



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2025 – 10:09 PM JST

PDB ID : 8ZB2
Title : L-Methionine oxidase from Burkholderiales bacterium
Authors : Kawamura, Y.; Chisuga, T.; Nakano, S.
Deposited on : 2024-04-26
Resolution : 2.69 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.21
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.2

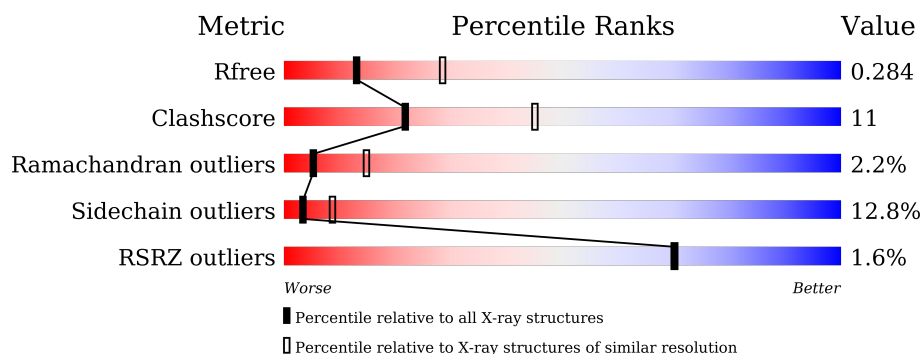
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


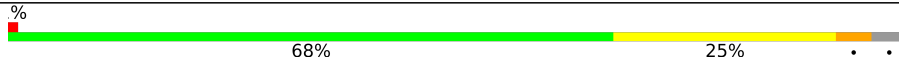
The reported resolution of this entry is 2.69 Å.

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}	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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	506	
1	B	506	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FAD	A	601	X	-	-	-
2	FAD	B	601	X	-	-	-

2 Entry composition [i](#)

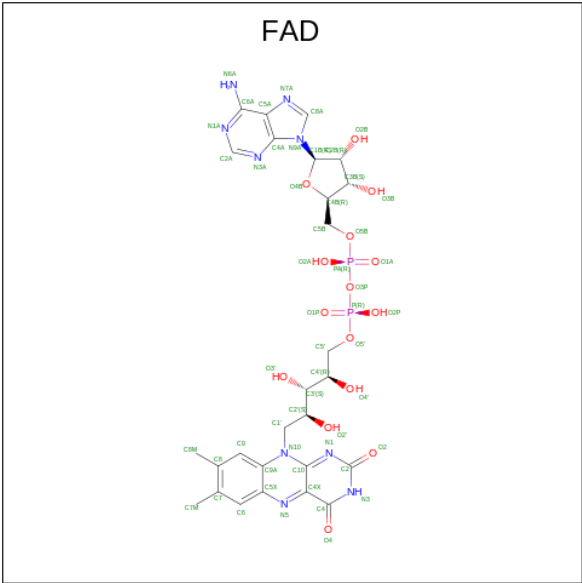
There are 3 unique types of molecules in this entry. The entry contains 7751 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FAD-binding protein.

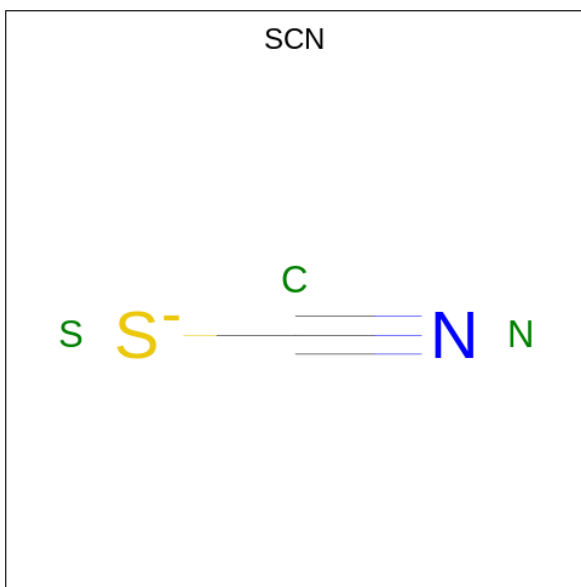
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	0	0
			3822	2436	690	680	16			
1	B	487	Total	C	N	O	S	0	0	0
			3817	2433	689	679	16			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).



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 THIOCYANATE ION (three-letter code: SCN) (formula: CNS).

