Full wwPDB X-ray Structure Validation Report (i)

Nov 2, 2023 – 06:06 PM EDT

PDB ID	:	8T3P
Title	:	Crystal structure of MonC1 (a flavin-dependent monooxygenase)
Authors	:	Wang, Q.; Mathews, I.I.; Kim, C.Y.
Deposited on	:	2023-06-07
Resolution	:	1.90 Å(reported)

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

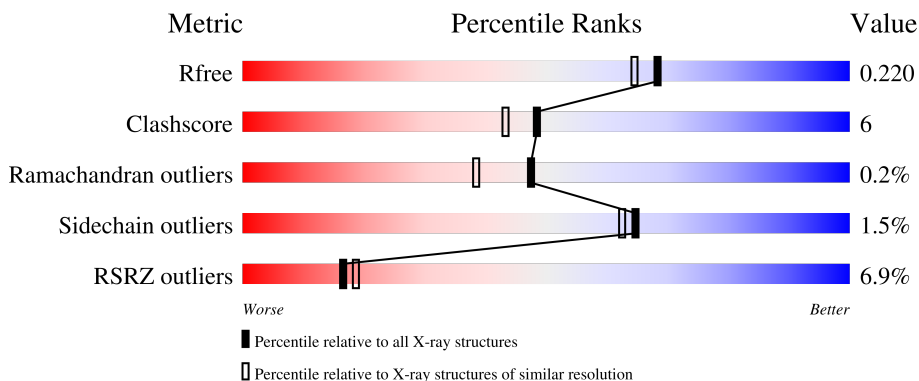|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.90 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	Percentile Ranks	Value
Rfree		0.220
Clashscore		6
Ramachandran outliers		0.2%
Sidechain outliers		1.5%
RSRZ outliers		6.9%

Worse   *Better*

▮ Percentile relative to all X-ray structures

⫿ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	512	3% / 84% 9% 7%
1	B	512	10% / 76% 15% 9%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8009 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 MonCI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total 3633	C 2266	N 673	O 685	S 9	0	4	0
1	B	468	Total 3547	C 2219	N 650	O 668	S 10	0	3	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP Q846W9
A	-14	ASN	-	expression tag	UNP Q846W9
A	-13	HIS	-	expression tag	UNP Q846W9
A	-12	LYS	-	expression tag	UNP Q846W9
A	-11	VAL	-	expression tag	UNP Q846W9
A	-10	HIS	-	expression tag	UNP Q846W9
A	-9	HIS	-	expression tag	UNP Q846W9
A	-8	HIS	-	expression tag	UNP Q846W9
A	-7	HIS	-	expression tag	UNP Q846W9
A	-6	HIS	-	expression tag	UNP Q846W9
A	-5	HIS	-	expression tag	UNP Q846W9
A	-4	ILE	-	expression tag	UNP Q846W9
A	-3	GLU	-	expression tag	UNP Q846W9
A	-2	GLY	-	expression tag	UNP Q846W9
A	-1	ARG	-	expression tag	UNP Q846W9
A	0	HIS	-	expression tag	UNP Q846W9
B	-15	MET	-	initiating methionine	UNP Q846W9
B	-14	ASN	-	expression tag	UNP Q846W9
B	-13	HIS	-	expression tag	UNP Q846W9
B	-12	LYS	-	expression tag	UNP Q846W9
B	-11	VAL	-	expression tag	UNP Q846W9
B	-10	HIS	-	expression tag	UNP Q846W9
B	-9	HIS	-	expression tag	UNP Q846W9
B	-8	HIS	-	expression tag	UNP Q846W9
B	-7	HIS	-	expression tag	UNP Q846W9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP Q846W9
B	-5	HIS	-	expression tag	UNP Q846W9
B	-4	ILE	-	expression tag	UNP Q846W9
B	-3	GLU	-	expression tag	UNP Q846W9
B	-2	GLY	-	expression tag	UNP Q846W9
B	-1	ARG	-	expression tag	UNP Q846W9
B	0	HIS	-	expression tag	UNP Q846W9

