Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 12:48 PM EDT

PDB ID	:	8TWF
Title	:	Crystal structure of tetracycline destructase Tet(56-3)
Authors	:	Kumar, H.; Tang, W.K.; Tolia, N.
Deposited on	:	2023-08-21
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:

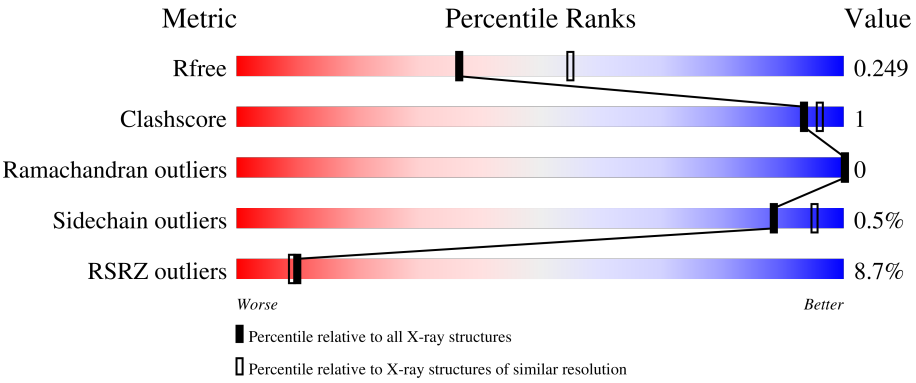
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 <=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	403	8% 90% · 6%
1	B	403	10% 88% · 7%
1	C	403	8% 92% · ·
1	D	403	7% 90% · 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 24320 atoms, of which 11898 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 6-hydroxynicotinate 3-monooxygenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	D	378	Total	C	H	N	O	S	0	0	0
			5957	1911	2943	519	569	15			
1	A	377	Total	C	H	N	O	S	0	0	0
			5932	1899	2934	517	567	15			
1	B	373	Total	C	H	N	O	S	0	0	0
			5885	1884	2916	512	558	15			
1	C	385	Total	C	H	N	O	S	0	0	0
			6051	1946	2981	531	578	15			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	MET	-	expression tag	UNP A0A078L5T0
D	-14	THR	-	expression tag	UNP A0A078L5T0
D	-13	GLY	-	expression tag	UNP A0A078L5T0
D	-12	SER	-	expression tag	UNP A0A078L5T0
D	-11	SER	-	expression tag	UNP A0A078L5T0
D	-10	HIS	-	expression tag	UNP A0A078L5T0
D	-9	HIS	-	expression tag	UNP A0A078L5T0
D	-8	HIS	-	expression tag	UNP A0A078L5T0
D	-7	HIS	-	expression tag	UNP A0A078L5T0
D	-6	HIS	-	expression tag	UNP A0A078L5T0
D	-5	HIS	-	expression tag	UNP A0A078L5T0
D	-4	SER	-	expression tag	UNP A0A078L5T0
D	-3	SER	-	expression tag	UNP A0A078L5T0
D	-2	GLY	-	expression tag	UNP A0A078L5T0
D	-1	LYS	-	expression tag	UNP A0A078L5T0
D	0	LEU	-	expression tag	UNP A0A078L5T0
A	-15	MET	-	expression tag	UNP A0A078L5T0
A	-14	THR	-	expression tag	UNP A0A078L5T0
A	-13	GLY	-	expression tag	UNP A0A078L5T0
A	-12	SER	-	expression tag	UNP A0A078L5T0
A	-11	SER	-	expression tag	UNP A0A078L5T0

Continued on next page...

Continued from previous page...

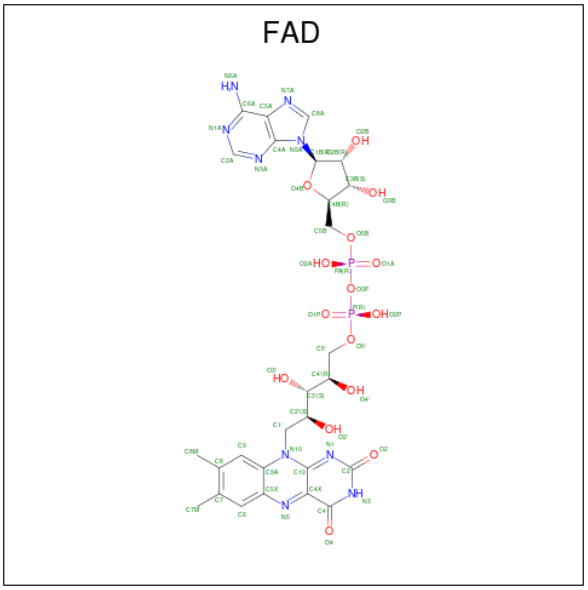
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	HIS	-	expression tag	UNP A0A078L5T0
A	-9	HIS	-	expression tag	UNP A0A078L5T0
A	-8	HIS	-	expression tag	UNP A0A078L5T0
A	-7	HIS	-	expression tag	UNP A0A078L5T0
A	-6	HIS	-	expression tag	UNP A0A078L5T0
A	-5	HIS	-	expression tag	UNP A0A078L5T0
A	-4	SER	-	expression tag	UNP A0A078L5T0
A	-3	SER	-	expression tag	UNP A0A078L5T0
A	-2	GLY	-	expression tag	UNP A0A078L5T0
A	-1	LYS	-	expression tag	UNP A0A078L5T0
A	0	LEU	-	expression tag	UNP A0A078L5T0
B	-15	MET	-	expression tag	UNP A0A078L5T0
B	-14	THR	-	expression tag	UNP A0A078L5T0
B	-13	GLY	-	expression tag	UNP A0A078L5T0
B	-12	SER	-	expression tag	UNP A0A078L5T0
B	-11	SER	-	expression tag	UNP A0A078L5T0
B	-10	HIS	-	expression tag	UNP A0A078L5T0
B	-9	HIS	-	expression tag	UNP A0A078L5T0
B	-8	HIS	-	expression tag	UNP A0A078L5T0
B	-7	HIS	-	expression tag	UNP A0A078L5T0
B	-6	HIS	-	expression tag	UNP A0A078L5T0
B	-5	HIS	-	expression tag	UNP A0A078L5T0
B	-4	SER	-	expression tag	UNP A0A078L5T0
B	-3	SER	-	expression tag	UNP A0A078L5T0
B	-2	GLY	-	expression tag	UNP A0A078L5T0
B	-1	LYS	-	expression tag	UNP A0A078L5T0
B	0	LEU	-	expression tag	UNP A0A078L5T0
C	-15	MET	-	expression tag	UNP A0A078L5T0
C	-14	THR	-	expression tag	UNP A0A078L5T0
C	-13	GLY	-	expression tag	UNP A0A078L5T0
C	-12	SER	-	expression tag	UNP A0A078L5T0
C	-11	SER	-	expression tag	UNP A0A078L5T0
C	-10	HIS	-	expression tag	UNP A0A078L5T0
C	-9	HIS	-	expression tag	UNP A0A078L5T0
C	-8	HIS	-	expression tag	UNP A0A078L5T0
C	-7	HIS	-	expression tag	UNP A0A078L5T0
C	-6	HIS	-	expression tag	UNP A0A078L5T0
C	-5	HIS	-	expression tag	UNP A0A078L5T0
C	-4	SER	-	expression tag	UNP A0A078L5T0
C	-3	SER	-	expression tag	UNP A0A078L5T0
C	-2	GLY	-	expression tag	UNP A0A078L5T0
C	-1	LYS	-	expression tag	UNP A0A078L5T0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	LEU	-	expression tag	UNP A0A078L5T0

