



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 7, 2020 – 03:53 am BST

PDB ID : 6FAH
Title : Molecular basis of the flavin-based electron-bifurcating caffeyl-CoA reductase reaction
Authors : Demmer, J.K.; Bertsch, J.; Oeppinger, C.; Wohlers, H.; Kayastha, K.; Demmer, U.; Ermler, U.; Mueller, V.
Deposited on : 2017-12-15
Resolution : 3.13 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 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 : 2.11
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) : 2.11

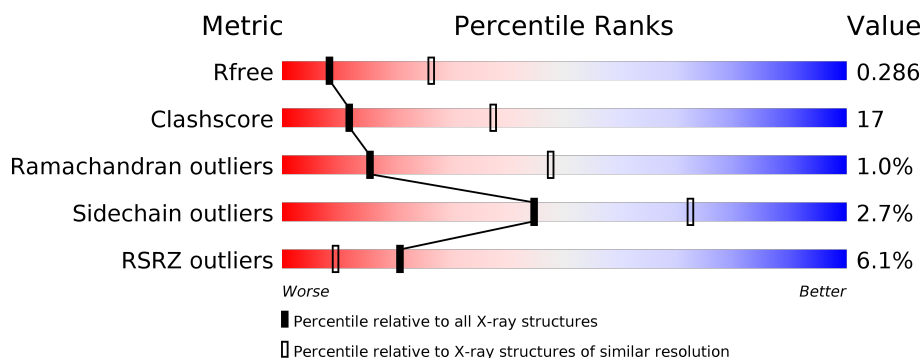
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.13 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	1626 (3.18-3.10)
Clashscore	141614	1735 (3.18-3.10)
Ramachandran outliers	138981	1677 (3.18-3.10)
Sidechain outliers	138945	1677 (3.18-3.10)
RSRZ outliers	127900	1588 (3.18-3.10)

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 on 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	396	<div> <div>10%</div> <div>56%</div> <div>34%</div> <div>6%</div> <div>• •</div> </div>
1	E	396	<div> <div>14%</div> <div>58%</div> <div>34%</div> <div>6%</div> <div>• •</div> </div>
2	B	262	<div> <div>5%</div> <div>65%</div> <div>34%</div> <div>•</div> </div>
2	F	262	<div> <div>6%</div> <div>65%</div> <div>34%</div> <div>•</div> </div>
3	C	379	<div> <div>77%</div> <div>22%</div> <div>•</div> </div>
3	D	379	<div> <div>75%</div> <div>25%</div> <div>•</div> </div>

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
6	SO4	D	403	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15985 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 Caffeyl-CoA reductase-Etf complex subunit CarE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			2915	1839	479	575	22			
1	E	393	Total	C	N	O	S	0	0	0
			2948	1861	484	581	22			

- Molecule 2 is a protein called Caffeyl-CoA reductase-Etf complex subunit CarD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	262	Total	C	N	O	S	0	0	0
			1970	1235	332	387	16			
2	F	262	Total	C	N	O	S	0	0	0
			1970	1235	332	387	16			

- Molecule 3 is a protein called Caffeyl-CoA reductase-Etf complex subunit CarC.

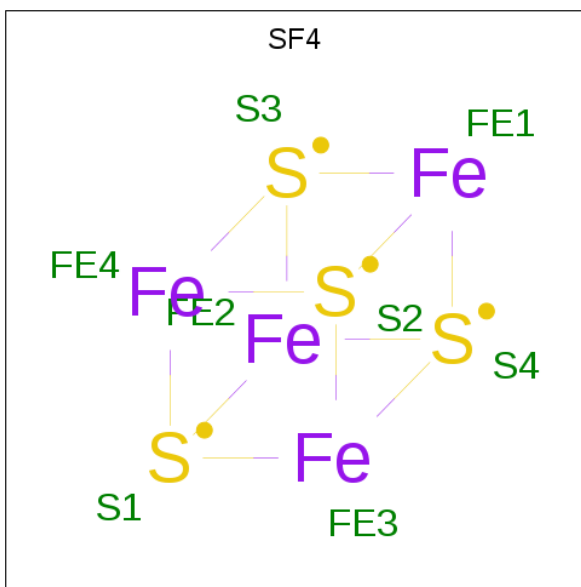
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	379	Total	C	N	O	S	0	1	0
			2903	1841	480	556	26			
3	D	379	Total	C	N	O	S	0	0	0
			2894	1833	480	555	26			

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



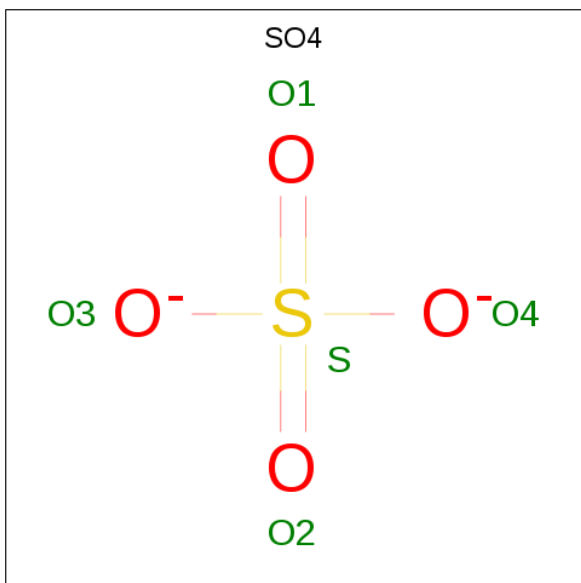
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			8	4	4		
5	A	1	Total	Fe	S	0	0
			8	4	4		
5	E	1	Total	Fe	S	0	0
			8	4	4		
5	E	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