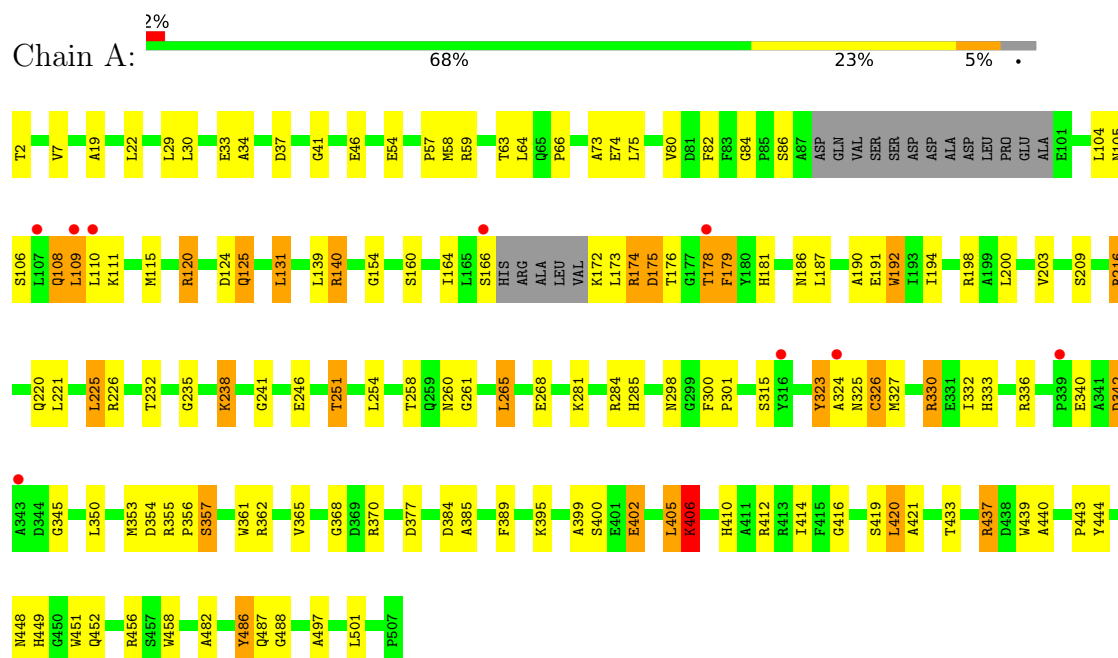


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	S	0	0
			3	1	1	1		
3	B	1	Total	C	N	S	0	0
			3	1	1	1		

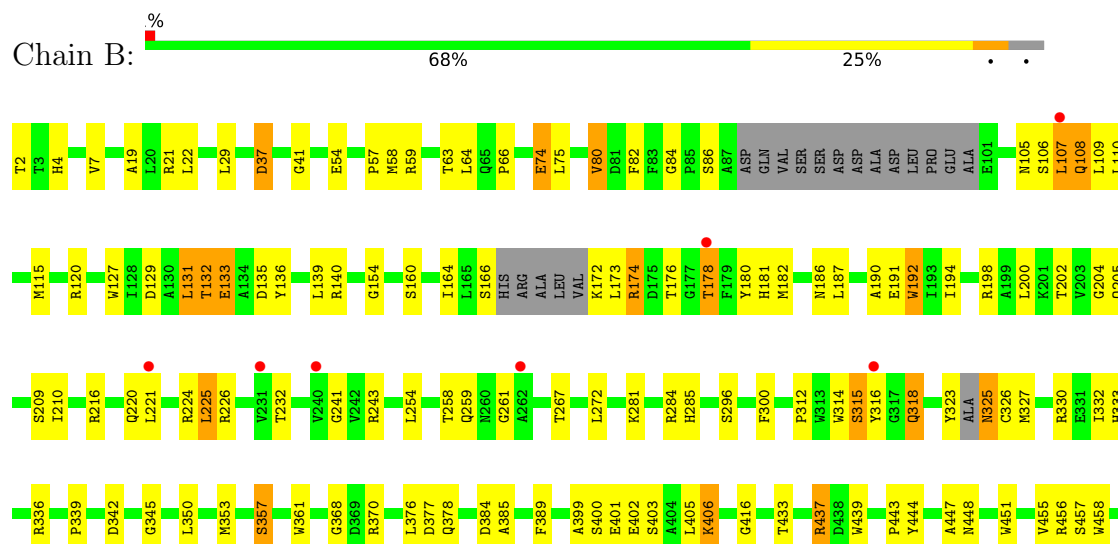
3 Residue-property plots [i](#)

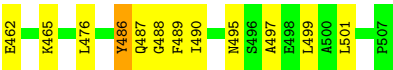
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: FAD-binding protein



• Molecule 1: FAD-binding protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	124.79Å 124.79Å 148.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.78 – 2.69 47.78 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.78-2.69) 99.8 (47.78-2.69)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.220 , 0.283 0.227 , 0.284	Depositor DCC
R_{free} test set	1774 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	82.2	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7751	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% 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, SCN

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	0.71	0/3917	0.88	0/5316
1	B	0.71	0/3911	0.89	0/5306
All	All	0.71	0/7828	0.88	0/10622

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
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	LEU	Peptide
1	B	108	GLN	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	3822	0	3777	74	0
1	B	3817	0	3771	90	0
2	A	53	0	31	2	0
2	B	53	0	31	6	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
All	All	7751	0	7610	162	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 11.

