Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 12:45 am BST

PDB ID	:	4BJY
Title	:	Crystal structure of 3-hydroxybenzoate 6-hydroxylase uncovers lipid- assisted flavoprotein strategy for regioselective aromatic hydroxylation: Platinum derivative
Authors	:	Orru, R.; Montersino, S.; Barendregt, A.; Westphal, A.H.; van Duijn, E.; Mattevi, A.; van Berkel, W.J.H.
Deposited on	:	2013-04-21
Resolution	:	1.52 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

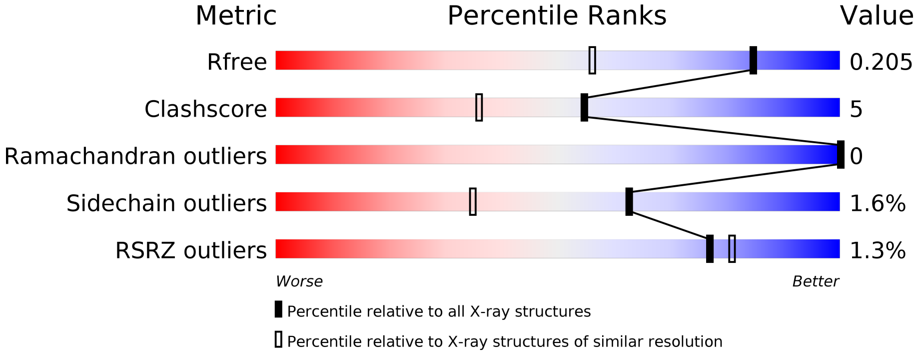
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.52 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	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)
RSRZ outliers	127900	3943 (1.54-1.50)

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 <=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	424	

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 3448 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 PROBABLE SALICYLATE MONOOXYGENASE.

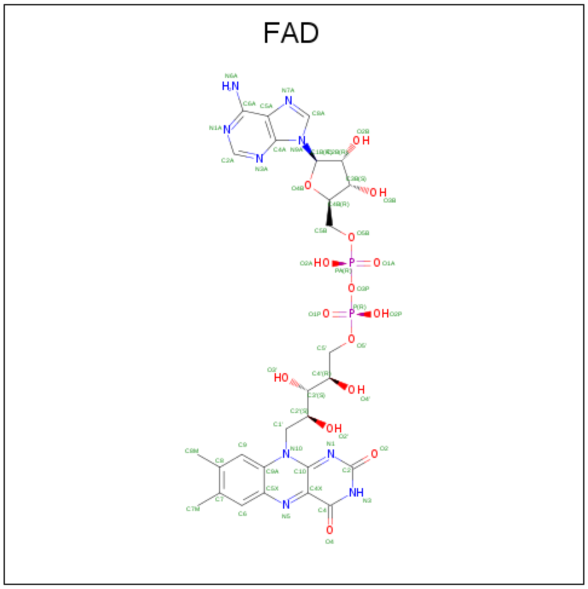
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	393	3067	1926	546	584	11	0	1	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	400	LYS	-	expression tag	UNP Q0SFK6
A	401	LEU	-	expression tag	UNP Q0SFK6
A	402	GLY	-	expression tag	UNP Q0SFK6
A	403	PRO	-	expression tag	UNP Q0SFK6
A	404	GLU	-	expression tag	UNP Q0SFK6
A	405	GLN	-	expression tag	UNP Q0SFK6
A	406	LYS	-	expression tag	UNP Q0SFK6
A	407	LEU	-	expression tag	UNP Q0SFK6
A	408	ILE	-	expression tag	UNP Q0SFK6
A	409	SER	-	expression tag	UNP Q0SFK6
A	410	GLU	-	expression tag	UNP Q0SFK6
A	411	GLU	-	expression tag	UNP Q0SFK6
A	412	ASP	-	expression tag	UNP Q0SFK6
A	413	LEU	-	expression tag	UNP Q0SFK6
A	414	ASN	-	expression tag	UNP Q0SFK6
A	415	SER	-	expression tag	UNP Q0SFK6
A	416	ALA	-	expression tag	UNP Q0SFK6
A	417	VAL	-	expression tag	UNP Q0SFK6
A	418	ASP	-	expression tag	UNP Q0SFK6
A	419	HIS	-	expression tag	UNP Q0SFK6
A	420	HIS	-	expression tag	UNP Q0SFK6
A	421	HIS	-	expression tag	UNP Q0SFK6
A	422	HIS	-	expression tag	UNP Q0SFK6
A	423	HIS	-	expression tag	UNP Q0SFK6
A	424	HIS	-	expression tag	UNP Q0SFK6

