wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 02:16 PM EDT

PDB ID	:	3I6D
Title	:	Crystal structure of PPO from bacillus subtilis with AF
Authors	:	Shen, Y.
Deposited on	:	2009-07-06
Resolution	:	2.90 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 (i) 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 (i)) were used in the production of this report:

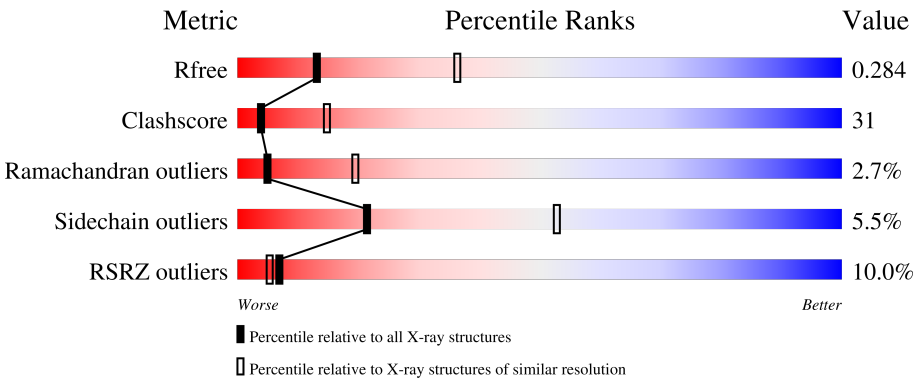
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	470	8% 47% 38% • 12%
1	B	470	9% 49% 37% • • 11%

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
3	ACJ	A	471	-	-	-	X

2 Entry composition (i)

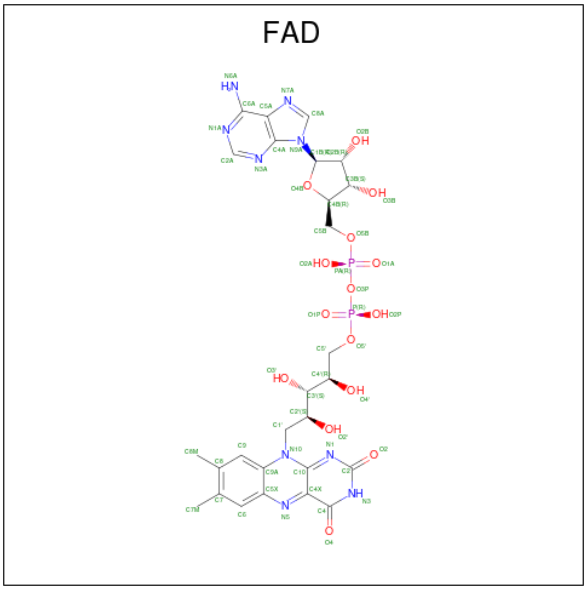
There are 5 unique types of molecules in this entry. The entry contains 6525 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Protoporphyrinogen oxidase.

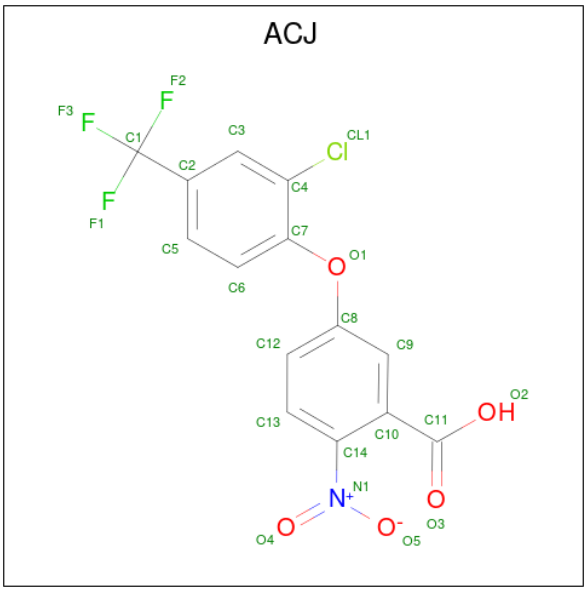
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	414	3162	2007	532	608	15	0	0	0
1	B	419	3188	2022	538	613	15	0	0	0

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



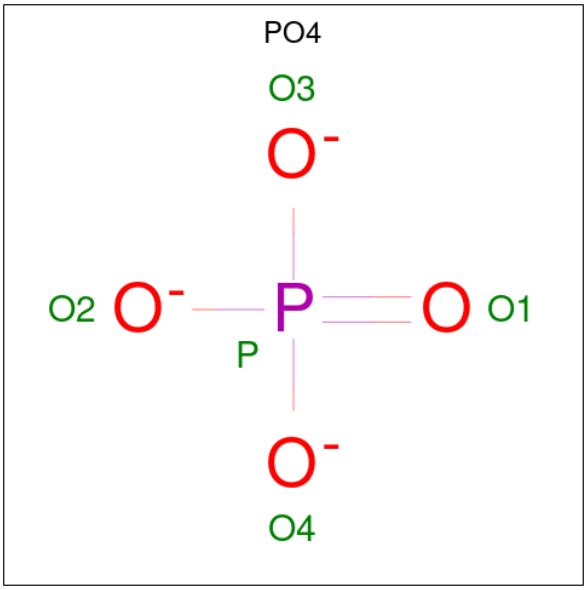
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	53	27	9	15	2	0	0
2	B	1	53	27	9	15	2	0	0

