Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2023 – 11:39 PM EDT

PDB ID	:	5DBJ
Title	:	Crystal structure of halogenase PltA
Authors	:	Pang, A.H.; Tsodikov, O.V.
Deposited on	:	2015-08-21
Resolution	:	2.75 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:

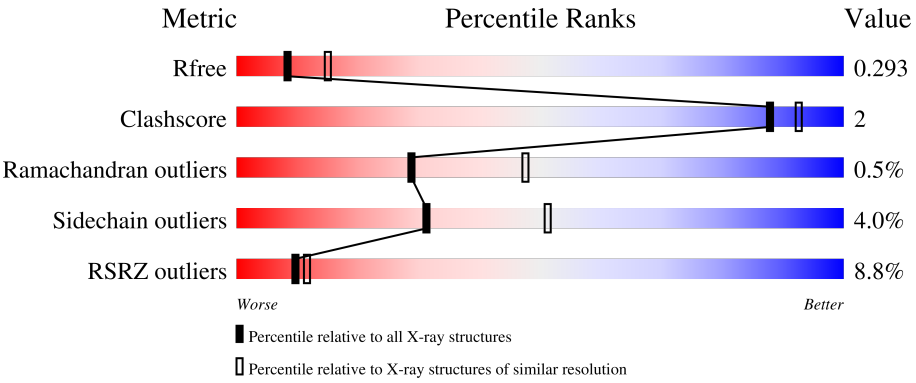
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	455	3% 88% 7%
1	B	455	19% 89% 6%
1	C	455	9% 87% 9%
1	D	455	9% 89% 6% 5%
1	E	455	% 86% 9%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17754 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 FADH2-dependent halogenase PltA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	437	Total	C	N	O	S	0	0	0
			3488	2234	591	653	10			
1	A	435	Total	C	N	O	S	0	0	0
			3468	2222	585	651	10			
1	B	435	Total	C	N	O	S	0	0	0
			3468	2222	585	651	10			
1	C	437	Total	C	N	O	S	0	0	0
			3488	2234	591	653	10			
1	D	433	Total	C	N	O	S	0	0	0
			3458	2217	583	648	10			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP Q4KCZ0
E	-1	PRO	-	expression tag	UNP Q4KCZ0
E	0	HIS	-	expression tag	UNP Q4KCZ0
E	450	GLU	-	expression tag	UNP Q4KCZ0
E	451	ASN	-	expression tag	UNP Q4KCZ0
E	452	ASP	-	expression tag	UNP Q4KCZ0
A	-2	GLY	-	expression tag	UNP Q4KCZ0
A	-1	PRO	-	expression tag	UNP Q4KCZ0
A	0	HIS	-	expression tag	UNP Q4KCZ0
A	450	GLU	-	expression tag	UNP Q4KCZ0
A	451	ASN	-	expression tag	UNP Q4KCZ0
A	452	ASP	-	expression tag	UNP Q4KCZ0
B	-2	GLY	-	expression tag	UNP Q4KCZ0
B	-1	PRO	-	expression tag	UNP Q4KCZ0
B	0	HIS	-	expression tag	UNP Q4KCZ0
B	450	GLU	-	expression tag	UNP Q4KCZ0
B	451	ASN	-	expression tag	UNP Q4KCZ0
B	452	ASP	-	expression tag	UNP Q4KCZ0
C	-2	GLY	-	expression tag	UNP Q4KCZ0

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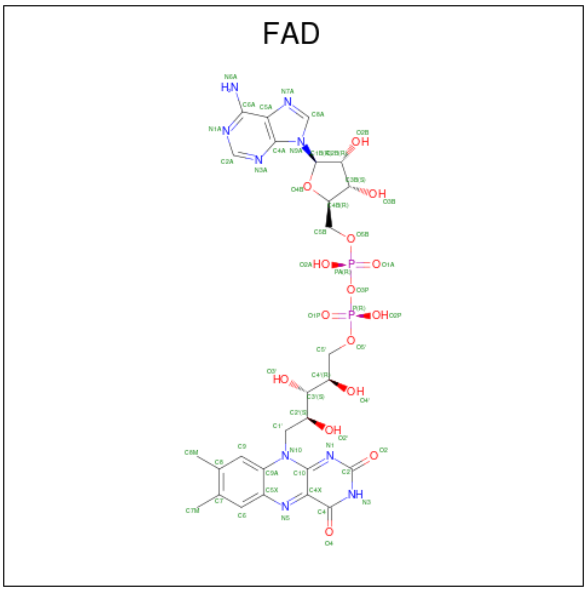
Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	PRO	-	expression tag	UNP Q4KCZ0
C	0	HIS	-	expression tag	UNP Q4KCZ0
C	450	GLU	-	expression tag	UNP Q4KCZ0
C	451	ASN	-	expression tag	UNP Q4KCZ0
C	452	ASP	-	expression tag	UNP Q4KCZ0
D	-2	GLY	-	expression tag	UNP Q4KCZ0
D	-1	PRO	-	expression tag	UNP Q4KCZ0
D	0	HIS	-	expression tag	UNP Q4KCZ0
D	450	GLU	-	expression tag	UNP Q4KCZ0
D	451	ASN	-	expression tag	UNP Q4KCZ0
D	452	ASP	-	expression tag	UNP Q4KCZ0

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	2	Total Cl 2 2	0	0
3	A	2	Total Cl 2 2	0	0
3	B	2	Total Cl 2 2	0	0
3	C	2	Total Cl 2 2	0	0
3	D	1	Total Cl 1 1	0	0

- Molecule 4 is water.

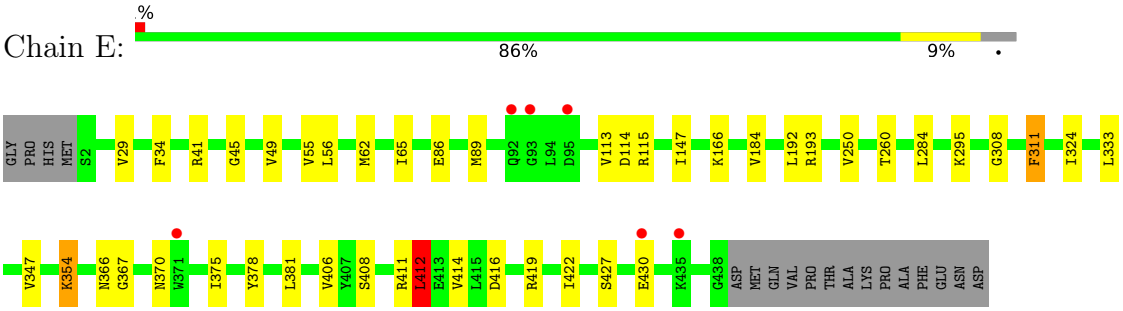
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	33	Total O 33 33	0	0
4	A	25	Total O 25 25	0	0
4	B	17	Total O 17 17	0	0
4	C	23	Total O 23 23	0	0
4	D	12	Total O 12 12	0	0

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.

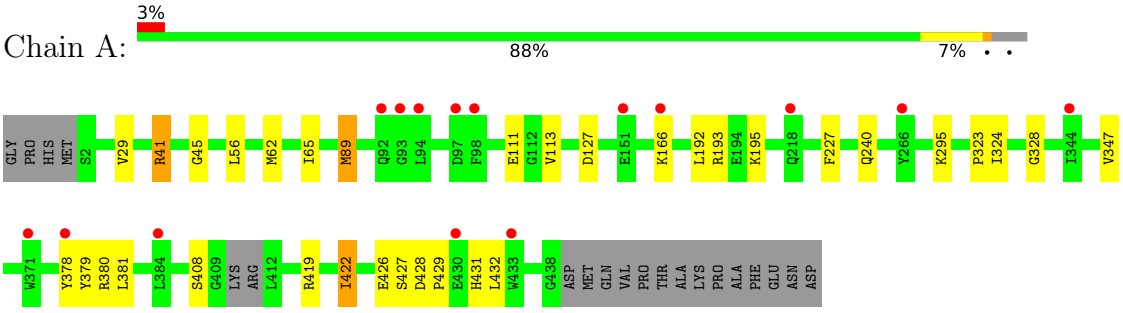
• Molecule 1: FADH2-dependent halogenase PltA

Chain E:



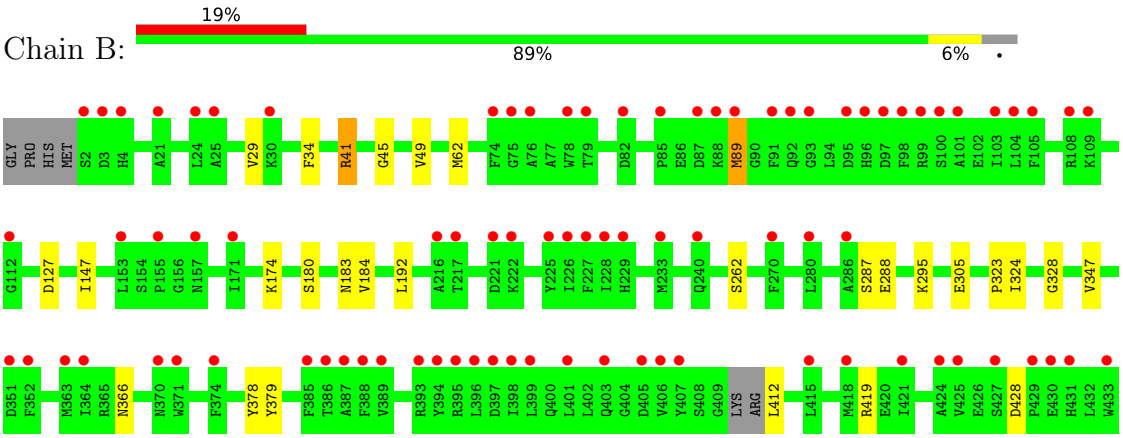
• Molecule 1: FADH2-dependent halogenase PltA

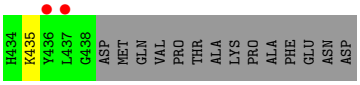
Chain A:



• Molecule 1: FADH2-dependent halogenase PltA

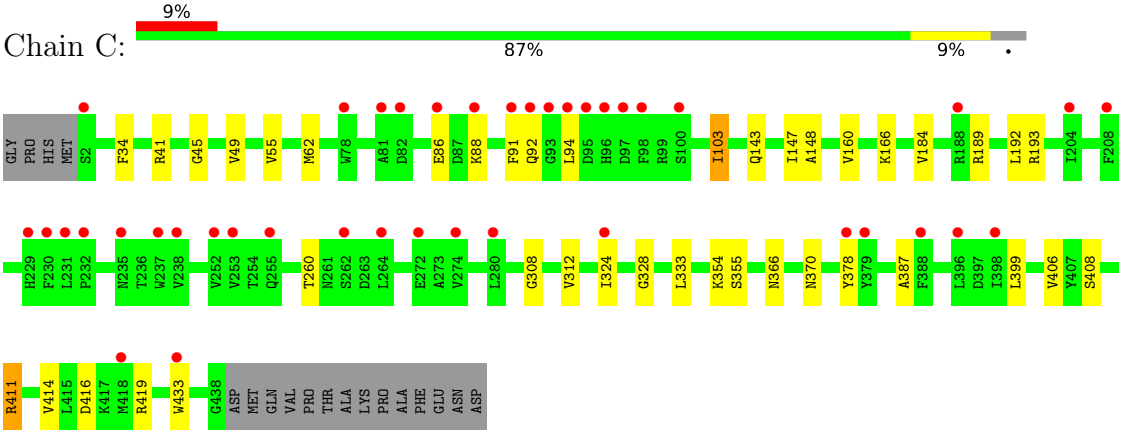
Chain B:





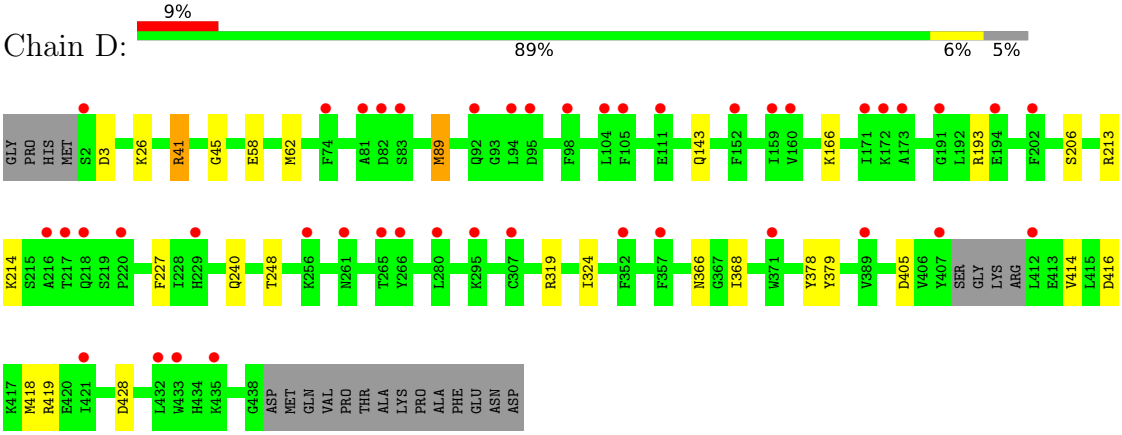
• Molecule 1: FADH2-dependent halogenase PltA

Chain C:



• Molecule 1: FADH2-dependent halogenase PltA

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	242.93Å 94.98Å 102.14Å 90.00° 91.21° 90.00°	Depositor
Resolution (Å)	40.00 – 2.75 47.43 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.2 (40.00-2.75) 93.2 (47.43-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.97 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.239 , 0.292 0.239 , 0.293	Depositor DCC
R_{free} test set	3021 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	59.8	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 38.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	17754	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: CL, 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	0.38	0/3548	0.64	0/4795
1	B	0.38	0/3548	0.62	0/4795
1	C	0.37	0/3569	0.63	0/4823
1	D	0.37	0/3538	0.59	0/4782
1	E	0.37	0/3569	0.64	0/4823
All	All	0.38	0/17772	0.63	0/24018

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	3468	0	3396	14	0
1	B	3468	0	3396	8	0
1	C	3488	0	3423	24	0
1	D	3458	0	3388	10	0
1	E	3488	0	3423	17	0
2	A	53	0	31	2	0
2	B	53	0	31	1	0
2	C	53	0	31	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	53	0	31	2	0
2	E	53	0	31	1	0
3	A	2	0	0	1	0
3	B	2	0	0	1	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
4	A	25	0	0	0	0
4	B	17	0	0	0	0
4	C	23	0	0	0	0
4	D	12	0	0	0	0
4	E	33	0	0	0	0
All	All	17754	0	17181	69	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 2.