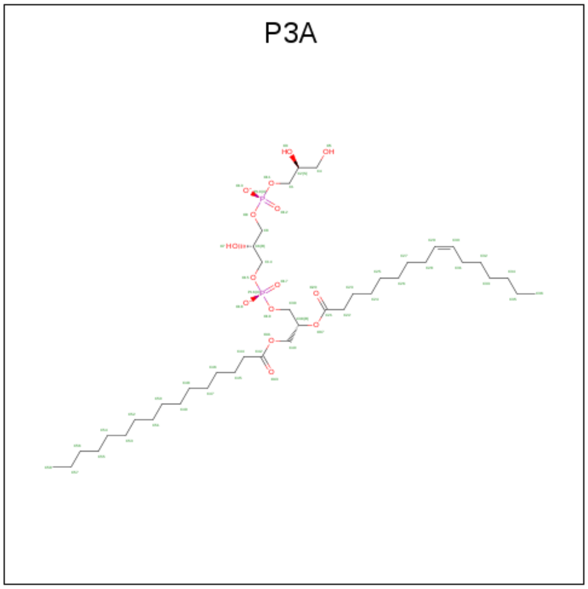
- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:

$C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is PHOSPHATIDYLGLYCEROL-PHOSPHOGLYCEROL (three-letter code: P3A) (formula: $C_{41}H_{78}O_{15}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
3	A	1	50	36	12	2	0	1

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0

- Molecule 5 is water.

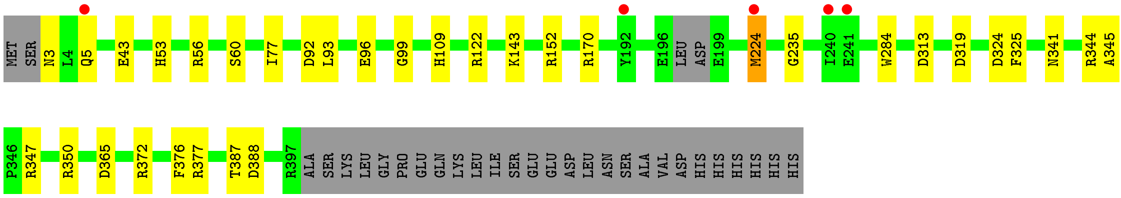
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	277	Total O 277 277	0	0

3 Residue-property plots ⓘ

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: PROBABLE SALICYLATE MONOOXYGENASE

Chain A:



4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	106.61Å 106.61Å 142.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.52 53.30 – 1.52	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-1.52) 100.0 (53.30-1.52)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.88 (at 1.52Å)	Xtriage
Refinement program	REFMAC 5.8.0033	Depositor
R, R_{free}	0.173 , 0.205 0.173 , 0.205	Depositor DCC
R_{free} test set	3168 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	14.7	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.6	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3448	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: P3A, FAD, CL

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	1.04	1/3141 (0.0%)	1.13	17/4262 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	MET	SD-CE	5.20	2.06	1.77

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	377	ARG	NE-CZ-NH2	-12.68	113.96	120.30
1	A	344	ARG	NE-CZ-NH2	-8.11	116.24	120.30
1	A	56	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	A	224	MET	CG-SD-CE	7.49	112.19	100.20
1	A	377	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	A	376	PHE	CB-CG-CD2	-6.98	115.91	120.80
1	A	388	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	A	170	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	152	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	92	ASP	CB-CG-OD1	6.13	123.82	118.30
1	A	152	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	319	ASP	CB-CG-OD2	-6.06	112.85	118.30
1	A	170	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	372	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	A	350	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	365	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	A	313	ASP	CB-CG-OD1	5.10	122.89	118.30

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	3067	0	2946	30	0
2	A	53	0	31	1	0
3	A	50	0	6	1	0
4	A	1	0	0	0	0
5	A	277	0	0	26	1
All	All	3448	0	2983	32	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 5.