- Molecule 3 is 5-[2-CHLORO-4-(TRIFLUOROMETHYL)PHENOXY]-2-NITROBENZOIC ACID (three-letter code: ACJ) (formula: $C_{14}H_7ClF_3NO_5$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	F	N	O		
3	A	1	24	14	1	3	1	5	0	0
			Total	C	Cl	F	N	O		
3	B	1	24	14	1	3	1	5	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 5 is water.

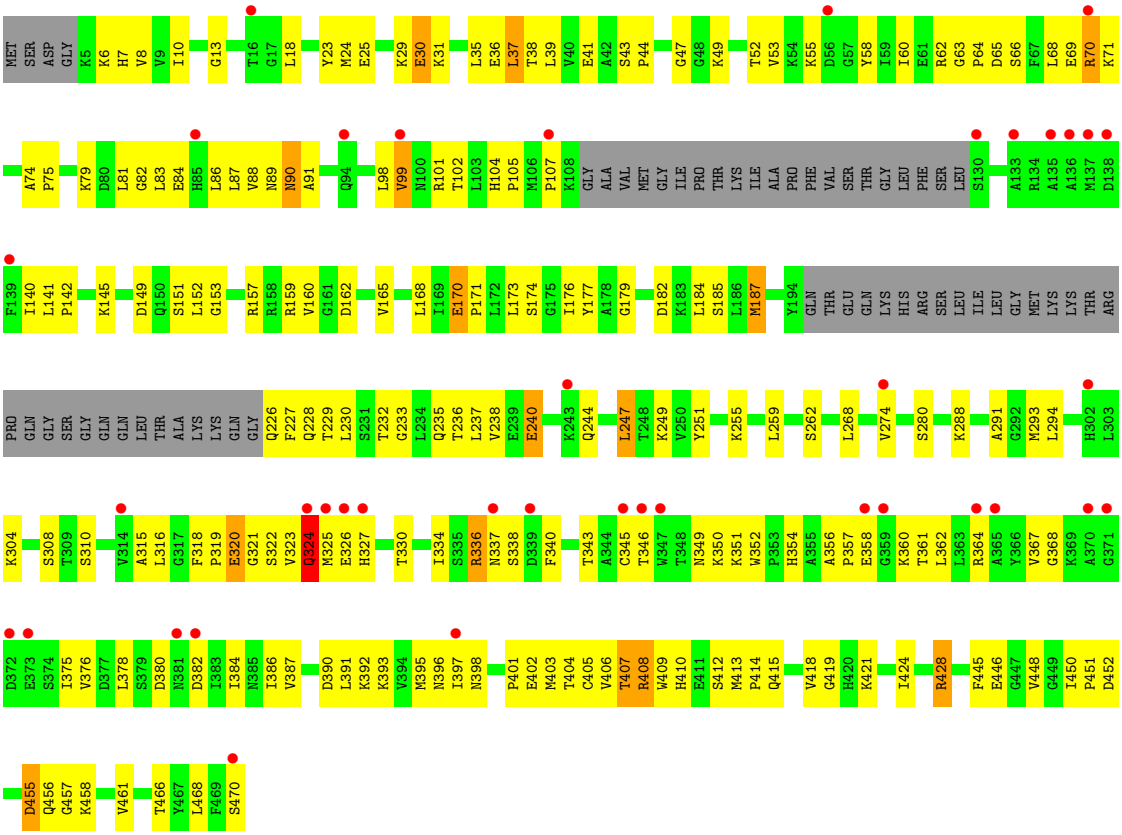
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	5	5	5	0	0
			Total	O		
5	B	6	6	6	0	0

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.

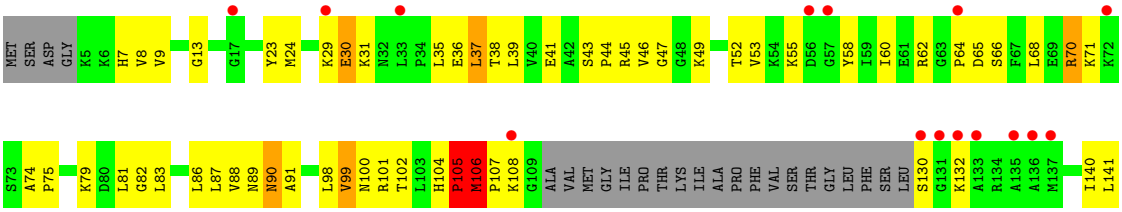
• Molecule 1: Protoporphyrinogen oxidase