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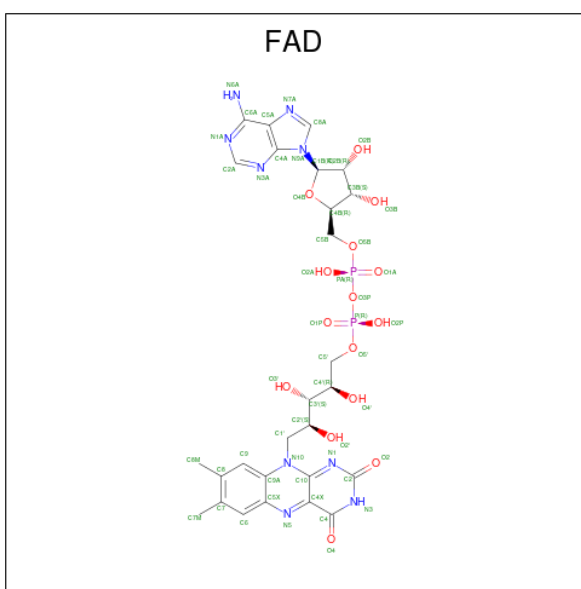
FAD

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	490	Total 501	O 501	0	11
4	B	219	Total 220	O 220	0	1

3 Residue-property plots ⓘ

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: MonCI

Chain A:

• Molecule 1: MonCI

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.15Å 52.35Å 141.56Å 90.00° 93.60° 90.00°	Depositor
Resolution (Å)	39.72 – 1.90 39.72 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.4 (39.72-1.90) 94.4 (39.72-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.181 , 0.222 0.180 , 0.220	Depositor DCC
R_{free} test set	3741 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	24.5	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.8	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8009	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% 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 $< |L| >$, $< L^2 >$ 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	0.46	0/3704	0.68	0/5047
1	B	0.38	0/3616	0.66	0/4926
All	All	0.42	0/7320	0.67	0/9973

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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	27	ARG	Sidechain
1	B	454	ARG	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	3633	0	3608	33	0
1	B	3547	0	3508	54	0
2	A	53	0	31	3	0
2	B	53	0	31	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	501	0	0	4	0
4	B	220	0	0	4	0
All	All	8009	0	7178	87	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 6.

