



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 09:13 AM EST

PDB ID : 4JNA  
Title : Crystal structure of the DepH complex with dimethyl-FK228  
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Deposited on : 2013-03-14  
Resolution : 2.00 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](mailto:validation@mail.wwpdb.org)

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<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>.

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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 : 2.36  
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

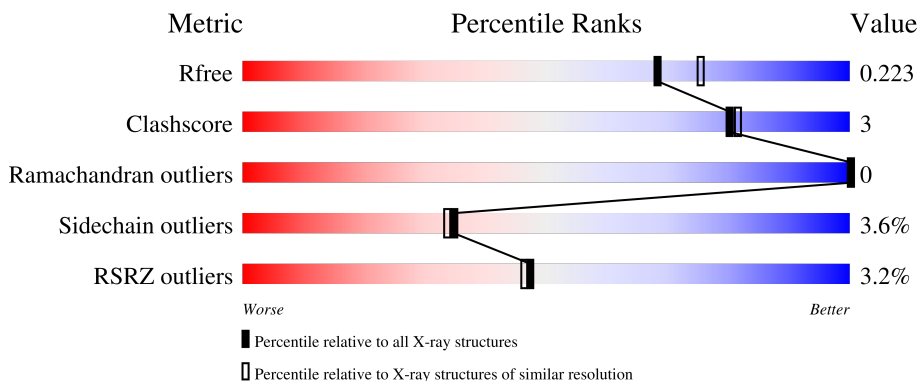
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	340	 2% 81% 6% • 13%
1	B	340	 3% 78% 7% • 14%
2	H	5	 20% 40% 60%
2	I	5	 40% 40% 20%

## 2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 5012 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 DepH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	296	2274	1411	422	428	13	0	4	0
1	B	293	2261	1402	426	422	11	0	4	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP A4ZPY8
A	2	GLY	-	expression tag	UNP A4ZPY8
A	3	SER	-	expression tag	UNP A4ZPY8
A	4	SER	-	expression tag	UNP A4ZPY8
A	5	HIS	-	expression tag	UNP A4ZPY8
A	6	HIS	-	expression tag	UNP A4ZPY8
A	7	HIS	-	expression tag	UNP A4ZPY8
A	8	HIS	-	expression tag	UNP A4ZPY8
A	9	HIS	-	expression tag	UNP A4ZPY8
A	10	HIS	-	expression tag	UNP A4ZPY8
A	11	SER	-	expression tag	UNP A4ZPY8
A	12	SER	-	expression tag	UNP A4ZPY8
A	13	GLY	-	expression tag	UNP A4ZPY8
A	14	LEU	-	expression tag	UNP A4ZPY8
A	15	VAL	-	expression tag	UNP A4ZPY8
A	16	PRO	-	expression tag	UNP A4ZPY8
A	17	ARG	-	expression tag	UNP A4ZPY8
A	18	GLY	-	expression tag	UNP A4ZPY8
A	19	SER	-	expression tag	UNP A4ZPY8
A	20	HIS	-	expression tag	UNP A4ZPY8
A	21	MET	-	expression tag	UNP A4ZPY8
B	1	MET	-	expression tag	UNP A4ZPY8
B	2	GLY	-	expression tag	UNP A4ZPY8
B	3	SER	-	expression tag	UNP A4ZPY8
B	4	SER	-	expression tag	UNP A4ZPY8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	5	HIS	-	expression tag	UNP A4ZPY8
B	6	HIS	-	expression tag	UNP A4ZPY8
B	7	HIS	-	expression tag	UNP A4ZPY8
B	8	HIS	-	expression tag	UNP A4ZPY8
B	9	HIS	-	expression tag	UNP A4ZPY8
B	10	HIS	-	expression tag	UNP A4ZPY8
B	11	SER	-	expression tag	UNP A4ZPY8
B	12	SER	-	expression tag	UNP A4ZPY8
B	13	GLY	-	expression tag	UNP A4ZPY8
B	14	LEU	-	expression tag	UNP A4ZPY8
B	15	VAL	-	expression tag	UNP A4ZPY8
B	16	PRO	-	expression tag	UNP A4ZPY8
B	17	ARG	-	expression tag	UNP A4ZPY8
B	18	GLY	-	expression tag	UNP A4ZPY8
B	19	SER	-	expression tag	UNP A4ZPY8
B	20	HIS	-	expression tag	UNP A4ZPY8
B	21	MET	-	expression tag	UNP A4ZPY8