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	D	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
2	A	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
2	B	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
2	C	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		

- Molecule 3 is water.

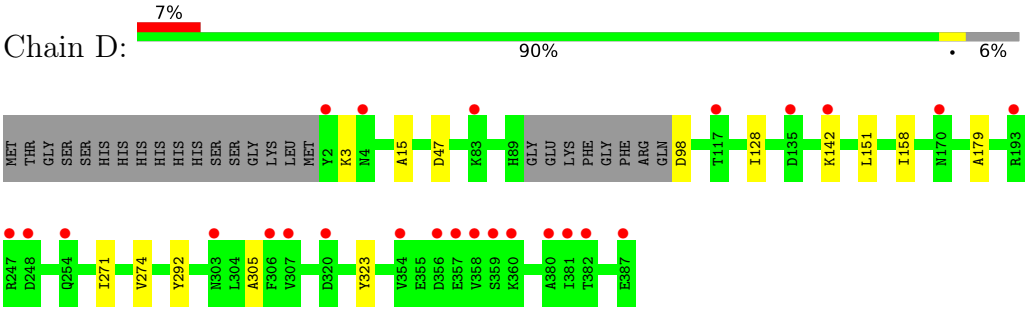
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	45	Total	O	0	0
			45	45		
3	A	37	Total	O	0	0
			37	37		
3	B	29	Total	O	0	0
			29	29		
3	C	48	Total	O	0	0
			48	48		

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.

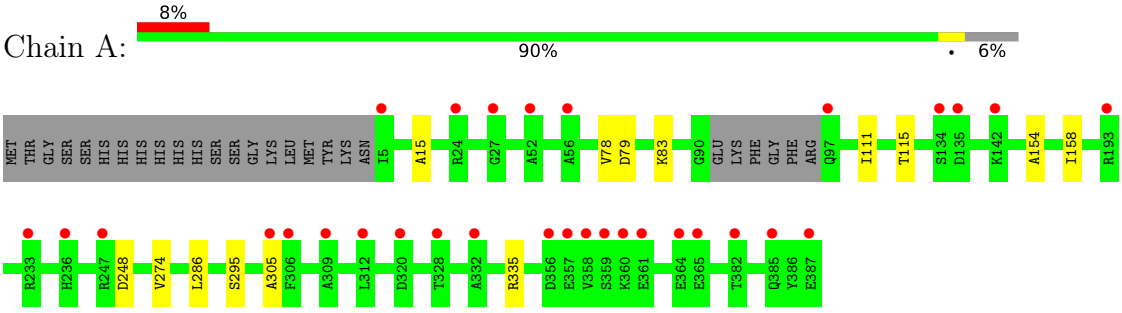
• Molecule 1: 6-hydroxynicotinate 3-monooxygenase

Chain D:



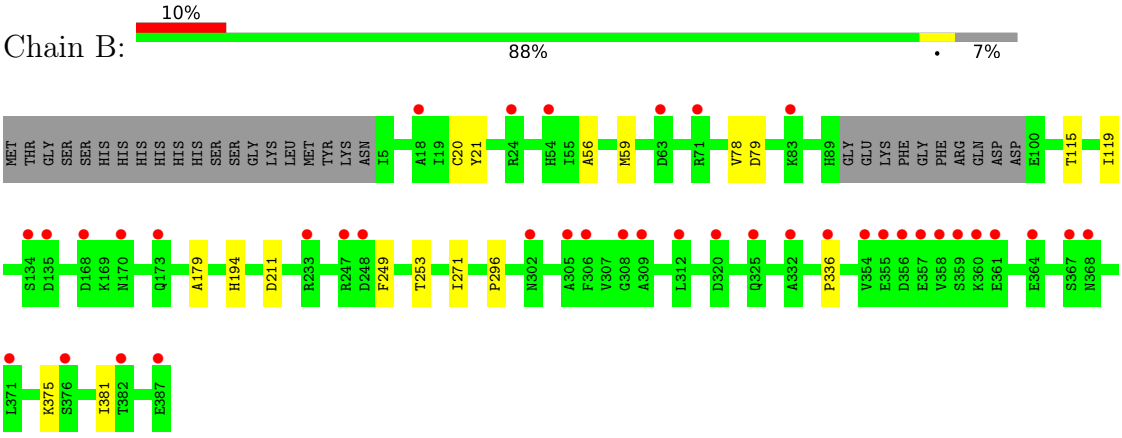
• Molecule 1: 6-hydroxynicotinate 3-monooxygenase

Chain A:



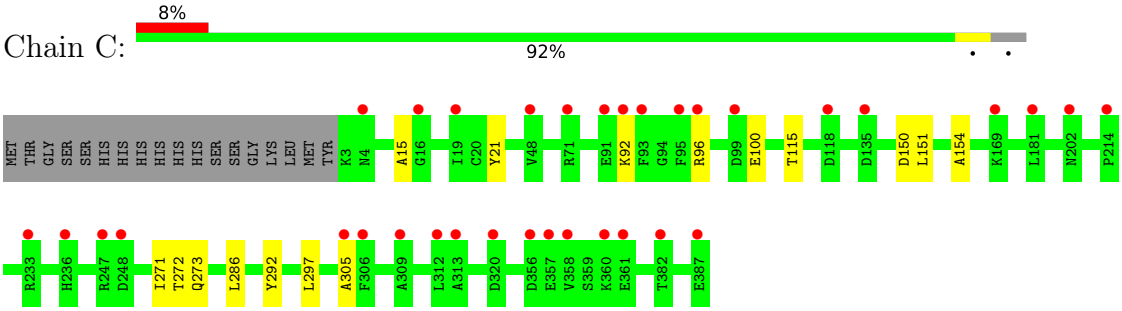
• Molecule 1: 6-hydroxynicotinate 3-monooxygenase