All (32) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:MET:SD	1:A:224:MET:CE	2.07	1.42
1:A:122:ARG:NH1	5:A:2083:HOH:O	1.65	1.30
1:A:60:SER:O	5:A:2032:HOH:O	1.67	1.12
1:A:60:SER:C	5:A:2032:HOH:O	1.85	1.11
1:A:325:PHE:HE2	5:A:2111:HOH:O	1.45	0.97
1:A:224:MET:HE3	5:A:2154:HOH:O	1.64	0.95
1:A:224:MET:CE	5:A:2154:HOH:O	2.20	0.89
1:A:224:MET:HE2	5:A:2156:HOH:O	1.72	0.88
1:A:224:MET:CE	5:A:2157:HOH:O	2.20	0.87
1:A:96:GLU:N	5:A:2066:HOH:O	1.96	0.86
1:A:224:MET:HE2	5:A:2157:HOH:O	1.79	0.80
1:A:224:MET:SD	5:A:2155:HOH:O	2.39	0.79
1:A:96:GLU:HG2	5:A:2066:HOH:O	1.83	0.79
1:A:224:MET:SD	5:A:2154:HOH:O	2.41	0.77
1:A:324:ASP:OD2	5:A:2206:HOH:O	2.08	0.72
1:A:224:MET:HG3	5:A:2155:HOH:O	1.91	0.70
1:A:224:MET:CG	5:A:2155:HOH:O	2.43	0.64
1:A:224:MET:HG3	5:A:2078:HOH:O	1.97	0.64
1:A:325:PHE:CE2	5:A:2111:HOH:O	2.32	0.64
1:A:99:GLY:N	5:A:2067:HOH:O	2.13	0.58
1:A:122:ARG:HD3	5:A:2082:HOH:O	2.03	0.58
3:A:600[B]:P3A:O17	5:A:2277:HOH:O	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:HIS:NE2	5:A:2078:HOH:O	2.28	0.57
1:A:235:GLY:HA3	5:A:2160:HOH:O	2.06	0.55
1:A:3:ASN:HD21	1:A:5:GLN:HE21	1.60	0.48
2:A:500:FAD:H8A	5:A:2017:HOH:O	2.13	0.48
1:A:3:ASN:ND2	1:A:5:GLN:HE21	2.13	0.46
1:A:224:MET:CE	5:A:2156:HOH:O	2.42	0.46
1:A:224:MET:HE3	5:A:2157:HOH:O	1.99	0.44
1:A:77:ILE:HG13	1:A:93:LEU:HD11	2.00	0.43
1:A:284:TRP:CZ2	1:A:345:ALA:HA	2.55	0.42

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)
5:A:2082:HOH:O	5:A:2089:HOH:O[15_555]	2.11	0.09

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	390/424 (92%)	383 (98%)	7 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	310/337 (92%)	305 (98%)	5 (2%)	62 35

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	53	HIS
1	A	143	LYS
1	A	341	ASN
1	A	347	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\#\|Z\| > 2$
3	P3A	A	600[B]	-	43,43,57	0.78	2 (4%)	47,48,67	1.01	5 (10%)
3	P3A	A	600[A]	-	43,43,57	0.78	2 (4%)	47,48,67	0.89	3 (6%)
2	FAD	A	500	-	51,58,58	2.37	12 (23%)	60,89,89	1.98	11 (18%)