- Molecule 2 is a protein called Dimethyl FK228.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	5	Total	C	N	O	S	0	0	0
			38	26	4	6	2			
2	I	5	Total	C	N	O	S	0	0	0
			38	26	4	6	2			

- Molecule 3 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
3	A	1	53	27	9	15	2	0	0
3	B	1	53	27	9	15	2	0	0

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

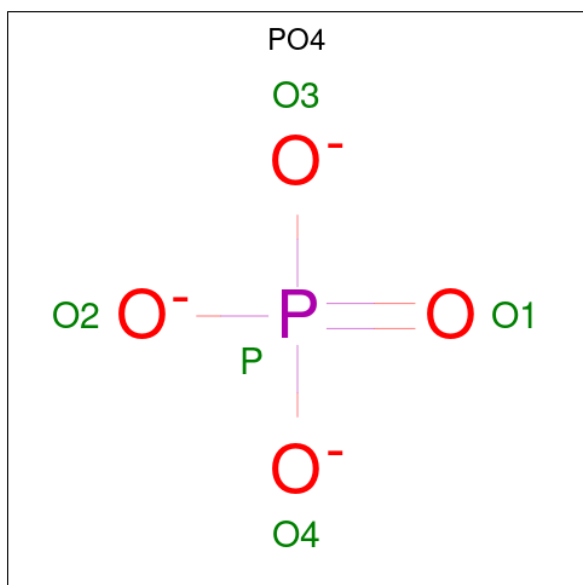
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	A	1	1	1	0	0
4	B	1	1	1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



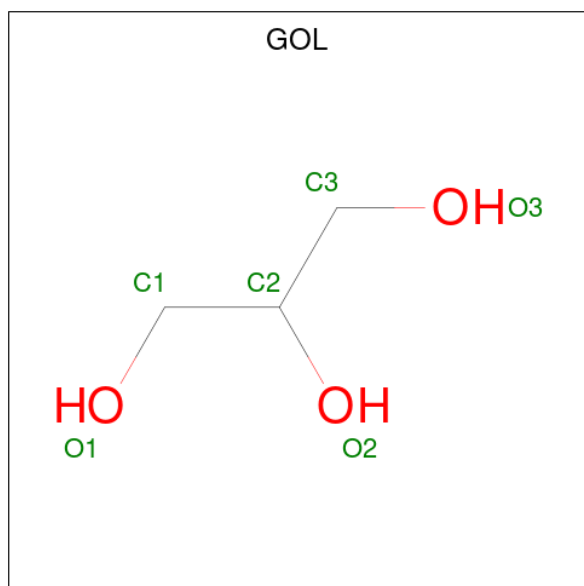
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		

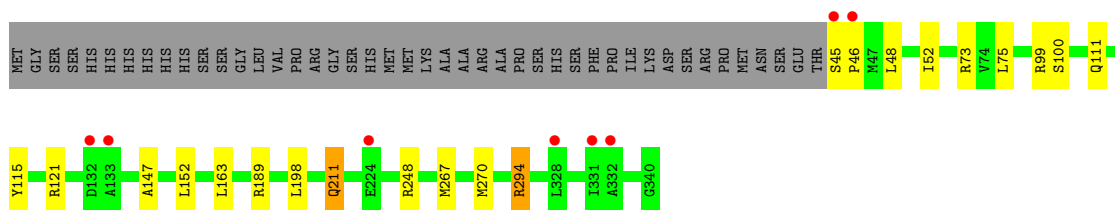
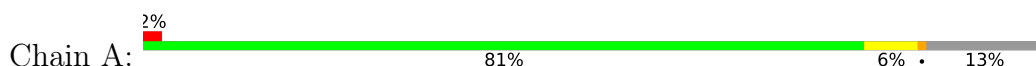
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	150	Total	O	0	0
			150	150		
8	B	110	Total	O	0	0
			110	110		
8	H	4	Total	O	0	0
			4	4		
8	I	2	Total	O	0	0
			2	2		