All (162) 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:179:PHE:O	1:A:330:ARG:NH2	2.15	0.79
1:A:115:MET:HE3	1:A:120:ARG:HB2	1.69	0.73
1:B:108:GLN:NE2	1:B:108:GLN:HA	2.02	0.73
1:A:241:GLY:HA2	1:A:285:HIS:CD2	2.23	0.73
1:B:115:MET:HE3	1:B:120:ARG:HB2	1.71	0.73
1:A:419:SER:O	1:A:421:ALA:N	2.22	0.72
1:B:456:ARG:HG2	1:B:458:TRP:CH2	2.24	0.72
1:A:456:ARG:HG2	1:A:458:TRP:CH2	2.26	0.71
1:B:82:PHE:CZ	1:B:84:GLY:HA3	2.26	0.70
1:A:173:LEU:O	1:A:174:ARG:NH1	2.25	0.69
1:A:140:ARG:HD3	1:A:191:GLU:OE2	1.93	0.68
1:A:41:GLY:HA2	1:A:444:TYR:OH	1.94	0.68
1:B:221:LEU:O	1:B:225:LEU:HB2	1.93	0.68
1:A:336:ARG:NH1	1:A:345:GLY:O	2.26	0.68
1:B:323:TYR:O	1:B:325:ASN:N	2.27	0.68
1:A:82:PHE:CZ	1:A:84:GLY:HA3	2.29	0.67
1:A:221:LEU:O	1:A:225:LEU:HB2	1.93	0.67
1:B:376:LEU:O	1:B:378:GLN:HG3	1.95	0.67
1:B:342:ASP:OD2	1:B:345:GLY:N	2.27	0.66
1:B:74:GLU:O	1:B:224:ARG:NH2	2.29	0.65
1:B:174:ARG:NE	1:B:174:ARG:HA	2.11	0.65
1:B:173:LEU:O	1:B:174:ARG:NH1	2.29	0.65
1:A:190:ALA:O	1:A:194:ILE:HG12	1.97	0.65
1:B:41:GLY:HA2	1:B:444:TYR:OH	1.97	0.64
1:B:315:SER:HB3	1:B:406:LYS:HB3	1.78	0.64
1:B:7:VAL:HG21	1:B:254:LEU:HD12	1.78	0.64
1:B:339:PRO:HA	1:B:342:ASP:HB2	1.78	0.64
1:A:173:LEU:O	1:A:174:ARG:CZ	2.45	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:TYR:CE2	1:A:332:ILE:HD13	2.34	0.63
1:A:342:ASP:OD2	1:A:345:GLY:HA2	1.97	0.63
1:B:190:ALA:O	1:B:194:ILE:HG12	1.99	0.63
1:B:173:LEU:O	1:B:174:ARG:CZ	2.47	0.63
1:B:108:GLN:HA	1:B:108:GLN:HE21	1.62	0.61
1:B:314:TRP:HB2	1:B:318:GLN:HG3	1.83	0.61
1:B:132:THR:HG22	1:B:135:ASP:OD2	2.03	0.58
1:B:490:ILE:HG12	2:B:601:FAD:H3'	1.85	0.58
1:B:107:LEU:HD12	1:B:108:GLN:HG2	1.86	0.58
1:B:166:SER:OG	1:B:172:LYS:HD2	2.03	0.58
1:B:178:THR:HB	1:B:181:HIS:CE1	2.39	0.57
1:A:7:VAL:HG21	1:A:254:LEU:HD12	1.88	0.56
1:A:166:SER:OG	1:A:172:LYS:HB3	2.06	0.56
1:A:57:PRO:HB3	2:A:601:FAD:C10	2.36	0.55
1:B:376:LEU:O	1:B:378:GLN:CG	2.54	0.55
1:A:175:ASP:C	1:A:175:ASP:OD2	2.44	0.55
1:A:325:ASN:O	1:B:172:LYS:HD3	2.07	0.55
1:B:109:LEU:HD12	1:B:110:LEU:N	2.21	0.55
1:A:7:VAL:HG21	1:A:254:LEU:CD1	2.37	0.54
1:B:107:LEU:HG	1:B:108:GLN:H	1.71	0.54
1:B:166:SER:OG	1:B:172:LYS:CD	2.55	0.54
1:B:447:ALA:HB1	2:B:601:FAD:HM83	1.90	0.53
1:B:224:ARG:HG3	1:B:224:ARG:O	2.08	0.53
1:B:451:TRP:CD1	1:B:487:GLN:OE1	2.62	0.53
1:A:353:MET:SD	1:A:361:TRP:CD1	3.01	0.53
2:B:601:FAD:H9	2:B:601:FAD:O2'	2.09	0.53
1:A:30:LEU:HD21	1:A:265:LEU:HD21	1.91	0.52
1:B:57:PRO:HB3	2:B:601:FAD:C10	2.39	0.52
1:A:33:GLU:HA	2:A:601:FAD:H8A	1.90	0.52
1:B:202:THR:O	1:B:204:GLY:O	2.27	0.52
1:A:377:ASP:OD1	1:A:433:THR:HA	2.10	0.52
1:A:451:TRP:CD1	1:A:487:GLN:OE1	2.63	0.52
1:A:327:MET:HG2	1:A:389:PHE:HB3	1.93	0.52
1:B:327:MET:HG2	1:B:389:PHE:HB3	1.92	0.52
1:B:133:GLU:HA	1:B:133:GLU:OE1	2.10	0.51
1:B:258:THR:HG22	1:B:261:GLY:O	2.11	0.51
1:B:108:GLN:HE21	1:B:108:GLN:CA	2.24	0.51
1:A:333:HIS:HB2	1:A:350:LEU:HB3	1.92	0.50
1:B:353:MET:SD	1:B:361:TRP:CD1	3.05	0.50
1:B:7:VAL:HG21	1:B:254:LEU:CD1	2.41	0.50
1:B:140:ARG:HD3	1:B:191:GLU:OE2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:SER:HA	1:A:172:LYS:HB3	1.94	0.49
1:B:198:ARG:HD2	1:B:486:TYR:CZ	2.47	0.49
1:B:54:GLU:HG3	1:B:58:MET:HA	1.94	0.49
1:A:258:THR:HG22	1:A:261:GLY:O	2.12	0.49
1:A:400:SER:C	1:A:402:GLU:H	2.16	0.49
1:B:241:GLY:HA2	1:B:285:HIS:CD2	2.47	0.48
1:B:108:GLN:NE2	1:B:108:GLN:CA	2.74	0.48
1:A:54:GLU:HG3	1:A:58:MET:HA	1.96	0.48
1:A:323:TYR:O	1:A:325:ASN:OD1	2.32	0.48
1:A:172:LYS:HE2	1:B:325:ASN:O	2.14	0.47
1:A:120:ARG:NH1	1:A:124:ASP:OD2	2.47	0.47
1:B:54:GLU:HB2	1:B:58:MET:HG2	1.95	0.47
1:B:368:GLY:O	1:B:370:ARG:N	2.44	0.47
1:A:174:ARG:NE	1:A:174:ARG:HA	2.29	0.47