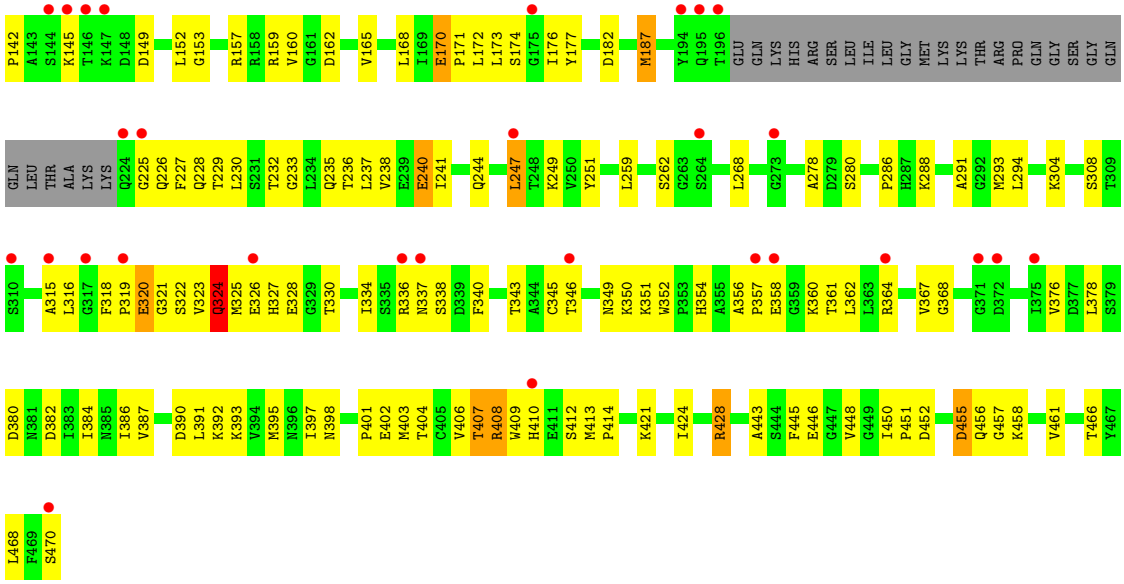
Chain A:



• Molecule 1: Protoporphyrinogen oxidase

Chain B:




P142 A143 S144 K145 T146 K147 D148 D149 L152 G153 R157 R158 R159 V160 G161 D162 V165 L168 I169 E170 P171 L172 L173 S174 G175 I176 Y177 D182 M187 Y194 Q195 T196 GLU GLN LYS HIS ARG SER LEU ILE LEU GLY MET LYS LYS THR ARG PRO GLN GLY SER GLY GLN
GLN LEU THR ALA LYS LYS Q224 G225 Q226 F227 Q228 T229 L230 S231 T232 G233 L234 Q235 T236 L237 V238 E239 E240 I241 Q244 L247 T248 K249 V250 Y251 L259 S262 G263 S264 L268 G273 A278 D279 S280 P286 H287 K288 A291 G292 M293 L294 K304 S308 T309
S310 A315 L316 G317 F318 P319 E320 G321 S322 V323 Q324 M325 E326 H327 E328 G329 T330 I334 S335 R336 N337 S338 D339 F340 T343 A344 C345 T346 N349 K350 K351 W352 P353 H354 A355 A356 P357 E358 G359 K360 T361 L362 L363 R364 V367 G368 G371 D372 I375 V376 D377 L378 S379
D380 N381 D382 I383 I384 N385 I386 V387 D390 L391 K392 K393 V394 M395 N396 I397 N398 P401 E402 M403 T404 G405 V406 T407 R408 W409 H410 E411 S412 M413 P414 K421 I424 R428 A443 S444 F445 E446 G447 V448 G449 I450 P451 D452 D455 Q456 G457 K458 V461 T466 Y467
L468 F469 S470

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	96.17Å 96.17Å 299.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.92 – 2.90 29.92 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.9 (29.92-2.90) 93.6 (29.92-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 2.80Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.272 , 0.293 0.265 , 0.284	Depositor DCC
R_{free} test set	1742 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	70.1	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6525	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, FAD, ACJ

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	0.41	0/3220	0.61	0/4353
1	B	0.42	0/3246	0.67	3/4388 (0.1%)
All	All	0.42	0/6466	0.64	3/8741 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	106	MET	C-N-CD	-14.43	88.86	120.60
1	B	106	MET	C-N-CA	6.91	151.03	122.00
1	B	105	PRO	N-CA-C	-5.31	98.30	112.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	3162	0	3178	211	0
1	B	3188	0	3193	192	1
2	A	53	0	31	18	0
2	B	53	0	31	7	0
3	A	24	0	6	1	0
3	B	24	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	5	0	0	0	0
5	B	6	0	0	0	0
All	All	6525	0	6445	396	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 31.

