



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:12 AM UTC

PDB ID : 4IV9 / pdb_00004iv9
Title : Structure of the Flavoprotein Tryptophan-2-Monooxygenase
Authors : Gaweska, H.M.; Taylor, A.B.; Hart, P.J.; Fitzpatrick, P.F.
Deposited on : 2013-01-22
Resolution : 1.95 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

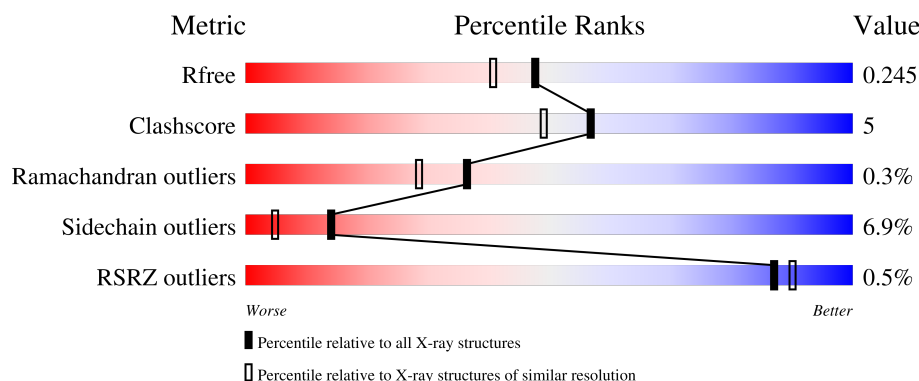
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	557	% 86% 11% ..
1	B	557	 82% 14% ...

2 Entry composition [i](#)

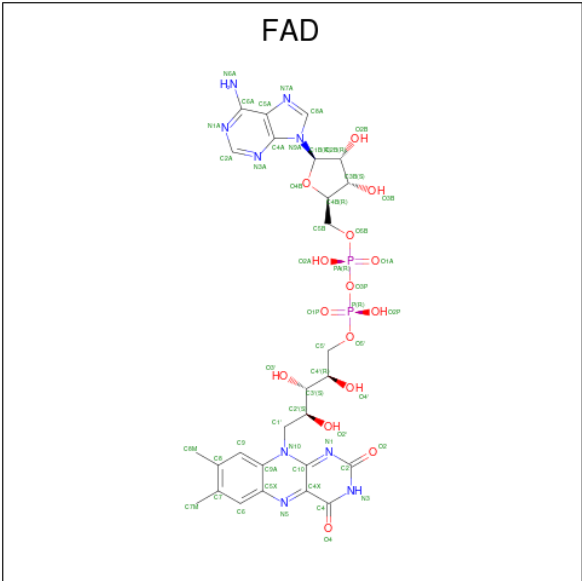
There are 6 unique types of molecules in this entry. The entry contains 9537 atoms, of which 0 are hydrogens and 0 are deuteriums.

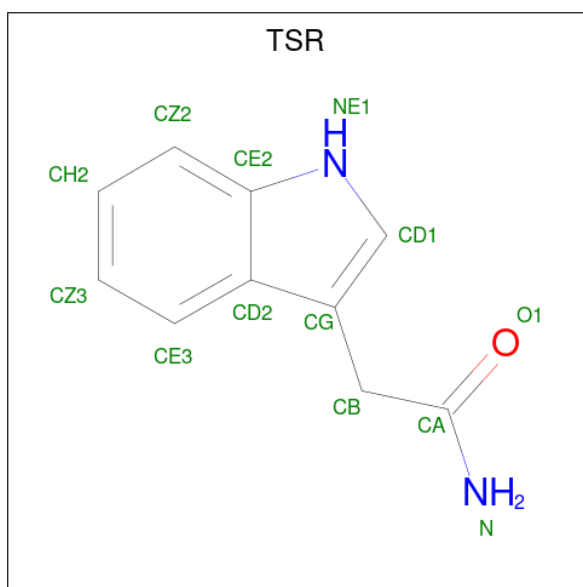
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tryptophan 2-monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	2	0
			4324	2750	753	800	21			
1	B	552	Total	C	N	O	S	0	1	0
			4320	2747	753	799	21			

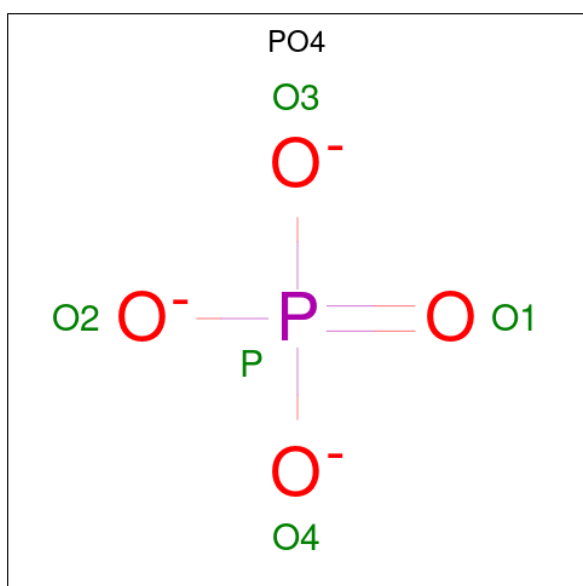
- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).