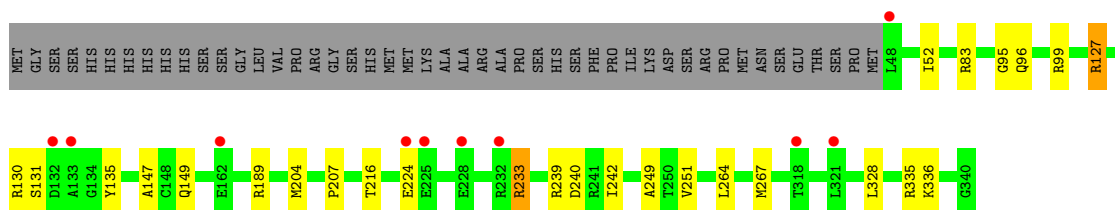
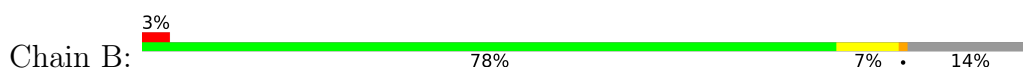
### 3 Residue-property plots [i](#)

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.

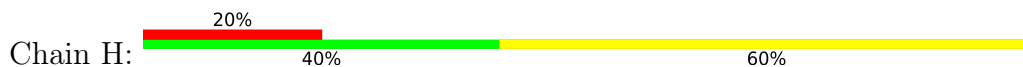
- Molecule 1: DepH



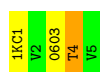
- Molecule 1: DepH



- Molecule 2: Dimethyl FK228



- Molecule 2: Dimethyl FK228





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.28Å 154.28Å 71.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.98 – 2.00 33.98 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.6 (33.98-2.00) 96.5 (33.98-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.26 (at 2.00Å)	Xtrriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, $R_{free}$	0.152 , 0.222 0.154 , 0.223	Depositor DCC
$R_{free}$ test set	2905 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.7	Xtrriage
Anisotropy	0.344	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5012	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, DVA, EDO, FAD, CL, 1KC, DBU, GOL, 060

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	0.36	0/2315	0.50	0/3130
1	B	0.33	0/2302	0.49	0/3111
2	H	0.70	0/6	1.97	0/7
2	I	0.76	0/6	2.46	0/7
All	All	0.35	0/4629	0.51	0/6255

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
2	H	0	2
2	I	0	2
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	1	1KC	Mainchain,Peptide
2	I	1	1KC	Mainchain,Peptide

## 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	2274	0	2223	11	0
1	B	2261	0	2216	16	0
2	H	38	0	30	0	0
2	I	38	0	30	1	0
3	A	53	0	31	0	0
3	B	53	0	31	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	8	0	12	1	0
5	B	8	0	12	0	0
6	A	5	0	0	0	0
7	B	6	0	8	0	0
8	A	150	0	0	2	0
8	B	110	0	0	2	0
8	H	4	0	0	0	0
8	I	2	0	0	0	0
All	All	5012	0	4593	25	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 3.

All (25) 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:335:ARG:HG3	2:I:4:DBU:HG2	1.77	0.64
1:A:48:LEU:O	1:A:73:ARG:NH1	2.37	0.58
1:B:207:PRO:HG2	1:B:233:ARG:HG2	1.85	0.57
1:A:52:ILE:HG13	1:A:147:ALA:HB2	1.87	0.56
1:B:52:ILE:HG13	1:B:147:ALA:HB2	1.88	0.56
1:B:130:ARG:NH1	1:B:135:TYR:OH	2.41	0.54
1:A:75:LEU:HD11	1:A:121:ARG:HG2	1.91	0.52
1:A:211[B]:GLN:HE21	1:A:211[B]:GLN:HA	1.74	0.51
1:A:111:GLN:OE1	1:B:95:GLY:N	2.45	0.49
1:B:96:GLN:OE1	1:B:99[A]:ARG:NH1	2.43	0.47
1:A:189:ARG:HG3	8:A:580:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:ILE:HG23	1:B:251:VAL:HG13	1.98	0.45
1:B:249:ALA:HB1	1:B:264:LEU:HG	1.98	0.45
1:B:240:ASP:HB3	8:B:559:HOH:O	2.18	0.44
1:B:216:THR:OG1	1:B:239:ARG:HA	2.18	0.43
1:B:96:GLN:OE1	1:B:99[A]:ARG:HD3	2.18	0.43
1:A:115:TYR:CE2	5:A:404:EDO:H12	2.54	0.42
1:B:127[B]:ARG:NH2	8:B:577:HOH:O	2.52	0.42
1:B:83:ARG:HG2	3:B:401:FAD:HM81	2.01	0.42
1:B:149:GLN:NE2	1:B:336:LYS:HG2	2.36	0.41
1:B:204:MET:O	1:B:233:ARG:NH1	2.51	0.41
1:A:99:ARG:HD2	8:A:593:HOH:O	2.20	0.41
1:A:45:SER:N	1:A:46:PRO:HD2	2.35	0.41
1:A:111:GLN:HE22	1:B:99[B]:ARG:NH1	2.18	0.41
1:A:294:ARG:HB3	1:A:294:ARG:NH2	2.36	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	298/340 (88%)	291 (98%)	7 (2%)	0	100	100
1	B	295/340 (87%)	285 (97%)	10 (3%)	0	100	100
All	All	593/680 (87%)	576 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	228/263 (87%)	217 (95%)	11 (5%)	25	22
1	B	226/263 (86%)	217 (96%)	9 (4%)	31	29
2	H	1/1 (100%)	1 (100%)	0	100	100
2	I	1/1 (100%)	1 (100%)	0	100	100
All	All	456/528 (86%)	436 (96%)	20 (4%)	35	25