The worst 5 of 396 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ASN:HD22	1:B:90:ASN:H	1.09	0.98
1:B:446:GLU:H	1:B:456:GLN:HE22	1.12	0.97
1:A:247:LEU:HD12	1:A:247:LEU:H	1.30	0.97
1:A:90:ASN:H	1:A:90:ASN:HD22	1.11	0.96
1:A:65:ASP:HB2	1:A:364:ARG:HH12	1.28	0.93

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)
1:B:328:GLU:OE2	1:B:328:GLU:OE2[7_645]	1.91	0.29

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	408/470 (87%)	358 (88%)	40 (10%)	10 (2%)	5 21
1	B	413/470 (88%)	359 (87%)	42 (10%)	12 (3%)	4 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	821/940 (87%)	717 (87%)	82 (10%)	22 (3%)	5 19

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	320	GLU
1	A	324	GLN
1	B	107	PRO
1	B	320	GLU
1	B	324	GLN

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	344/393 (88%)	325 (94%)	19 (6%)	21 53
1	B	344/393 (88%)	325 (94%)	19 (6%)	21 53
All	All	688/786 (88%)	650 (94%)	38 (6%)	21 53

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	247	LEU
1	B	421	LYS
1	B	288	LYS
1	B	343	THR
1	B	455	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	90	ASN
1	B	244	GLN
1	B	228	GLN

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Mol	Chain	Res	Type
1	B	261	HIS
1	A	244	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	$\#\|Z\| > 2$
4	PO4	B	472	-	4,4,4	2.20	1 (25%)	6,6,6	0.45	0
4	PO4	A	472	-	4,4,4	2.22	1 (25%)	6,6,6	0.38	0
2	FAD	A	600	-	54,58,58	1.37	7 (12%)	71,89,89	1.17	7 (9%)
3	ACJ	B	471	-	25,25,25	2.24	12 (48%)	34,37,37	1.11	2 (5%)
3	ACJ	A	471	-	25,25,25	2.22	12 (48%)	34,37,37	1.05	0
2	FAD	B	700	-	54,58,58	1.37	7 (12%)	71,89,89	1.17	7 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	600	-	-	0/30/50/50	0/6/6/6
2	FAD	B	700	-	-	0/30/50/50	0/6/6/6
3	ACJ	B	471	-	-	2/16/18/18	0/2/2/2
3	ACJ	A	471	-	-	4/16/18/18	0/2/2/2

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	C4X-N5	4.89	1.41	1.30
2	B	700	FAD	C4X-N5	4.87	1.41	1.30
3	A	471	ACJ	C14-N1	4.35	1.53	1.45
3	B	471	ACJ	C14-N1	4.35	1.53	1.45
4	B	472	PO4	P-O1	3.81	1.59	1.50

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	FAD	C4B-O4B-C1B	-3.36	106.84	109.92
2	B	700	FAD	C4B-O4B-C1B	-3.26	106.94	109.92
2	B	700	FAD	C5A-C6A-N6A	2.71	124.43	120.31
2	A	600	FAD	C5A-C6A-N6A	2.69	124.42	120.31
2	B	700	FAD	C9A-C5X-N5	-2.60	119.69	122.45

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	471	ACJ	C14-C10-C11-O3
3	A	471	ACJ	C14-C10-C11-O2
3	B	471	ACJ	C14-C10-C11-O2
3	B	471	ACJ	C14-C10-C11-O3
3	A	471	ACJ	C9-C10-C11-O3

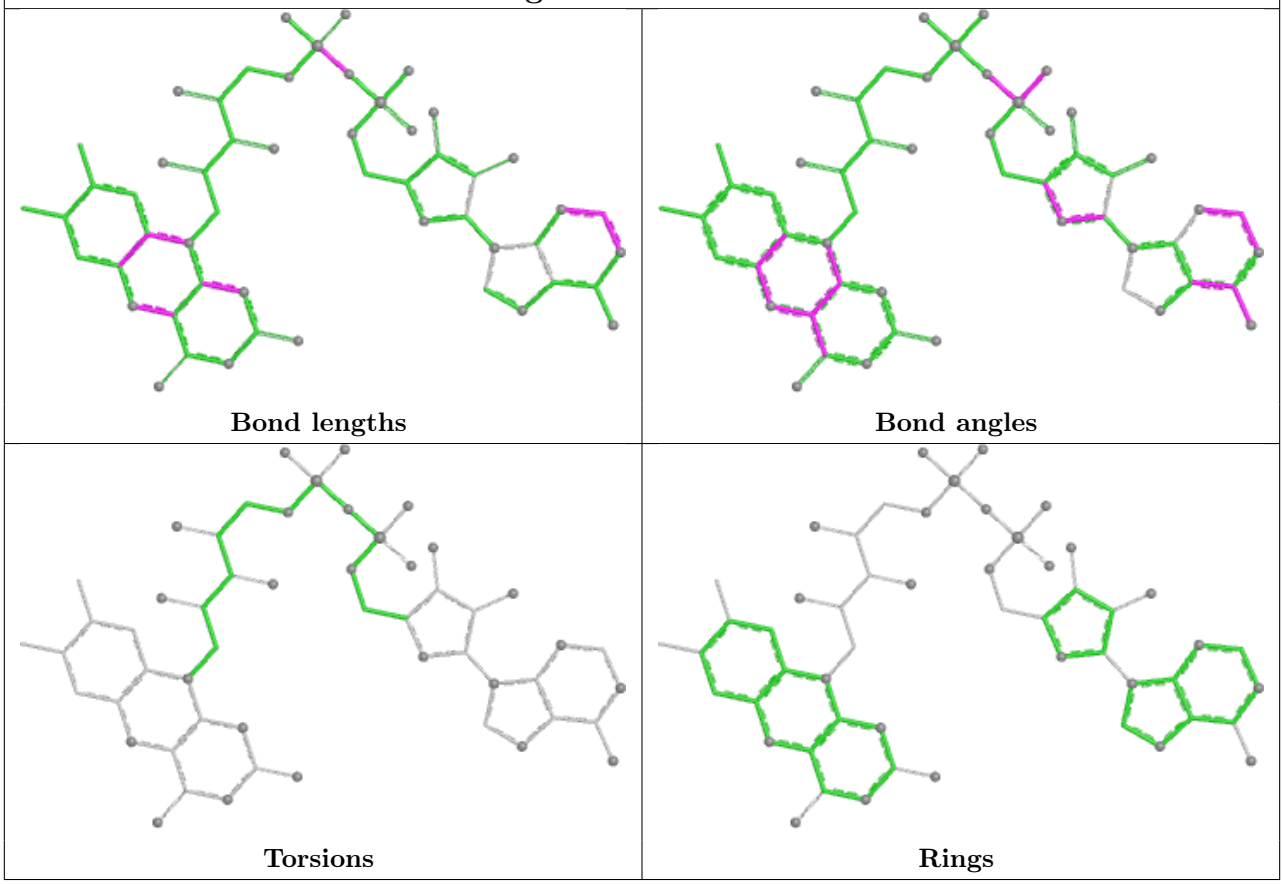
There are no ring outliers.