Chain B:



• Molecule 1: 6-hydroxynicotinate 3-monooxygenase

Chain C:


8%
92%
MET THR GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LYS LEU MET TYR K3 N4 A15 G16 I19 C20 Y21 V48 R71 E91 K92 F93 G94 F95 R96 D99 E100 T115 D118 D135 D150 L151 A154 K169 L181 N202 P214
R233 H236 R247 D248 I271 T272 Q273 L286 Y292 L297 A305 F306 A309 L312 A313 D320 D356 E357 V358 S359 K360 E361 T382 E387

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.96Å 134.28Å 165.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.74 – 2.40 19.74 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.74-2.40) 99.8 (19.74-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.72 (at 2.41Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.219 , 0.248 0.219 , 0.249	Depositor DCC
R_{free} test set	1999 reflections (2.92%)	wwPDB-VP
Wilson B-factor (Å^2)	39.3	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.47 , 57.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	24320	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.59 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.5752e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.26	0/3057	0.49	0/4131
1	B	0.26	0/3028	0.49	0/4092
1	C	0.26	0/3132	0.50	0/4230
1	D	0.27	0/3074	0.50	0/4154
All	All	0.26	0/12291	0.49	0/16607

There are no bond length outliers.

There are no bond angle outliers.

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	2998	2934	2933	8	0
1	B	2969	2916	2914	9	0
1	C	3070	2981	3006	9	0
1	D	3014	2943	2950	8	0
2	A	53	31	31	0	0
2	B	53	31	31	0	0
2	C	53	31	31	0	0
2	D	53	31	31	0	0
3	A	37	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	29	0	0	0	0
3	C	48	0	0	0	0
3	D	45	0	0	0	0
All	All	12422	11898	11927	34	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 1.

All (34) 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:D:179:ALA:HB3	1:D:271:ILE:HD12	1.72	0.72
1:C:92:LYS:HE3	1:C:96:ARG:NH2	2.13	0.64
1:C:96:ARG:HD3	1:C:100:GLU:OE2	2.02	0.59
1:D:128:ILE:HD11	1:D:142:LYS:HA	1.85	0.57
1:B:336:PRO:HB2	1:B:381:ILE:HD13	1.86	0.56
1:C:150:ASP:C	1:C:151:LEU:HD22	2.25	0.56
1:D:151:LEU:HD21	1:D:323:TYR:HB3	1.88	0.55
1:D:179:ALA:CB	1:D:271:ILE:HD12	2.36	0.55
1:A:154:ALA:HB3	1:A:286:LEU:HD23	1.91	0.53
1:A:335:ARG:NH2	3:A:502:HOH:O	2.38	0.52
1:B:21:TYR:CD1	1:B:115:THR:HG22	2.45	0.51
1:B:20:CYS:HB3	1:B:119:ILE:HD13	1.92	0.51
1:B:78:VAL:HG12	1:B:79:ASP:O	2.12	0.50
1:A:15:ALA:HB2	1:A:305:ALA:HB1	1.93	0.49
1:B:249:PHE:HB3	1:B:253:THR:HG21	1.95	0.48
1:B:194:HIS:ND1	1:B:211:ASP:O	2.48	0.46
1:C:21:TYR:CD1	1:C:115:THR:HG22	2.50	0.46
1:B:179:ALA:HB3	1:B:271:ILE:HD12	1.97	0.46
1:C:92:LYS:HE3	1:C:96:ARG:CZ	2.47	0.45
1:B:56:ALA:HA	1:B:59:MET:HE3	1.99	0.45
1:C:271:ILE:HG21	1:C:297:LEU:HG	1.98	0.45
1:D:158:ILE:HD12	1:D:274:VAL:CG2	2.48	0.44
1:D:15:ALA:HB2	1:D:305:ALA:HB1	1.99	0.44
1:A:111:ILE:O	1:A:115:THR:HG23	2.18	0.44
1:A:158:ILE:HD12	1:A:274:VAL:HG23	1.99	0.44
1:B:271:ILE:HG23	1:B:296:PRO:HD2	1.99	0.44
1:A:78:VAL:HG12	1:A:79:ASP:O	2.19	0.43
1:A:248:ASP:OD1	1:A:248:ASP:N	2.51	0.43
1:C:154:ALA:HB3	1:C:286:LEU:HD23	2.02	0.42
1:C:272:THR:HG22	1:C:273:GLN:N	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:ALA:HB2	1:C:305:ALA:HB1	2.01	0.42
1:D:158:ILE:HD12	1:D:274:VAL:HG23	2.01	0.41
1:A:79:ASP:OD1	1:A:83:LYS:N	2.53	0.41
1:D:151:LEU:HD21	1:D:323:TYR:CB	2.50	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	373/403 (93%)	361 (97%)	12 (3%)	0	100	100
1	B	369/403 (92%)	350 (95%)	19 (5%)	0	100	100
1	C	383/403 (95%)	368 (96%)	15 (4%)	0	100	100
1	D	374/403 (93%)	354 (95%)	20 (5%)	0	100	100
All	All	1499/1612 (93%)	1433 (96%)	66 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	322/345 (93%)	321 (100%)	1 (0%)	92	97
1	B	319/345 (92%)	318 (100%)	1 (0%)	92	97

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	329/345 (95%)	328 (100%)	1 (0%)	92 97
1	D	324/345 (94%)	320 (99%)	4 (1%)	71 85
All	All	1294/1380 (94%)	1287 (100%)	7 (0%)	88 95

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	3	LYS
1	D	47	ASP
1	D	98	ASP
1	D	292	TYR
1	A	295	SER
1	B	375	LYS
1	C	292	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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	401	-	53,58,58	0.48	0	68,89,89	0.49	1 (1%)
2	FAD	A	401	-	53,58,58	0.47	0	68,89,89	0.52	1 (1%)
2	FAD	C	401	-	53,58,58	0.46	0	68,89,89	0.52	1 (1%)
2	FAD	D	401	-	53,58,58	0.46	0	68,89,89	0.52	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	401	-	-	8/30/50/50	0/6/6/6
2	FAD	A	401	-	-	8/30/50/50	0/6/6/6
2	FAD	C	401	-	-	8/30/50/50	0/6/6/6
2	FAD	D	401	-	-	9/30/50/50	0/6/6/6

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	FAD	C5A-C6A-N6A	2.24	123.75	120.35
2	D	401	FAD	C5A-C6A-N6A	2.23	123.74	120.35
2	C	401	FAD	C5A-C6A-N6A	2.19	123.68	120.35
2	B	401	FAD	C5A-C6A-N6A	2.00	123.40	120.35

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	FAD	C5'-O5'-P-O1P
2	A	401	FAD	C5'-O5'-P-O1P
2	B	401	FAD	C5'-O5'-P-O1P
2	C	401	FAD	C5'-O5'-P-O1P
2	B	401	FAD	C2'-C3'-C4'-O4'
2	B	401	FAD	O3'-C3'-C4'-C5'
2	D	401	FAD	C2'-C3'-C4'-C5'

Continued on next page...