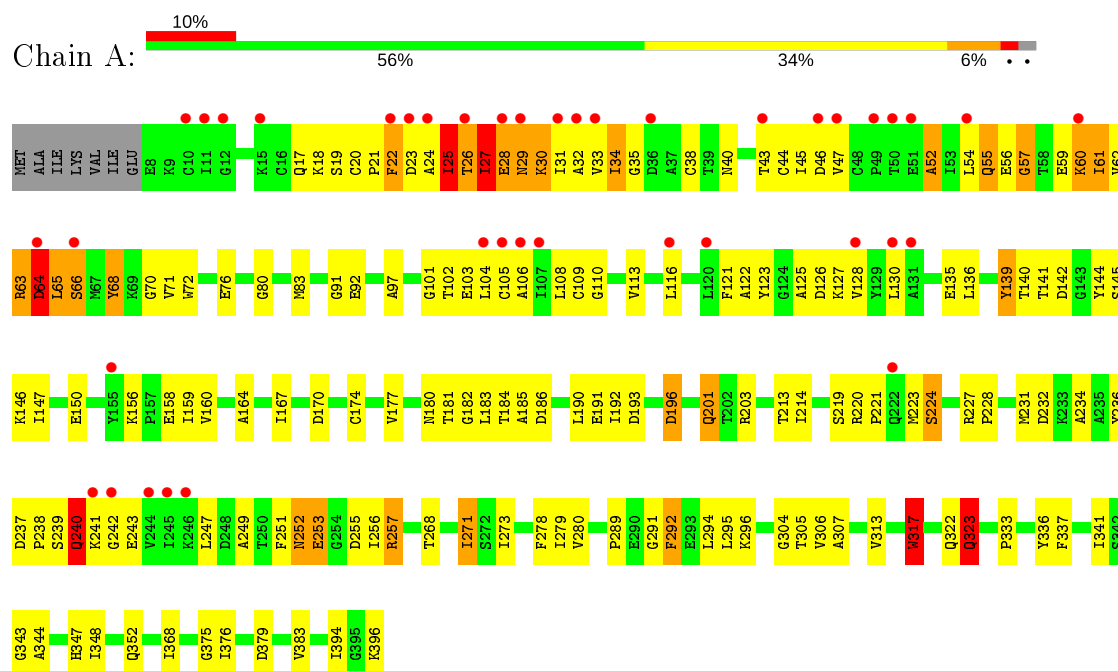


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

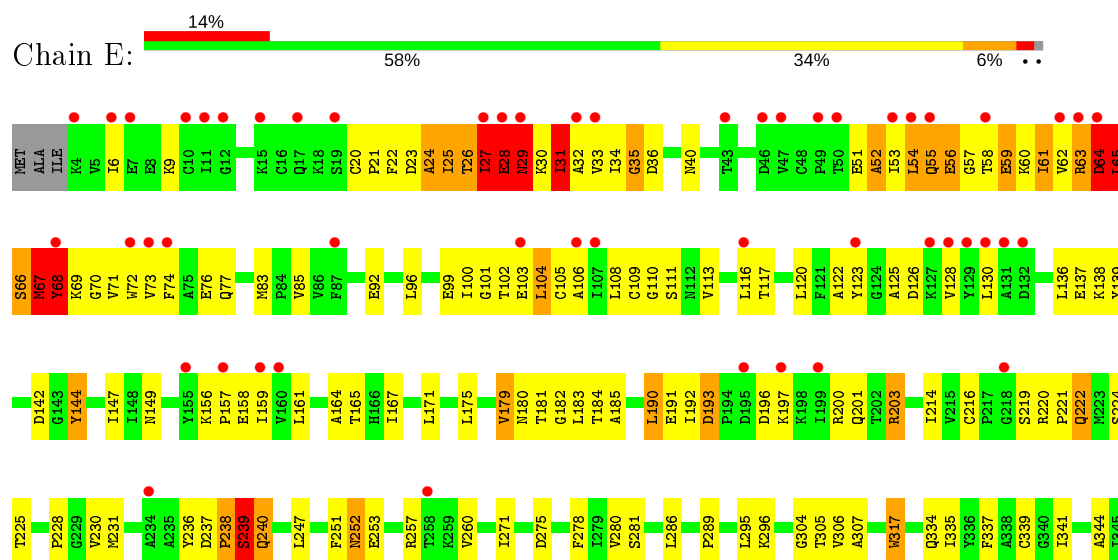
3 Residue-property plots [i](#)

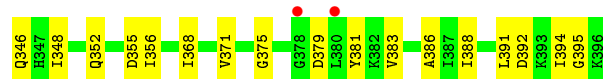
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Caffeyl-CoA reductase-Etf complex subunit CarE

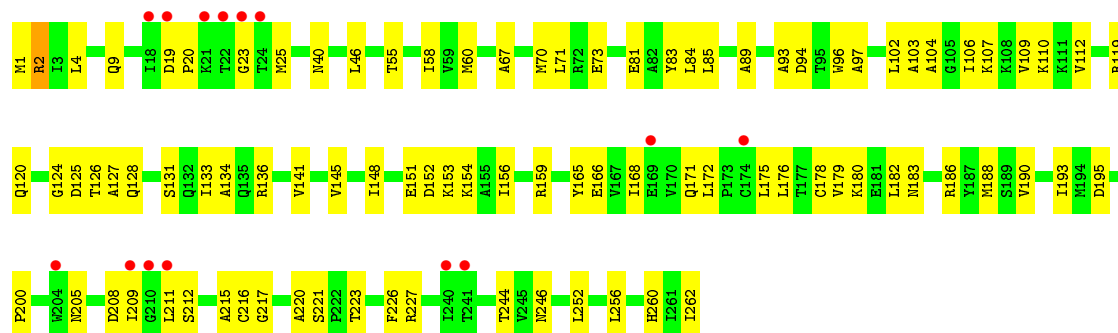


- Molecule 1: Caffeyl-CoA reductase-Etf complex subunit CarE

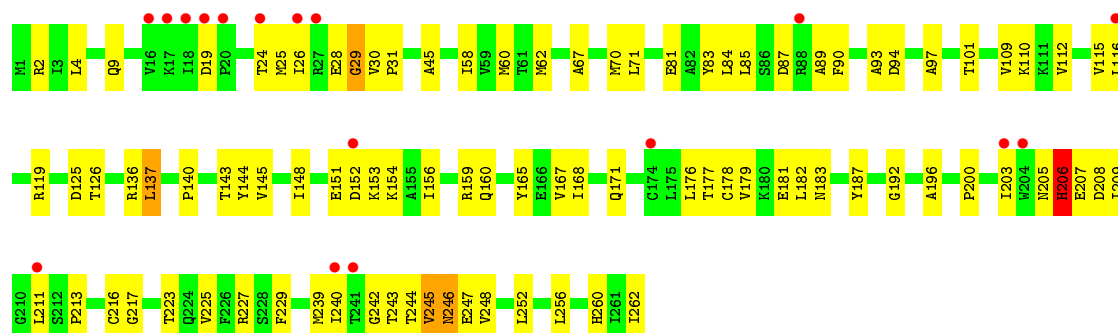




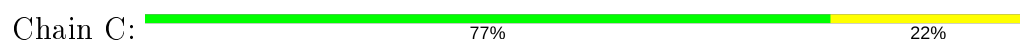
• Molecule 2: Caffeyl-CoA reductase-Etf complex subunit CarD



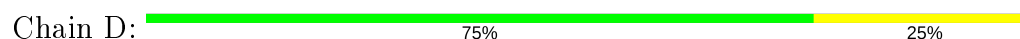
• Molecule 2: Caffeyl-CoA reductase-Etf complex subunit CarD

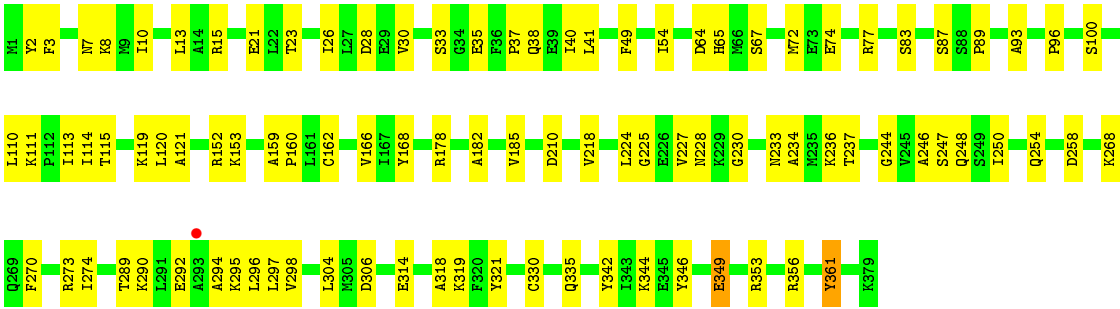


• Molecule 3: Caffeyl-CoA reductase-Etf complex subunit CarC



• Molecule 3: Caffeyl-CoA reductase-Etf complex subunit CarC





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	213.74Å 144.26Å 102.84Å 90.00° 98.93° 90.00°	Depositor
Resolution (Å)	49.52 – 3.13 49.52 – 3.13	Depositor EDS
% Data completeness (in resolution range)	75.2 (49.52-3.13) 75.2 (49.52-3.13)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.234 , 0.286 0.234 , 0.286	Depositor DCC
R_{free} test set	2057 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	85.3	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 108.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	15985	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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: SF4, SO4, 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	0.74	8/2958 (0.3%)	1.25	46/4004 (1.1%)
1	E	0.72	8/2991 (0.3%)	1.26	49/4048 (1.2%)
2	B	0.45	0/1999	0.66	0/2710
2	F	0.56	2/1999 (0.1%)	0.98	9/2710 (0.3%)
3	C	0.63	0/2948	0.66	1/3947 (0.0%)
3	D	0.62	0/2935	0.66	1/3929 (0.0%)
All	All	0.64	18/15830 (0.1%)	0.97	106/21348 (0.5%)