All (69) 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:C:91:PHE:CD1	1:C:387:ALA:HB1	2.15	0.81
1:C:91:PHE:CE2	1:C:433:TRP:HH2	2.06	0.72
1:C:91:PHE:CE1	1:C:387:ALA:HB1	2.25	0.72
1:C:91:PHE:CE2	1:C:433:TRP:CH2	2.78	0.71
1:D:41:ARG:NH1	2:D:501:FAD:O3B	2.27	0.67
1:C:148:ALA:O	1:C:189:ARG:NH1	2.33	0.62
1:A:324:ILE:HD11	1:A:379:TYR:CE2	2.36	0.61
1:A:324:ILE:HD13	1:A:378:TYR:CD1	2.36	0.60
1:B:45:GLY:HA2	2:B:501:FAD:C4X	2.33	0.59
1:C:91:PHE:CE1	1:C:387:ALA:CB	2.87	0.57
1:D:45:GLY:HA2	2:D:501:FAD:C4X	2.35	0.57
1:A:41:ARG:NH2	1:A:127:ASP:OD1	2.34	0.56
1:E:430:GLU:CD	1:C:92:GLN:HG3	2.27	0.54
1:C:91:PHE:HB3	1:C:94:LEU:HD11	1.89	0.54
1:E:370:ASN:HB2	1:E:406:VAL:HG13	1.90	0.54
1:E:324:ILE:HD13	1:E:378:TYR:CD1	2.44	0.53
1:C:91:PHE:HB3	1:C:94:LEU:CD1	2.40	0.52
1:A:380:ARG:NE	1:A:426:GLU:OE2	2.44	0.50
1:C:411:ARG:NH2	1:C:416:ASP:OD1	2.45	0.50
1:E:29:VAL:HG22	1:E:347:VAL:HG21	1.93	0.50
1:E:411:ARG:O	1:E:412:LEU:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:GLN:HB2	1:D:143:GLN:HB2	1.94	0.49
1:B:324:ILE:HD13	1:B:378:TYR:CD1	2.48	0.49
1:C:34:PHE:CG	1:C:147:ILE:HD11	2.48	0.49
1:C:45:GLY:HA2	2:C:501:FAD:C4X	2.43	0.48
1:C:370:ASN:HB2	1:C:406:VAL:HG13	1.95	0.48
1:C:308:GLY:HA2	1:C:354:LYS:HG3	1.95	0.48
1:E:55:VAL:HG11	1:E:333:LEU:HB3	1.95	0.48
1:D:324:ILE:HD13	1:D:378:TYR:CD1	2.49	0.48
1:E:45:GLY:HA2	2:E:501:FAD:C4X	2.43	0.48
1:C:91:PHE:CE1	1:C:387:ALA:C	2.87	0.47
1:D:324:ILE:HD11	1:D:379:TYR:CE2	2.49	0.47
1:E:381:LEU:HG	1:E:422:ILE:HD11	1.96	0.47
1:C:147:ILE:HD12	1:C:160:VAL:CG1	2.44	0.46
1:E:56:LEU:HD22	1:E:65:ILE:CD1	2.46	0.46
1:E:367:GLY:HA2	1:E:406:VAL:HG12	1.97	0.46
1:D:213:ARG:NH1	1:D:248:THR:OG1	2.49	0.46
1:A:428:ASP:OD2	1:A:431:HIS:N	2.49	0.45
1:A:45:GLY:HA2	2:A:501:FAD:C4X	2.47	0.45
1:A:381:LEU:HG	1:A:422:ILE:HD11	1.98	0.45
1:B:41:ARG:NH2	1:B:127:ASP:OD1	2.42	0.44
1:A:328:GLY:N	3:A:502:CL:CL	2.83	0.43
1:B:328:GLY:N	3:B:503:CL:CL	2.83	0.43
1:C:91:PHE:CB	1:C:94:LEU:HD11	2.47	0.43
1:A:227:PHE:HB2	1:A:240:GLN:HB3	2.01	0.43
1:C:184:VAL:O	1:C:184:VAL:HG12	2.19	0.43
1:E:34:PHE:CG	1:E:147:ILE:HD11	2.54	0.43
1:E:427:SER:O	1:C:88:LYS:NZ	2.50	0.42
1:B:34:PHE:CG	1:B:147:ILE:HD11	2.54	0.42
1:E:308:GLY:HA3	1:E:311:PHE:CE2	2.54	0.42
1:D:319:ARG:HG2	1:D:368:ILE:HD12	2.01	0.42
1:E:250:VAL:HG21	1:E:284:LEU:HD21	2.01	0.42
1:C:55:VAL:HG11	1:C:333:LEU:HB3	2.01	0.42
1:B:29:VAL:HG22	1:B:347:VAL:HG21	2.02	0.41
1:A:56:LEU:HD22	1:A:65:ILE:CD1	2.50	0.41
1:C:103:ILE:HG12	1:C:399:LEU:HD13	2.02	0.41
1:C:328:GLY:HA3	2:C:501:FAD:H1'2	2.02	0.41
1:E:308:GLY:HA2	1:E:354:LYS:HG3	2.02	0.41
1:D:227:PHE:HB2	1:D:240:GLN:HB3	2.03	0.41
1:C:324:ILE:HD13	1:C:378:TYR:CD1	2.55	0.41
1:E:114:ASP:OD1	1:E:115:ARG:NH1	2.54	0.41
1:E:324:ILE:HD11	1:E:375:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:SER:OG	1:B:183:ASN:HB2	2.21	0.41
1:D:26:LYS:NZ	1:D:58:GLU:O	2.54	0.41
1:A:323:PRO:HB3	2:A:501:FAD:C5X	2.50	0.40
1:B:324:ILE:HD11	1:B:379:TYR:CE2	2.57	0.40
1:A:29:VAL:HG22	1:A:347:VAL:HG21	2.02	0.40
1:A:427:SER:O	1:A:429:PRO:HD3	2.22	0.40
1:A:111:GLU:HG2	1:D:214:LYS:HB3	2.02	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	431/455 (95%)	404 (94%)	25 (6%)	2 (0%)	29 47
1	B	431/455 (95%)	405 (94%)	22 (5%)	4 (1%)	17 31
1	C	435/455 (96%)	416 (96%)	19 (4%)	0	100 100
1	D	429/455 (94%)	404 (94%)	24 (6%)	1 (0%)	47 69
1	E	435/455 (96%)	409 (94%)	23 (5%)	3 (1%)	22 39
All	All	2161/2275 (95%)	2038 (94%)	113 (5%)	10 (0%)	29 47

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	MET
1	B	89	MET
1	D	89	MET
1	E	408	SER
1	A	408	SER
1	E	412	LEU
1	B	262	SER

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Mol	Chain	Res	Type
1	B	323	PRO
1	E	184	VAL
1	B	184	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	371/388 (96%)	359 (97%)	12 (3%)	39	59
1	B	371/388 (96%)	356 (96%)	15 (4%)	31	51
1	C	373/388 (96%)	357 (96%)	16 (4%)	29	48
1	D	370/388 (95%)	356 (96%)	14 (4%)	33	53
1	E	373/388 (96%)	355 (95%)	18 (5%)	25	44
All	All	1858/1940 (96%)	1783 (96%)	75 (4%)	31	51

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	41	ARG
1	E	49	VAL
1	E	62	MET
1	E	86	GLU
1	E	89	MET
1	E	113	VAL
1	E	166	LYS
1	E	192	LEU
1	E	193	ARG
1	E	260	THR
1	E	295	LYS
1	E	311	PHE
1	E	354	LYS
1	E	366	ASN
1	E	412	LEU
1	E	414	VAL

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Mol	Chain	Res	Type
1	E	416	ASP
1	E	419	ARG
1	A	41	ARG
1	A	62	MET
1	A	89	MET
1	A	113	VAL
1	A	166	LYS
1	A	192	LEU
1	A	193	ARG
1	A	195	LYS
1	A	295	LYS
1	A	419	ARG
1	A	422	ILE
1	A	432	LEU
1	B	41	ARG
1	B	49	VAL
1	B	62	MET
1	B	89	MET
1	B	174	LYS
1	B	192	LEU
1	B	287	SER
1	B	288	GLU
1	B	295	LYS
1	B	305	GLU
1	B	366	ASN
1	B	412	LEU
1	B	419	ARG
1	B	428	ASP
1	B	435	LYS
1	C	41	ARG
1	C	49	VAL
1	C	62	MET
1	C	86	GLU
1	C	103	ILE
1	C	166	LYS
1	C	192	LEU
1	C	193	ARG
1	C	260	THR
1	C	312	VAL
1	C	355	SER
1	C	366	ASN
1	C	408	SER

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Mol	Chain	Res	Type
1	C	411	ARG
1	C	414	VAL
1	C	419	ARG
1	D	3	ASP
1	D	41	ARG
1	D	62	MET
1	D	89	MET
1	D	166	LYS
1	D	193	ARG
1	D	206	SER
1	D	366	ASN
1	D	405	ASP
1	D	414	VAL
1	D	416	ASP
1	D	418	MET
1	D	419	ARG
1	D	428	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	258	ASN
1	B	161	ASN
1	B	258	ASN
1	C	258	ASN
1	C	431	HIS
1	D	258	ASN

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)

Of 14 ligands modelled in this entry, 9 are monoatomic - leaving 5 for Mogul analysis.

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	C	501	-	53,58,58	1.37	7 (13%)	68,89,89	1.33	9 (13%)
2	FAD	E	501	-	53,58,58	1.34	7 (13%)	68,89,89	1.36	9 (13%)
2	FAD	D	501	-	53,58,58	1.41	7 (13%)	68,89,89	1.32	9 (13%)
2	FAD	A	501	-	53,58,58	1.34	6 (11%)	68,89,89	1.38	11 (16%)
2	FAD	B	501	-	53,58,58	1.40	7 (13%)	68,89,89	1.28	9 (13%)

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	C	501	-	-	5/30/50/50	0/6/6/6
2	FAD	E	501	-	-	1/30/50/50	0/6/6/6
2	FAD	D	501	-	-	4/30/50/50	0/6/6/6
2	FAD	A	501	-	-	12/30/50/50	0/6/6/6
2	FAD	B	501	-	-	2/30/50/50	0/6/6/6

