.97	0.05	28,40,67,74	0

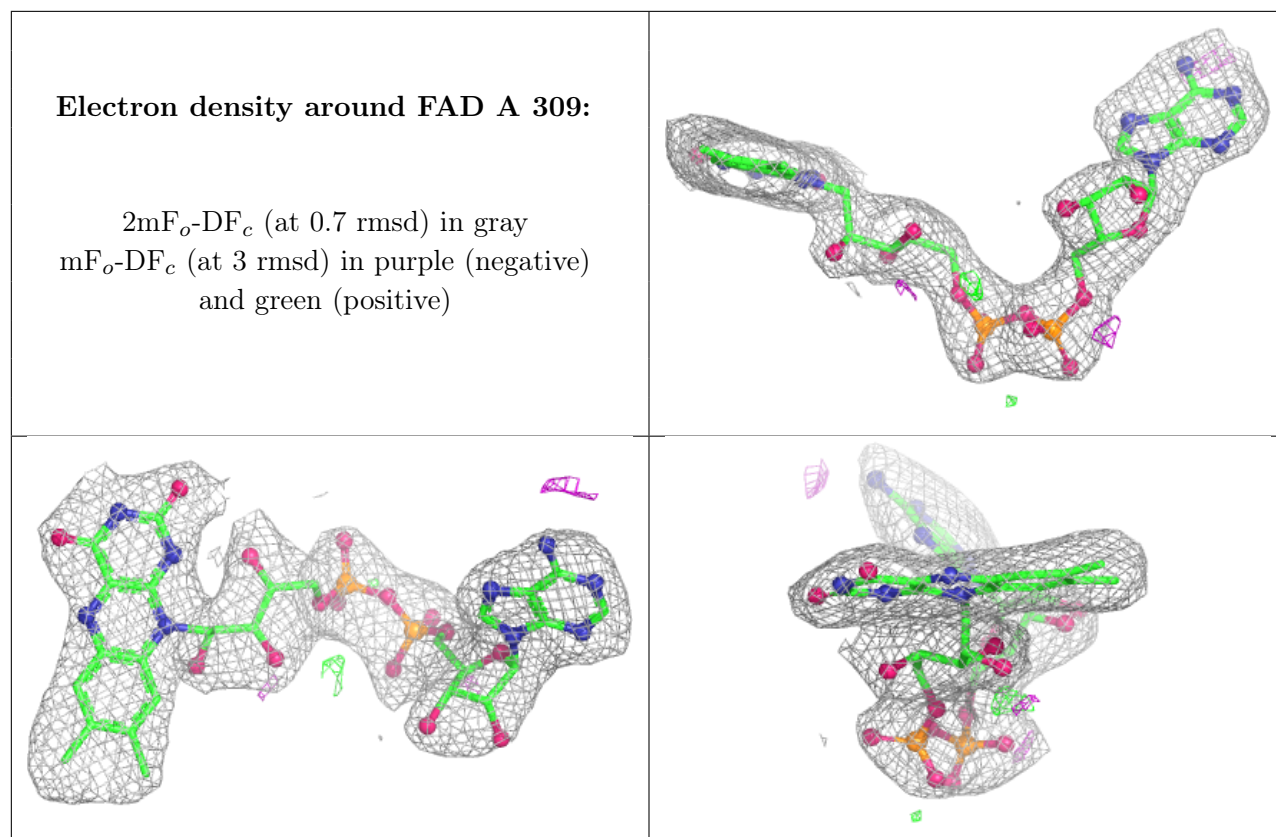
The following is a graphical depiction of the model fit to experimental electron density of all

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 B 1309:

$2mF_o-DF_c$ (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.