1:B:315:SER:CB	1:B:406:LYS:HD3	2.45	0.47
1:B:57:PRO:HB3	2:B:601:FAD:C4X	2.44	0.47
1:B:353:MET:HB2	1:B:357:SER:HB2	1.96	0.47
1:B:462:GLU:HA	1:B:465:LYS:HE3	1.96	0.47
1:A:323:TYR:CD2	1:A:332:ILE:HG21	2.49	0.47
1:A:187:LEU:HD12	1:A:192:TRP:CE2	2.50	0.47
1:A:452:GLN:HA	1:A:452:GLN:OE1	2.15	0.47
1:B:139:LEU:HB3	1:B:194:ILE:HD11	1.97	0.47
1:A:330:ARG:HG3	1:A:354:ASP:OD1	2.15	0.47
1:A:22:LEU:HB3	1:A:29:LEU:HD21	1.96	0.46
1:A:385:ALA:O	1:A:389:PHE:CD1	2.68	0.46
1:B:166:SER:OG	1:B:172:LYS:HB3	2.15	0.46
1:B:400:SER:C	1:B:402:GLU:H	2.18	0.46
1:A:19:ALA:HA	1:A:29:LEU:HD13	1.97	0.46
1:A:368:GLY:O	1:A:370:ARG:N	2.44	0.46
1:B:312:PRO:HB2	1:B:336:ARG:NH1	2.30	0.46
1:B:187:LEU:HD12	1:B:192:TRP:CE2	2.51	0.46
1:A:198:ARG:CD	1:A:486:TYR:CZ	2.99	0.46
1:B:495:ASN:O	1:B:499:LEU:HD23	2.16	0.46
1:A:325:ASN:O	1:B:172:LYS:NZ	2.47	0.45
1:B:131:LEU:HD12	1:B:131:LEU:HA	1.87	0.45
1:B:465:LYS:HE2	1:B:499:LEU:HD12	1.99	0.45
1:B:22:LEU:HB3	1:B:29:LEU:HD21	1.98	0.45
1:B:377:ASP:OD1	1:B:433:THR:HA	2.16	0.45
1:A:131:LEU:HD12	1:A:131:LEU:HA	1.87	0.45
1:A:198:ARG:HD2	1:A:486:TYR:CZ	2.52	0.45
1:B:198:ARG:CD	1:B:486:TYR:CZ	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:MET:HB2	1:A:357:SER:HB2	1.99	0.44
1:B:385:ALA:O	1:B:389:PHE:HD2	2.01	0.44
1:B:19:ALA:HA	1:B:29:LEU:HD13	2.00	0.44
1:B:209:SER:OG	1:B:210:ILE:N	2.49	0.44
2:B:601:FAD:H9	2:B:601:FAD:C2'	2.47	0.44
1:A:178:THR:HB	1:A:181:HIS:CD2	2.52	0.44
1:B:376:LEU:HD12	1:B:376:LEU:N	2.33	0.44
1:B:140:ARG:HD3	1:B:457:SER:HG	1.83	0.44
1:A:139:LEU:HB3	1:A:194:ILE:HD11	2.00	0.44
1:A:54:GLU:HB2	1:A:58:MET:HG2	1.99	0.43
1:A:160:SER:HB3	1:B:389:PHE:CZ	2.52	0.43
1:A:154:GLY:HA3	1:A:186:ASN:OD1	2.19	0.43
1:A:323:TYR:O	1:A:325:ASN:N	2.45	0.43
1:B:486:TYR:CE1	1:B:489:PHE:HD2	2.37	0.43
1:A:410:HIS:O	1:A:414:ILE:HG12	2.19	0.43
1:A:365:VAL:HG23	1:A:365:VAL:O	2.19	0.42
1:A:75:LEU:HD12	1:A:220:GLN:C	2.40	0.42
1:A:449:HIS:HB2	1:A:482:ALA:HA	2.01	0.42
1:B:109:LEU:HD12	1:B:109:LEU:C	2.39	0.42
1:A:216:ARG:HD2	1:A:216:ARG:HA	1.92	0.42
1:B:315:SER:OG	1:B:316:TYR:N	2.52	0.42
1:B:497:ALA:O	1:B:501:LEU:HG	2.20	0.42
1:A:34:ALA:HB1	1:A:238:LYS:HG3	2.02	0.42
1:B:4:HIS:O	1:B:267:THR:HA	2.19	0.42
1:A:73:ALA:O	1:A:75:LEU:N	2.53	0.42
1:A:437:ARG:NH1	1:A:439:TRP:CZ3	2.88	0.42
1:B:174:ARG:N	1:B:174:ARG:HD2	2.34	0.42
1:B:333:HIS:HB2	1:B:350:LEU:HB3	2.01	0.42
1:A:64:LEU:O	1:A:66:PRO:HD2	2.20	0.42
1:A:315:SER:OG	1:A:406:LYS:HD3	2.20	0.41
1:A:448:ASN:CG	1:A:488:GLY:HA2	2.40	0.41
1:A:251:THR:HG23	1:A:268:GLU:OE2	2.20	0.41
1:A:325:ASN:CG	1:A:326:CYS:H	2.23	0.41
1:B:75:LEU:HD12	1:B:220:GLN:C	2.40	0.41
1:B:405:LEU:HD13	1:B:405:LEU:HA	1.95	0.41
1:B:296:SER:HB2	1:B:455:VAL:HG11	2.03	0.41
1:B:64:LEU:O	1:B:66:PRO:HD2	2.20	0.41
1:B:166:SER:OG	1:B:172:LYS:CG	2.68	0.41
1:B:323:TYR:CD2	1:B:332:ILE:HG21	2.55	0.41
1:B:120:ARG:NH1	1:B:127:TRP:CD1	2.89	0.41
1:B:37:ASP:N	1:B:37:ASP:OD1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:GLY:HA3	1:B:186:ASN:OD1	2.21	0.40
1:B:132:THR:O	1:B:135:ASP:HB2	2.20	0.40
1:A:301:PRO:HB3	1:A:440:ALA:HB2	2.03	0.40
1:A:405:LEU:O	1:A:406:LYS:C	2.60	0.40
1:A:497:ALA:O	1:A:501:LEU:HG	2.21	0.40
1:B:448:ASN:CG	1:B:488:GLY:HA2	2.41	0.40
1:A:355:ARG:HA	1:A:356:PRO:HA	1.92	0.40
1:A:405:LEU:HD22	1:A:405:LEU:HA	1.91	0.40
1:B:133:GLU:OE1	1:B:136:TYR:HD2	2.03	0.40
1:A:198:ARG:HD3	1:A:486:TYR:CZ	2.57	0.40
1:B:437:ARG:NH1	1:B:439:TRP:CZ3	2.90	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	482/506 (95%)	412 (86%)	56 (12%)	14 (3%)	3	9
1	B	479/506 (95%)	413 (86%)	59 (12%)	7 (2%)	8	22
All	All	961/1012 (95%)	825 (86%)	115 (12%)	21 (2%)	5	15