All (87) 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:151:GLY:HA2	1:A:362:ARG:HH12	1.32	0.92
1:A:231:ASP:HB2	1:A:278:ASN:HD21	1.54	0.72
1:B:92:LEU:HG	1:B:225:ALA:HB3	1.72	0.71
1:B:93:VAL:HG22	1:B:226:VAL:HG22	1.74	0.68
1:A:153:ARG:HG3	1:A:316:ASP:HB2	1.77	0.65
1:B:263:LEU:HD12	1:B:264:PRO:HD2	1.79	0.65
1:A:287:ARG:HG3	1:A:287:ARG:HH11	1.63	0.64
1:B:150:SER:OG	1:B:151:GLY:N	2.31	0.64
1:B:428:SER:O	1:B:432:THR:HG23	1.98	0.63
1:B:271:ILE:HD12	1:B:271:ILE:H	1.63	0.63
1:B:160:ARG:HE	1:B:167:GLN:HE21	1.48	0.62
1:B:153:ARG:HG3	1:B:316:ASP:HB2	1.81	0.61
1:B:468:LEU:HD23	1:B:469:PRO:HD2	1.83	0.61
1:A:214:LYS:HG2	1:A:292:LEU:HD21	1.82	0.60
1:B:211:ARG:HH21	1:B:294:PRO:HA	1.66	0.59
1:A:208:TYR:OH	1:A:331:ILE:HG13	2.03	0.59
1:B:243:VAL:HG23	1:B:282:LEU:HD22	1.85	0.59
1:B:330:PRO:HB3	2:B:501:FAD:C6	2.32	0.58
1:A:56:ALA:HB1	1:A:244:TYR:HD2	1.70	0.57
1:B:137:ARG:HB3	1:B:162:LEU:HD11	1.87	0.57
1:B:332:TYR:CE1	1:B:386:LYS:HD3	2.40	0.57
1:A:150:SER:O	1:A:362:ARG:NH1	2.39	0.56
1:A:287:ARG:NH1	4:A:607:HOH:O	2.34	0.56
1:B:470:GLU:OE1	1:B:470:GLU:N	2.19	0.56
1:A:334:HIS:CE1	1:A:382:LEU:HD13	2.40	0.56
1:A:330:PRO:HB3	2:A:501:FAD:C5X	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:SER:HB3	1:B:247:GLU:OE2	2.08	0.54
1:B:52:GLN:HB2	2:B:501:FAD:HM82	1.91	0.53
1:B:336:MET:HB2	2:B:501:FAD:O2	2.09	0.53
1:A:330:PRO:HB3	2:A:501:FAD:C6	2.38	0.52
1:B:137:ARG:O	1:B:162:LEU:HG	2.10	0.52
1:B:133:THR:HG23	4:B:755:HOH:O	2.10	0.52
1:A:267:GLU:OE1	4:A:601:HOH:O	2.19	0.51
1:A:152:GLY:N	1:A:362:ARG:HH22	2.08	0.51
1:B:212:LEU:HB2	1:B:293:THR:HG23	1.93	0.51
1:A:312:GLU:O	1:A:366:ARG:NH2	2.45	0.50
1:A:214:LYS:HG2	1:A:292:LEU:HD11	1.95	0.49
1:B:43:GLU:O	1:B:45:GLN:N	2.46	0.49
1:A:37:ARG:HG3	1:A:162:LEU:HD11	1.95	0.48
1:B:138:THR:HG22	1:B:159:VAL:HG22	1.95	0.48
1:B:179:THR:OG1	1:B:183:SER:HB2	2.14	0.48
1:B:330:PRO:HB3	2:B:501:FAD:C5X	2.43	0.47
1:A:52:GLN:HB2	2:A:501:FAD:HM82	1.96	0.47
1:B:150:SER:N	1:B:362:ARG:HH12	2.12	0.47
1:B:160:ARG:NE	1:B:167:GLN:HE21	2.12	0.47
1:B:215:ALA:HB1	1:B:219:ALA:HB3	1.96	0.47
1:A:233:ARG:HB2	1:A:236:GLU:HG3	1.95	0.47
1:B:93:VAL:HG12	1:B:103:ARG:HD2	1.97	0.47
1:B:468:LEU:CD2	1:B:469:PRO:HD2	2.44	0.47
1:A:214:LYS:NZ	4:A:620:HOH:O	2.49	0.46
1:A:287:ARG:HG3	1:A:287:ARG:NH1	2.29	0.46
1:A:142:GLU:HA	1:A:188:TRP:CD1	2.50	0.46
1:B:264:PRO:HD3	1:B:273:PHE:CD2	2.51	0.46
1:B:160:ARG:HE	1:B:167:GLN:NE2	2.12	0.45
1:B:37:ARG:O	1:B:137:ARG:HA	2.16	0.45
1:B:65:ARG:HD2	4:B:704:HOH:O	2.15	0.45
1:B:210:THR:O	1:B:295:VAL:HA	2.17	0.45
1:A:114:SER:HB3	1:A:246:ILE:HD12	1.99	0.44
1:B:4:THR:OG1	1:B:5:ARG:N	2.46	0.44
1:A:316:ASP:OD1	1:A:362:ARG:NE	2.50	0.44
1:B:66:LEU:HD23	1:B:66:LEU:HA	1.83	0.44
1:B:454:ARG:O	1:B:454:ARG:HD3	2.17	0.44
1:B:316:ASP:OD1	1:B:362:ARG:NE	2.40	0.43
1:A:382:LEU:C	1:A:382:LEU:HD23	2.38	0.43
1:B:327:ALA:HA	4:B:607:HOH:O	2.19	0.43
1:B:93:VAL:HA	4:B:624:HOH:O	2.18	0.42
1:B:199:GLU:HB2	1:B:306:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ARG:NE	1:B:77:ARG:HA	2.32	0.42
1:B:48:LYS:HE3	1:B:48:LYS:HB3	1.90	0.42
1:B:114:SER:OG	1:B:116:PRO:HD2	2.19	0.42
1:A:112[B]:VAL:HG11	1:A:244:TYR:HB3	2.01	0.42
1:A:421:SER:O	1:A:428:SER:HB2	2.19	0.42
1:B:13:GLY:O	1:B:18:GLY:HA3	2.19	0.42
1:B:320:VAL:HG22	1:B:325:LEU:HB2	2.02	0.42
1:A:58:LEU:HD21	1:A:244:TYR:CZ	2.55	0.41
1:A:230:ALA:HA	4:A:931:HOH:O	2.20	0.41
1:B:388:ILE:HD12	1:B:402:LEU:HB3	2.02	0.41
1:A:257:CYS:SG	1:A:263:LEU:HG	2.60	0.41
1:A:176:ILE:HD12	1:A:319:LEU:HB2	2.03	0.41
1:B:57:HIS:HA	2:B:501:FAD:O4	2.21	0.41
1:B:211:ARG:HD3	1:B:291:PRO:HB3	2.02	0.41
1:B:95:LEU:HB2	1:B:100:TRP:CZ3	2.56	0.41
1:A:301:GLY:HA2	1:A:330:PRO:HD3	2.02	0.41
1:A:334:HIS:HE1	1:A:382:LEU:HD13	1.84	0.40
1:B:82:GLY:HA3	1:B:247:GLU:HB2	2.03	0.40
1:B:421:SER:O	1:B:428:SER:HB2	2.21	0.40
1:B:176:ILE:CD1	1:B:319:LEU:HB2	2.52	0.40