Continued from previous page...

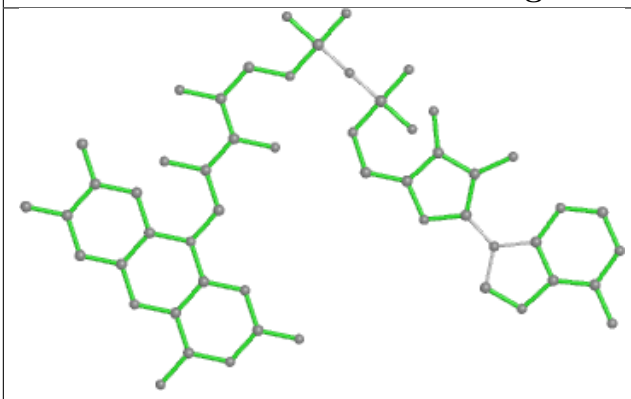
Mol	Chain	Res	Type	Atoms
2	B	401	FAD	C2'-C3'-C4'-C5'
2	C	401	FAD	C2'-C3'-C4'-C5'
2	D	401	FAD	C2'-C3'-C4'-O4'
2	C	401	FAD	C2'-C3'-C4'-O4'
2	D	401	FAD	O3'-C3'-C4'-C5'
2	A	401	FAD	O3'-C3'-C4'-C5'
2	C	401	FAD	O3'-C3'-C4'-C5'
2	A	401	FAD	C2'-C3'-C4'-C5'
2	D	401	FAD	O3'-C3'-C4'-O4'
2	A	401	FAD	O3'-C3'-C4'-O4'
2	B	401	FAD	O3'-C3'-C4'-O4'
2	C	401	FAD	O3'-C3'-C4'-O4'
2	A	401	FAD	C2'-C3'-C4'-O4'
2	D	401	FAD	O4B-C4B-C5B-O5B
2	D	401	FAD	C5'-O5'-P-O3P
2	A	401	FAD	C5'-O5'-P-O3P
2	B	401	FAD	C5'-O5'-P-O3P
2	C	401	FAD	C5'-O5'-P-O3P
2	D	401	FAD	C5'-O5'-P-O2P
2	A	401	FAD	C5'-O5'-P-O2P
2	B	401	FAD	C5'-O5'-P-O2P
2	C	401	FAD	C5'-O5'-P-O2P
2	A	401	FAD	O4B-C4B-C5B-O5B
2	C	401	FAD	O4B-C4B-C5B-O5B
2	D	401	FAD	C3B-C4B-C5B-O5B
2	B	401	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

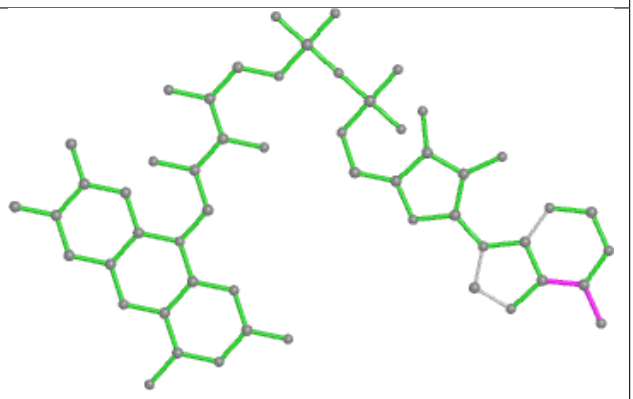
No monomer is involved in short contacts.

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 then 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.