3 monomers are involved in 26 short contacts:

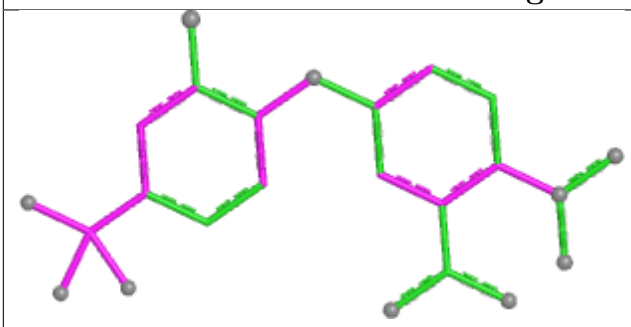
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FAD	18	0
3	A	471	ACJ	1	0
2	B	700	FAD	7	0

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.

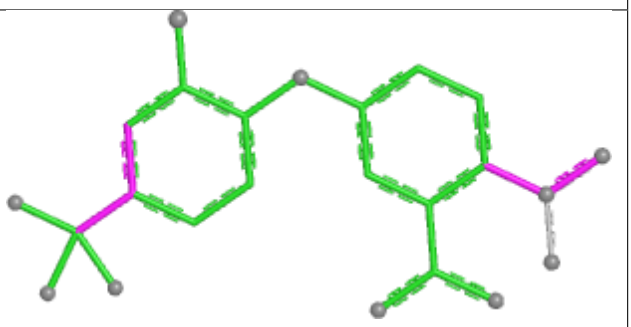
Ligand FAD A 600



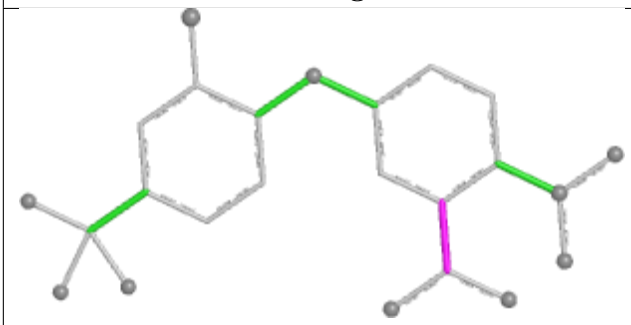
Ligand ACJ B 471



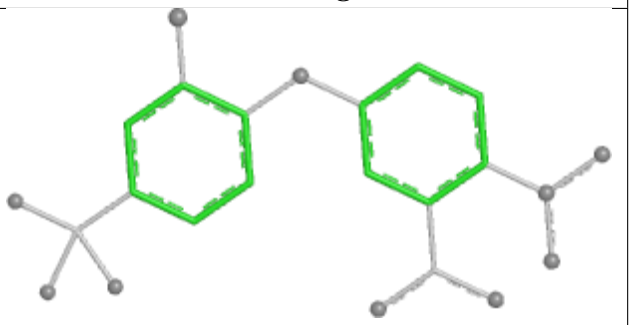
Bond lengths



Bond angles

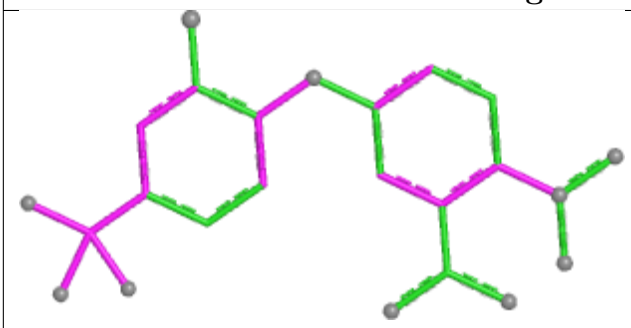


Torsions

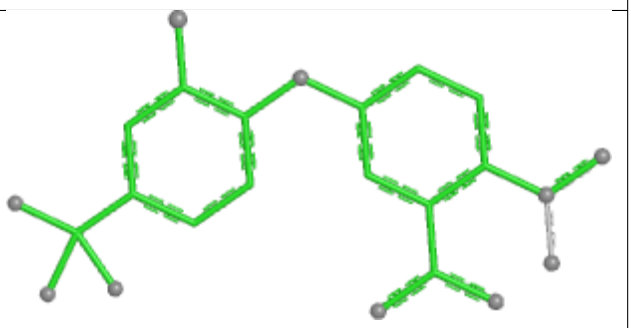


Rings

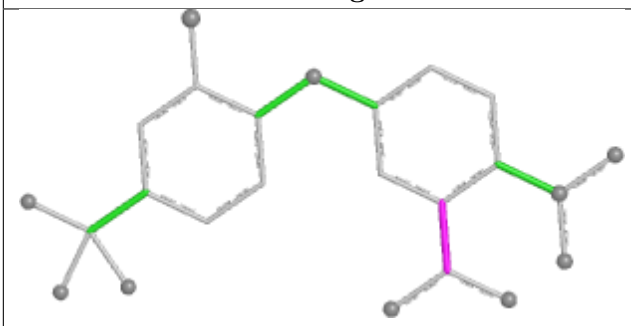
Ligand ACJ A 471