There are no symmetry-related clashes.

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	479/512 (94%)	472 (98%)	5 (1%)	2 (0%)	34	24
1	B	465/512 (91%)	454 (98%)	11 (2%)	0	100	100
All	All	944/1024 (92%)	926 (98%)	16 (2%)	2 (0%)	47	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	GLY
1	A	150	SER

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	371/402 (92%)	368 (99%)	3 (1%)	81	82
1	B	361/402 (90%)	353 (98%)	8 (2%)	52	47
All	All	732/804 (91%)	721 (98%)	11 (2%)	65	62

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	GLN
1	A	451	MET
1	A	453	MET
1	B	77	ARG
1	B	186	LYS
1	B	187	GLN
1	B	300	SER
1	B	370	LYS
1	B	394	ARG
1	B	406	ASP
1	B	451	MET

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

Mol	Chain	Res	Type
1	A	101	GLN
1	A	222	HIS
1	A	278	ASN
1	A	409	GLN
1	B	167	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	B	501	-	53,58,58	0.50	0	68,89,89	0.60	1 (1%)
2	FAD	A	501	-	53,58,58	0.58	1 (1%)	68,89,89	0.63	2 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	B	501	-	-	5/30/50/50	0/6/6/6
2	FAD	A	501	-	-	5/30/50/50	0/6/6/6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FAD	P-O2P	-2.30	1.44	1.55

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	FAD	O5'-P-O1P	2.48	118.77	109.07
2	A	501	FAD	C5A-C6A-N6A	2.32	123.87	120.35
2	B	501	FAD	C5A-C6A-N6A	2.26	123.78	120.35