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	FAD	C9A-C5X	5.78	1.50	1.41
2	B	501	FAD	C9A-C5X	5.78	1.50	1.41
2	D	501	FAD	C9A-C5X	5.69	1.50	1.41
2	A	501	FAD	C9A-C5X	5.56	1.50	1.41
2	E	501	FAD	C9A-C5X	5.43	1.50	1.41
2	D	501	FAD	C8-C7	3.64	1.50	1.40
2	C	501	FAD	C8-C7	3.56	1.49	1.40
2	B	501	FAD	C8-C7	3.56	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	FAD	C8-C7	3.51	1.49	1.40
2	A	501	FAD	C8-C7	3.47	1.49	1.40
2	B	501	FAD	C4X-N5	2.69	1.36	1.30
2	C	501	FAD	C4X-N5	2.60	1.35	1.30
2	D	501	FAD	C4X-N5	2.56	1.35	1.30
2	E	501	FAD	C4X-N5	2.55	1.35	1.30
2	D	501	FAD	C5A-C4A	2.55	1.47	1.40
2	A	501	FAD	C4X-N5	2.52	1.35	1.30
2	E	501	FAD	C5A-C4A	2.39	1.47	1.40
2	C	501	FAD	C5A-C4A	2.38	1.47	1.40
2	B	501	FAD	C5A-C4A	2.35	1.47	1.40
2	D	501	FAD	C10-N10	2.33	1.42	1.37
2	D	501	FAD	C4-N3	-2.30	1.34	1.38
2	A	501	FAD	C5A-C4A	2.27	1.46	1.40
2	B	501	FAD	C4-N3	-2.26	1.34	1.38
2	D	501	FAD	C2A-N3A	2.23	1.35	1.32
2	C	501	FAD	C10-N10	2.20	1.42	1.37
2	E	501	FAD	C10-N10	2.15	1.42	1.37
2	B	501	FAD	C2A-N3A	2.12	1.35	1.32
2	E	501	FAD	C2A-N3A	2.10	1.35	1.32
2	E	501	FAD	C4-N3	-2.10	1.34	1.38
2	B	501	FAD	C10-N10	2.05	1.41	1.37
2	C	501	FAD	C2A-N3A	2.03	1.35	1.32
2	C	501	FAD	C4-N3	-2.03	1.35	1.38
2	A	501	FAD	C4-N3	-2.01	1.35	1.38
2	A	501	FAD	C10-N10	2.01	1.41	1.37

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	FAD	N3A-C2A-N1A	-3.85	122.66	128.68
2	B	501	FAD	N3A-C2A-N1A	-3.76	122.80	128.68
2	D	501	FAD	N3A-C2A-N1A	-3.70	122.89	128.68
2	E	501	FAD	N3A-C2A-N1A	-3.63	123.00	128.68
2	A	501	FAD	N3A-C2A-N1A	-3.62	123.02	128.68
2	E	501	FAD	C4-C4X-N5	3.41	123.09	118.23
2	E	501	FAD	P-O3P-PA	-3.28	121.56	132.83
2	C	501	FAD	P-O3P-PA	-3.08	122.26	132.83
2	B	501	FAD	C4-C4X-N5	3.06	122.59	118.23
2	B	501	FAD	P-O3P-PA	-3.02	122.46	132.83
2	A	501	FAD	C4-C4X-N5	2.95	122.42	118.23
2	C	501	FAD	C4-C4X-N5	2.92	122.39	118.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	FAD	C4X-C10-N1	-2.88	118.06	124.73
2	E	501	FAD	C4X-C10-N1	-2.80	118.23	124.73
2	A	501	FAD	C4X-C10-N1	-2.74	118.38	124.73
2	C	501	FAD	C4X-C10-N1	-2.72	118.41	124.73
2	D	501	FAD	C4-C4X-N5	2.71	122.09	118.23
2	B	501	FAD	C4A-C5A-N7A	-2.69	106.59	109.40
2	B	501	FAD	C4X-C10-N1	-2.69	118.50	124.73
2	D	501	FAD	P-O3P-PA	-2.66	123.69	132.83
2	E	501	FAD	C10-N1-C2	2.62	122.14	116.90
2	A	501	FAD	C10-N1-C2	2.60	122.10	116.90
2	A	501	FAD	C4A-C5A-N7A	-2.56	106.73	109.40
2	C	501	FAD	C4A-C5A-N7A	-2.56	106.73	109.40
2	E	501	FAD	O2-C2-N1	-2.56	117.59	121.83
2	A	501	FAD	P-O3P-PA	-2.53	124.16	132.83
2	E	501	FAD	C4X-C10-N10	2.49	120.13	116.48
2	C	501	FAD	C10-N1-C2	2.46	121.82	116.90
2	B	501	FAD	C10-N1-C2	2.42	121.73	116.90
2	D	501	FAD	C10-N1-C2	2.41	121.72	116.90
2	D	501	FAD	C4A-C5A-N7A	-2.35	106.95	109.40
2	A	501	FAD	O4-C4-C4X	-2.33	120.43	126.60
2	A	501	FAD	O2-C2-N1	-2.20	118.18	121.83
2	A	501	FAD	C5X-N5-C4X	2.18	121.70	118.07
2	C	501	FAD	C4X-C10-N10	2.18	119.67	116.48
2	A	501	FAD	C5'-C4'-C3'	2.15	116.35	112.20
2	C	501	FAD	O2-C2-N1	-2.13	118.29	121.83
2	E	501	FAD	C4A-C5A-N7A	-2.13	107.18	109.40
2	B	501	FAD	C4X-C10-N10	2.12	119.58	116.48
2	C	501	FAD	O4-C4-C4X	-2.12	120.98	126.60
2	A	501	FAD	C4X-C10-N10	2.11	119.57	116.48
2	E	501	FAD	C10-C4X-N5	-2.11	120.38	124.86
2	D	501	FAD	O4-C4-C4X	-2.07	121.12	126.60
2	D	501	FAD	C4X-C4-N3	2.06	118.42	113.19
2	B	501	FAD	C4X-C4-N3	2.04	118.37	113.19
2	D	501	FAD	C4X-C10-N10	2.02	119.44	116.48
2	B	501	FAD	O4-C4-C4X	-2.01	121.27	126.60

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FAD	O4'-C4'-C5'-O5'
2	A	501	FAD	C5'-O5'-P-O3P

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Mol	Chain	Res	Type	Atoms
2	A	501	FAD	C3'-C4'-C5'-O5'
2	A	501	FAD	O3'-C3'-C4'-C5'
2	A	501	FAD	PA-O3P-P-O5'
2	C	501	FAD	PA-O3P-P-O5'
2	B	501	FAD	O4B-C4B-C5B-O5B
2	A	501	FAD	C5'-O5'-P-O1P
2	A	501	FAD	C2'-C3'-C4'-C5'
2	E	501	FAD	O4B-C4B-C5B-O5B
2	A	501	FAD	P-O3P-PA-O2A
2	A	501	FAD	O3'-C3'-C4'-O4'
2	C	501	FAD	O4B-C4B-C5B-O5B
2	D	501	FAD	O4B-C4B-C5B-O5B
2	A	501	FAD	C2'-C3'-C4'-O4'
2	A	501	FAD	P-O3P-PA-O1A
2	C	501	FAD	P-O3P-PA-O2A
2	D	501	FAD	P-O3P-PA-O2A
2	C	501	FAD	O2'-C2'-C3'-O3'
2	A	501	FAD	O4B-C4B-C5B-O5B
2	B	501	FAD	C3B-C4B-C5B-O5B
2	C	501	FAD	C1'-C2'-C3'-O3'
2	D	501	FAD	C1'-C2'-C3'-O3'
2	D	501	FAD	O2'-C2'-C3'-O3'

There are no ring outliers.

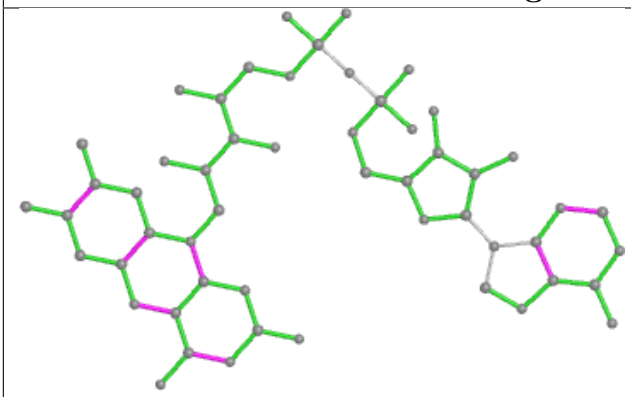
5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	FAD	2	0
2	E	501	FAD	1	0
2	D	501	FAD	2	0
2	A	501	FAD	2	0
2	B	501	FAD	1	0

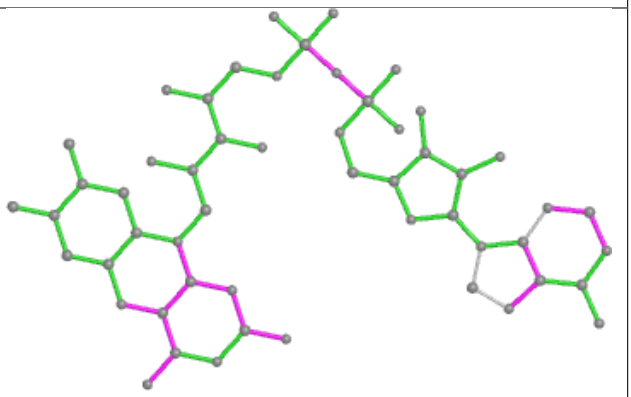
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