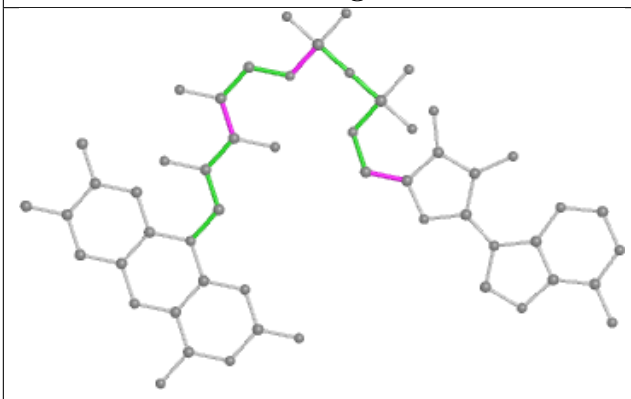
Ligand FAD B 401



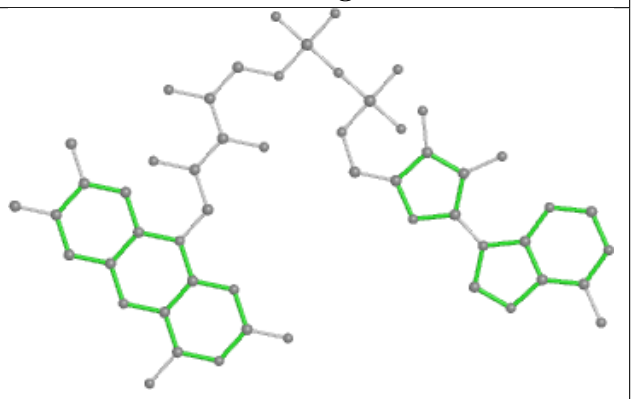
Bond lengths



Bond angles

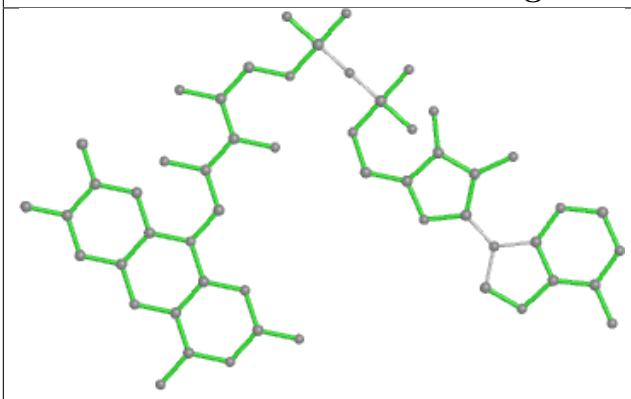


Torsions

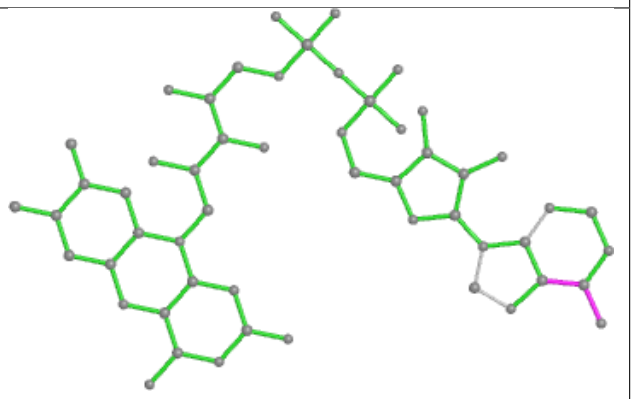


Rings

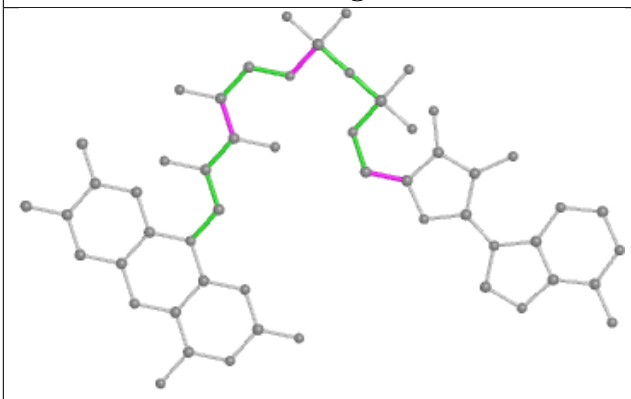
Ligand FAD A 401



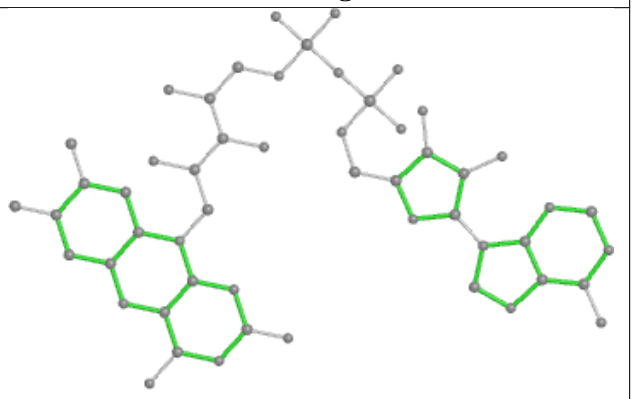
Bond lengths



Bond angles

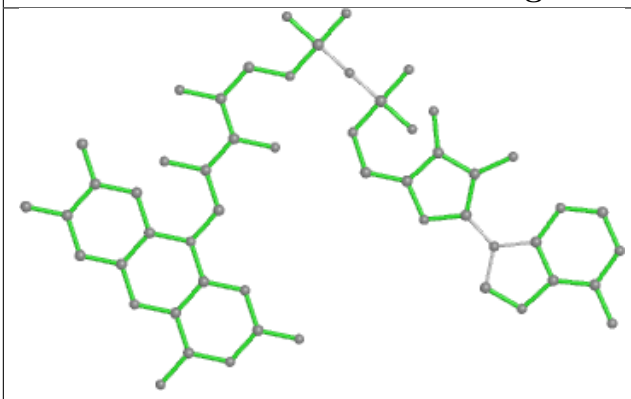


Torsions

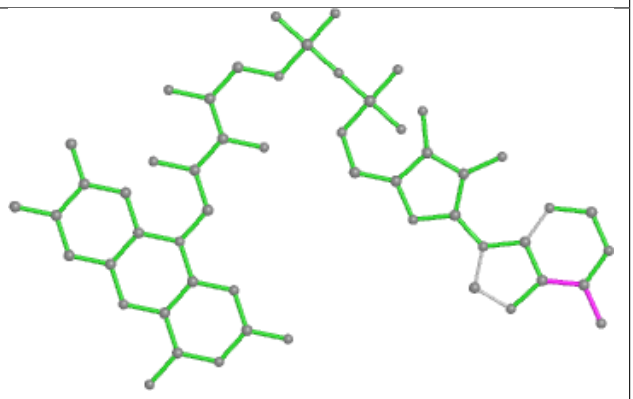


Rings

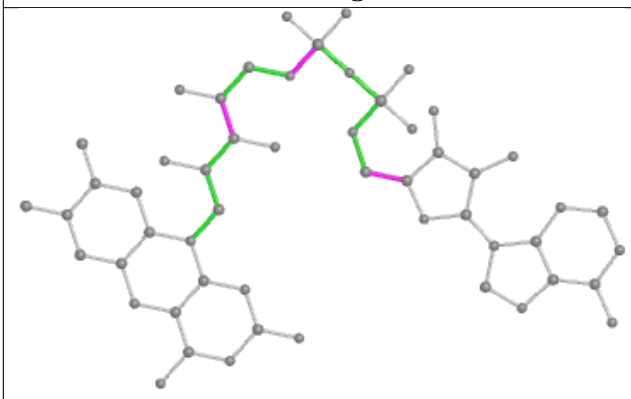
Ligand FAD C 401



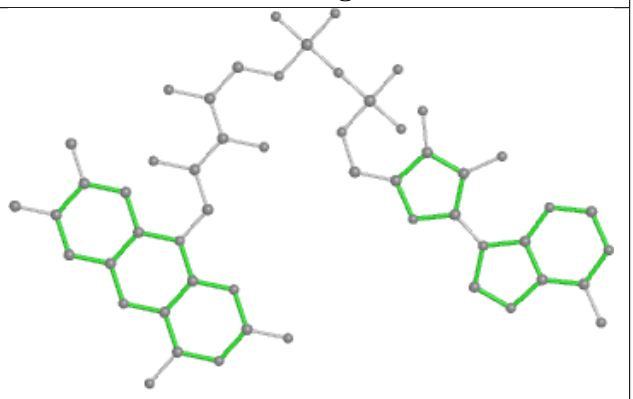
Bond lengths



Bond angles

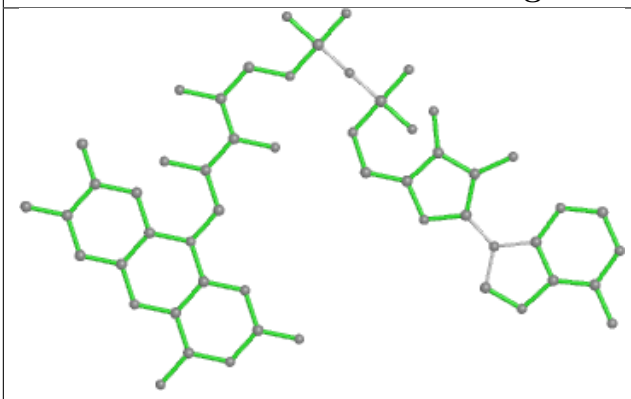


Torsions

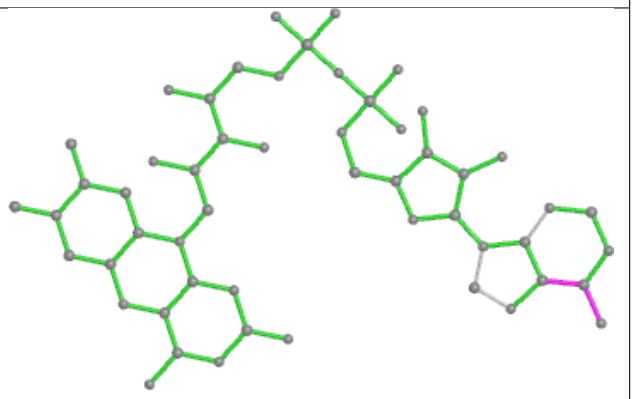


Rings

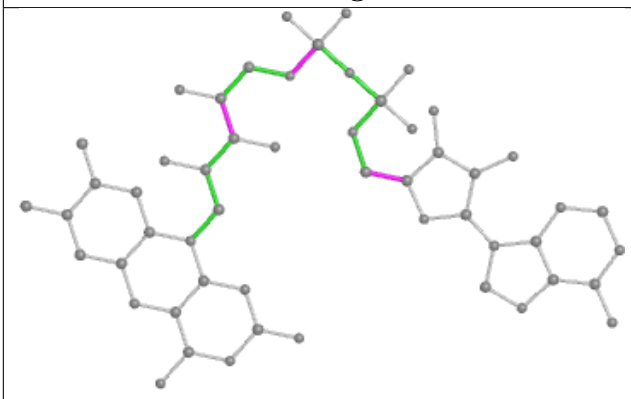
Ligand FAD D 401



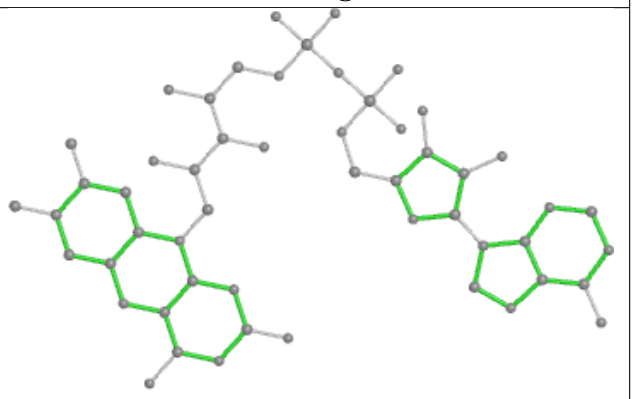
Bond lengths



Bond angles



Torsions



Rings

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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	377/403 (93%)	0.41	31 (8%) 11 10	28, 40, 62, 84	0
1	B	373/403 (92%)	0.66	39 (10%) 6 5	28, 47, 68, 95	0
1	C	385/403 (95%)	0.48	34 (8%) 10 9	27, 44, 64, 87	0
1	D	378/403 (93%)	0.43	28 (7%) 14 13	26, 42, 64, 83	0
All	All	1513/1612 (93%)	0.49	132 (8%) 10 9	26, 43, 65, 95	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	356	ASP	10.2
1	B	368	ASN	7.1
1	D	360	LYS	6.9
1	B	360	LYS	6.9
1	C	357	GLU	6.5
1	B	371	LEU	6.2
1	D	357	GLU	5.4
1	A	360	LYS	5.2
1	B	357	GLU	4.9
1	A	357	GLU	4.5
1	C	361	GLU	4.5
1	D	4	ASN	4.4
1	B	364	GLU	4.3
1	B	361	GLU	4.2
1	C	360	LYS	4.2
1	D	2	TYR	4.1
1	B	134	SER	4.1
1	B	135	ASP	4.0
1	A	233	ARG	4.0
1	B	382	THR	3.8
1	B	71	ARG	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	4	ASN	3.7
1	C	236	HIS	3.7
1	A	97	GLN	3.7
1	D	247	ARG	3.6
1	B	320	ASP	3.6
1	C	96	ARG	3.6
1	D	358	VAL	3.6