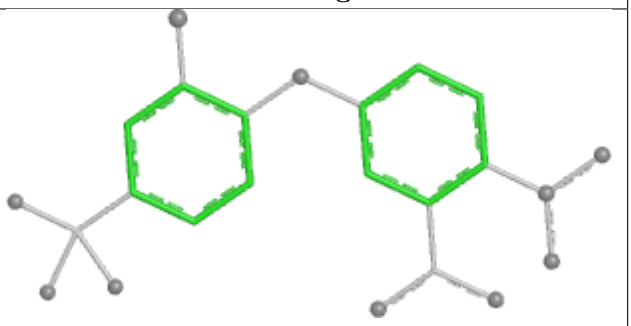
Bond lengths



Bond angles

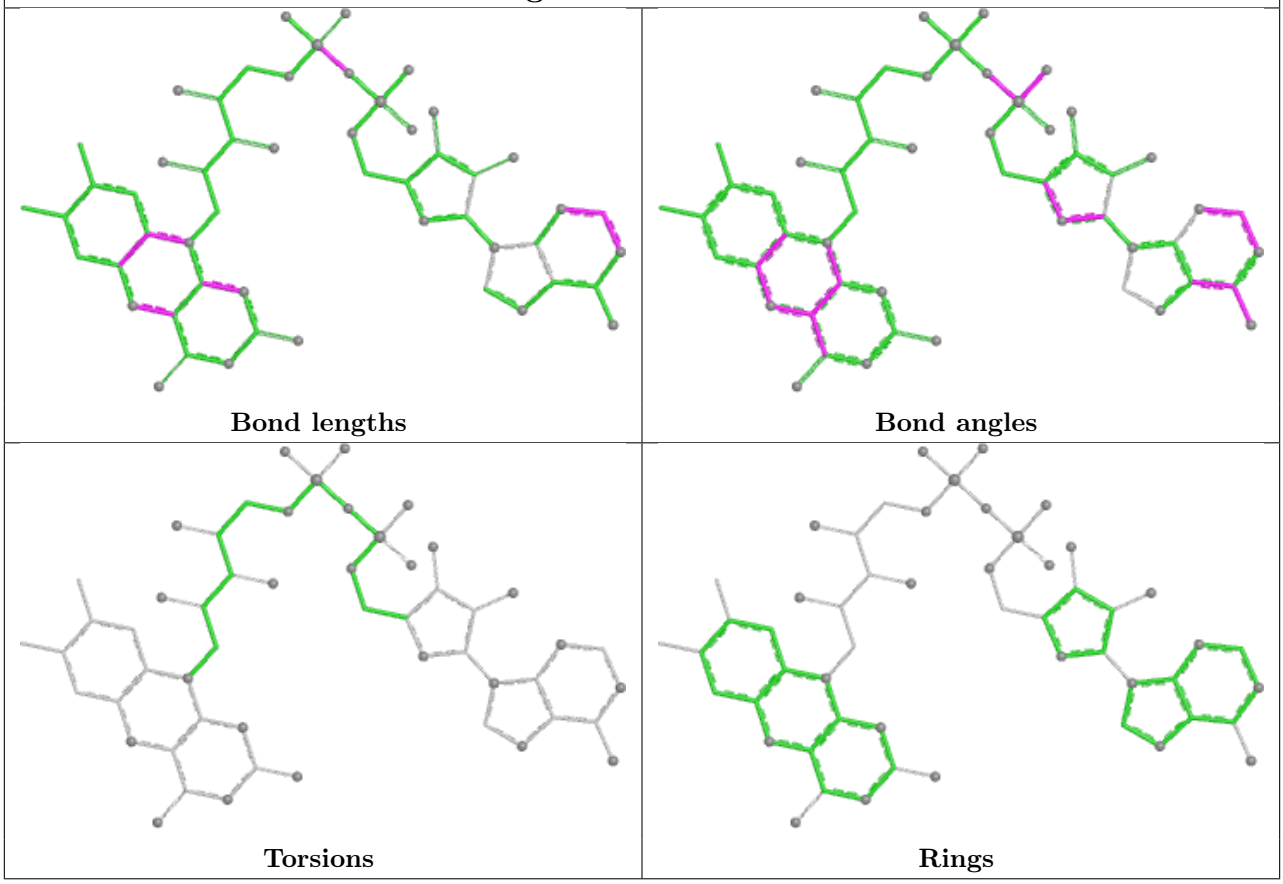


Torsions



Rings

Ligand FAD B 700



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	414/470 (88%)	0.53	39 (9%) 8 6	44, 78, 102, 116	0
1	B	419/470 (89%)	0.64	44 (10%) 6 5	43, 80, 102, 115	0
All	All	833/940 (88%)	0.59	83 (9%) 7 5	43, 79, 102, 116	0

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	371	GLY	5.7
1	B	470	SER	5.5
1	B	135	ALA	5.3
1	A	56	ASP	4.4
1	A	327	HIS	4.1

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 monosaccharides in this entry.

6.4 Ligands (i)