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	SER
1	A	152	LEU
1	A	163	LEU
1	A	198	LEU
1	A	211[A]	GLN
1	A	211[B]	GLN
1	A	248	ARG
1	A	267	MET
1	A	270[A]	MET
1	A	270[B]	MET
1	A	294	ARG
1	B	127[A]	ARG
1	B	127[B]	ARG
1	B	131	SER
1	B	189[A]	ARG
1	B	189[B]	ARG
1	B	224	GLU
1	B	233	ARG
1	B	267	MET
1	B	328	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	143	GLN
1	B	149	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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
2	060	H	3	2	5,6,7	0.81	0	2,6,8	3.68	1 (50%)
2	060	I	3	2	5,6,7	0.80	0	2,6,8	3.46	1 (50%)
2	DBU	H	4	2	4,5,6	3.19	2 (50%)	2,5,7	3.97	2 (100%)
2	DBU	I	4	2	4,5,6	3.43	2 (50%)	2,5,7	3.10	2 (100%)

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	060	H	3	2	-	0/3/5/7	-
2	060	I	3	2	-	1/3/5/7	-
2	DBU	H	4	2	-	1/1/4/6	-
2	DBU	I	4	2	-	0/1/4/6	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	4	DBU	C-CA	4.88	1.53	1.45
2	I	4	DBU	CA-N	4.82	1.47	1.35
2	H	4	DBU	CA-N	4.70	1.47	1.35
2	H	4	DBU	C-CA	4.28	1.52	1.45

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	3	060	CS-S-C1	5.00	110.49	101.30
2	I	3	060	CS-S-C1	4.75	110.03	101.30
2	H	4	DBU	CG-CB-CA	-4.07	121.10	126.38
2	H	4	DBU	O-C-CA	-3.86	120.48	125.39
2	I	4	DBU	O-C-CA	-3.31	121.17	125.39
2	I	4	DBU	CG-CB-CA	-2.86	122.68	126.38

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	4	DBU	O-C-CA-CB
2	I	3	060	CA-C1-S-CS

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	4	DBU	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	$\# Z  > 2$
6	PO4	A	405	-	4,4,4	0.70	0	6,6,6	0.60	0
3	FAD	A	401	-	53,58,58	1.83	13 (24%)	68,89,89	1.45	15 (22%)
5	EDO	B	403	-	3,3,3	0.57	0	2,2,2	0.71	0
7	GOL	B	405	-	5,5,5	0.74	0	5,5,5	1.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	A	403	-	3,3,3	0.54	0	2,2,2	0.94	0
5	EDO	B	404	-	3,3,3	0.58	0	2,2,2	0.75	0
5	EDO	A	404	-	3,3,3	0.56	0	2,2,2	0.90	0
3	FAD	B	401	-	53,58,58	1.86	14 (26%)	68,89,89	1.42	11 (16%)

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	FAD	A	401	-	-	1/30/50/50	0/6/6/6
5	EDO	B	403	-	-	0/1/1/1	-
7	GOL	B	405	-	-	1/4/4/4	-
5	EDO	A	403	-	-	1/1/1/1	-
5	EDO	B	404	-	-	1/1/1/1	-
5	EDO	A	404	-	-	0/1/1/1	-
3	FAD	B	401	-	-	1/30/50/50	0/6/6/6