1	B	358	VAL	3.6
1	B	247	ARG	3.5
1	A	52	ALA	3.5
1	B	332	ALA	3.5
1	B	233	ARG	3.4
1	B	387	GLU	3.4
1	D	135	ASP	3.4
1	D	117	THR	3.4
1	A	356	ASP	3.3
1	D	142	LYS	3.3
1	C	233	ARG	3.3
1	B	354	VAL	3.3
1	C	387	GLU	3.2
1	A	134	SER	3.2
1	A	306	PHE	3.2
1	B	248	ASP	3.2
1	A	385	GLN	3.1
1	D	193	ARG	3.1
1	C	248	ASP	3.1
1	A	309	ALA	3.0
1	B	170	ASN	3.0
1	C	306	PHE	3.0
1	A	247	ARG	3.0
1	D	248	ASP	3.0
1	C	214	PRO	3.0
1	B	306	PHE	3.0
1	A	135	ASP	3.0
1	B	309	ALA	3.0
1	A	305	ALA	3.0
1	A	359	SER	2.9
1	D	354	VAL	2.9
1	C	91	GLU	2.9
1	D	170	ASN	2.9
1	D	320	ASP	2.9
1	B	54	HIS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	93	PHE	2.9
1	B	18	ALA	2.9
1	B	83	LYS	2.9
1	B	173	GLN	2.8
1	A	364	GLU	2.8
1	C	356	ASP	2.8
1	A	365	GLU	2.8
1	D	387	GLU	2.8
1	A	142	LYS	2.7
1	C	169	LYS	2.7
1	B	367	SER	2.7
1	A	320	ASP	2.7
1	D	380	ALA	2.7
1	B	359	SER	2.7
1	C	305	ALA	2.7
1	C	95	PHE	2.7
1	B	24	ARG	2.6
1	C	135	ASP	2.6
1	A	5	ILE	2.5
1	A	361	GLU	2.5
1	D	303	ASN	2.5
1	D	83	LYS	2.5
1	C	247	ARG	2.5
1	A	27	GLY	2.5
1	C	313	ALA	2.5
1	B	308	GLY	2.4
1	A	236	HIS	2.4
1	C	382	THR	2.4
1	A	387	GLU	2.4
1	B	305	ALA	2.4
1	A	358	VAL	2.4
1	B	168	ASP	2.4
1	B	376	SER	2.4
1	B	336	PRO	2.4
1	B	325	GLN	2.4
1	D	381	ILE	2.4
1	D	306	PHE	2.4
1	C	99	ASP	2.4
1	C	312	LEU	2.4
1	B	312	LEU	2.3
1	C	16	GLY	2.3
1	C	320	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	19	ILE	2.3
1	C	309	ALA	2.3
1	A	24	ARG	2.3
1	D	356	ASP	2.3
1	A	312	LEU	2.3
1	D	307	VAL	2.3
1	C	358	VAL	2.3
1	C	48	VAL	2.2
1	A	382	THR	2.2
1	D	254	GLN	2.2
1	C	118	ASP	2.2
1	C	181	LEU	2.2
1	D	359	SER	2.2
1	D	213	ASP	2.2
1	A	193	ARG	2.2
1	D	214	PRO	2.1
1	C	92	LYS	2.1
1	A	328	THR	2.1
1	C	202	ASN	2.1
1	C	71	ARG	2.1
1	A	56	ALA	2.1
1	D	215	GLU	2.1
1	B	355	GLU	2.1
1	B	63	ASP	2.0
1	B	302	ASN	2.0
1	A	332	ALA	2.0
1	D	382	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,