There are no chirality outliers.
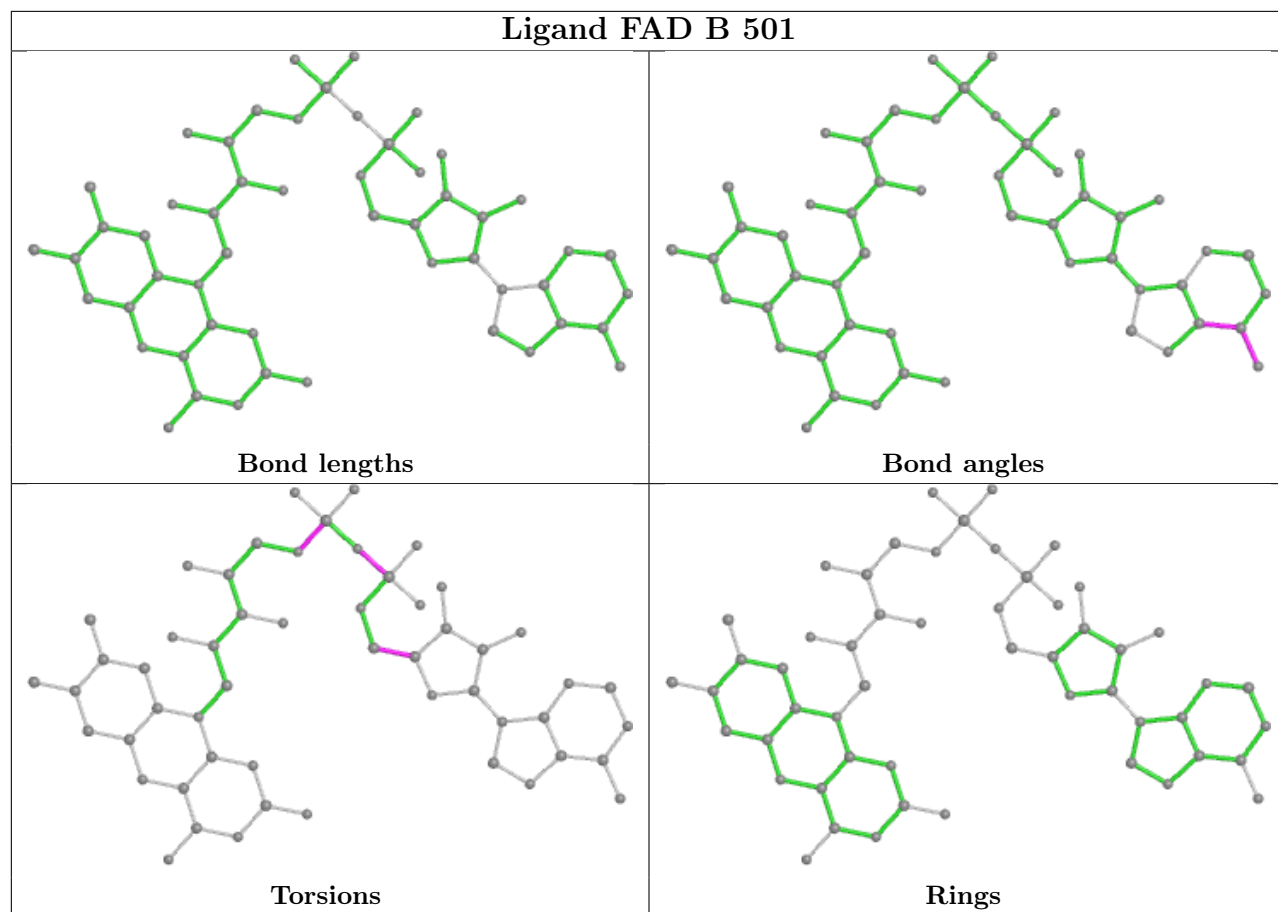
All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FAD	C5'-O5'-P-O2P
2	A	501	FAD	C5'-O5'-P-O3P
2	B	501	FAD	C5'-O5'-P-O2P
2	B	501	FAD	C5'-O5'-P-O3P
2	B	501	FAD	P-O3P-PA-O1A
2	B	501	FAD	O4B-C4B-C5B-O5B
2	A	501	FAD	P-O3P-PA-O2A
2	B	501	FAD	P-O3P-PA-O2A
2	A	501	FAD	O4B-C4B-C5B-O5B
2	A	501	FAD	P-O3P-PA-O1A

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	FAD	5	0
2	A	501	FAD	3	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 B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD A 501