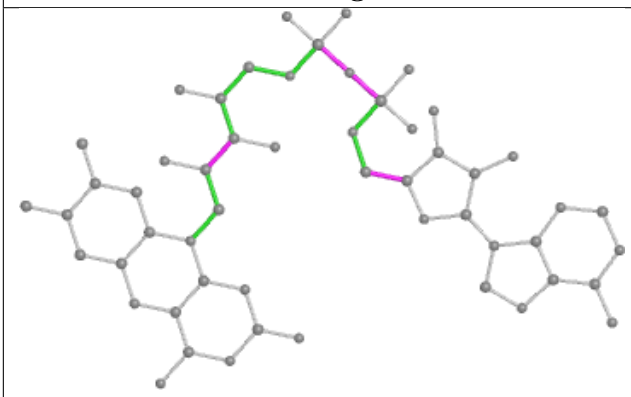
Ligand FAD C 501



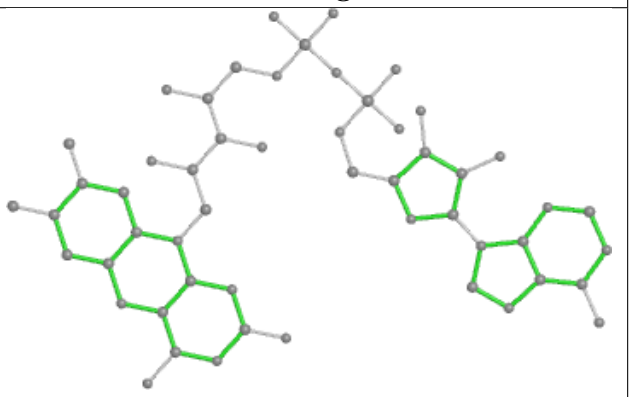
Bond lengths



Bond angles

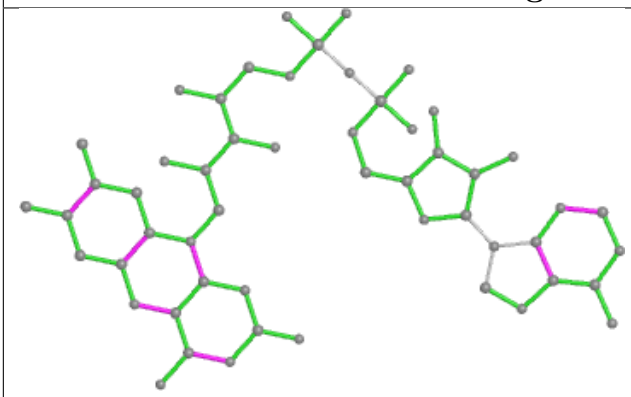


Torsions

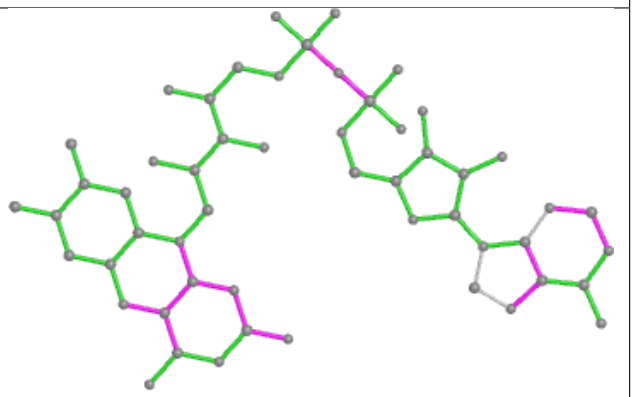


Rings

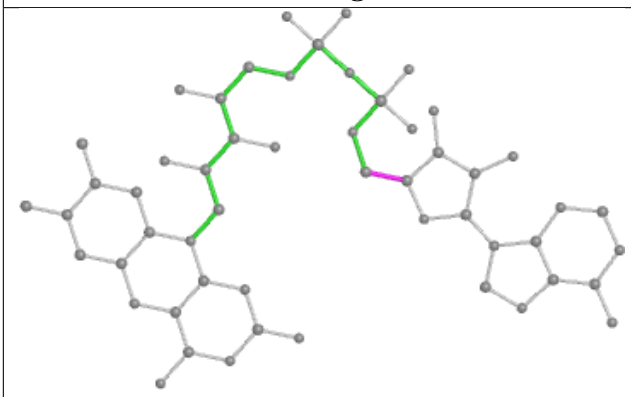
Ligand FAD E 501



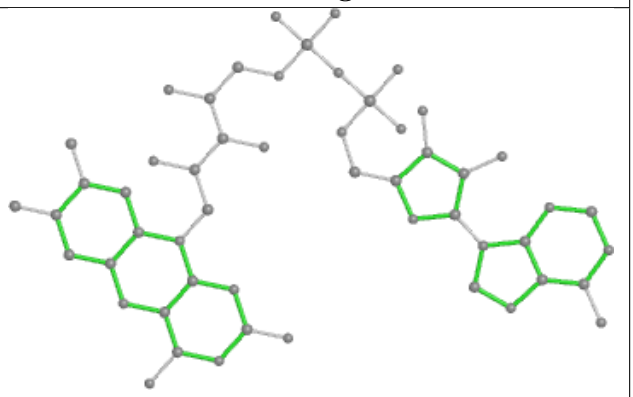
Bond lengths



Bond angles

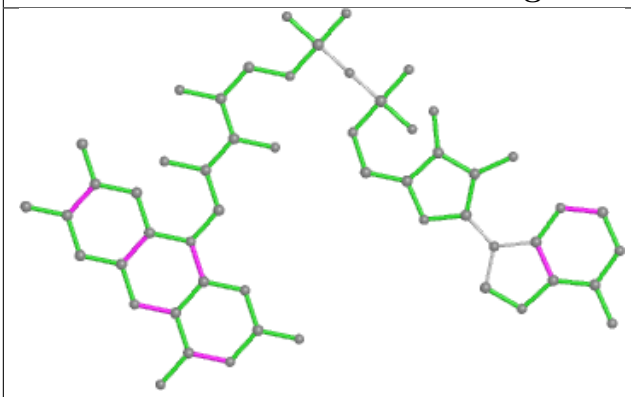


Torsions

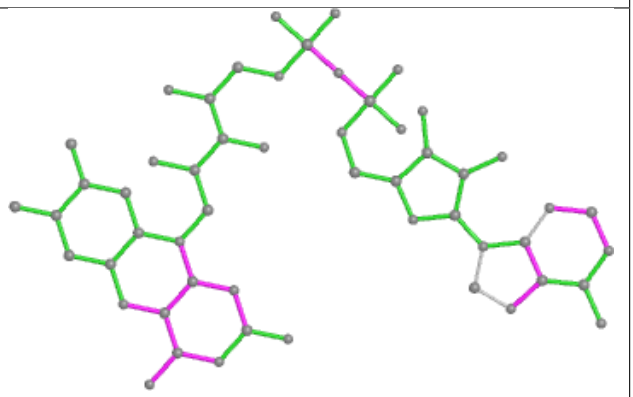


Rings

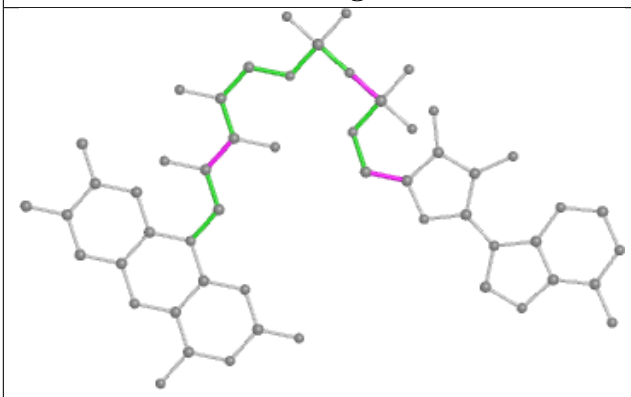
Ligand FAD D 501



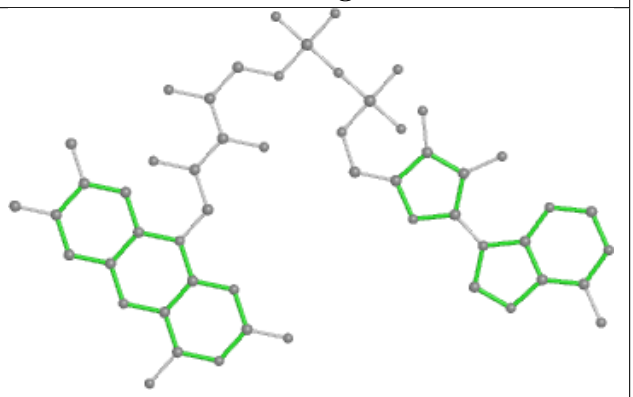
Bond lengths



Bond angles

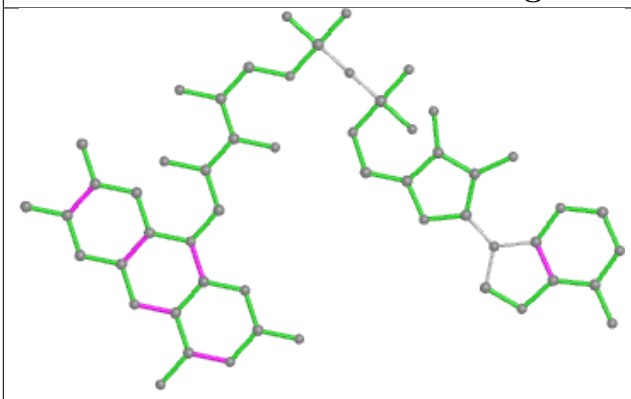


Torsions