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
3	P3A	A	600[B]	-	-	8/45/45/65	-
3	P3A	A	600[A]	-	-	6/45/45/65	-
2	FAD	A	500	-	-	3/30/50/50	0/6/6/6

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	FAD	C4X-C10	10.75	1.49	1.38
2	A	500	FAD	O4B-C1B	7.66	1.51	1.41
2	A	500	FAD	C9A-N10	3.57	1.43	1.38
2	A	500	FAD	C8-C7	3.22	1.48	1.40
2	A	500	FAD	C9-C9A	-3.21	1.34	1.40
2	A	500	FAD	C2B-C1B	-2.97	1.49	1.53
2	A	500	FAD	C9A-C5X	2.91	1.48	1.42
3	A	600[B]	P3A	O37-C21	2.76	1.42	1.34
3	A	600[A]	P3A	O37-C21	2.76	1.42	1.34
2	A	500	FAD	C5'-C4'	-2.16	1.48	1.51
2	A	500	FAD	C4X-N5	2.16	1.36	1.33
2	A	500	FAD	O2B-C2B	2.12	1.48	1.43
3	A	600[B]	P3A	O41-C42	2.11	1.39	1.33
3	A	600[A]	P3A	O41-C42	2.11	1.39	1.33
2	A	500	FAD	C4-C4X	2.10	1.45	1.41
2	A	500	FAD	C10-N1	2.03	1.35	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	FAD	C4-N3-C2	9.23	122.93	115.14
2	A	500	FAD	C4-C4X-C10	-5.53	116.29	119.95
2	A	500	FAD	N3A-C2A-N1A	-3.86	122.65	128.68
2	A	500	FAD	C4X-C4-N3	-3.41	118.77	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	FAD	C4A-C5A-N7A	3.23	112.76	109.40
2	A	500	FAD	C4-C4X-N5	3.17	122.22	118.60
3	A	600[B]	P3A	O19-P16-O17	2.96	114.78	106.47
2	A	500	FAD	C1'-N10-C10	2.77	120.89	118.41
2	A	500	FAD	O4B-C4B-C3B	2.74	110.54	105.11
2	A	500	FAD	C4X-N5-C5X	2.73	119.50	116.77
2	A	500	FAD	C2A-N1A-C6A	2.52	123.06	118.75
3	A	600[B]	P3A	P16-O19-C39	2.30	124.63	118.30
3	A	600[B]	P3A	O43-C42-C44	2.07	131.82	123.73
3	A	600[A]	P3A	O43-C42-C44	2.07	131.82	123.73
3	A	600[B]	P3A	C46-C45-C44	-2.07	105.77	113.19
3	A	600[A]	P3A	C46-C45-C44	-2.07	105.77	113.19
3	A	600[B]	P3A	O41-C42-O43	-2.06	118.39	123.59
3	A	600[A]	P3A	O41-C42-O43	-2.06	118.39	123.59
2	A	500	FAD	O4'-C4'-C3'	-2.03	104.17	109.10

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	600[B]	P3A	C39-O19-P16-O18
3	A	600[B]	P3A	C39-O19-P16-O15
3	A	600[B]	P3A	C30-C31-C32-C33
3	A	600[A]	P3A	C30-C31-C32-C33
3	A	600[B]	P3A	C25-C26-C27-C28
3	A	600[A]	P3A	C25-C26-C27-C28
3	A	600[B]	P3A	C53-C54-C55-C56
3	A	600[A]	P3A	C53-C54-C55-C56
3	A	600[B]	P3A	C49-C50-C51-C52
3	A	600[A]	P3A	C49-C50-C51-C52
3	A	600[B]	P3A	C44-C45-C46-C47
3	A	600[A]	P3A	C44-C45-C46-C47
3	A	600[B]	P3A	C45-C46-C47-C48
3	A	600[A]	P3A	C45-C46-C47-C48
2	A	500	FAD	O2'-C2'-C3'-C4'
2	A	500	FAD	O2'-C2'-C3'-O3'
2	A	500	FAD	O4B-C4B-C5B-O5B