Bond lengths

Bond angles

Torsions

Rings
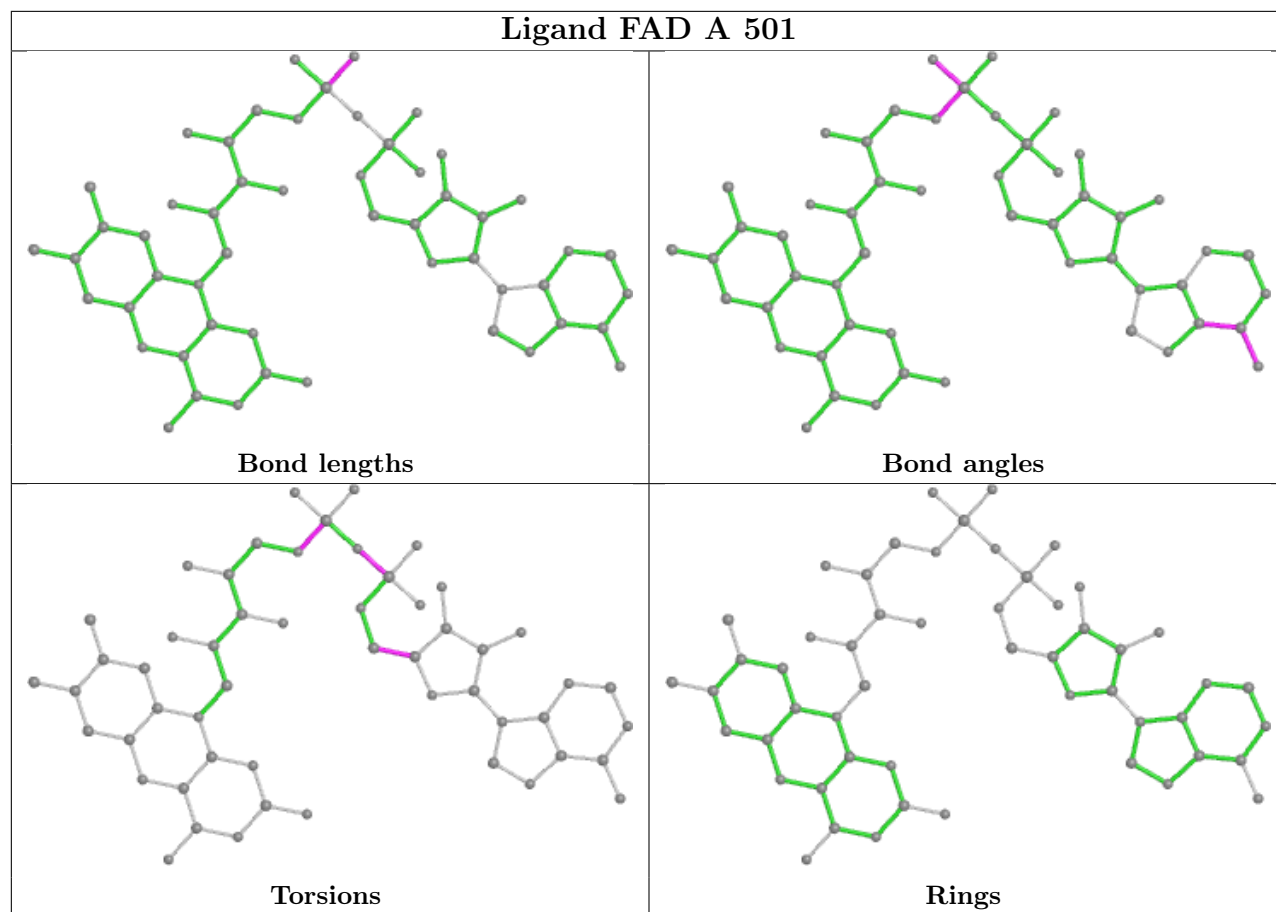
5.7 Other polymers ⓘ

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, 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	477/512 (93%)	0.02	14 (2%)	51	54	12, 22, 44, 88	0
1	B	468/512 (91%)	0.63	51 (10%)	5	6	20, 43, 71, 91	0
All	All	945/1024 (92%)	0.32	65 (6%)	16	19	12, 31, 64, 91	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	473	ALA	6.8
1	A	232	ASP	5.7
1	B	476	GLY	5.0
1	B	474	VAL	4.5
1	A	151	GLY	4.4
1	B	464	ALA	4.2
1	B	262	GLN	4.2
1	B	394	ARG	3.8
1	B	268	ASP	3.8
1	A	233	ARG	3.6
1	B	191	ALA	3.6
1	B	158	VAL	3.5
1	B	392	ASN	3.4
1	B	470	GLU	3.2
1	A	363	ALA	3.2
1	B	435[A]	MET	3.2
1	B	164	SER	3.1
1	A	234	VAL	3.0
1	B	280	PRO	3.0
1	B	469	PRO	2.9
1	B	162	LEU	2.9
1	A	478	ASP	2.9
1	A	480	ALA	2.9
1	B	288	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	163	ASP	2.7
1	A	479	ALA	2.7
1	B	260	GLY	2.7
1	B	391	VAL	2.7
1	B	395	VAL	2.7
1	B	468	LEU	2.7
1	A	150	SER	2.6
1	A	358	THR	2.6
1	B	234	VAL	2.6
1	B	463	THR	2.6
1	B	348[A]	ARG	2.5
1	A	361	ALA	2.5
1	B	271	ILE	2.5
1	B	472	LEU	2.5
1	B	120	LEU	2.4
1	B	166	ARG	2.4
1	B	222	HIS	2.4
1	A	362	ARG	2.4
1	B	287	ARG	2.4
1	B	261	ALA	2.4
1	B	77	ARG	2.4
1	B	169	GLN	2.3
1	B	190	ALA	2.3
1	B	160	ARG	2.3
1	B	236	GLU	2.2
1	B	194	VAL	2.2
1	A	230	ALA	2.2
1	B	273	PHE	2.2
1	B	168	GLU	2.1
1	B	146	SER	2.1
1	B	165	GLY	2.1
1	B	290	GLU	2.1
1	B	150	SER	2.1
1	B	286	LEU	2.1
1	A	149	GLY	2.1
1	B	229	ALA	2.0
1	B	477	LEU	2.0
1	B	265	THR	2.0
1	B	41	PRO	2.0
1	B	129	ALA	2.0
1	B	275	GLU	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 monosaccharides 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
2	FAD	B	501	53/53	0.96	0.10	27,36,40,43	0
3	CL	B	502	1/1	0.97	0.16	57,57,57,57	0
2	FAD	A	501	53/53	0.98	0.10	14,18,21,22	0
3	CL	A	502	1/1	1.00	0.14	27,27,27,27	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.