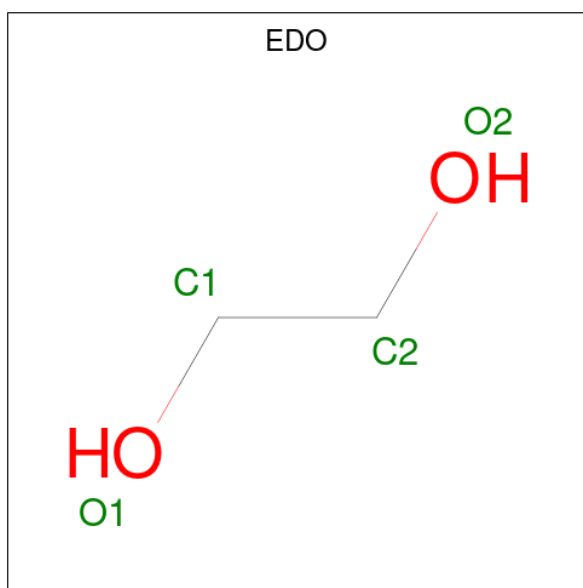
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			13	10	2	1		
3	B	1	Total	C	N	O	0	0
			13	10	2	1		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	394	Total	O	0	0
			394	394		
6	B	353	Total	O	0	0
			353	353		

- Molecule 1: Tryptophan 2-monooxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	111.14Å 122.21Å 76.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.03 – 1.95 28.03 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.4 (28.03-1.95) 99.4 (28.03-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1161)	Depositor
R, R_{free}	0.187 , 0.245 0.189 , 0.245	Depositor DCC
R_{free} test set	3809 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9537	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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: EDO, PO4, FAD, TSR

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	0.48	1/4439 (0.0%)	0.82	4/6019 (0.1%)
1	B	0.49	1/4431 (0.0%)	0.84	5/6007 (0.1%)
All	All	0.49	2/8870 (0.0%)	0.83	9/12026 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	425	MET	CA-CB	5.73	1.56	1.52
1	B	425	MET	CA-CB	5.28	1.56	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	GLY	N-CA-C	-8.78	102.99	114.85
1	B	424	ALA	N-CA-C	-6.73	101.64	110.53
1	A	424	ALA	N-CA-C	-6.25	102.47	110.53
1	B	317	GLY	N-CA-C	-6.22	106.53	114.37
1	B	380	LEU	N-CA-C	5.53	117.76	110.36
1	A	10	ILE	N-CA-C	5.47	116.20	110.62
1	A	380	LEU	N-CA-C	5.39	117.34	109.84
1	B	499	SER	CA-C-N	5.04	125.32	119.47
1	B	499	SER	C-N-CA	5.04	125.32	119.47

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	4324	0	4247	33	0
1	B	4320	0	4247	47	0
2	A	53	0	31	2	0
2	B	53	0	31	5	0
3	A	13	0	10	0	0
3	B	13	0	10	0	0
4	A	10	0	0	0	0
5	A	4	0	6	0	0
6	A	394	0	0	5	0
6	B	353	0	0	5	0
All	All	9537	0	8582	79	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 5.