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	5
1	E	0	6
All	All	0	11

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	246	ASN	CG-ND2	9.97	1.57	1.32
1	A	323	GLN	CD-OE1	-9.75	1.02	1.24
1	E	179	VAL	CB-CG2	-8.29	1.35	1.52
1	A	240	GLN	CG-CD	8.02	1.69	1.51
1	E	28	GLU	CB-CG	7.26	1.66	1.52

The worst 5 of 106 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	246	ASN	CB-CG-OD1	29.19	179.98	121.60
1	E	65	LEU	CB-CG-CD2	-16.16	83.54	111.00
2	F	246	ASN	OD1-CG-ND2	-12.75	92.58	121.90
2	F	246	ASN	CB-CG-ND2	-12.20	87.43	116.70
1	E	36	ASP	CB-CG-OD1	12.17	129.25	118.30

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	GLN	Sidechain,Mainchain
1	A	26	THR	Mainchain
1	A	323	GLN	Sidechain
1	A	52	ALA	Mainchain
1	E	29	ASN	Sidechain

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	2915	0	2933	149	0
1	E	2948	0	2973	150	0
2	B	1970	0	2005	68	0
2	F	1970	0	2005	83	0
3	C	2903	0	2952	61	0
3	D	2894	0	2943	57	1
4	A	53	0	31	3	0
4	B	53	0	31	5	0
4	C	53	0	31	5	0
4	D	53	0	31	4	0
4	E	53	0	31	5	0
4	F	53	0	31	7	0
5	A	16	0	0	1	0
5	E	16	0	0	0	0
6	C	25	0	0	0	0
6	D	10	0	0	0	0
All	All	15985	0	15997	554	1

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 17.

The worst 5 of 554 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:E:65:LEU:HD21	1:E:68:TYR:OH	1.42	1.19
1:A:201:GLN:HE22	1:A:224:SER:HB3	1.05	1.16
1:A:26:THR:HG23	1:A:31:ILE:HA	1.31	1.12
1:E:77:GLN:NE2	1:E:109:CYS:O	1.81	1.10
1:E:99:GLU:HB3	1:E:192:ILE:HD11	1.31	1.07

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:321:TYR:OH	3:D:321:TYR:OH[2_555]	2.00	0.20

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	387/396 (98%)	332 (86%)	45 (12%)	10 (3%)	5	24
1	E	391/396 (99%)	333 (85%)	50 (13%)	8 (2%)	7	29
2	B	260/262 (99%)	247 (95%)	13 (5%)	0	100	100
2	F	260/262 (99%)	245 (94%)	14 (5%)	1 (0%)	34	67
3	C	378/379 (100%)	359 (95%)	19 (5%)	0	100	100
3	D	377/379 (100%)	358 (95%)	18 (5%)	1 (0%)	41	72
All	All	2053/2074 (99%)	1874 (91%)	159 (8%)	20 (1%)	15	47

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	ILE
1	A	27	ILE
1	A	52	ALA
1	A	64	ASP
1	A	65	LEU

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	315/321 (98%)	307 (98%)	8 (2%)	47	74
1	E	319/321 (99%)	305 (96%)	14 (4%)	28	59
2	B	216/216 (100%)	212 (98%)	4 (2%)	57	80
2	F	216/216 (100%)	210 (97%)	6 (3%)	43	71
3	C	307/306 (100%)	301 (98%)	6 (2%)	55	79
3	D	306/306 (100%)	299 (98%)	7 (2%)	50	75
All	All	1679/1686 (100%)	1634 (97%)	45 (3%)	44	72

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	119	LYS
1	E	55	GLN
2	F	200	PRO
3	D	349	GLU
1	E	63	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	GLN
1	E	180	ASN
1	E	240	GLN
2	F	206	HIS

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Mol	Chain	Res	Type
2	F	246	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

17 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	$\# Z > 2$
6	SO4	C	405	-	4,4,4	0.23	0	6,6,6	0.08	0
4	FAD	E	401	-	51,58,58	1.24	4 (7%)	60,89,89	2.26	7 (11%)
4	FAD	C	401	-	51,58,58	1.43	5 (9%)	60,89,89	2.26	8 (13%)
4	FAD	A	401	-	51,58,58	1.24	3 (5%)	60,89,89	2.29	9 (15%)
6	SO4	D	402	-	4,4,4	0.21	0	6,6,6	0.21	0
5	SF4	E	403	1	0,12,12	0.00	-	-		
5	SF4	E	402	1	0,12,12	0.00	-	-		
4	FAD	B	301	-	51,58,58	1.25	4 (7%)	60,89,89	2.25	8 (13%)
6	SO4	C	403	-	4,4,4	0.31	0	6,6,6	0.18	0
6	SO4	C	404	-	4,4,4	0.20	0	6,6,6	0.27	0
4	FAD	F	301	-	51,58,58	1.28	4 (7%)	60,89,89	2.25	8 (13%)
6	SO4	C	406	-	4,4,4	0.25	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	D	403	-	4,4,4	0.19	0	6,6,6	0.11	0
5	SF4	A	402	1	0,12,12	0.00	-	-		
6	SO4	C	402	-	4,4,4	0.20	0	6,6,6	0.09	0
4	FAD	D	401	-	51,58,58	1.37	6 (11%)	60,89,89	2.30	8 (13%)
5	SF4	A	403	1	0,12,12	0.00	-	-		

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
4	FAD	E	401	-	-	7/30/50/50	0/6/6/6
4	FAD	C	401	-	-	8/30/50/50	0/6/6/6
4	FAD	A	401	-	-	9/30/50/50	0/6/6/6
5	SF4	E	402	1	-	-	0/6/5/5
4	FAD	B	301	-	-	8/30/50/50	0/6/6/6
5	SF4	E	403	1	-	-	0/6/5/5
4	FAD	F	301	-	-	9/30/50/50	0/6/6/6
5	SF4	A	402	1	-	-	0/6/5/5
4	FAD	D	401	-	-	10/30/50/50	0/6/6/6
5	SF4	A	403	1	-	-	0/6/5/5

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	301	FAD	C4X-C10	5.25	1.44	1.38
4	E	401	FAD	C4X-C10	5.19	1.44	1.38
4	A	401	FAD	C4X-C10	5.13	1.43	1.38
4	D	401	FAD	C4X-C10	5.09	1.43	1.38
4	B	301	FAD	C4X-C10	5.06	1.43	1.38