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	FAD	C10-N1	5.20	1.43	1.33
3	A	401	FAD	C10-N1	4.95	1.43	1.33
3	A	401	FAD	P-O1P	4.02	1.65	1.50
3	B	401	FAD	P-O1P	3.98	1.65	1.50
3	B	401	FAD	C2B-C3B	-3.71	1.43	1.53
3	A	401	FAD	C1'-C2'	3.62	1.57	1.52
3	A	401	FAD	C2B-C3B	-3.55	1.43	1.53
3	B	401	FAD	C1'-C2'	3.51	1.57	1.52
3	A	401	FAD	C6A-N6A	3.50	1.46	1.34
3	B	401	FAD	C6A-N6A	3.48	1.46	1.34
3	B	401	FAD	C2-N1	3.43	1.44	1.36
3	B	401	FAD	C9A-N10	-3.39	1.35	1.41
3	A	401	FAD	C9A-N10	-3.36	1.35	1.41
3	A	401	FAD	C2-N1	3.25	1.44	1.36
3	A	401	FAD	O4-C4	-3.10	1.17	1.23
3	A	401	FAD	C5X-N5	-2.68	1.34	1.39
3	B	401	FAD	C5X-N5	-2.67	1.34	1.39
3	B	401	FAD	O2-C2	2.62	1.29	1.24
3	B	401	FAD	O4-C4	-2.58	1.18	1.23
3	B	401	FAD	C4X-N5	2.56	1.35	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	FAD	C9A-C5X	-2.55	1.36	1.41
3	B	401	FAD	C9A-C5X	-2.37	1.37	1.41
3	A	401	FAD	C7M-C7	2.36	1.55	1.51
3	A	401	FAD	C4X-N5	2.36	1.35	1.30
3	B	401	FAD	C2-N3	2.31	1.44	1.39
3	B	401	FAD	C7M-C7	2.15	1.55	1.51
3	A	401	FAD	C2-N3	2.06	1.43	1.39

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	FAD	N3A-C2A-N1A	-4.87	121.07	128.68
3	A	401	FAD	N3A-C2A-N1A	-4.46	121.71	128.68
3	A	401	FAD	C10-C4X-N5	-3.17	118.13	124.86
3	A	401	FAD	C4X-C10-N10	3.10	121.02	116.48
3	A	401	FAD	C1'-C2'-C3'	3.07	118.38	109.79
3	B	401	FAD	C10-C4X-N5	-2.99	118.52	124.86
3	B	401	FAD	C1'-C2'-C3'	2.96	118.06	109.79
3	B	401	FAD	O2P-P-O5'	-2.96	94.00	107.75
3	A	401	FAD	O2P-P-O5'	-2.78	94.85	107.75
3	B	401	FAD	C4X-C10-N10	2.64	120.33	116.48
3	A	401	FAD	C4-N3-C2	-2.58	120.87	125.64
3	A	401	FAD	O5'-P-O1P	-2.45	99.49	109.07
3	A	401	FAD	C4-C4X-N5	2.43	121.69	118.23
3	A	401	FAD	O5'-C5'-C4'	2.41	115.80	109.36
3	B	401	FAD	O5'-P-O1P	-2.35	99.90	109.07
3	A	401	FAD	C1'-N10-C9A	2.31	124.37	120.51
3	A	401	FAD	O4B-C4B-C5B	2.20	116.61	109.37
3	B	401	FAD	C4-C4X-C10	2.17	120.43	116.79
3	B	401	FAD	O2P-P-O1P	2.15	122.88	112.24
3	B	401	FAD	C4-N3-C2	-2.13	121.71	125.64
3	B	401	FAD	O4B-C4B-C5B	2.12	116.36	109.37
3	A	401	FAD	O2P-P-O1P	2.10	122.61	112.24
3	B	401	FAD	O4-C4-C4X	-2.09	121.04	126.60
3	A	401	FAD	C4A-C5A-N7A	-2.08	107.23	109.40
3	A	401	FAD	C4X-C4-N3	2.02	118.33	113.19
3	A	401	FAD	C4-C4X-C10	2.02	120.18	116.79

There are no chirality outliers.