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	420	LEU
1	A	324	ALA
1	A	362	ARG
1	A	399	ALA
1	A	74	GLU
1	A	125	GLN
1	A	260	ASN

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Mol	Chain	Res	Type
1	A	384	ASP
1	B	180	TYR
1	B	384	ASP
1	A	108	GLN
1	B	74	GLU
1	B	399	ALA
1	A	164	ILE
1	A	406	LYS
1	A	235	GLY
1	B	164	ILE
1	A	416	GLY
1	A	203	VAL
1	B	416	GLY
1	B	80	VAL

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	384/399 (96%)	331 (86%)	53 (14%)	3	7
1	B	384/399 (96%)	339 (88%)	45 (12%)	4	11
All	All	768/798 (96%)	670 (87%)	98 (13%)	3	9

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	37	ASP
1	A	46	GLU
1	A	59	ARG
1	A	63	THR
1	A	80	VAL
1	A	86	SER
1	A	104	LEU
1	A	105	ASN

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Mol	Chain	Res	Type
1	A	106	SER
1	A	108	GLN
1	A	109	LEU
1	A	110	LEU
1	A	111	LYS
1	A	120	ARG
1	A	125	GLN
1	A	131	LEU
1	A	140	ARG
1	A	174	ARG
1	A	175	ASP
1	A	176	THR
1	A	178	THR
1	A	179	PHE
1	A	192	TRP
1	A	200	LEU
1	A	209	SER
1	A	216	ARG
1	A	225	LEU
1	A	226	ARG
1	A	232	THR
1	A	238	LYS
1	A	246	GLU
1	A	251	THR
1	A	265	LEU
1	A	281	LYS
1	A	284	ARG
1	A	298	ASN
1	A	300	PHE
1	A	323	TYR
1	A	326	CYS
1	A	330	ARG
1	A	340	GLU
1	A	342	ASP
1	A	357	SER
1	A	395	LYS
1	A	402	GLU
1	A	405	LEU
1	A	406	LYS
1	A	412	ARG
1	A	420	LEU
1	A	437	ARG

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Mol	Chain	Res	Type
1	A	443	PRO
1	A	486	TYR
1	B	2	THR
1	B	21	ARG
1	B	37	ASP
1	B	59	ARG
1	B	63	THR
1	B	80	VAL
1	B	86	SER
1	B	105	ASN
1	B	106	SER
1	B	107	LEU
1	B	129	ASP
1	B	131	LEU
1	B	132	THR
1	B	133	GLU
1	B	160	SER
1	B	174	ARG
1	B	176	THR
1	B	178	THR
1	B	182	MET
1	B	192	TRP
1	B	200	LEU
1	B	205	GLN
1	B	216	ARG
1	B	225	LEU
1	B	226	ARG
1	B	232	THR
1	B	243	ARG
1	B	259	GLN
1	B	272	LEU
1	B	281	LYS
1	B	284	ARG
1	B	300	PHE
1	B	315	SER
1	B	318	GLN
1	B	325	ASN
1	B	326	CYS
1	B	330	ARG
1	B	357	SER
1	B	401	GLU
1	B	403	SER

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Mol	Chain	Res	Type
1	B	406	LYS
1	B	437	ARG
1	B	443	PRO
1	B	476	LEU
1	B	486	TYR

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	125	GLN
1	A	206	GLN
1	A	285	HIS
1	A	298	ASN
1	B	108	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](#)

4 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	601	-	53,58,58	0.70	0	68,89,89	1.05	5 (7%)
3	SCN	A	602	-	1,2,2	0.86	0	0,1,1	-	-
2	FAD	A	601	-	53,58,58	0.76	1 (1%)	68,89,89	0.86	4 (5%)
3	SCN	B	602	-	1,2,2	1.01	0	0,1,1	-	-

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	601	-	2/2/9/9	19/30/50/50	0/6/6/6
2	FAD	A	601	-	1/1/9/9	18/30/50/50	0/6/6/6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C1'-C2'	-2.20	1.49	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	C1'-N10-C9A	3.13	125.72	120.51
2	A	601	FAD	C1'-C2'-C3'	-2.86	101.80	109.79
2	B	601	FAD	C9-C9A-N10	2.62	125.37	121.84
2	B	601	FAD	C4'-C3'-C2'	2.47	118.50	113.36
2	A	601	FAD	O4B-C1B-C2B	-2.21	103.70	106.93
2	A	601	FAD	C5A-C6A-N6A	2.16	123.64	120.35
2	B	601	FAD	C4-N3-C2	-2.15	121.67	125.64
2	B	601	FAD	C5A-C6A-N6A	2.08	123.51	120.35
2	A	601	FAD	C4-N3-C2	-2.00	121.94	125.64

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	601	FAD	C2B
2	B	601	FAD	C2B
2	B	601	FAD	C4'