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	FAD	C4-N3-C2	13.11	126.21	115.14
4	E	401	FAD	C4-N3-C2	13.01	126.12	115.14
4	D	401	FAD	C4-N3-C2	12.91	126.04	115.14
4	B	301	FAD	C4-N3-C2	12.90	126.03	115.14
4	F	301	FAD	C4-N3-C2	12.85	125.99	115.14

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

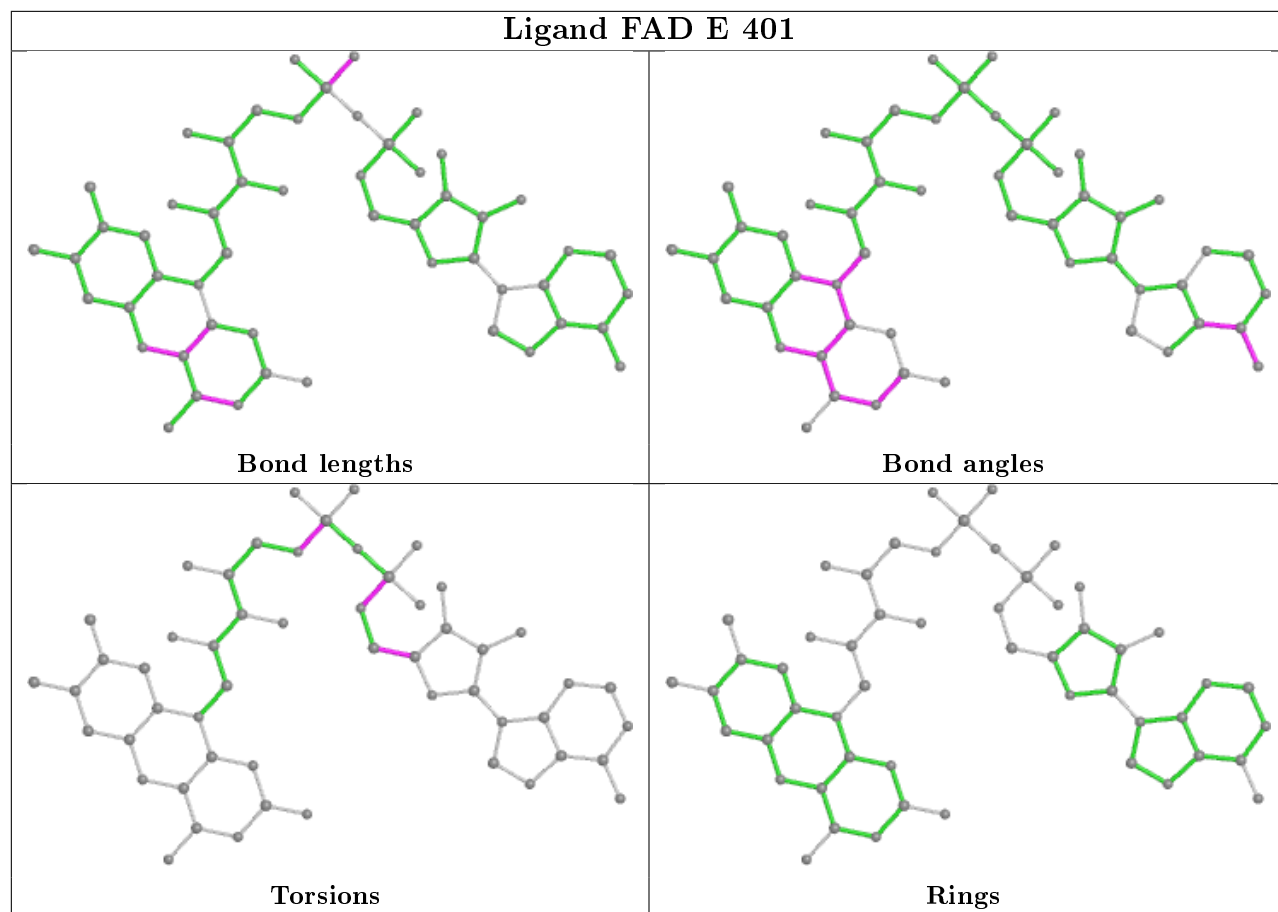
Mol	Chain	Res	Type	Atoms
4	E	401	FAD	C5B-O5B-PA-O1A
4	E	401	FAD	C5B-O5B-PA-O2A
4	E	401	FAD	C3B-C4B-C5B-O5B
4	E	401	FAD	C5'-O5'-P-O1P
4	E	401	FAD	C5'-O5'-P-O3P

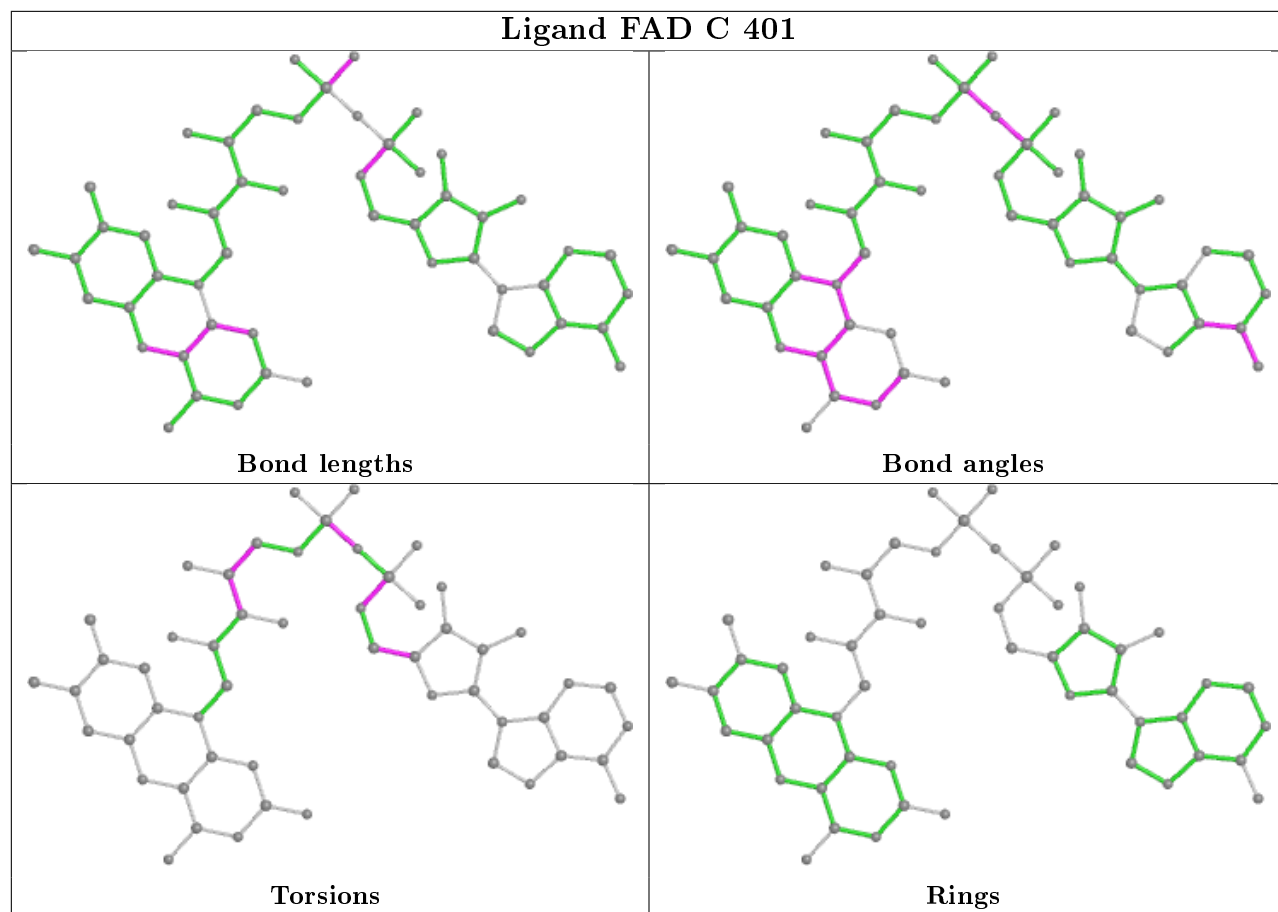
There are no ring outliers.