All (79) 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:341:THR:HG23	1:B:352:ALA:HB1	1.49	0.92
1:B:477:LYS:HG3	1:B:517:GLY:HA3	1.78	0.64
1:B:42:ALA:HB3	1:B:325:VAL:HG22	1.79	0.64
1:B:379:LYS:HG2	1:B:380:LEU:HD13	1.80	0.63
1:B:523:ALA:HB2	2:B:601:FAD:H5'2	1.79	0.63
1:A:13:LEU:HD11	1:A:191:ALA:HB2	1.78	0.63
1:B:25:MET:HB3	1:B:26:THR:HG23	1.80	0.63
1:B:145:LYS:NZ	6:B:914:HOH:O	2.33	0.60
1:B:353:ARG:NH1	1:B:486:TYR:OH	2.34	0.60
1:B:96:ALA:HA	2:B:601:FAD:C4X	2.33	0.58
1:B:86:THR:HG22	1:B:87:ARG:HG3	1.84	0.58
1:A:310:ILE:HD12	1:A:346:PHE:HE1	1.69	0.58
1:B:312:ILE:HD11	1:B:325:VAL:HG21	1.87	0.57
1:A:78:VAL:HG13	1:A:274:ILE:HG23	1.86	0.56
1:B:378:ASN:HB2	1:B:380:LEU:HD22	1.88	0.56
1:B:20:LEU:HD21	1:B:528:LEU:HD11	1.88	0.56
1:A:299:ARG:NH2	1:A:337:ILE:HD12	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ARG:HH21	1:A:337:ILE:HD12	1.71	0.55
1:A:391:ARG:NH2	1:B:357:GLU:OE2	2.37	0.55
1:B:214:PHE:CE1	1:B:220:PRO:HG2	2.42	0.55
1:B:215:THR:HA	1:B:224:ARG:HG3	1.89	0.55
1:A:138:TYR:CZ	1:A:149:LEU:HD12	2.44	0.53
1:A:429:LYS:HB2	6:A:1028:HOH:O	2.07	0.53
1:A:477:LYS:HG3	1:A:517:GLY:HA3	1.91	0.52
1:A:96:ALA:HA	2:A:601:FAD:C4X	2.40	0.52
1:A:305:ARG:NH1	1:A:504:THR:O	2.43	0.51
1:B:318:GLU:HG2	1:B:320:ARG:NH1	2.26	0.50
1:A:299:ARG:NH1	6:A:1041:HOH:O	2.43	0.50
1:B:518:GLY:C	2:B:601:FAD:H1'2	2.37	0.50
1:B:341:THR:HG21	1:B:356:ARG:CD	2.42	0.49
1:B:341:THR:O	1:B:341:THR:HG22	2.12	0.49
1:A:378:ASN:HB2	1:A:380:LEU:HD22	1.94	0.49
1:B:341:THR:HG21	1:B:356:ARG:HG3	1.95	0.49
1:B:177:ASP:O	1:B:181:MET:HG3	2.13	0.48
1:B:391:ARG:HD2	1:B:418:ASP:OD2	2.13	0.48
1:B:341:THR:HG21	1:B:356:ARG:HD3	1.96	0.48
1:B:339:CYS:HB3	1:B:342:ASP:OD2	2.14	0.47
1:A:391:ARG:HE	1:A:418:ASP:CG	2.22	0.47
1:A:477:LYS:HG2	1:A:512:SER:HA	1.97	0.47
1:B:335:GLN:CD	1:B:356:ARG:HG2	2.40	0.47
1:A:367:PHE:CZ	1:A:410:LEU:HD13	2.50	0.46
1:B:77:ARG:O	1:B:95:GLY:HA3	2.14	0.46
1:B:13:LEU:HD11	1:B:191:ALA:HB2	1.98	0.46
1:B:71:ARG:NH2	1:B:469:ASP:OD1	2.42	0.46
1:A:375:TRP:CD2	1:A:395:CYS:HB3	2.51	0.45
1:B:521:GLU:O	1:B:525:GLN:HG3	2.17	0.45
1:A:390:VAL:HG22	1:A:411:LEU:O	2.17	0.45
1:B:300:VAL:HG13	1:B:312:ILE:HG23	1.98	0.45
1:A:421:LYS:HE2	1:B:332:ARG:NH1	2.32	0.44
1:B:371:ARG:HD2	6:B:1021:HOH:O	2.18	0.44
1:B:374:PHE:HA	1:B:377:LYS:HE2	1.99	0.44
1:A:63:LYS:HE3	1:A:63:LYS:HB3	1.78	0.44
1:B:293:ASP:OD2	6:B:842:HOH:O	2.21	0.44
1:A:49:SER:HB2	1:A:523:ALA:HB1	1.99	0.44
1:A:341:THR:HG21	1:A:356:ARG:HD3	1.98	0.44
1:B:103:ALA:HB1	1:B:521:GLU:HB2	2.00	0.44
1:A:8:PRO:O	1:A:182:LEU:HG	2.18	0.44
1:A:425:MET:HE1	1:A:434:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:ALA:O	1:B:425:MET:HG2	2.18	0.43
1:A:518:GLY:C	2:A:601:FAD:H1'2	2.42	0.43
1:B:78:VAL:HG13	1:B:274:ILE:HG23	2.01	0.43
1:A:24:GLU:O	1:A:59:ARG:NH2	2.52	0.42
1:B:299:ARG:NH2	1:B:337:ILE:HD12	2.34	0.42
1:B:238:GLY:HA3	1:B:242:GLY:O	2.18	0.42
1:B:459:ARG:NH1	6:B:943:HOH:O	2.28	0.42
1:A:40:ARG:HG2	1:A:322:PHE:CD1	2.55	0.42
1:A:377:LYS:HE3	6:A:1001:HOH:O	2.19	0.42
1:A:256:LEU:HD12	1:A:256:LEU:HA	1.92	0.42
1:B:8:PRO:O	1:B:182:LEU:HG	2.19	0.41
1:B:523:ALA:CB	2:B:601:FAD:H5'2	2.49	0.41
2:B:601:FAD:HM73	2:B:601:FAD:HM81	1.84	0.41
1:A:232:GLU:OE2	6:A:1054:HOH:O	2.21	0.41
1:B:369:LEU:O	1:B:453:VAL:HG23	2.21	0.41
1:A:167:LEU:HB3	6:A:983:HOH:O	2.20	0.41
1:B:283:ASP:OD1	1:B:292:ARG:NH1	2.43	0.41
1:A:429:LYS:HG2	1:A:457:TYR:CG	2.55	0.41
1:B:21:LYS:NZ	6:B:851:HOH:O	2.53	0.41
1:B:282:ALA:HA	1:B:291:LEU:HB3	2.04	0.40
1:A:207:TYR:O	1:A:211:VAL:HG23	2.21	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	552/557 (99%)	537 (97%)	14 (2%)	1 (0%)	43	36
1	B	551/557 (99%)	534 (97%)	15 (3%)	2 (0%)	30	21
All	All	1103/1114 (99%)	1071 (97%)	29 (3%)	3 (0%)	36	28