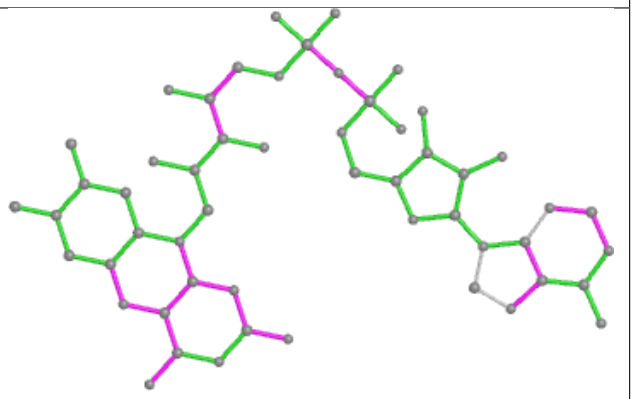


Rings

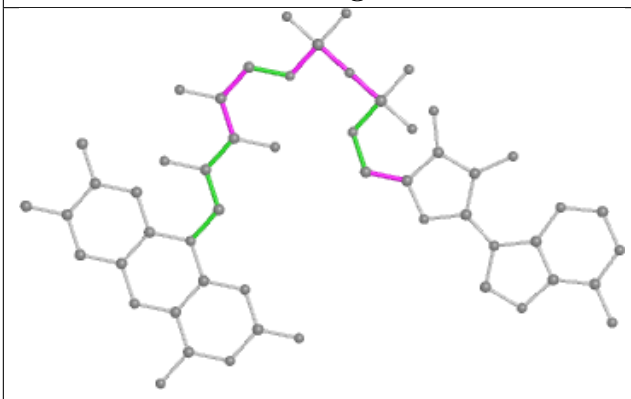
Ligand FAD A 501



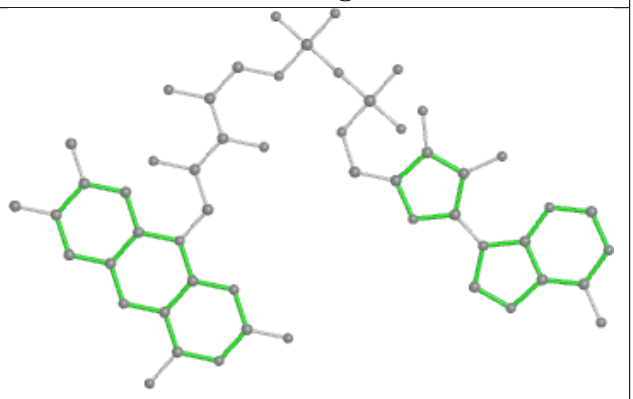
Bond lengths



Bond angles

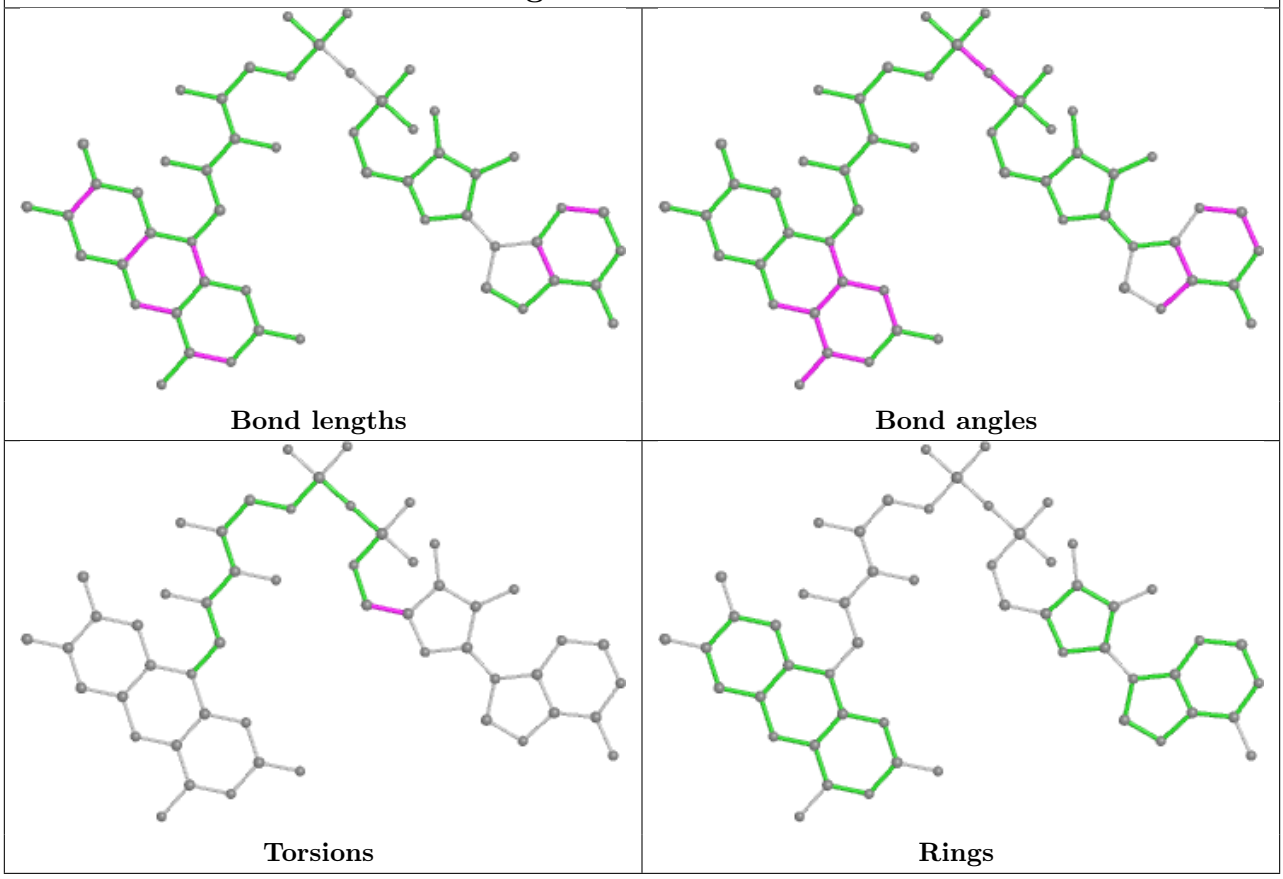


Torsions



Rings

Ligand FAD B 501



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	435/455 (95%)	0.27	15 (3%) 45 53	47, 70, 98, 118	0
1	B	435/455 (95%)	1.19	87 (20%) 1 1	54, 97, 153, 194	0
1	C	437/455 (96%)	0.48	41 (9%) 8 10	52, 71, 107, 122	0
1	D	433/455 (95%)	0.61	43 (9%) 7 8	55, 84, 130, 150	0
1	E	437/455 (96%)	0.18	6 (1%) 75 82	41, 62, 93, 111	0
All	All	2177/2275 (95%)	0.55	192 (8%) 10 11	41, 75, 129, 194	0