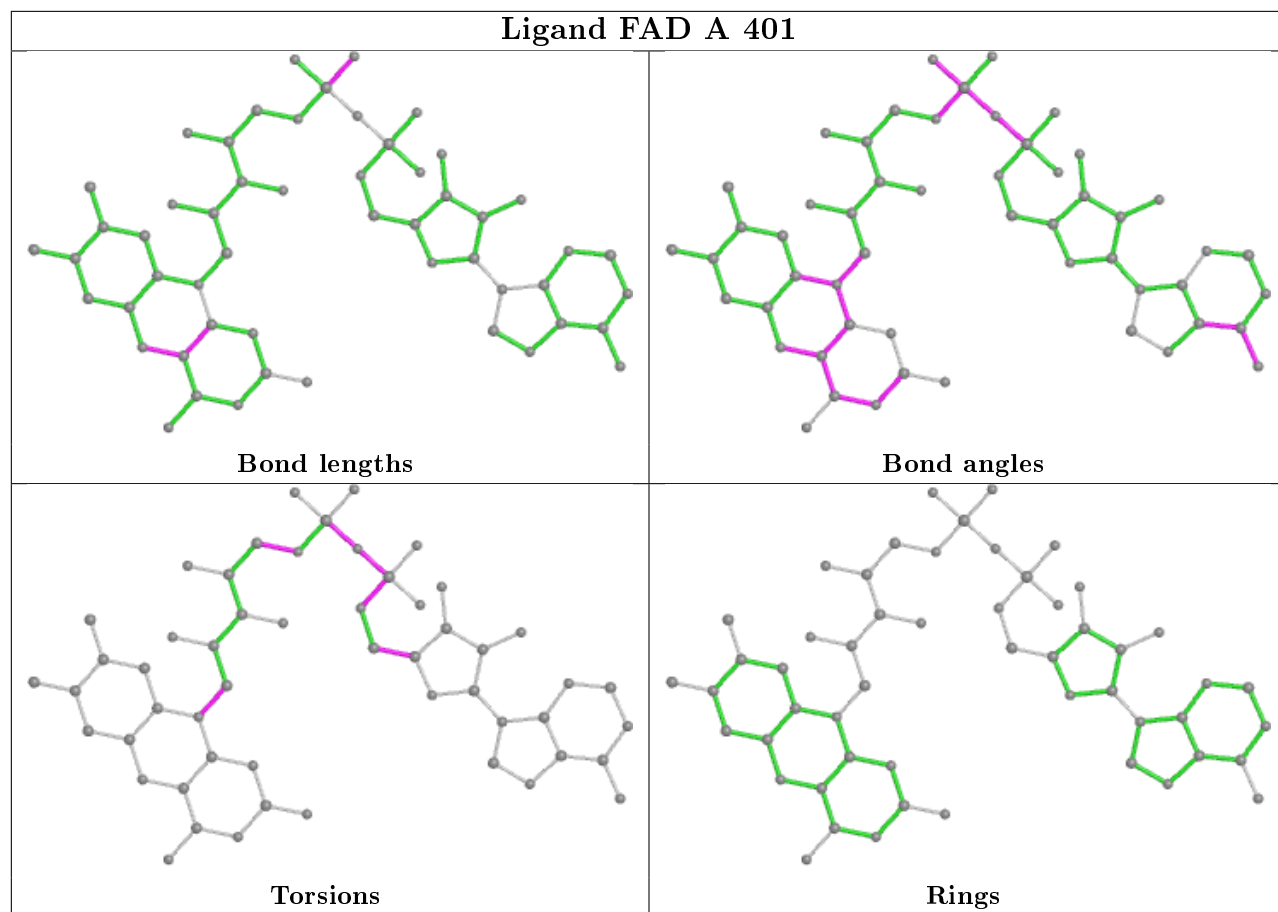
7 monomers are involved in 30 short contacts:

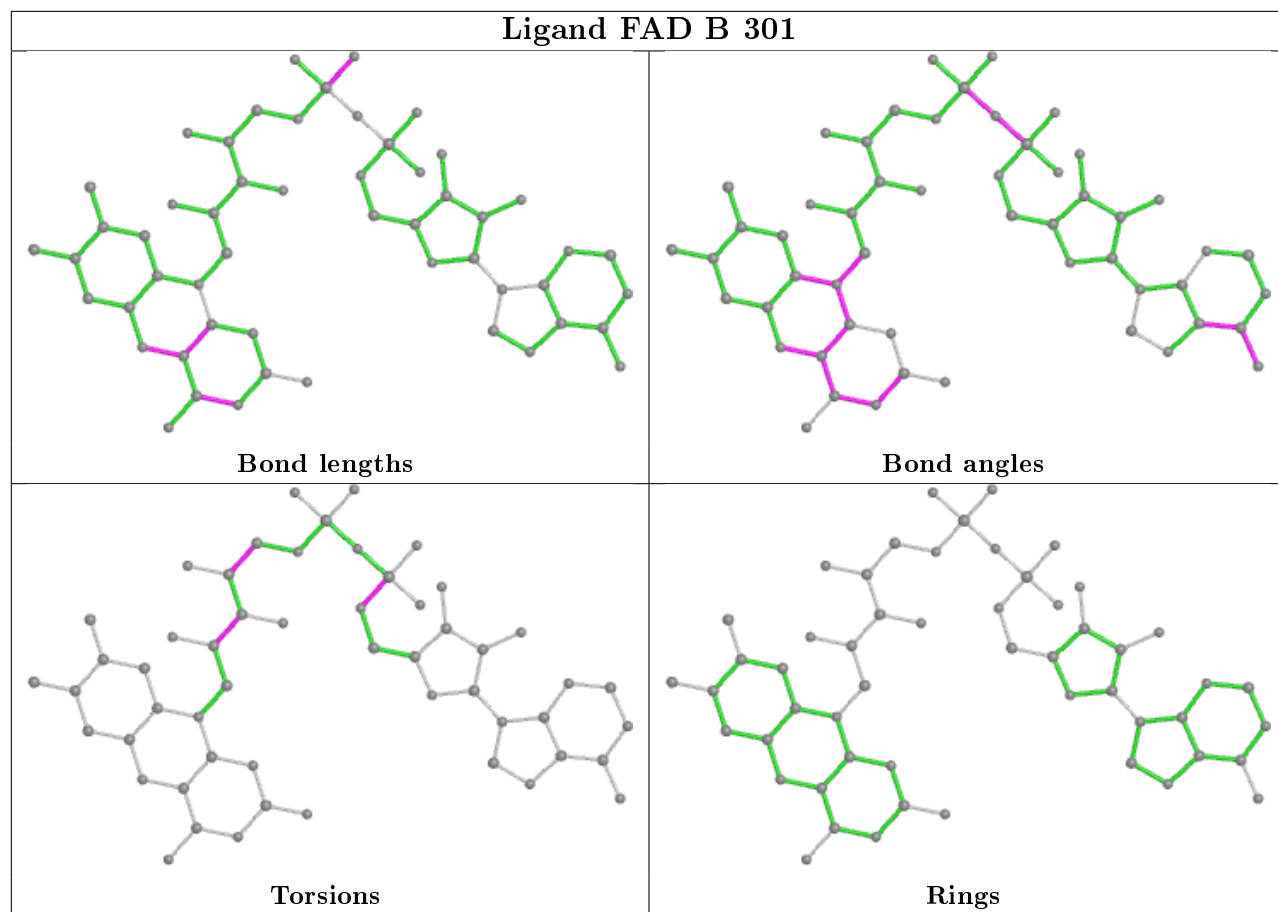
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	401	FAD	5	0
4	C	401	FAD	5	0
4	A	401	FAD	3	0
4	B	301	FAD	5	0
4	F	301	FAD	7	0
4	D	401	FAD	4	0
5	A	403	SF4	1	0