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	391	ARG
1	B	318	GLU
1	B	391	ARG

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	459/462 (99%)	430 (94%)	29 (6%)	16	6
1	B	458/462 (99%)	424 (93%)	34 (7%)	13	4
All	All	917/924 (99%)	854 (93%)	63 (7%)	14	5

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	LYS
1	A	65	VAL
1	A	66	VAL
1	A	74	ILE
1	A	119	THR
1	A	120	THR
1	A	149	LEU
1	A	160	LEU
1	A	167	LEU
1	A	182	LEU
1	A	223	ASP
1	A	256	LEU
1	A	269	LEU
1	A	289	LYS
1	A	291	LEU
1	A	309	LYS
1	A	315	GLU
1	A	341	THR
1	A	379	LYS
1	A	380	LEU

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Mol	Chain	Res	Type
1	A	390	VAL
1	A	396	LEU
1	A	420	GLN
1	A	458	GLU
1	A	459	ARG
1	A	477	LYS
1	A	478	LEU
1	A	535	LEU
1	A	541	GLN
1	B	9	SER
1	B	25	MET
1	B	65	VAL
1	B	66	VAL
1	B	74	ILE
1	B	86	THR
1	B	119	THR
1	B	149	LEU
1	B	171	SER
1	B	182	LEU
1	B	256	LEU
1	B	280	ARG
1	B	291	LEU
1	B	309	LYS
1	B	312	ILE
1	B	318	GLU
1	B	319	GLN
1	B	321	VAL
1	B	358	THR
1	B	371	ARG
1	B	377	LYS
1	B	379	LYS
1	B	380	LEU
1	B	390	VAL
1	B	391	ARG
1	B	396	LEU
1	B	404	GLU
1	B	420	GLN
1	B	429	LYS
1	B	442	ILE
1	B	477	LYS
1	B	478	LEU
1	B	501	ASN

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Mol	Chain	Res	Type
1	B	541	GLN

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	81	GLN
1	A	85	GLN
1	A	208	ASN
1	A	218	HIS
1	A	249	GLN
1	A	319	GLN
1	A	399	GLN
1	B	108	HIS
1	B	385	GLN
1	B	406	HIS

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](#)

7 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	601	-	58,58,58	1.90	13 (22%)	85,89,89	1.67	18 (21%)
3	TSR	A	602	-	14,14,14	1.63	3 (21%)	19,19,19	1.06	1 (5%)
4	PO4	A	604	-	4,4,4	1.16	0	6,6,6	0.74	0
3	TSR	B	602	-	14,14,14	1.70	3 (21%)	19,19,19	1.12	2 (10%)
5	EDO	A	605	-	3,3,3	0.52	0	2,2,2	0.33	0
4	PO4	A	603	-	4,4,4	0.62	0	6,6,6	0.47	0
2	FAD	B	601	-	58,58,58	1.90	12 (20%)	85,89,89	1.66	17 (20%)

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	601	-	-	7/34/50/50	0/6/6/6
3	TSR	B	602	-	-	0/4/4/4	0/2/2/2
5	EDO	A	605	-	-	1/1/1/1	-
3	TSR	A	602	-	-	0/4/4/4	0/2/2/2
2	FAD	B	601	-	-	8/34/50/50	0/6/6/6

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C8M-C8	-6.52	1.38	1.51
2	A	601	FAD	C7M-C7	-6.19	1.39	1.51
2	B	601	FAD	C7M-C7	-6.13	1.39	1.51
2	B	601	FAD	C8M-C8	-6.10	1.39	1.51
2	A	601	FAD	C9A-N10	-3.73	1.34	1.41
2	B	601	FAD	C9A-N10	-3.68	1.34	1.41
2	B	601	FAD	C5A-N7A	-3.66	1.32	1.39
3	B	602	TSR	CA-N	3.44	1.43	1.32
2	A	601	FAD	C5A-N7A	-3.31	1.33	1.39
2	B	601	FAD	C10-N1	3.25	1.39	1.33
2	B	601	FAD	C5A-C4A	-3.21	1.33	1.39
3	A	602	TSR	CA-N	3.17	1.43	1.32
2	B	601	FAD	C8A-N9A	-3.00	1.32	1.37
2	A	601	FAD	C5A-C4A	-2.93	1.33	1.39
2	A	601	FAD	C8A-N9A	-2.92	1.32	1.37
2	B	601	FAD	C2A-N1A	2.90	1.39	1.33
3	A	602	TSR	CD2-CE2	-2.81	1.37	1.41
2	A	601	FAD	C2A-N1A	2.79	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C2A-N3A	2.79	1.38	1.33
2	A	601	FAD	C10-N1	2.79	1.38	1.33
2	A	601	FAD	C5X-N5	-2.73	1.34	1.39
2	B	601	FAD	C2A-N3A	2.70	1.38	1.33
2	B	601	FAD	C5X-N5	-2.70	1.34	1.39
3	B	602	TSR	CD2-CE2	-2.62	1.38	1.41
2	A	601	FAD	C5A-C6A	-2.62	1.33	1.41
3	B	602	TSR	CB-CA	-2.61	1.49	1.52
2	B	601	FAD	C5A-C6A	-2.54	1.33	1.41
2	B	601	FAD	C4A-N9A	-2.52	1.32	1.37
2	A	601	FAD	C4A-N9A	-2.45	1.32	1.37
3	A	602	TSR	CB-CA	-2.43	1.50	1.52
2	A	601	FAD	P-O2P	-2.13	1.45	1.55