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C5B-O5B-PA-O1A
2	A	601	FAD	C5B-O5B-PA-O2A
2	A	601	FAD	C2'-C3'-C4'-C5'
2	A	601	FAD	O3'-C3'-C4'-C5'
2	A	601	FAD	C3'-C4'-C5'-O5'
2	A	601	FAD	O4'-C4'-C5'-O5'
2	A	601	FAD	C5'-O5'-P-O1P
2	A	601	FAD	C5'-O5'-P-O2P
2	A	601	FAD	PA-O3P-P-O5'
2	B	601	FAD	C5B-O5B-PA-O1A
2	B	601	FAD	C2'-C1'-N10-C9A
2	B	601	FAD	C2'-C1'-N10-C10
2	B	601	FAD	N10-C1'-C2'-O2'
2	B	601	FAD	N10-C1'-C2'-C3'
2	B	601	FAD	C1'-C2'-C3'-O3'
2	B	601	FAD	C2'-C3'-C4'-O4'
2	B	601	FAD	C2'-C3'-C4'-C5'
2	B	601	FAD	O3'-C3'-C4'-C5'
2	B	601	FAD	C5'-O5'-P-O2P
2	B	601	FAD	C5'-O5'-P-O3P
2	A	601	FAD	O3'-C3'-C4'-O4'
2	B	601	FAD	O3'-C3'-C4'-O4'
2	A	601	FAD	O4B-C4B-C5B-O5B
2	A	601	FAD	C3B-C4B-C5B-O5B
2	B	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	C3B-C4B-C5B-O5B
2	A	601	FAD	C2'-C3'-C4'-O4'
2	B	601	FAD	O2'-C2'-C3'-O3'
2	B	601	FAD	C5'-O5'-P-O1P
2	A	601	FAD	O2'-C2'-C3'-C4'
2	A	601	FAD	O2'-C2'-C3'-O3'
2	B	601	FAD	O2'-C2'-C3'-C4'
2	A	601	FAD	C5B-O5B-PA-O3P
2	A	601	FAD	C5'-O5'-P-O3P
2	B	601	FAD	C5B-O5B-PA-O3P
2	B	601	FAD	PA-O3P-P-O1P
2	A	601	FAD	C1'-C2'-C3'-O3'

There are no ring outliers.

2 monomers are involved in 8 short contacts:

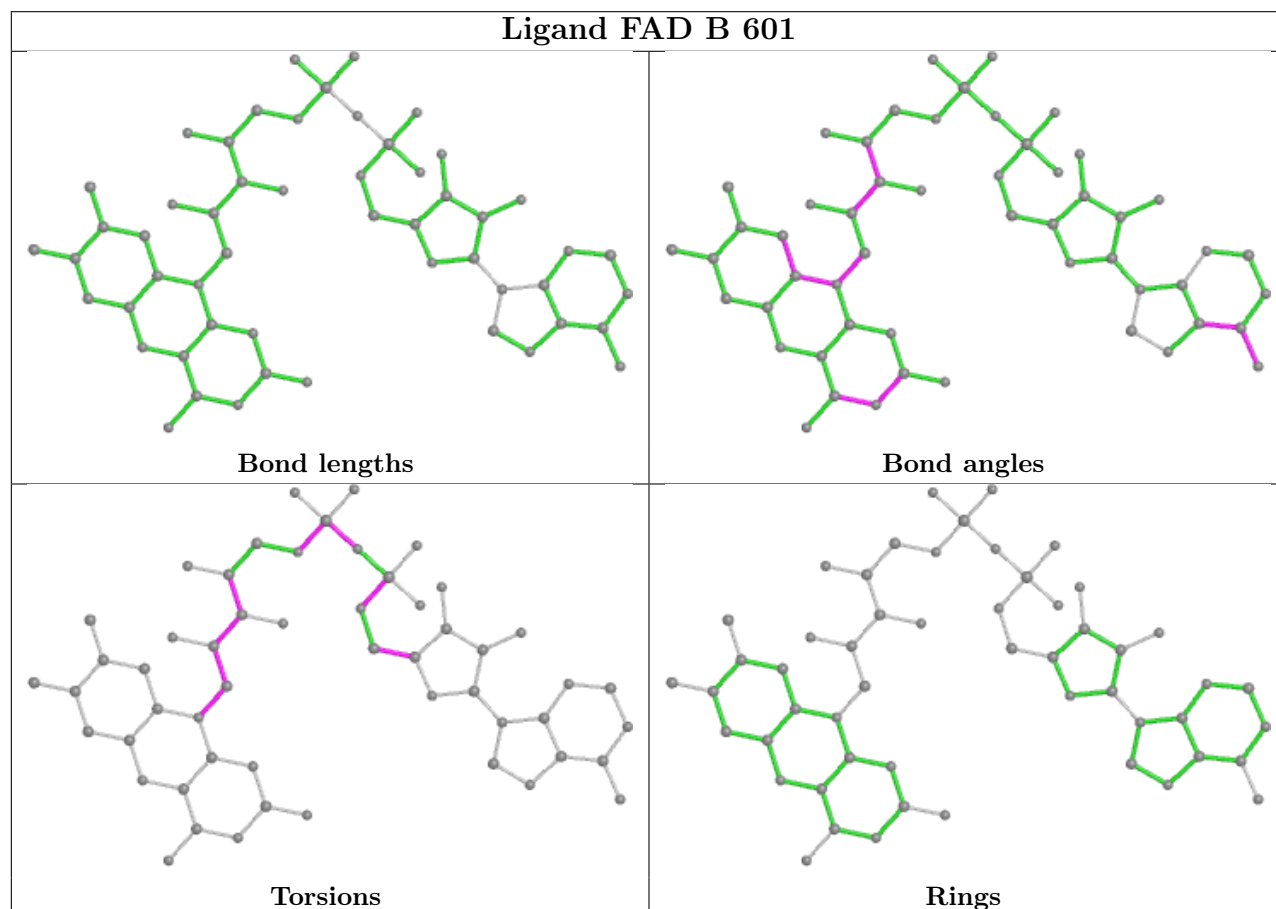
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	FAD	6	0