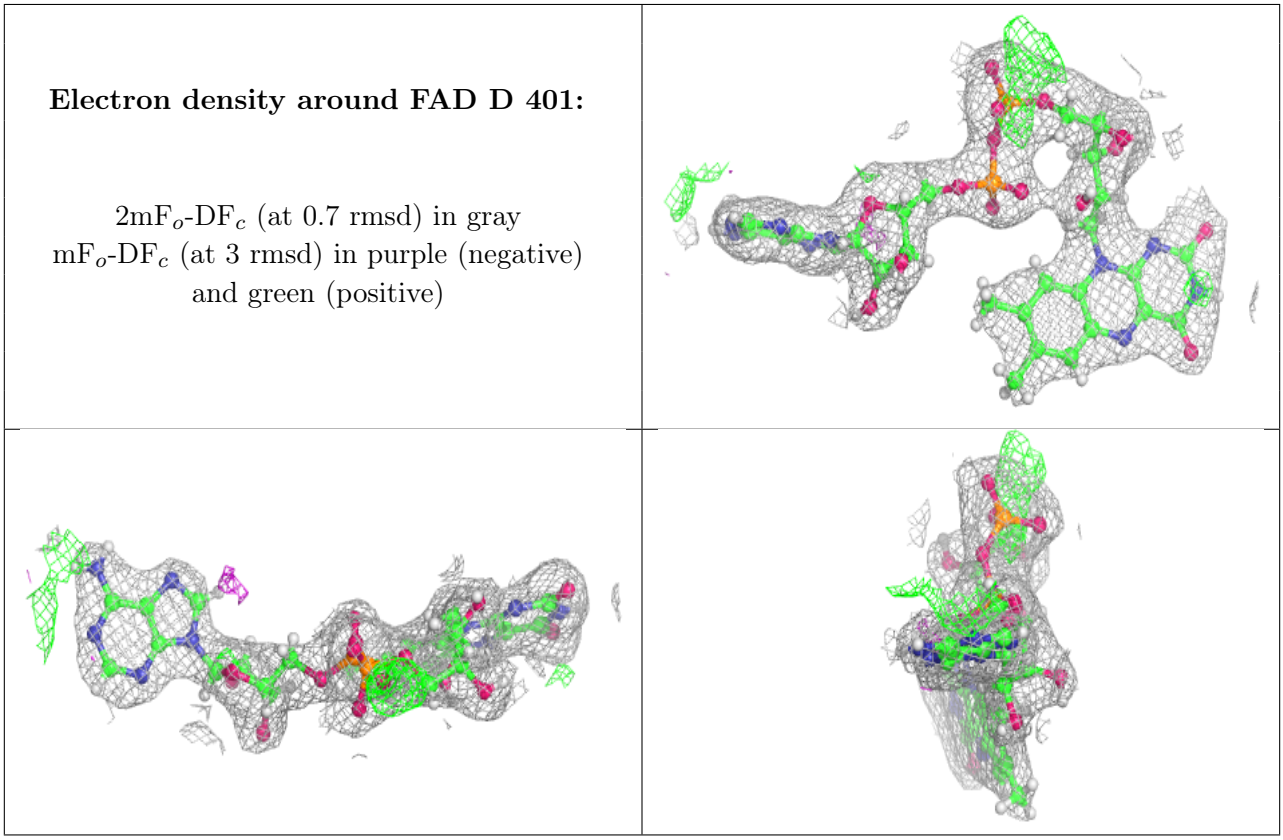
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FAD	D	401	53/53	0.94	0.15	26,34,40,44	0
2	FAD	A	401	53/53	0.95	0.14	22,31,36,39	0
2	FAD	B	401	53/53	0.95	0.14	26,34,39,41	0
2	FAD	C	401	53/53	0.95	0.14	24,31,36,38	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.