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	N3A-C2A-N1A	-6.70	118.44	128.58
2	A	601	FAD	N3A-C2A-N1A	-6.45	118.81	128.58
2	B	601	FAD	C5A-C4A-N3A	-4.45	120.59	126.72
2	B	601	FAD	N9A-C8A-N7A	-4.33	107.79	113.94
2	A	601	FAD	C5A-C4A-N3A	-4.25	120.87	126.72
2	A	601	FAD	N9A-C8A-N7A	-4.12	108.09	113.94
2	B	601	FAD	C2A-N3A-C4A	3.29	119.87	111.83
2	B	601	FAD	C5A-N7A-C8A	3.29	108.62	103.45
2	A	601	FAD	C4-N3-C2	-3.17	120.02	125.64
2	A	601	FAD	C5A-N7A-C8A	3.11	108.34	103.45
2	A	601	FAD	C2A-N3A-C4A	3.10	119.41	111.83
2	A	601	FAD	C5'-C4'-C3'	-3.01	106.55	112.22
2	B	601	FAD	C4A-C5A-N7A	-2.92	107.24	110.58
2	A	601	FAD	C4X-C10-N10	2.85	120.56	116.48
3	A	602	TSR	CB-CA-N	2.81	119.60	116.75
2	A	601	FAD	C4A-C5A-N7A	-2.77	107.42	110.58
2	B	601	FAD	C10-C4X-N5	-2.77	119.16	124.81
2	A	601	FAD	C10-C4X-N5	-2.72	119.25	124.81
2	B	601	FAD	C6A-C5A-C4A	2.69	120.86	117.18
2	A	601	FAD	C9A-C5X-N5	-2.69	119.60	122.45
2	B	601	FAD	C4-N3-C2	-2.58	121.06	125.64
2	B	601	FAD	C9A-C5X-N5	-2.55	119.75	122.45
2	B	601	FAD	C4X-C10-N10	2.53	120.11	116.48
2	B	601	FAD	C5A-C6A-N6A	-2.51	117.06	123.29
2	A	601	FAD	C5A-C6A-N6A	-2.51	117.07	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	TSR	CB-CA-N	2.50	119.28	116.75
2	A	601	FAD	C4X-C4-N3	2.48	119.58	113.25
2	B	601	FAD	C4X-C4-N3	2.48	119.57	113.25
3	B	602	TSR	CZ2-CE2-CD2	-2.37	119.90	122.19
2	A	601	FAD	N3A-C4A-N9A	2.36	131.18	127.17
2	A	601	FAD	C4A-N9A-C8A	2.35	108.20	105.74
2	A	601	FAD	C6A-C5A-C4A	2.33	120.36	117.18
2	B	601	FAD	C5A-C4A-N9A	2.31	108.33	105.81
2	B	601	FAD	N3A-C4A-N9A	2.30	131.07	127.17
2	B	601	FAD	C4A-N9A-C8A	2.17	108.02	105.74
2	A	601	FAD	C5X-C9A-N10	2.15	119.91	117.97
2	B	601	FAD	C4-C4X-N5	2.13	121.15	118.21
2	A	601	FAD	O4-C4-C4X	-2.09	121.02	126.53

There are no chirality outliers.

All (16) torsion outliers are listed below:

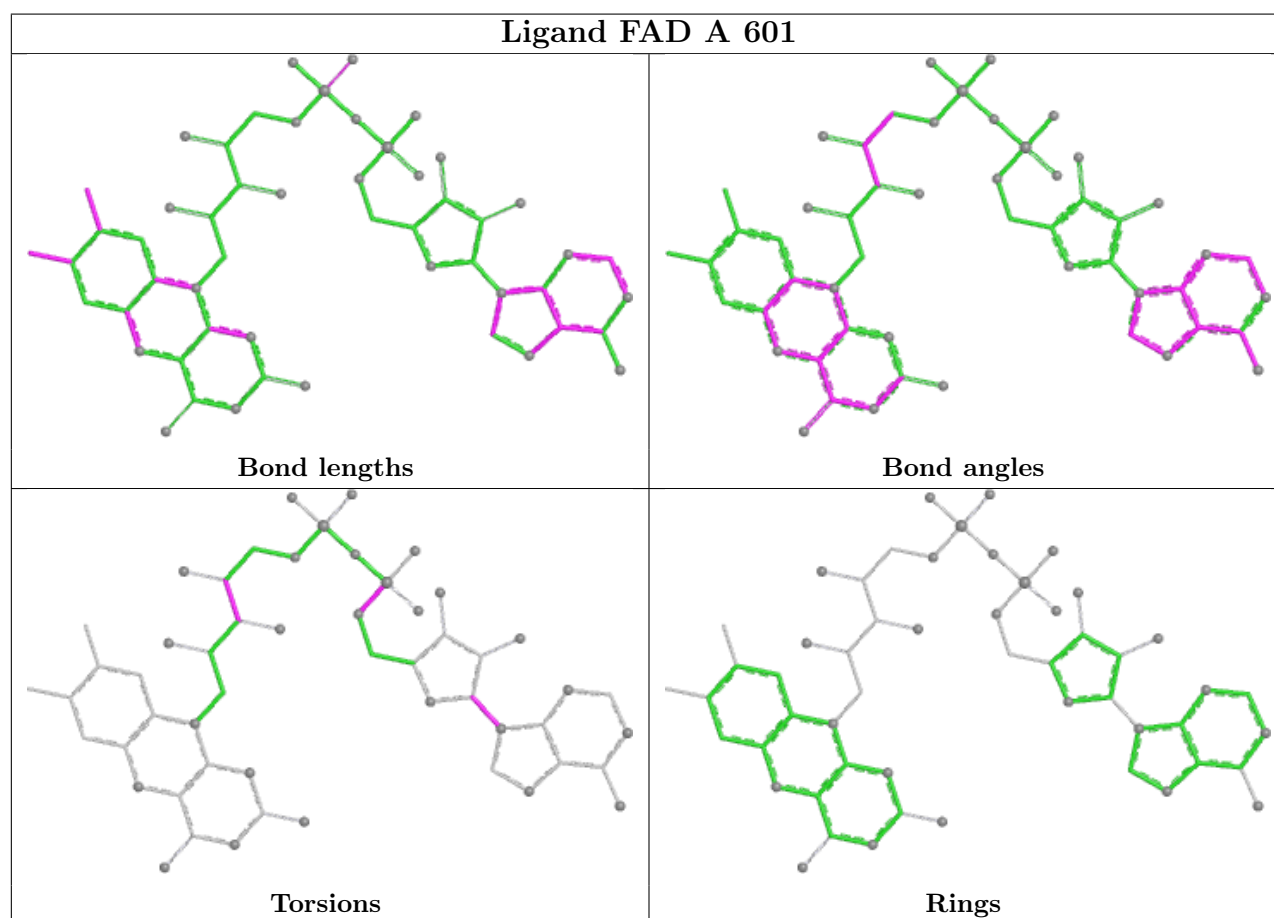
Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C5B-O5B-PA-O2A
2	B	601	FAD	C3'-C4'-C5'-O5'
2	B	601	FAD	O4'-C4'-C5'-O5'
2	B	601	FAD	C5'-O5'-P-O1P
2	B	601	FAD	C5'-O5'-P-O2P
2	B	601	FAD	C5'-O5'-P-O3P
5	A	605	EDO	O1-C1-C2-O2
2	A	601	FAD	C2'-C3'-C4'-C5'
2	A	601	FAD	C2'-C3'-C4'-O4'
2	B	601	FAD	PA-O3P-P-O5'
2	A	601	FAD	C5B-O5B-PA-O1A
2	A	601	FAD	C5B-O5B-PA-O3P
2	A	601	FAD	C2B-C1B-N9A-C8A
2	A	601	FAD	O3'-C3'-C4'-C5'
2	B	601	FAD	C2B-C1B-N9A-C8A
2	B	601	FAD	O4B-C4B-C5B-O5B