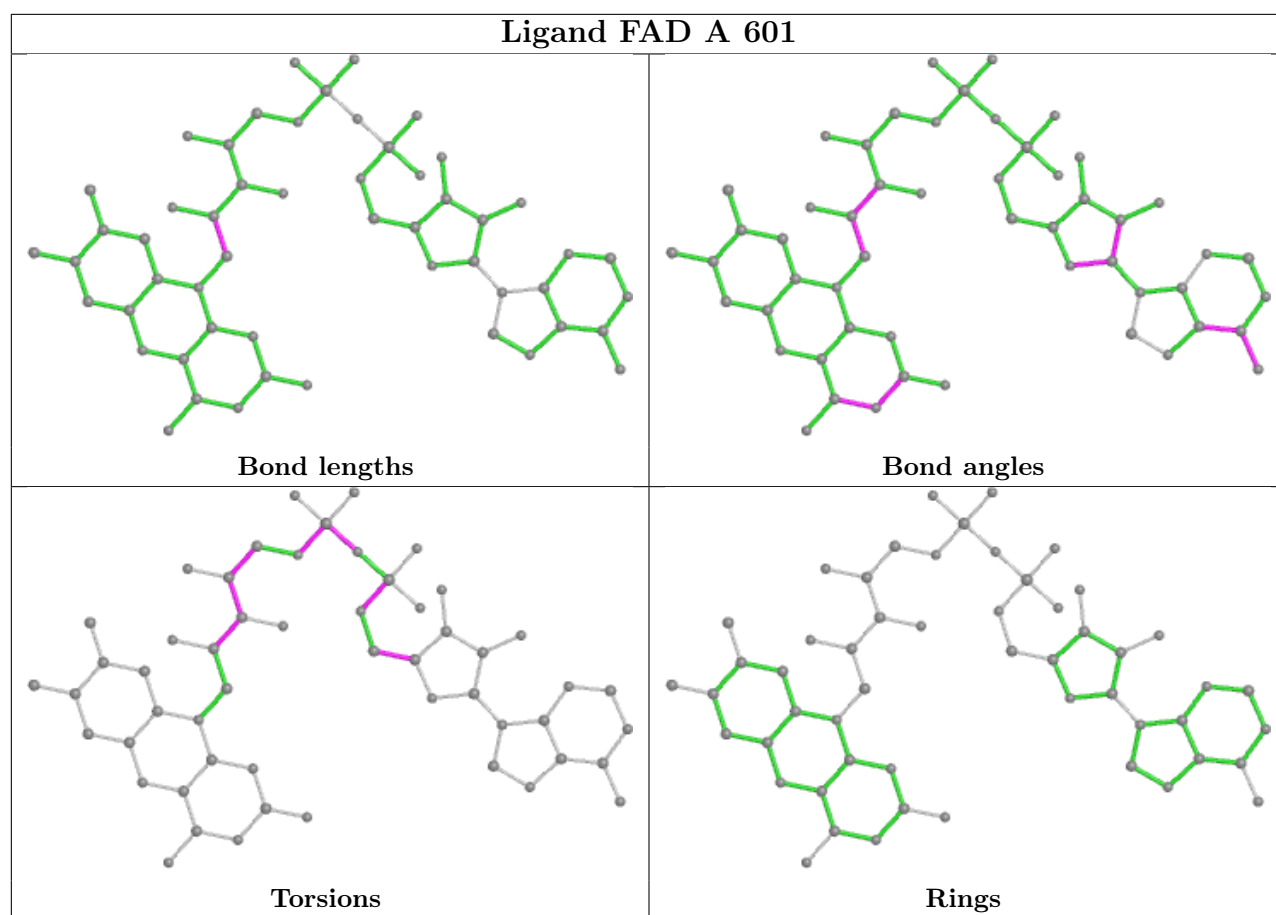
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FAD	2	0

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	488/506 (96%)	0.07	9 (1%) 67 67	50, 88, 138, 170	0
1	B	487/506 (96%)	0.05	7 (1%) 73 73	51, 91, 135, 172	0
All	All	975/1012 (96%)	0.06	16 (1%) 70 70	50, 90, 138, 172	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	107	LEU	4.0
1	B	262	ALA	3.4
1	A	109	LEU	3.3
1	B	178	THR	3.2
1	A	324	ALA	2.9
1	A	316	TYR	2.5
1	B	316	TYR	2.4
1	A	110	LEU	2.3
1	B	231	VAL	2.3
1	B	107	LEU	2.3
1	B	240	VAL	2.2
1	A	343	ALA	2.2
1	A	339	PRO	2.1
1	A	166	SER	2.1
1	B	221	LEU	2.0
1	A	178	THR	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](#)