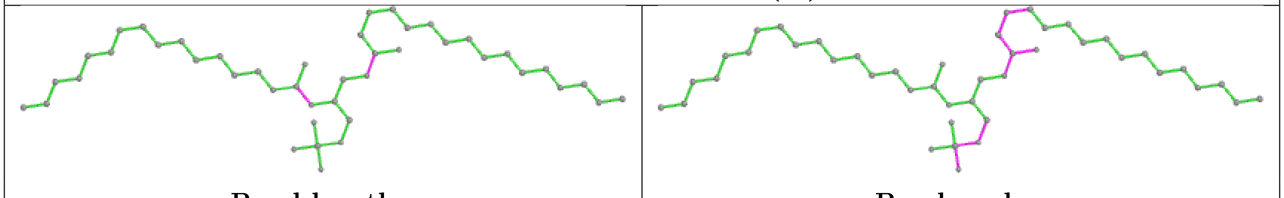
There are no ring outliers.

2 monomers are involved in 2 short contacts:

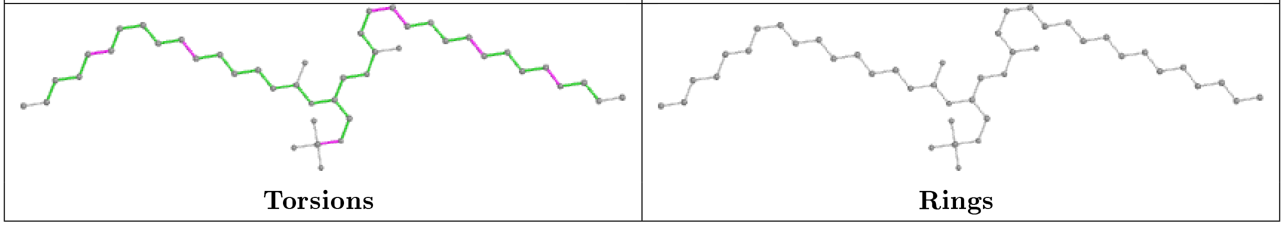
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600[B]	P3A	1	0
2	A	500	FAD	1	0

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 P3A A 600 (B)

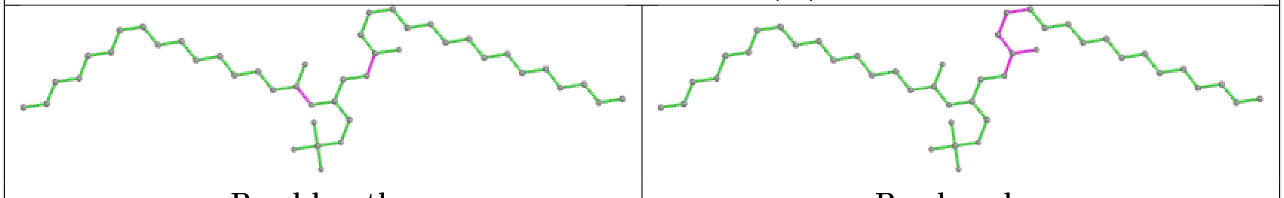


Bond lengths **Bond angles**

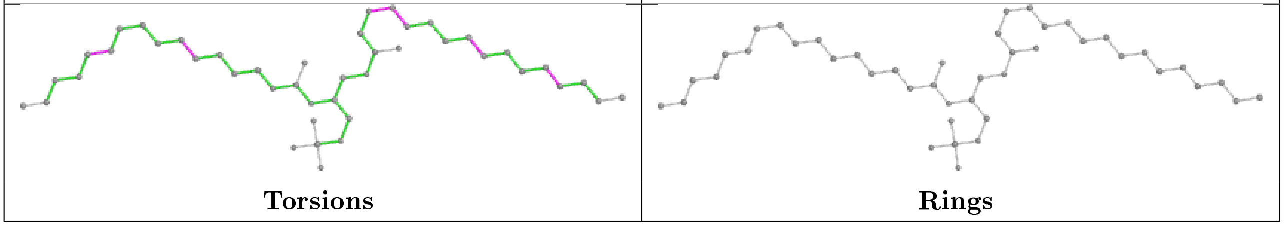


Torsions **Rings**

Ligand P3A A 600 (A)