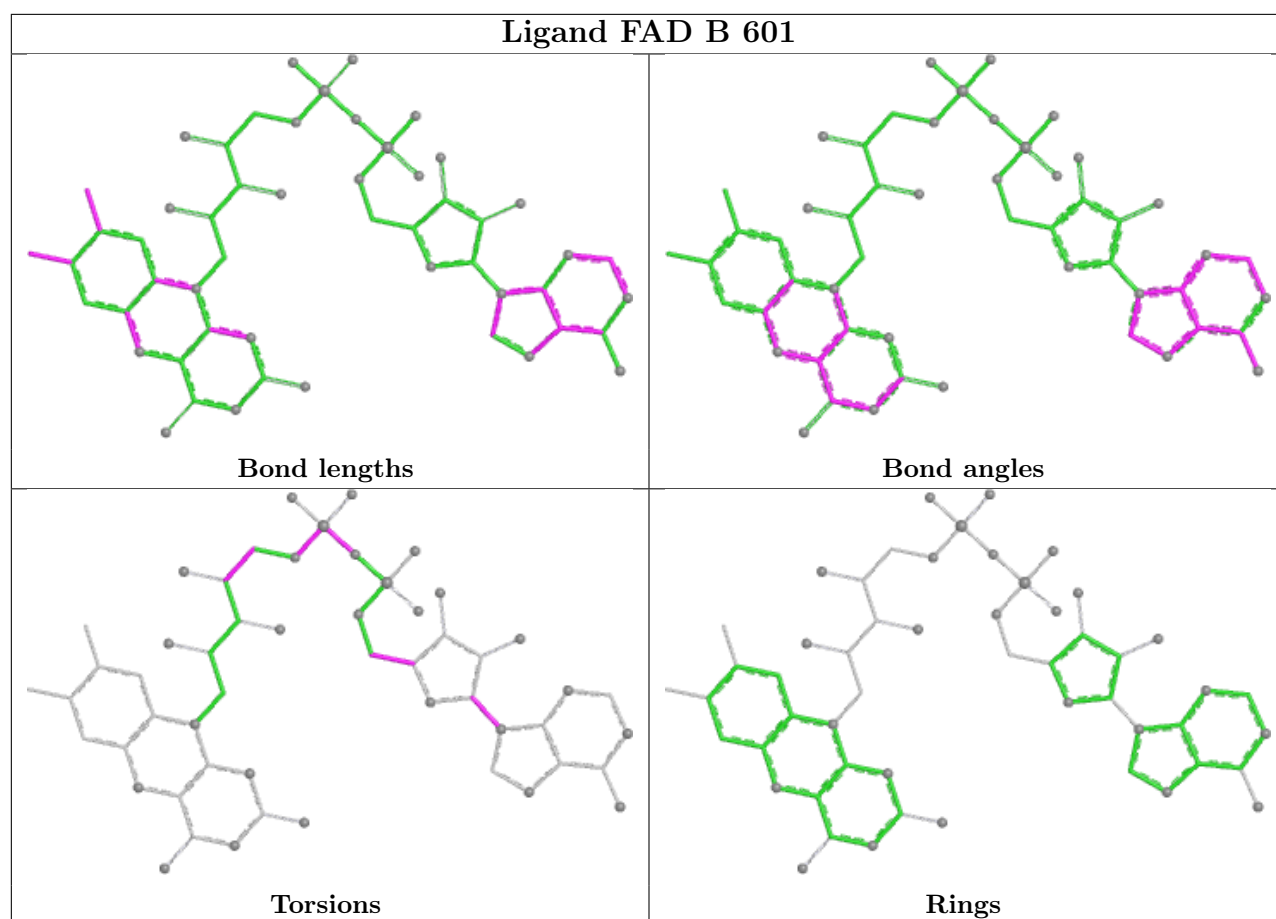
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FAD	2	0
2	B	601	FAD	5	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	552/557 (99%)	-0.51	3 (0%)	87 90	7, 13, 24, 43	2 (0%)
1	B	552/557 (99%)	-0.43	2 (0%)	88 91	7, 14, 26, 44	1 (0%)
All	All	1104/1114 (99%)	-0.47	5 (0%)	87 90	7, 13, 25, 44	3 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	379	LYS	3.0
1	B	169	GLY	2.8
1	B	25	MET	2.7
1	A	315	GLU	2.3
1	A	316	ALA	2.2

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](#)

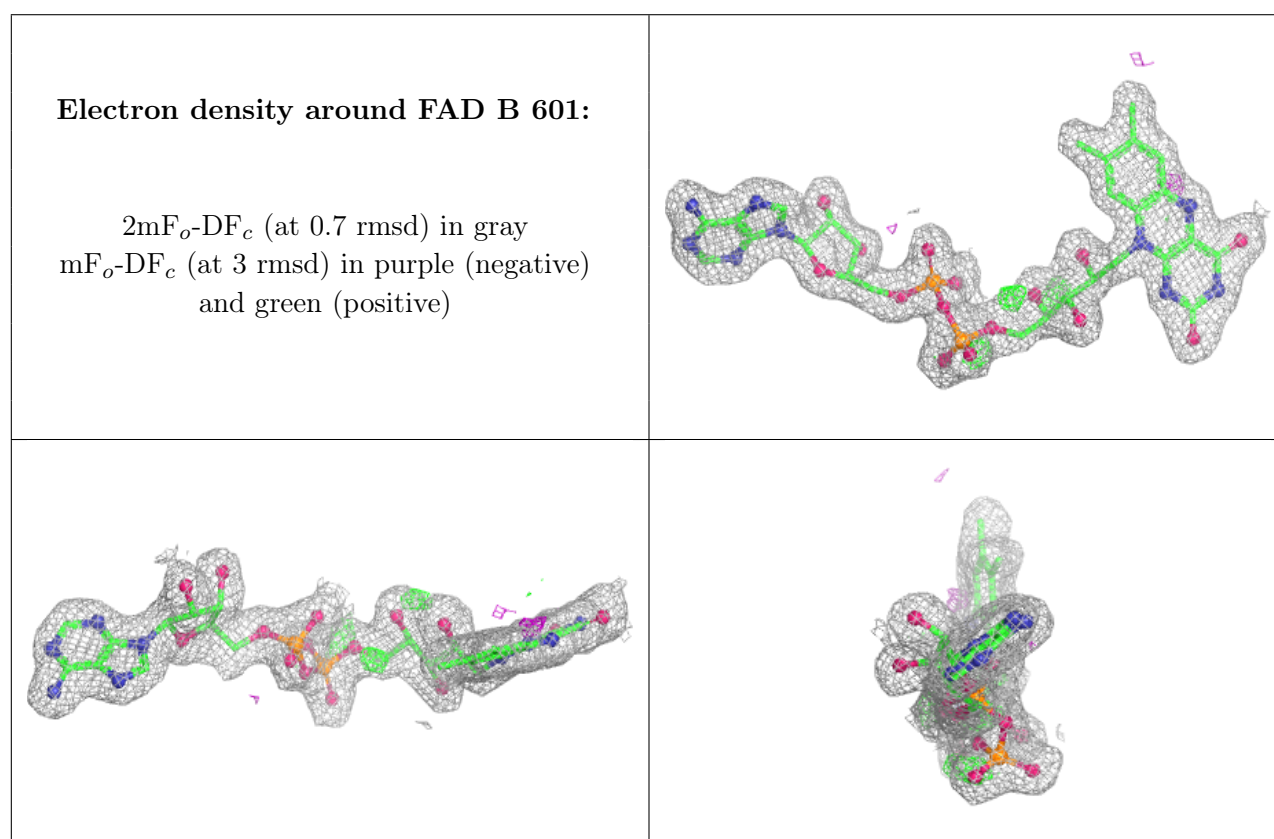
There are no oligosaccharides in this entry.