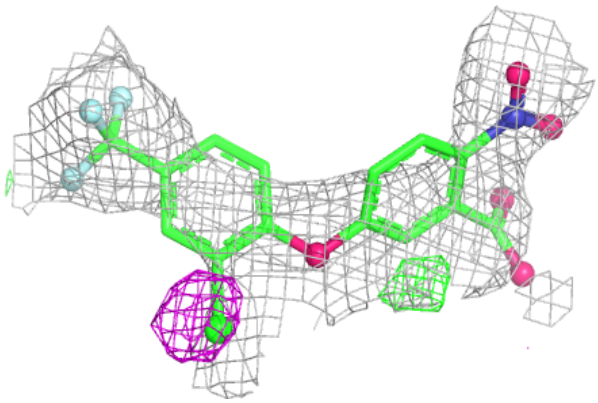
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

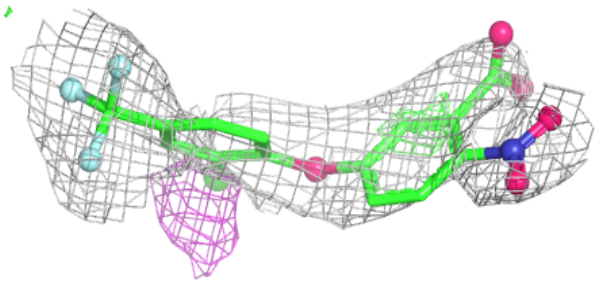
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ACJ	A	471	24/24	0.63	0.41	113,114,116,117	0
3	ACJ	B	471	24/24	0.67	0.38	103,106,107,108	0
2	FAD	A	600	53/53	0.86	0.31	55,68,83,83	0
2	FAD	B	700	53/53	0.88	0.32	60,67,81,81	0
4	PO4	A	472	5/5	0.88	0.29	112,113,114,114	0
4	PO4	B	472	5/5	0.93	0.27	103,104,104,105	0

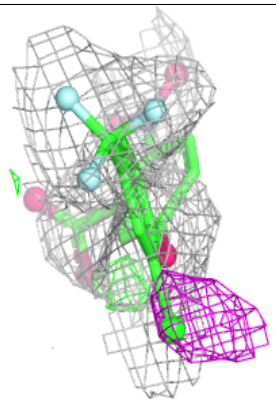
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACJ A 471:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