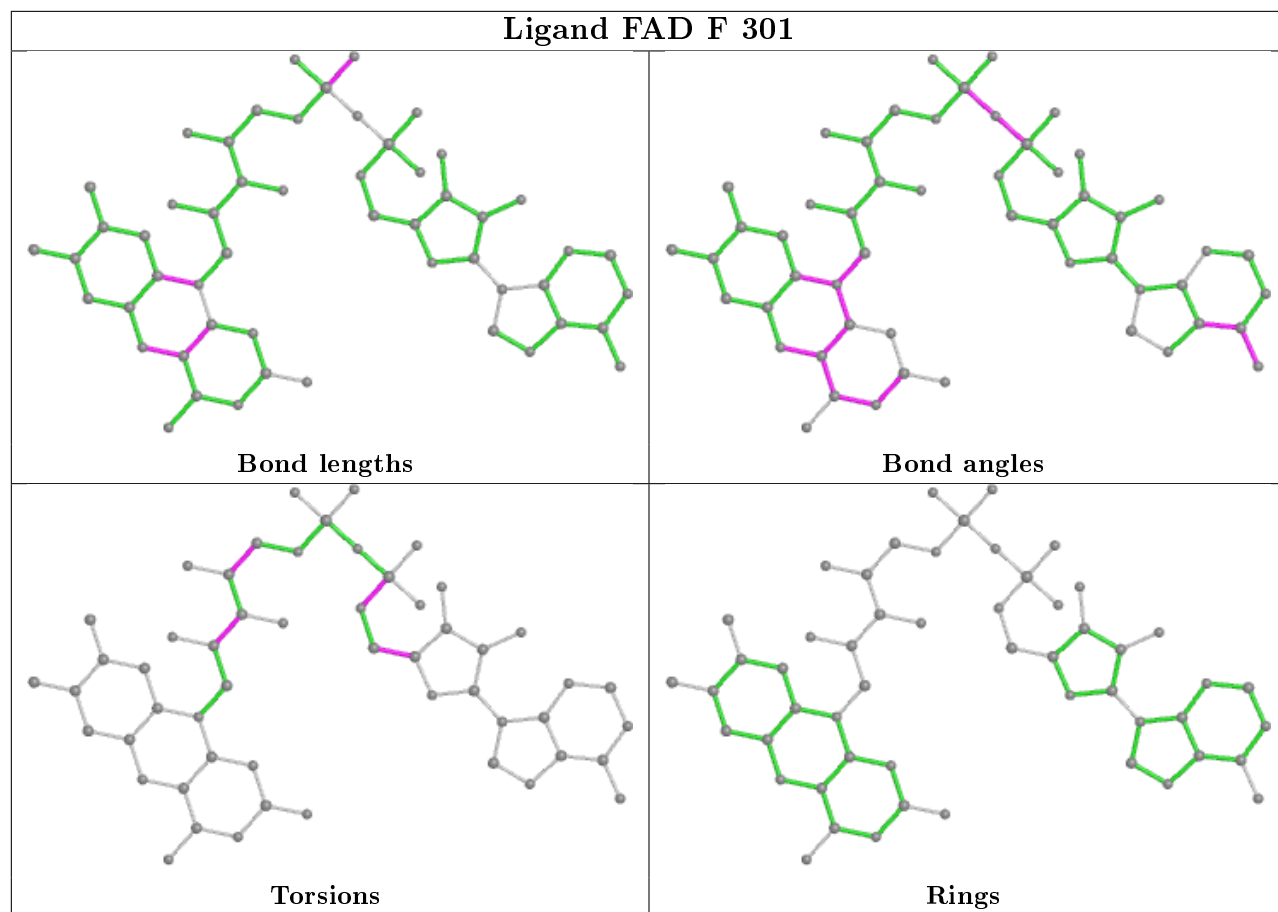
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