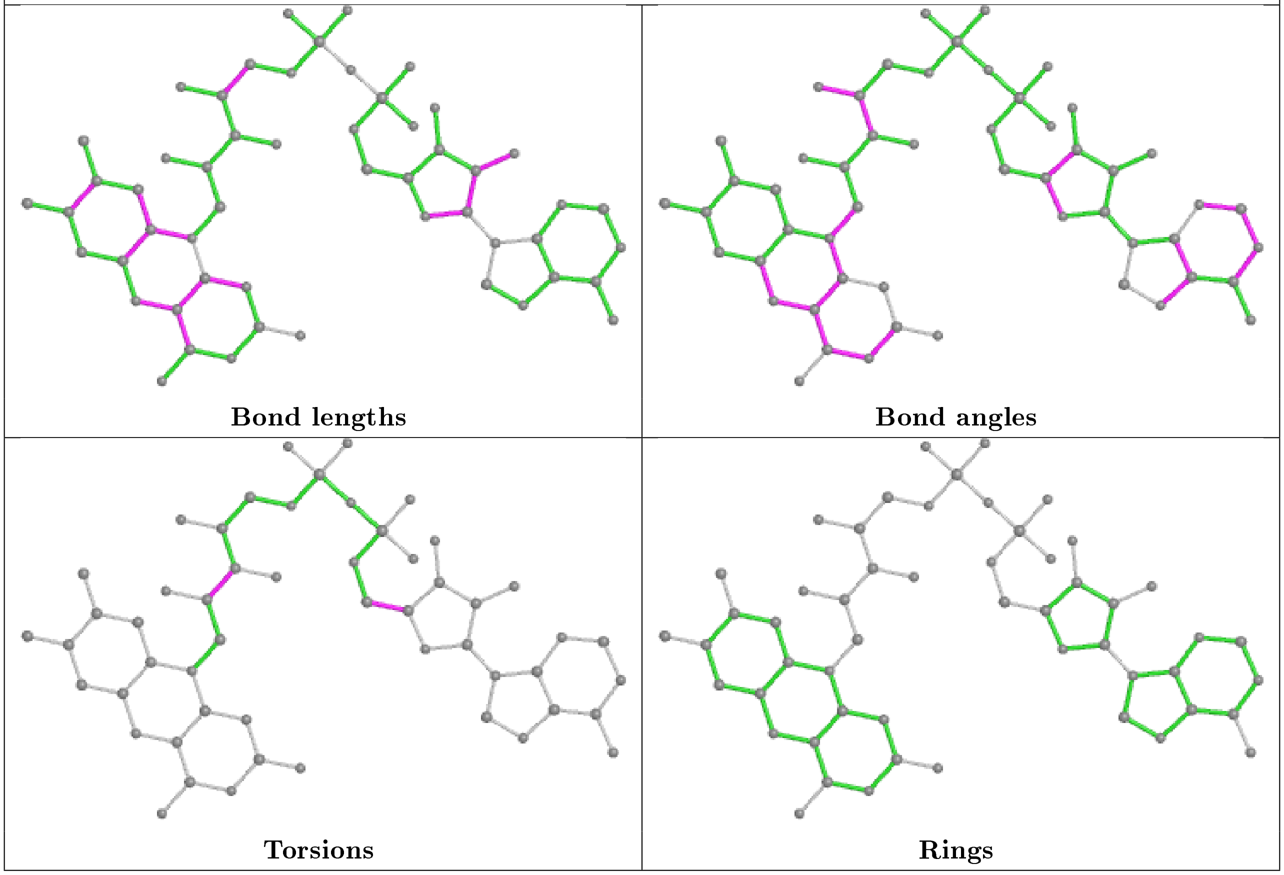


Bond lengths **Bond angles**



Torsions **Rings**

Ligand FAD A 500



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	393/424 (92%)	-0.21	5 (1%)	77	81	9, 17, 34, 53	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	241	GLU	2.8
1	A	5	GLN	2.5
1	A	240	ILE	2.4
1	A	192	TYR	2.1
1	A	224	MET	2.0