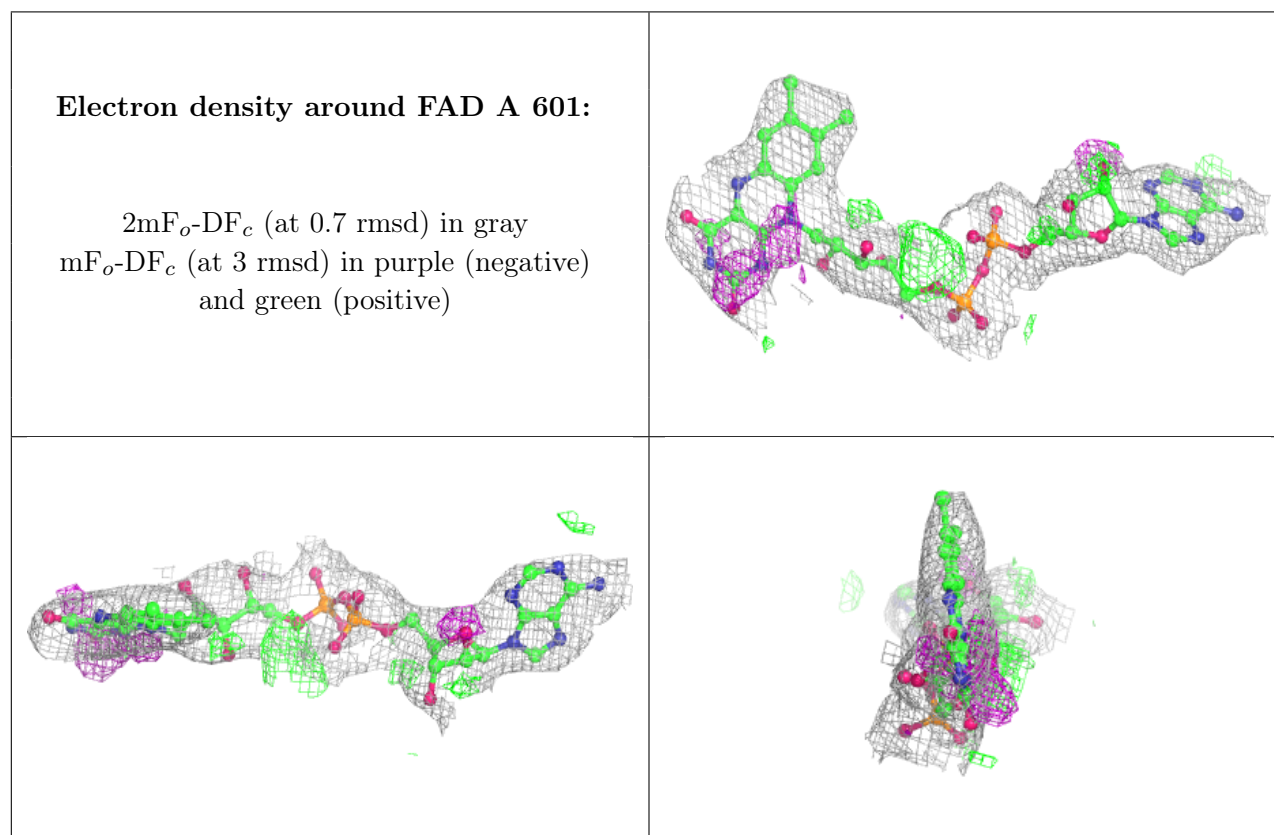
There are no monosaccharides in this entry.

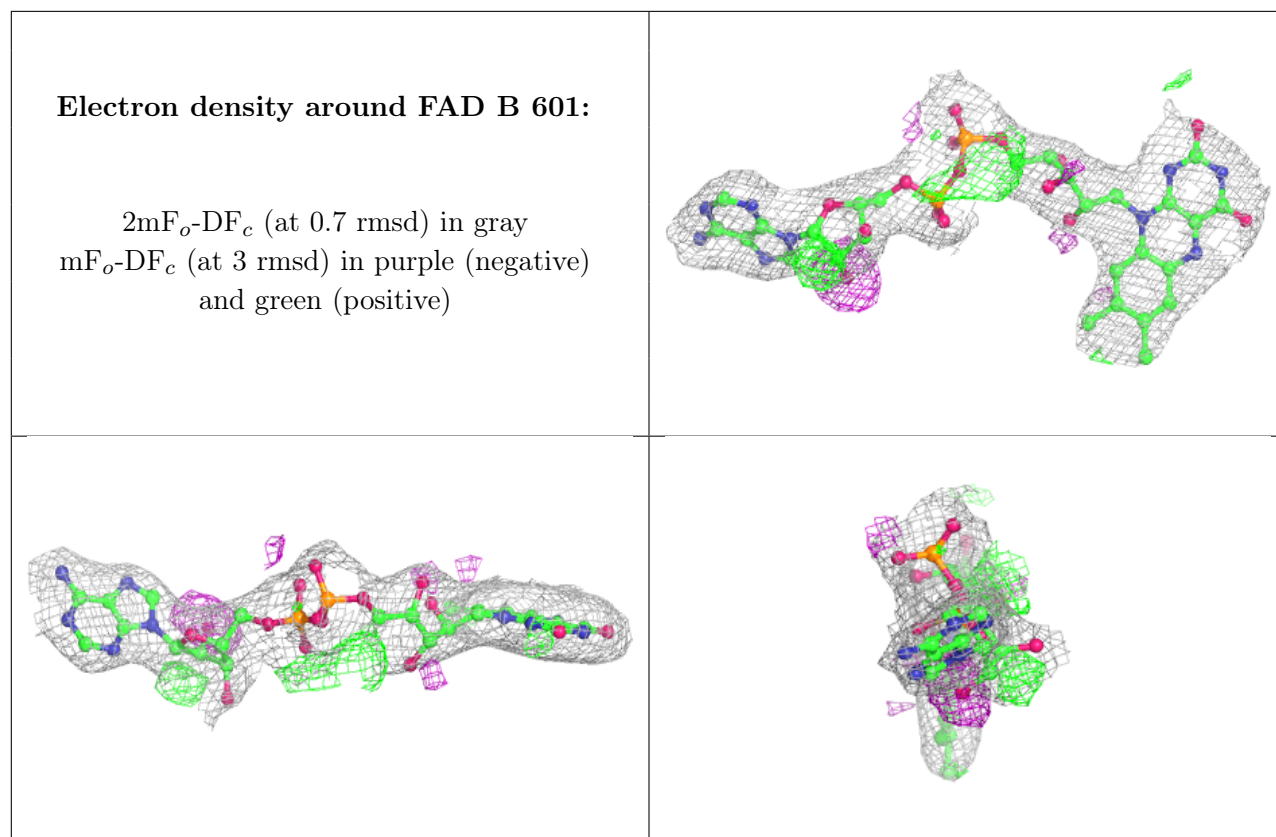
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
3	SCN	A	602	3/3	0.65	0.20	65,65,85,97	0
3	SCN	B	602	3/3	0.74	0.20	70,70,88,98	0
2	FAD	A	601	53/53	0.89	0.12	55,69,92,108	0
2	FAD	B	601	53/53	0.89	0.10	58,71,86,100	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.