All (5) torsion outliers are listed below:

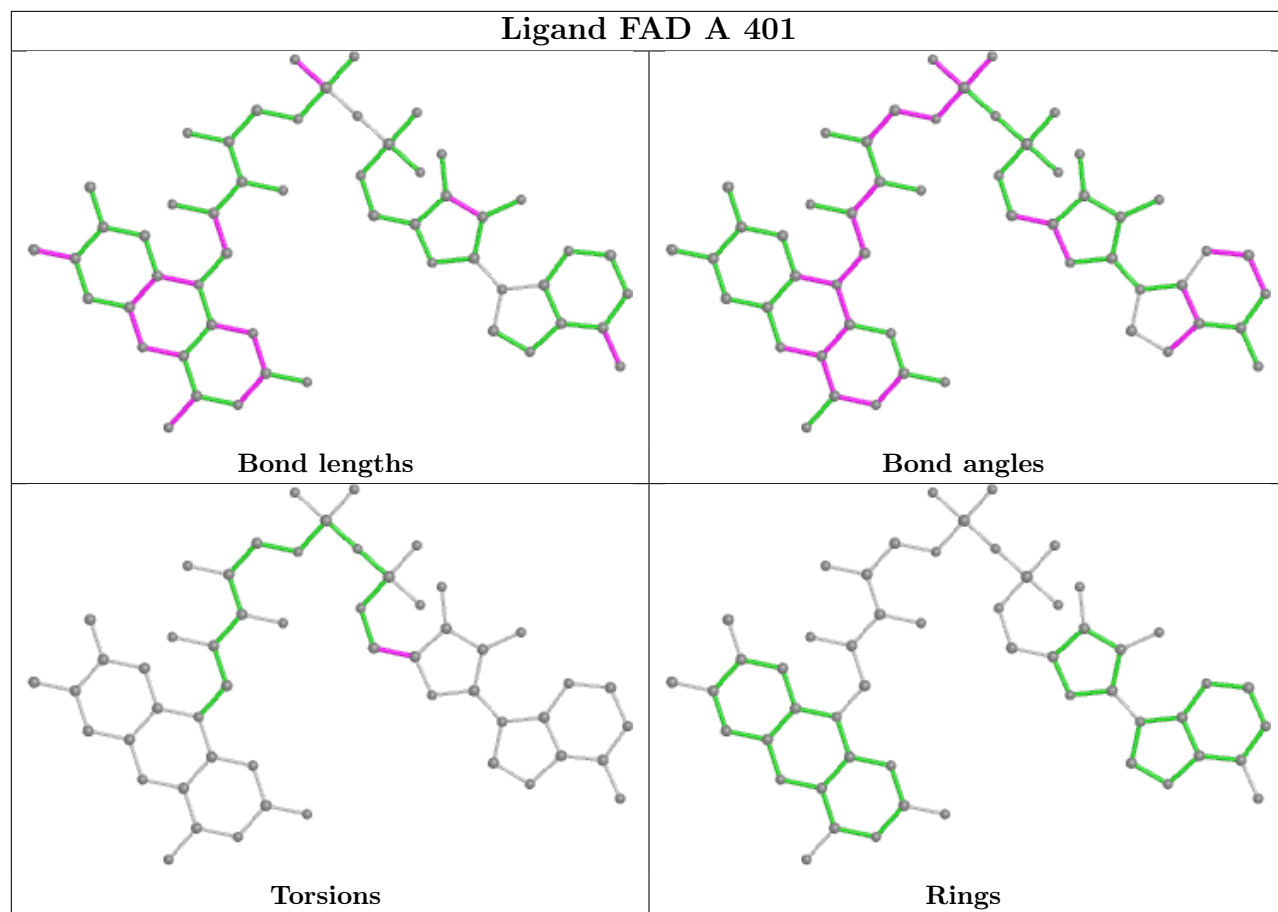
Mol	Chain	Res	Type	Atoms
5	B	404	EDO	O1-C1-C2-O2
5	A	403	EDO	O1-C1-C2-O2
3	A	401	FAD	O4B-C4B-C5B-O5B
7	B	405	GOL	O1-C1-C2-C3
3	B	401	FAD	O4B-C4B-C5B-O5B