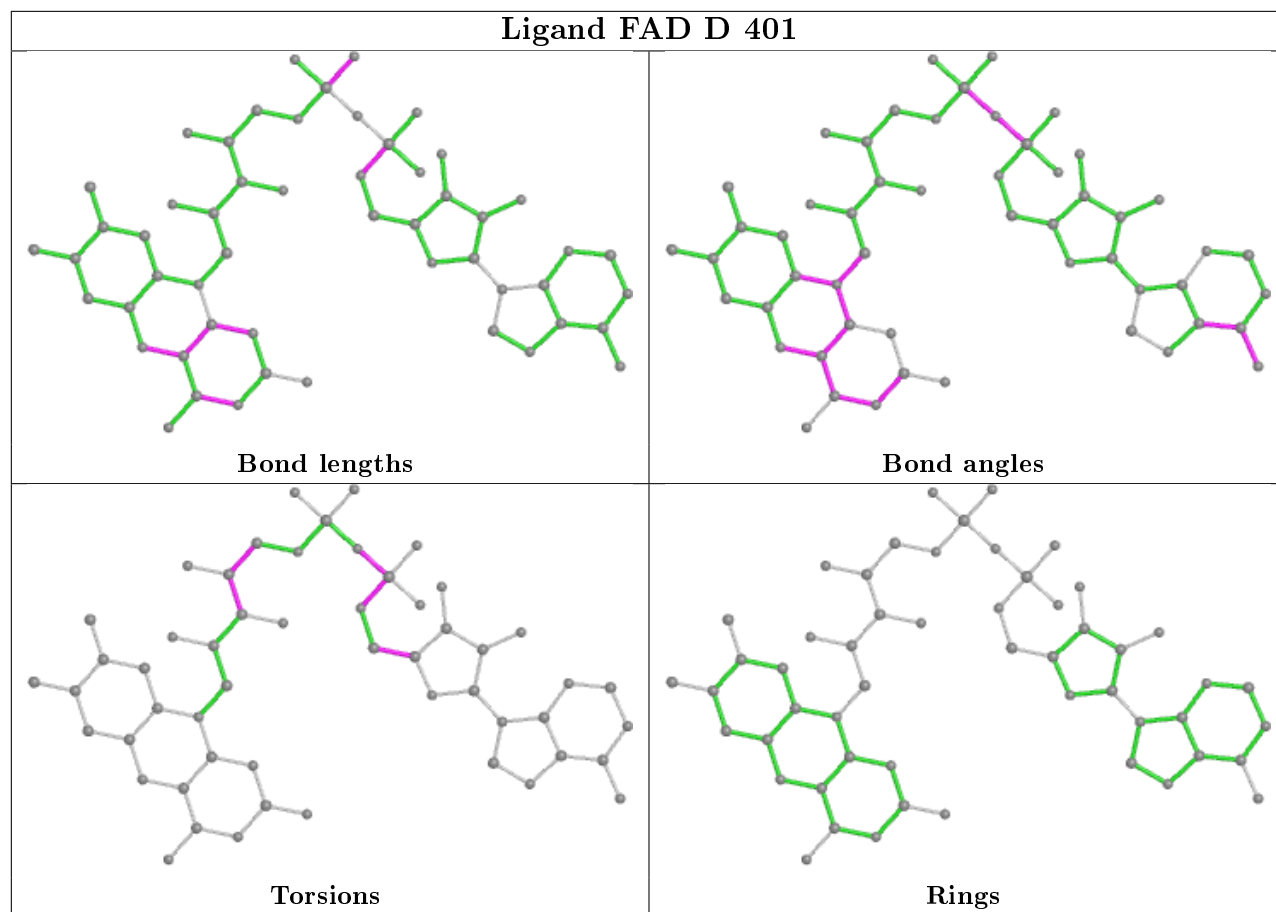












5.7 Other polymers [i](#)

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	389/396 (98%)	0.46	40 (10%) 6 2	33, 133, 234, 270	0
1	E	393/396 (99%)	0.70	54 (13%) 3 1	52, 156, 253, 314	0
2	B	262/262 (100%)	0.10	14 (5%) 26 12	64, 118, 177, 230	0
2	F	262/262 (100%)	0.25	17 (6%) 18 8	83, 134, 213, 260	0
3	C	379/379 (100%)	-0.44	0 100 100	26, 62, 103, 128	0
3	D	379/379 (100%)	-0.49	1 (0%) 94 89	22, 67, 104, 148	0
All	All	2064/2074 (99%)	0.09	126 (6%) 21 9	22, 101, 218, 314	0

The worst 5 of 126 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	106	ALA	12.7
2	F	18	ILE	9.3
1	A	43	THR	7.7
1	E	130	LEU	7.5
1	A	106	ALA	6.1

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 carbohydrates in this entry.

6.4 Ligands ⓘ

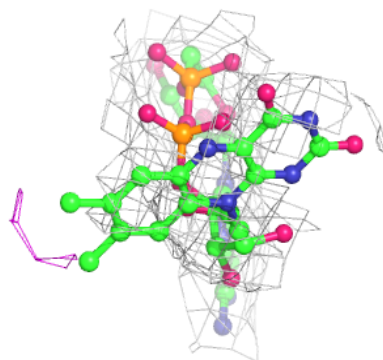
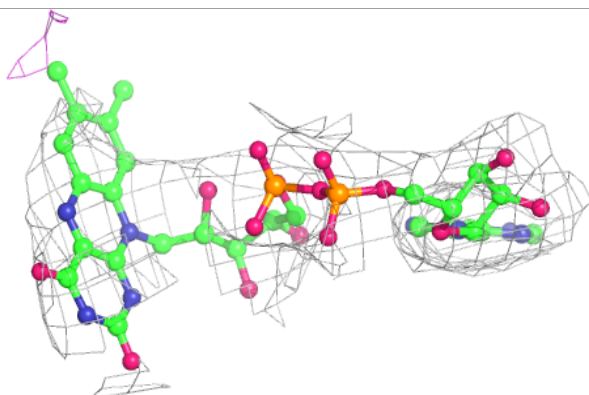
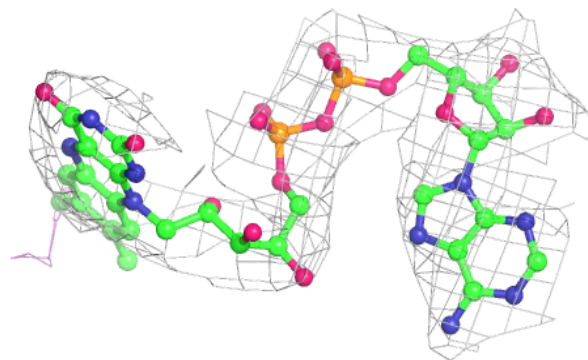
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SF4	E	402	8/8	0.69	0.11	347,351,352,352	0
6	SO4	D	403	5/5	0.77	1.18	304,305,306,311	0
6	SO4	C	406	5/5	0.84	0.32	129,131,136,138	0
6	SO4	C	404	5/5	0.84	0.26	100,117,124,128	0
5	SF4	A	402	8/8	0.86	0.08	257,267,273,273	0
5	SF4	A	403	8/8	0.87	0.09	237,240,244,247	0
6	SO4	D	402	5/5	0.88	0.32	168,170,172,173	0
6	SO4	C	405	5/5	0.89	0.27	139,143,145,146	0
6	SO4	C	402	5/5	0.91	0.20	134,140,146,147	0
5	SF4	E	403	8/8	0.91	0.08	238,241,245,249	0
4	FAD	F	301	53/53	0.92	0.16	67,109,135,144	0
4	FAD	E	401	53/53	0.92	0.16	41,79,98,111	0
4	FAD	A	401	53/53	0.93	0.16	32,68,85,104	0
6	SO4	C	403	5/5	0.95	0.20	90,95,105,108	0
4	FAD	B	301	53/53	0.95	0.16	44,95,122,134	0
4	FAD	D	401	53/53	0.96	0.19	10,41,67,79	0
4	FAD	C	401	53/53	0.97	0.18	13,39,58,61	0

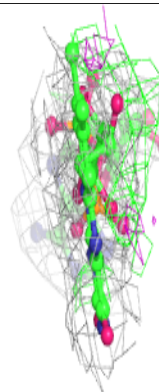
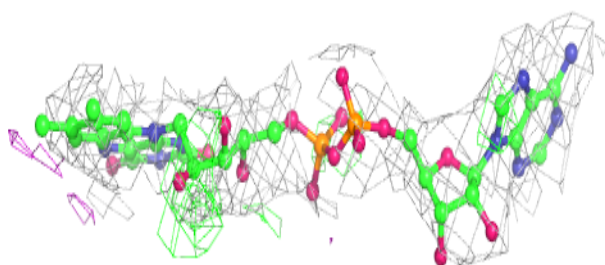
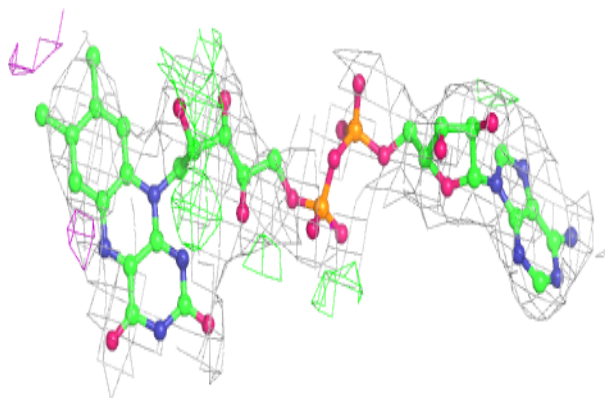
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD F 301:

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

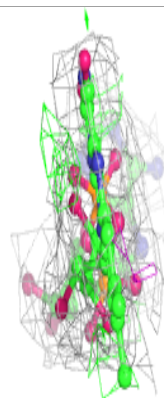
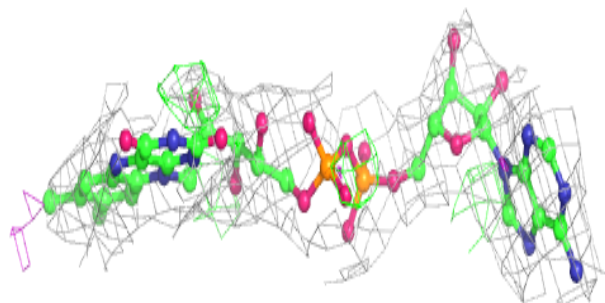
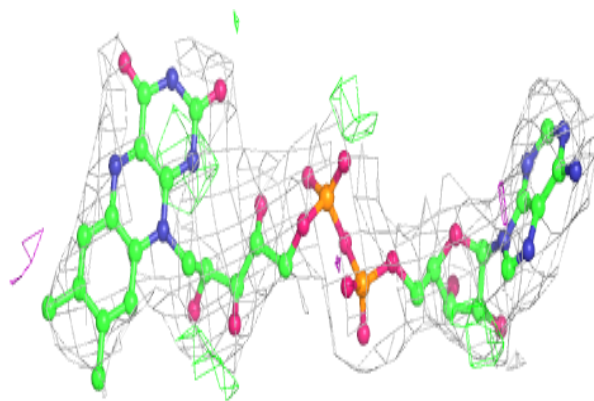
**Electron density around FAD E 401:**

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

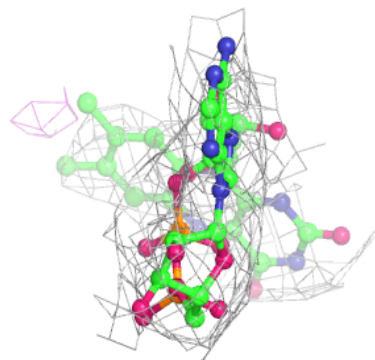
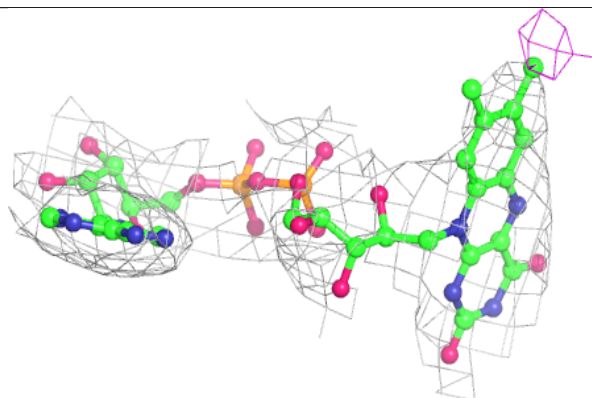
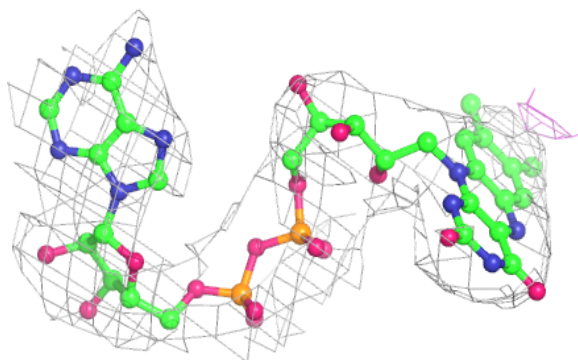


Electron density around FAD A 401:

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

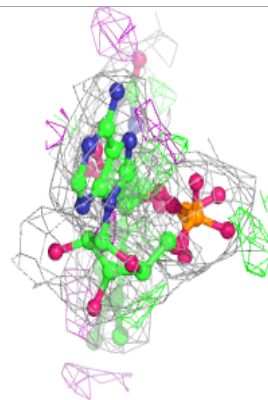
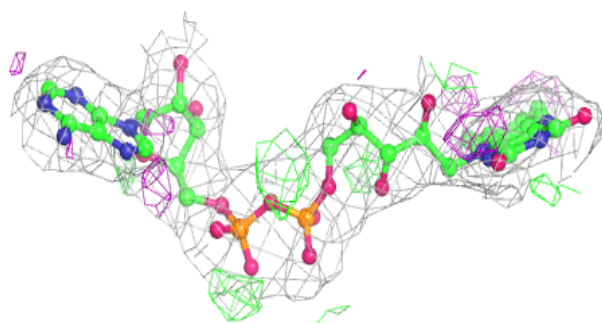
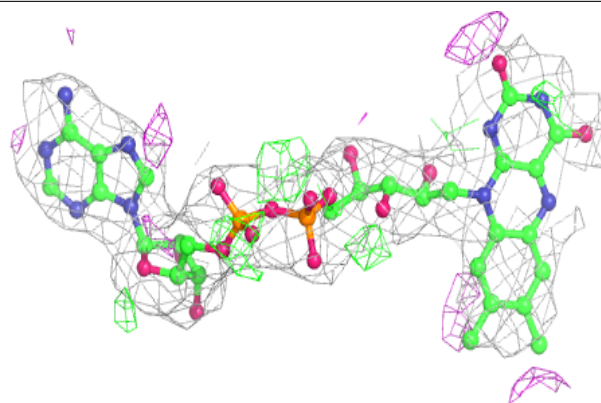
**Electron density around FAD B 301:**

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

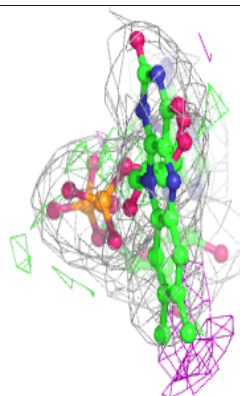
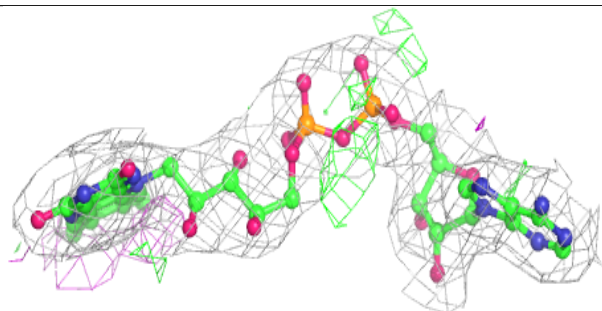
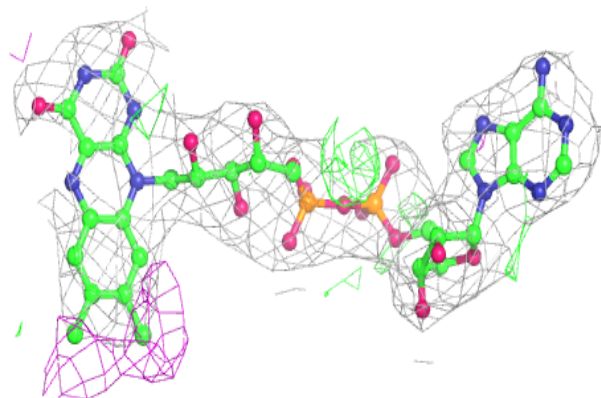


Electron density around FAD D 401:

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

**Electron density around FAD 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.