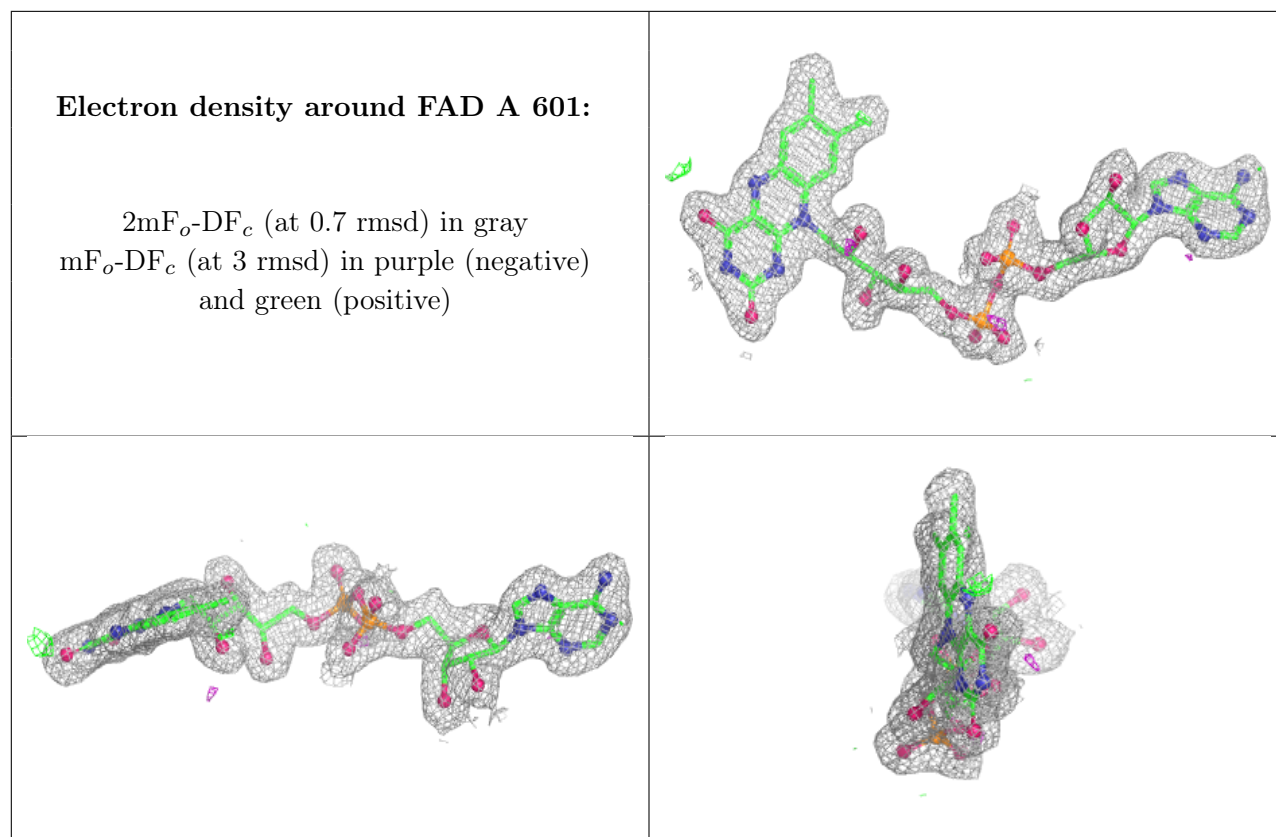
6.4 Ligands [i](#)

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
5	EDO	A	605	4/4	0.82	0.13	18,27,29,32	0
4	PO4	A	604	5/5	0.89	0.09	29,38,49,52	0
4	PO4	A	603	5/5	0.92	0.08	30,32,39,47	0
3	TSR	B	602	13/13	0.95	0.06	8,10,12,13	0
3	TSR	A	602	13/13	0.95	0.05	7,10,13,15	0
2	FAD	B	601	53/53	0.97	0.05	7,9,13,15	0
2	FAD	A	601	53/53	0.97	0.05	5,9,14,17	0

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





6.5 Other polymers [i](#)

There are no such residues in this entry.