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

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

6.3 Carbohydrates ⓘ

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, 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	P3A	A	600[B]	44/58	0.91	0.10	16,21,29,31	6
3	P3A	A	600[A]	44/58	0.91	0.10	16,21,28,31	6

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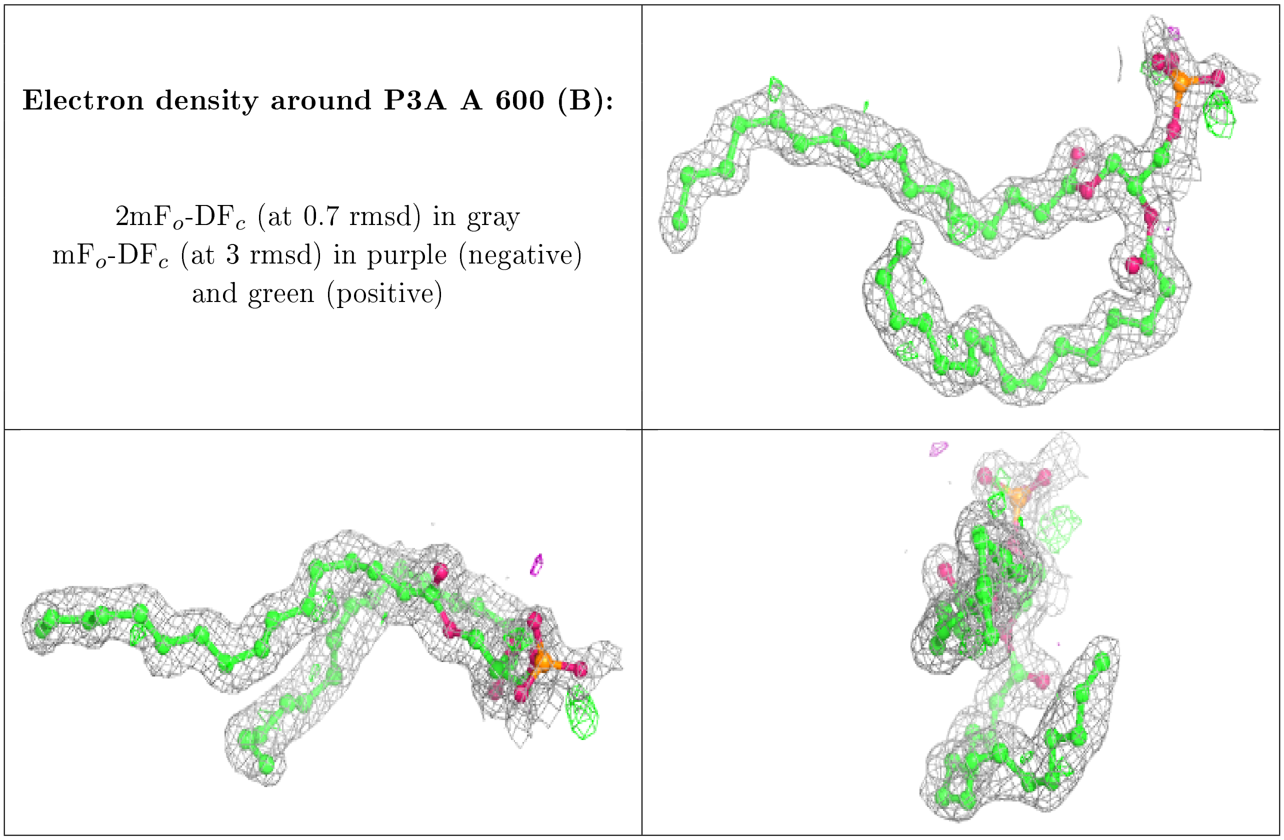
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\mathring{A}^2$)	Q<0.9
2	FAD	A	500	53/53	0.98	0.06	8,13,17,20	0
4	CL	A	1398	1/1	0.99	0.04	16,16,16,16	0

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.