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Electron density around FAD B 501:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
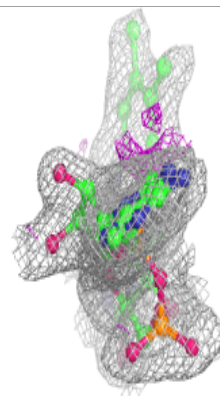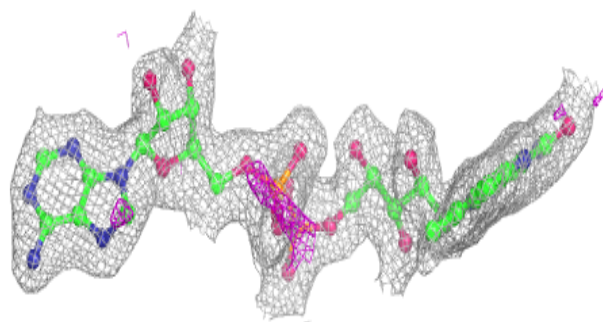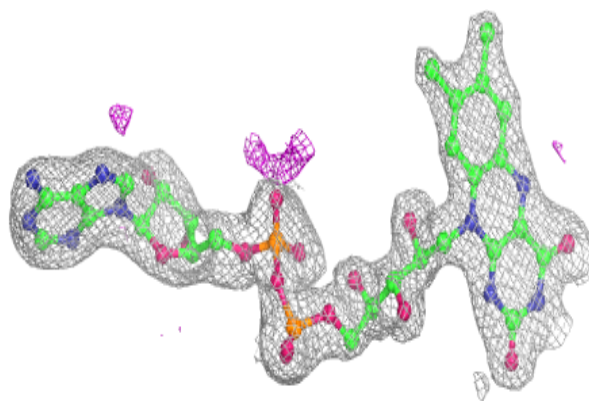
Electron density around FAD A 501:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
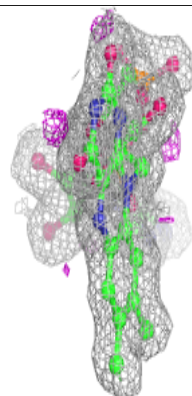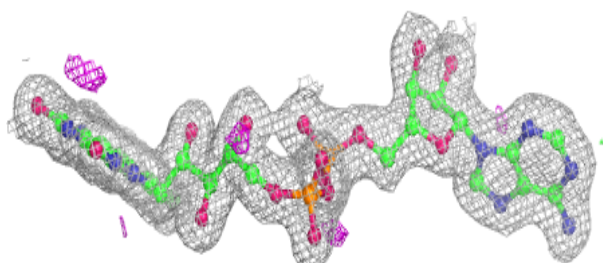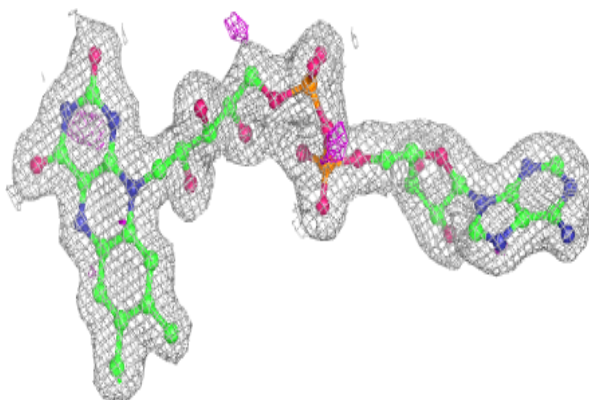
6.5 Other polymers (i)

There are no such residues in this entry.