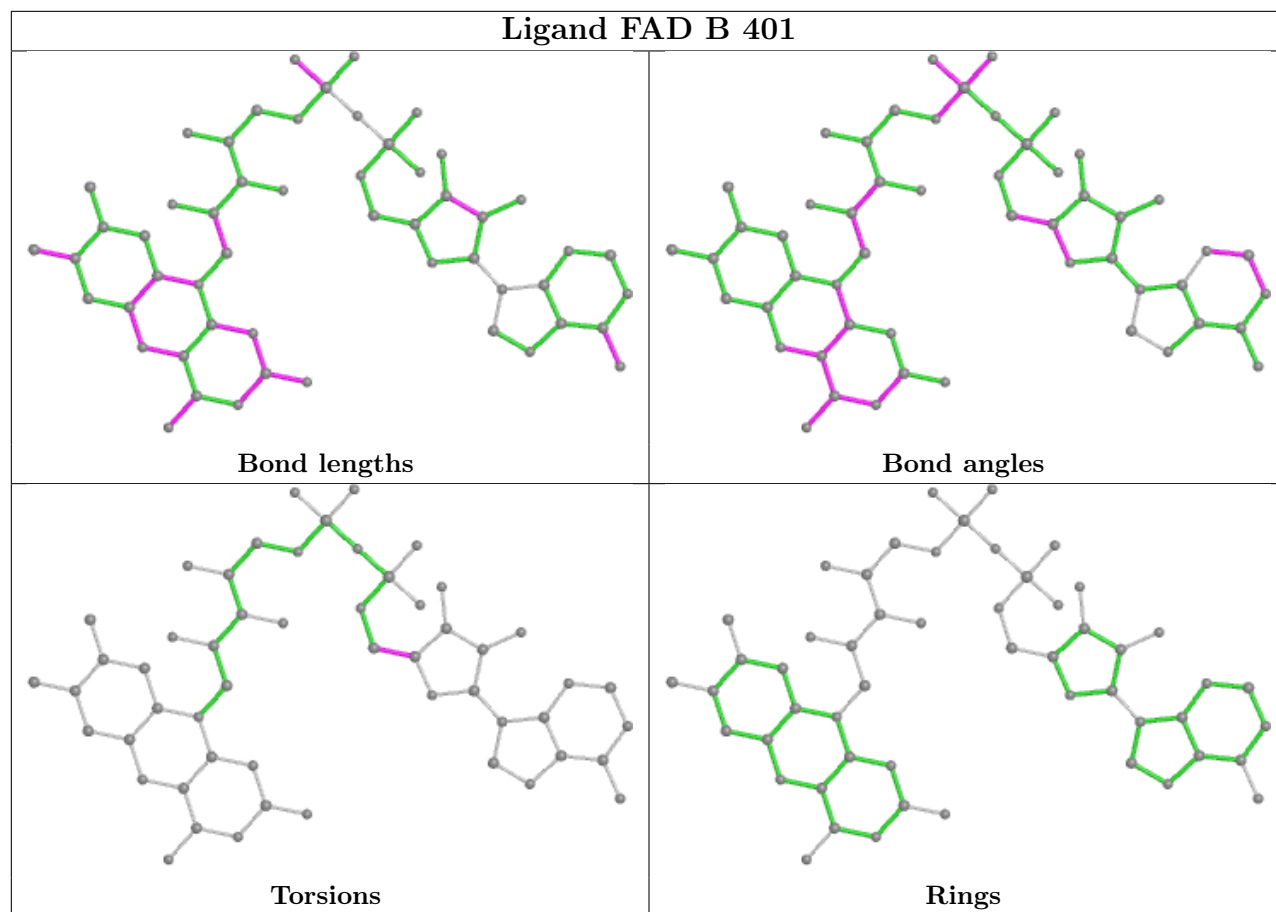
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	404	EDO	1	0
3	B	401	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	296/340 (87%)	-0.14	8 (2%) 54 53	19, 33, 65, 89	0
1	B	293/340 (86%)	-0.03	10 (3%) 45 44	20, 39, 75, 89	0
2	H	1/5 (20%)	2.32	1 (100%) 0 0	32, 32, 32, 32	0
2	I	1/5 (20%)	-0.16	0 100 100	65, 65, 65, 65	0
All	All	591/690 (85%)	-0.08	19 (3%) 47 46	19, 36, 68, 89	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	45	SER	3.9
1	B	162	GLU	3.7
1	B	132	ASP	3.6
1	A	133	ALA	3.5
1	B	232	ARG	3.5
1	A	132	ASP	3.4
1	B	224	GLU	3.3
1	B	228	GLU	3.3
1	B	133	ALA	3.3
1	B	321	LEU	3.0
1	A	331	ILE	2.8
1	B	48	LEU	2.6
1	A	46	PRO	2.6
1	A	224	GLU	2.6
1	B	225	GLU	2.4
2	H	5	VAL	2.3
1	A	328	LEU	2.2
1	A	332	ALA	2.1
1	B	318	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	DBU	I	4	6/7	0.94	0.14	60,64,65,66	0
2	DVA	I	2	7/8	0.94	0.19	75,80,82,83	0
2	060	I	3	7/8	0.94	0.16	68,74,82,83	0
2	DVA	H	2	7/8	0.97	0.20	32,36,42,50	0
2	060	H	3	7/8	0.98	0.18	29,32,46,48	0
2	DBU	H	4	6/7	0.99	0.21	28,31,33,36	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