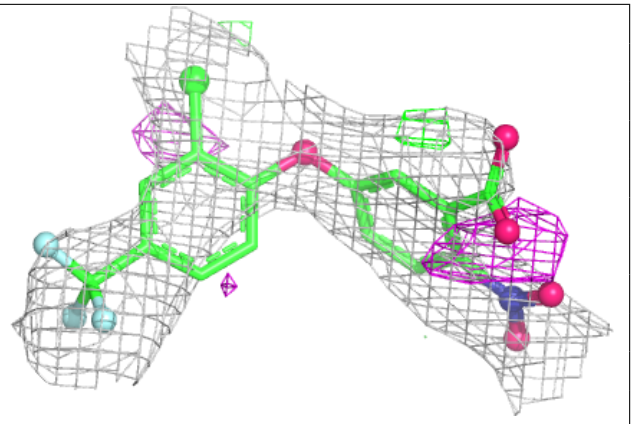


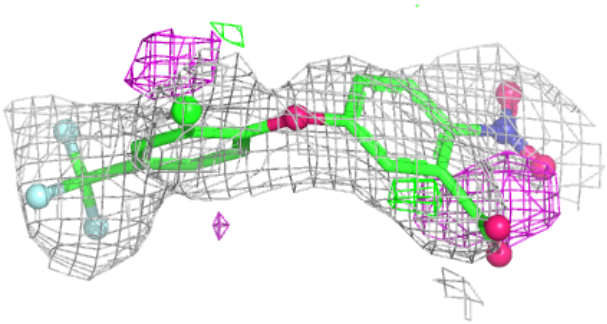


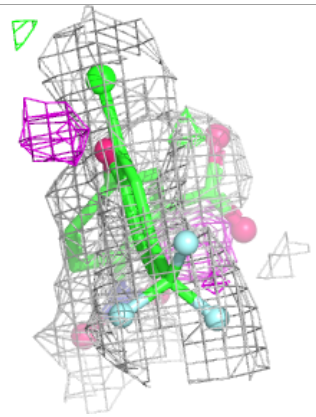


Electron density around ACJ B 471:

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

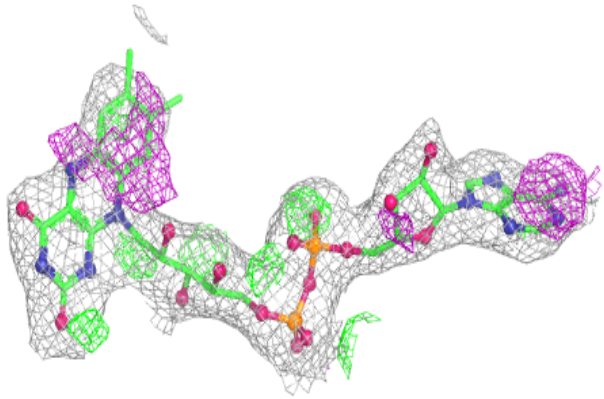


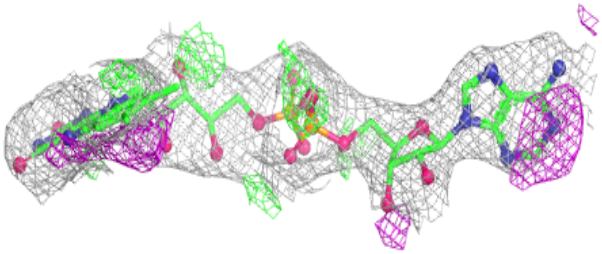


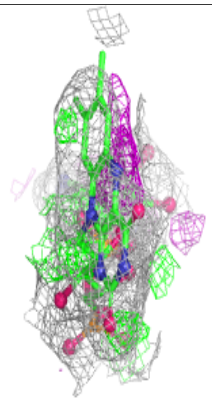


Electron density around FAD A 600:

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

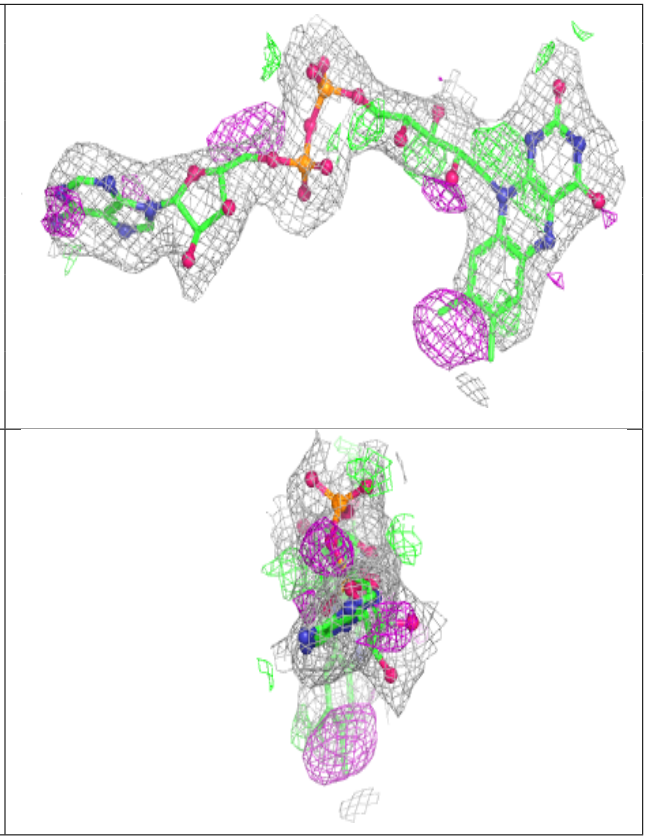






Electron density around FAD B 700:

$2mF_o$-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.