All (192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	103	ILE	7.0
1	B	398	ILE	6.7
1	B	92	GLN	6.6
1	B	401	LEU	6.1
1	B	394	TYR	6.1
1	B	91	PHE	5.8
1	B	433	TRP	5.8
1	B	109	LYS	5.6
1	B	389	VAL	5.5
1	B	396	LEU	5.4
1	C	95	ASP	5.1
1	B	415	LEU	4.9
1	C	88	LYS	4.8
1	C	94	LEU	4.8
1	B	403	GLN	4.7
1	B	74	PHE	4.7
1	E	92	GLN	4.7
1	B	93	GLY	4.6
1	B	427	SER	4.3
1	B	405	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	387	ALA	4.3
1	B	421	ILE	4.1
1	C	91	PHE	4.1
1	C	92	GLN	4.1
1	B	95	ASP	4.0
1	B	100	SER	4.0
1	B	397	ASP	4.0
1	D	159	ILE	4.0
1	B	228	ILE	3.9
1	B	153	LEU	3.9
1	B	85	PRO	3.9
1	C	379	TYR	3.8
1	B	101	ALA	3.8
1	B	105	PHE	3.8
1	A	92	GLN	3.8
1	B	157	ASN	3.8
1	C	98	PHE	3.8
1	B	79	THR	3.7
1	B	104	LEU	3.7
1	A	371	TRP	3.7
1	B	108	ARG	3.7
1	B	352	PHE	3.6
1	B	217	THR	3.6
1	B	395	ARG	3.6
1	B	240	GLN	3.6
1	C	82	ASP	3.6
1	B	76	ALA	3.6
1	D	357	PHE	3.6
1	C	2	SER	3.6
1	B	24	LEU	3.5
1	B	89	MET	3.5
1	C	229	HIS	3.5
1	B	97	ASP	3.5
1	B	75	GLY	3.4
1	B	385	PHE	3.4
1	A	166	LYS	3.4
1	B	98	PHE	3.4
1	B	78	TRP	3.4
1	B	3	ASP	3.3
1	D	92	GLN	3.3
1	C	378	TYR	3.3
1	A	94	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	231	LEU	3.3
1	B	21	ALA	3.3
1	D	74	PHE	3.3
1	B	25	ALA	3.3
1	B	406	VAL	3.3
1	B	436	TYR	3.2
1	C	97	ASP	3.2
1	B	82	ASP	3.2
1	D	2	SER	3.1
1	C	253	VAL	3.1
1	D	433	TRP	3.1
1	C	81	ALA	3.1
1	D	104	LEU	3.0
1	B	99	ARG	3.0
1	B	407	TYR	3.0
1	B	425	VAL	3.0
1	C	280	LEU	3.0
1	B	363	MET	3.0
1	B	374	PHE	3.0
1	D	266	TYR	2.9
1	D	94	LEU	2.9
1	A	218	GLN	2.9
1	C	188	ARG	2.9
1	D	435	LYS	2.9
1	D	98	PHE	2.9
1	D	432	LEU	2.9
1	E	93	GLY	2.9
1	C	272	GLU	2.9
1	A	98	PHE	2.9
1	A	97	ASP	2.8
1	D	256	LYS	2.8
1	C	93	GLY	2.8
1	B	216	ALA	2.8
1	D	216	ALA	2.8
1	B	229	HIS	2.8
1	D	82	ASP	2.7
1	B	431	HIS	2.7
1	D	81	ALA	2.7
1	B	370	ASN	2.7
1	C	255	GLN	2.7
1	B	4	HIS	2.7
1	A	384	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	412	LEU	2.7
1	B	270	PHE	2.7
1	C	388	PHE	2.7
1	B	430	GLU	2.7
1	A	344	ILE	2.6
1	D	421	ILE	2.6
1	C	252	VAL	2.6
1	C	230	PHE	2.6
1	D	352	PHE	2.6
1	D	217	THR	2.6
1	D	407	TYR	2.6
1	E	435	LYS	2.6
1	C	418	MET	2.6
1	D	371	TRP	2.6
1	C	324	ILE	2.6
1	C	396	LEU	2.6
1	D	111	GLU	2.6
1	B	388	PHE	2.5
1	D	307	CYS	2.5
1	D	389	VAL	2.5
1	D	172	LYS	2.5
1	E	95	ASP	2.5
1	B	280	LEU	2.5
1	C	433	TRP	2.5
1	D	152	PHE	2.5
1	B	424	ALA	2.5
1	C	264	LEU	2.5
1	B	96	HIS	2.5
1	B	227	PHE	2.5
1	A	433	TRP	2.4
1	B	221	ASP	2.4
1	A	378	TYR	2.4
1	E	371	TRP	2.4
1	B	88	LYS	2.4
1	D	191	GLY	2.4
1	A	266	TYR	2.4
1	B	286	ALA	2.4
1	B	399	LEU	2.4
1	B	386	THR	2.3
1	C	100	SER	2.3
1	D	261	ASN	2.3
1	C	78	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	171	ILE	2.3
1	C	235	ASN	2.3
1	D	218	GLN	2.3
1	D	202	PHE	2.3
1	B	371	TRP	2.3
1	D	280	LEU	2.3
1	D	295	LYS	2.3
1	D	95	ASP	2.3
1	C	237	TRP	2.3
1	B	112	GLY	2.2
1	A	151	GLU	2.2
1	A	430	GLU	2.2
1	E	430	GLU	2.2
1	D	229	HIS	2.2
1	B	226	ILE	2.2
1	B	351	ASP	2.2
1	C	204	ILE	2.2
1	B	429	PRO	2.2
1	B	393	ARG	2.2
1	B	30	LYS	2.2
1	C	232	PRO	2.1
1	B	222	LYS	2.1
1	D	194	GLU	2.1
1	D	220	PRO	2.1
1	D	83	SER	2.1
1	B	225	TYR	2.1
1	C	398	ILE	2.1
1	B	364	ILE	2.1
1	C	238	VAL	2.1
1	C	208	PHE	2.1
1	A	93	GLY	2.1
1	B	155	PRO	2.1
1	B	87	ASP	2.1
1	B	233	MET	2.1
1	D	105	PHE	2.1
1	B	437	LEU	2.0
1	D	173	ALA	2.0
1	C	262	SER	2.0
1	B	2	SER	2.0
1	D	265	THR	2.0
1	B	418	MET	2.0
1	C	96	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	171	ILE	2.0
1	C	86	GLU	2.0
1	C	274	VAL	2.0
1	D	160	VAL	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)

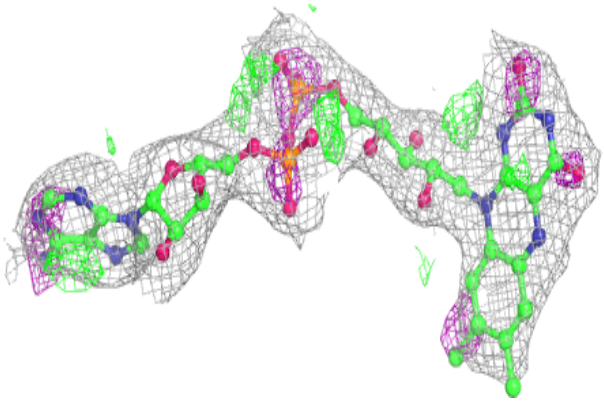
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

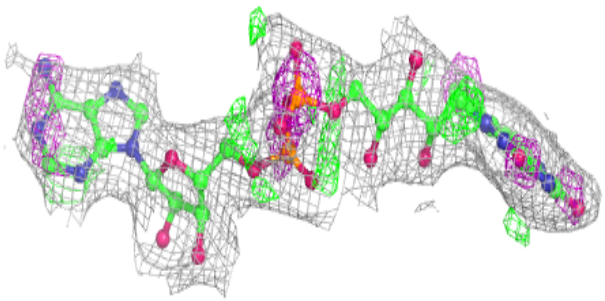
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CL	C	502	1/1	0.65	0.11	118,118,118,118	0
3	CL	A	503	1/1	0.68	0.16	99,99,99,99	0
3	CL	B	502	1/1	0.75	0.16	102,102,102,102	0
3	CL	E	503	1/1	0.78	0.15	75,75,75,75	0
3	CL	B	503	1/1	0.83	0.37	132,132,132,132	0
3	CL	D	502	1/1	0.89	0.17	100,100,100,100	0
3	CL	A	502	1/1	0.91	0.12	70,70,70,70	0
3	CL	C	503	1/1	0.92	0.24	82,82,82,82	0
2	FAD	B	501	53/53	0.93	0.16	31,32,37,37	0
2	FAD	C	501	53/53	0.94	0.15	32,34,36,36	0
2	FAD	D	501	53/53	0.94	0.13	35,37,38,39	0
2	FAD	E	501	53/53	0.95	0.16	30,32,40,41	0
2	FAD	A	501	53/53	0.96	0.14	26,29,33,34	0
3	CL	E	502	1/1	0.96	0.30	74,74,74,74	0

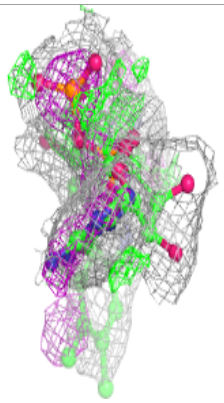
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 501:

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

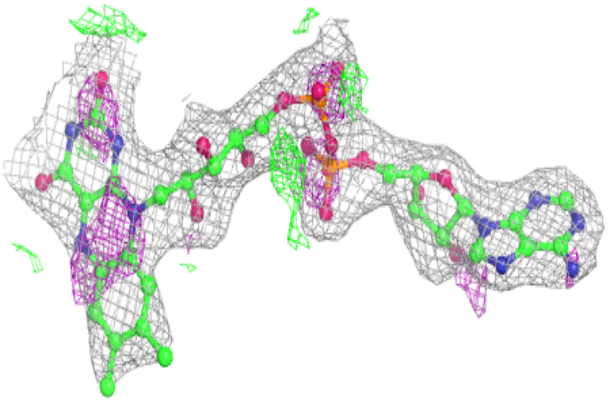


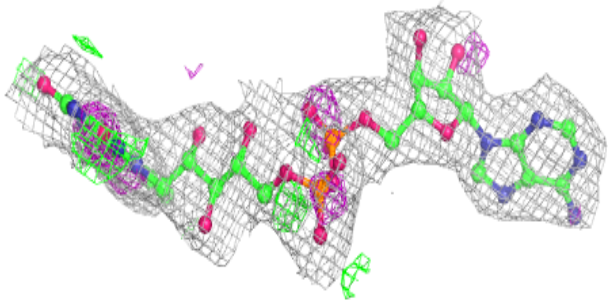


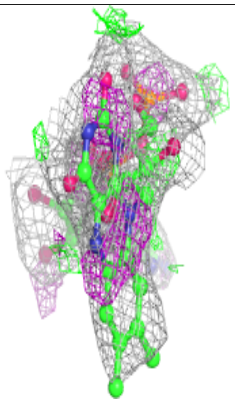


Electron density around FAD C 501:

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

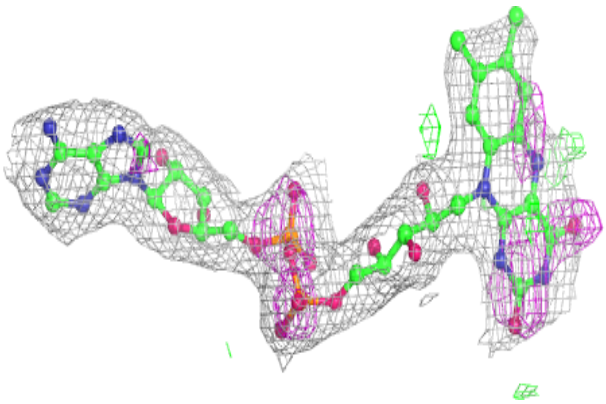


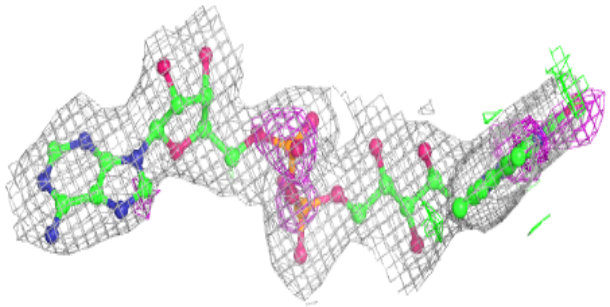


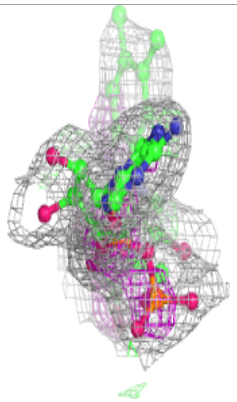


Electron density around FAD D 501:

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

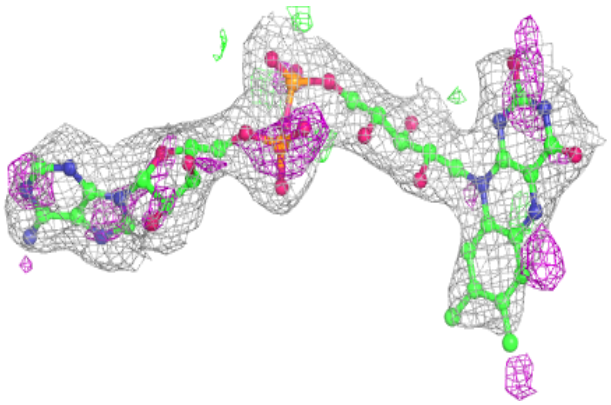


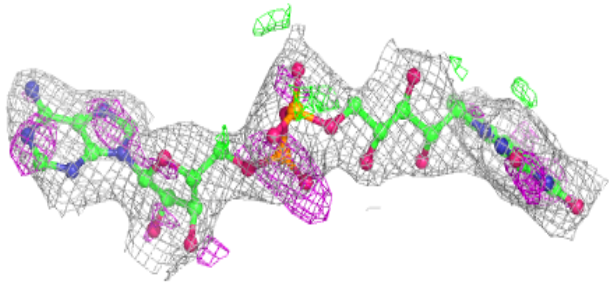


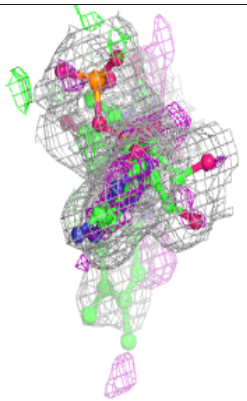


Electron density around FAD E 501:

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

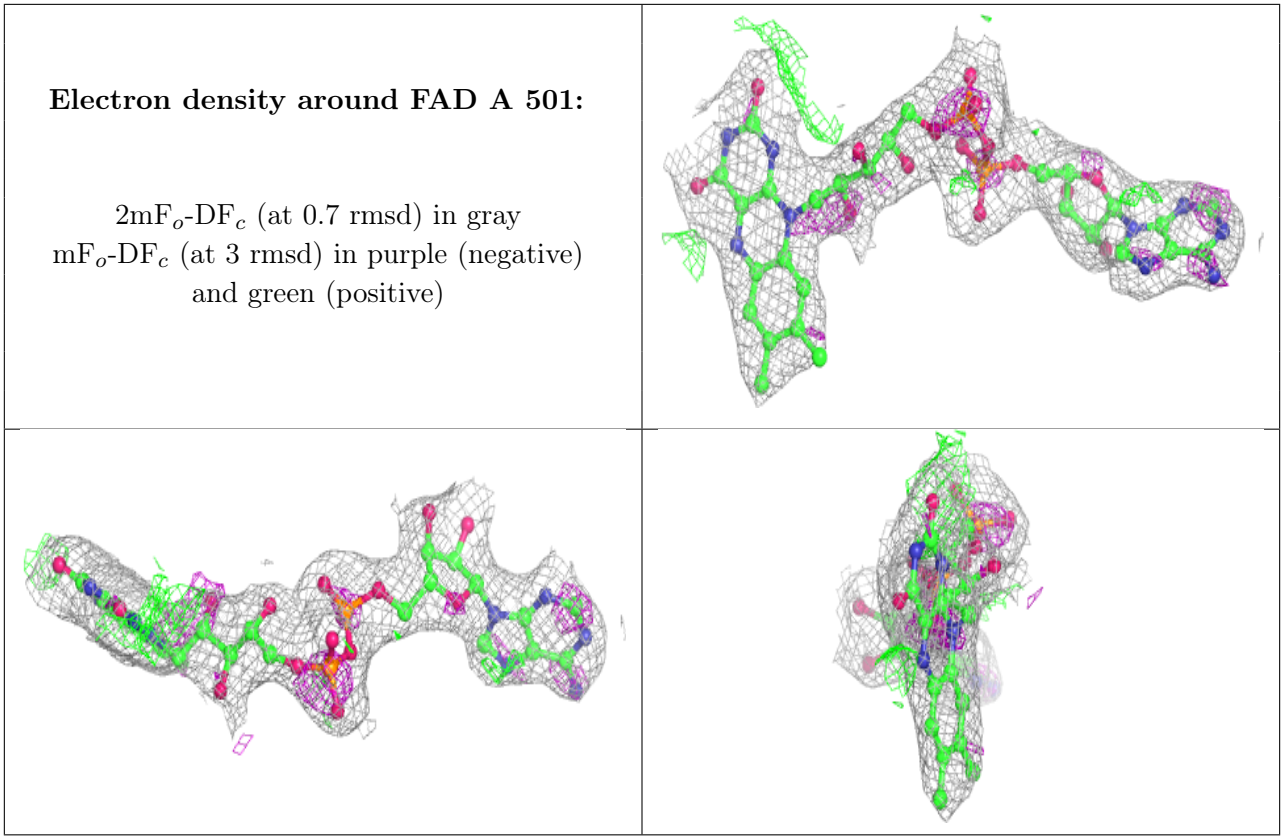






Electron density around FAD A 501:

$2mF_o$-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.