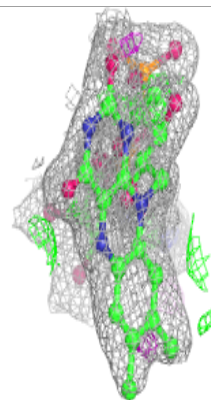
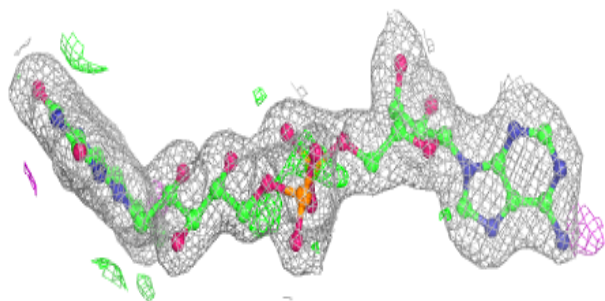
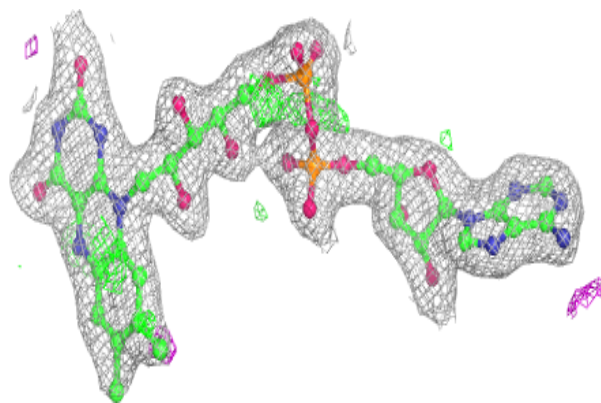
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	GOL	B	405	6/6	0.84	0.22	73,76,76,77	0
5	EDO	B	404	4/4	0.91	0.18	61,61,63,66	0
5	EDO	A	403	4/4	0.92	0.17	66,69,69,72	0
6	PO4	A	405	5/5	0.95	0.17	51,51,58,63	0
5	EDO	A	404	4/4	0.95	0.28	59,59,61,62	0
5	EDO	B	403	4/4	0.98	0.16	54,55,56,59	0
3	FAD	B	401	53/53	0.98	0.13	21,28,36,42	0
3	FAD	A	401	53/53	0.99	0.10	18,25,32,36	0
4	CL	A	402	1/1	0.99	0.12	46,46,46,46	0
4	CL	B	402	1/1	0.99	0.08	44,44,44,44	0

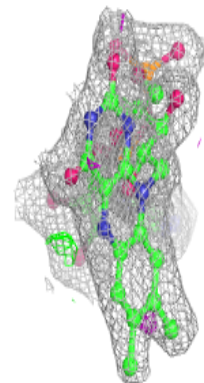
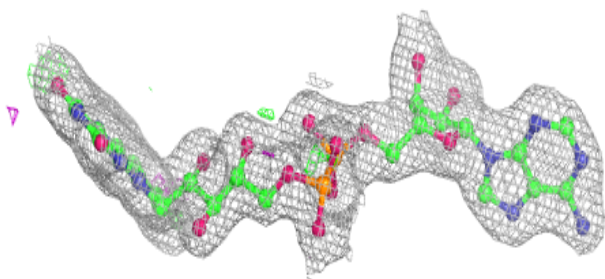
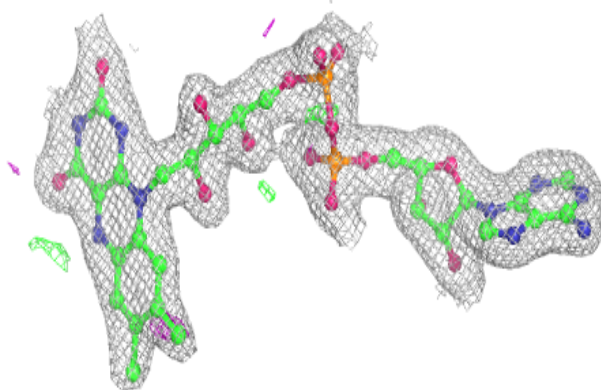
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around FAD B 401:**

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

**Electron density around FAD A 401:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.