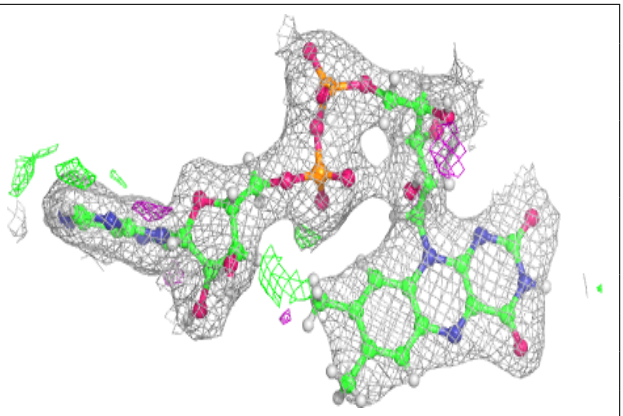
Electron density around FAD D 401:

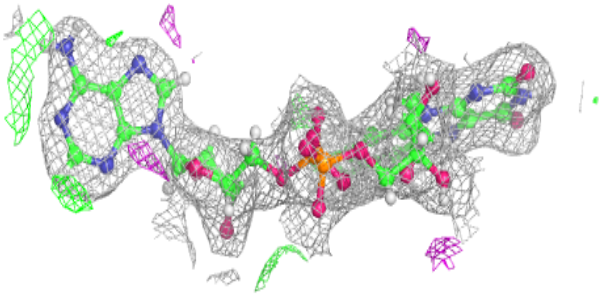
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

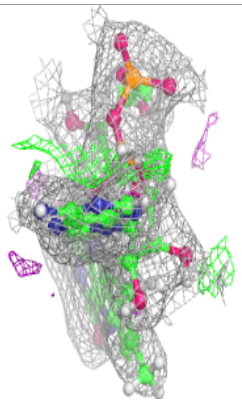


Electron density around FAD A 401:

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

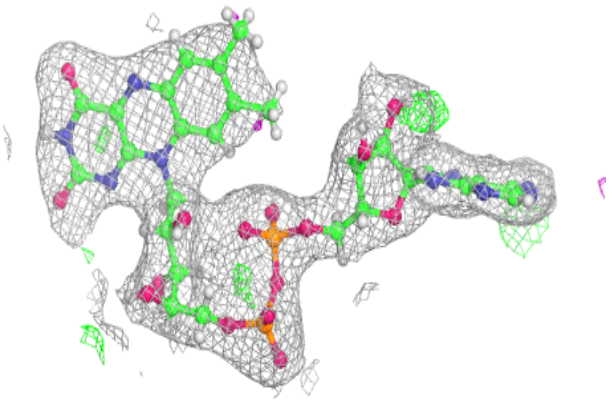


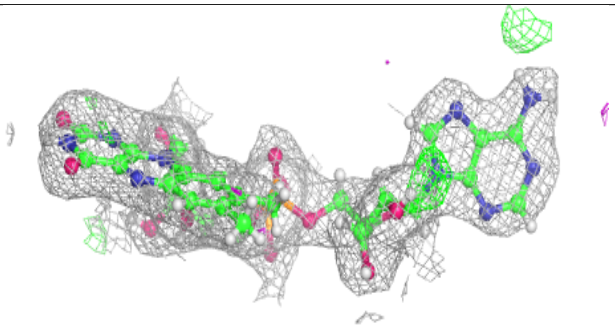


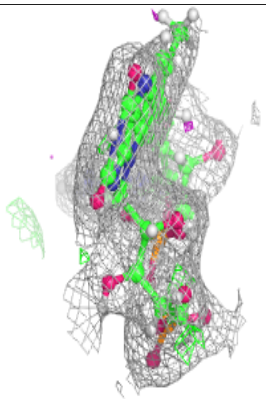


Electron density around FAD B 401:

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

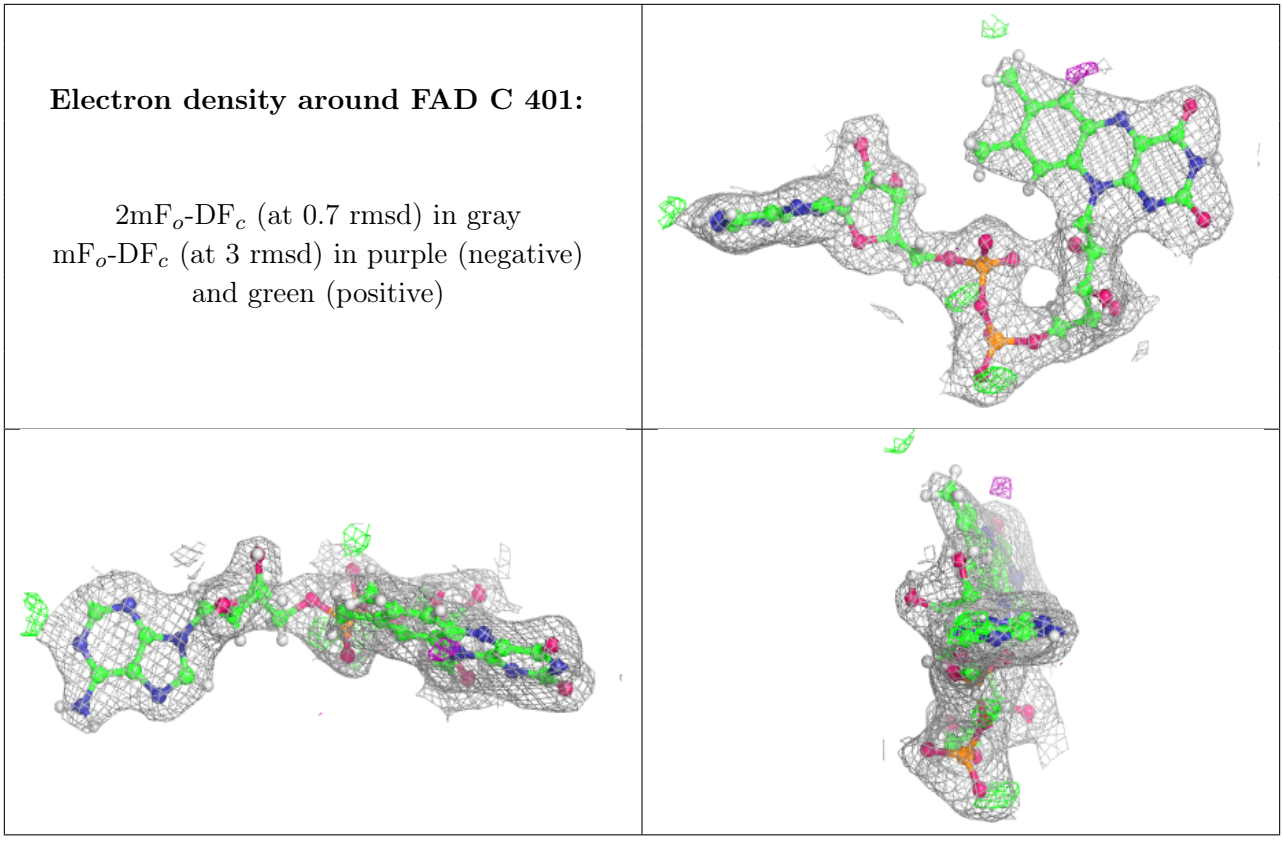






Electron density around FAD C 401:

$2mF_o$-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.