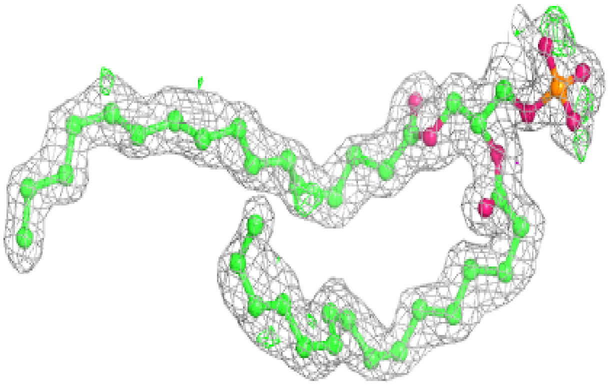


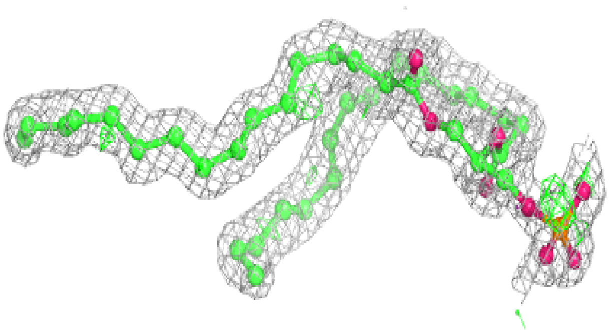
Electron density around P3A A 600 (B):

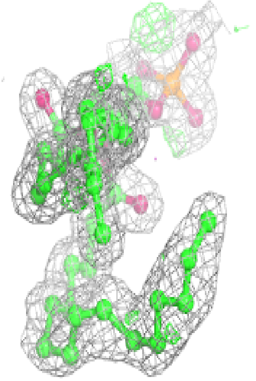
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around P3A A 600 (A):

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

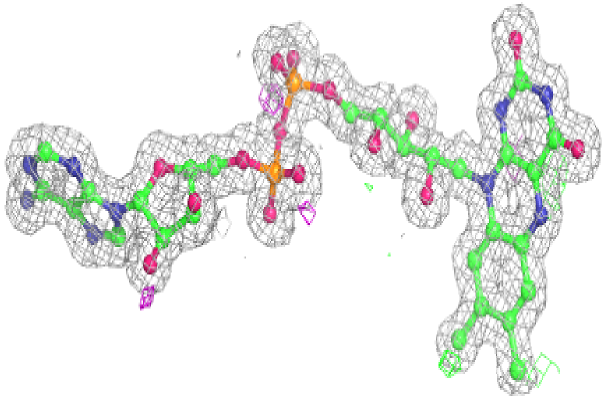


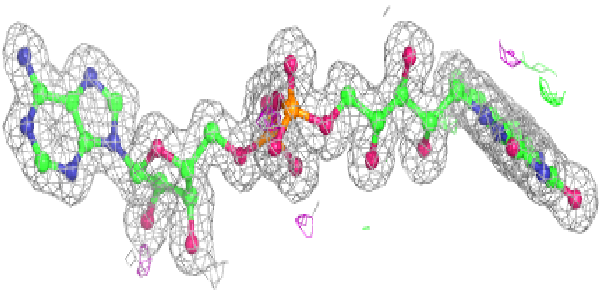


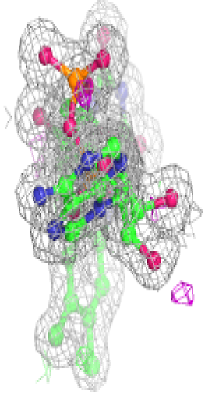


Electron density around FAD A 500:

$2mF_o$-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 ⓘ

There are no such residues in this entry.