



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 04:48 pm BST

PDB ID : 6EV3  
Title : Structure of wild type *A. niger* Fdc1 that has been illuminated with UV light, with prFMN in the iminium and ketimine form  
Authors : Bailey, S.S.; David, L.; Payne, K.A.P.  
Deposited on : 2017-11-01  
Resolution : 1.30 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)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 2.11  
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

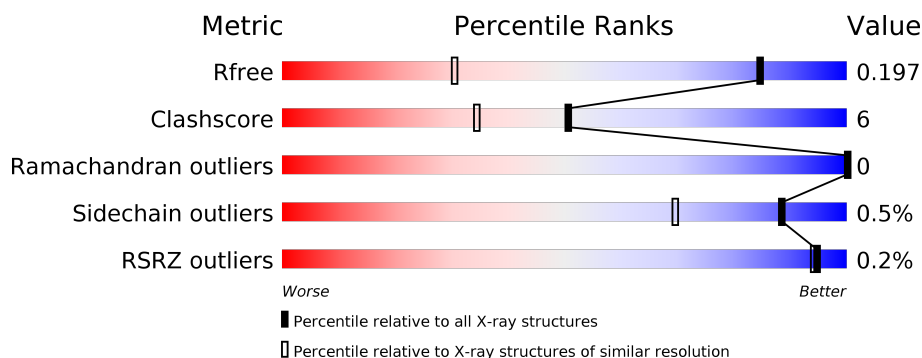
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.30 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	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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  $\geq 3$ , 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	508	 87% 10% ..

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4932 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.

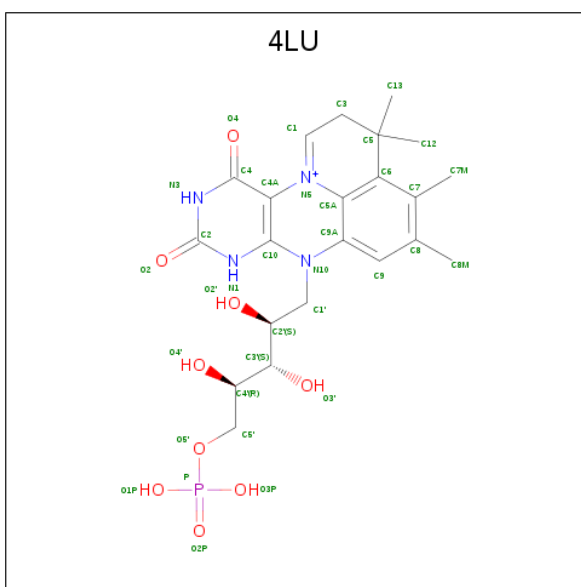
- Molecule 1 is a protein called Ferulic acid decarboxylase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	500	4122	2609	709	774	30	0	35	1

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	499B	LEU	-	expression tag	UNP A2QHE5
A	499C	GLU	-	expression tag	UNP A2QHE5
A	502	HIS	-	expression tag	UNP A2QHE5
A	503	HIS	-	expression tag	UNP A2QHE5
A	504	HIS	-	expression tag	UNP A2QHE5
A	505	HIS	-	expression tag	UNP A2QHE5
A	506	HIS	-	expression tag	UNP A2QHE5
A	507	HIS	-	expression tag	UNP A2QHE5

- Molecule 2 is 1-deoxy-5-O-phosphono-1-(3,3,4,5-tetramethyl-9,11-dioxo-2,3,8,9,10,11-hexahydro-7H-quinolino[1,8-fg]pteridin-12-ium-7-yl)-D-ribitol (three-letter code: 4LU) (formula:  $C_{22}H_{30}N_4O_9P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			36	22	4	9	1		

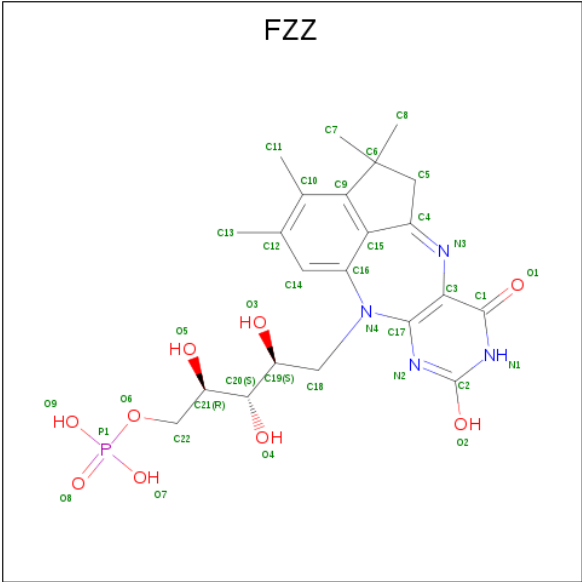
- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mn 1 1	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total K 2 2	0	0

- Molecule 5 is 1-deoxy-5-O-phosphono-1-[(10aR)-2,2,3,4-tetramethyl-8,10-dioxo-1,2,8,9,10,10a-hexahydro-6H-indeno[1,7-e]pyrimido[4,5-b][1,4]diazepin-6-yl]-D-ribitol (three-letter code: FZZ) (formula: C<sub>22</sub>H<sub>29</sub>N<sub>4</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	1
			36	22	4	9	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	735	Total	O	0	0
			735	735		

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- Molecule 1: Ferulic acid decarboxylase 1

[illegible]

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.13Å 63.91Å 87.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.85 – 1.30 64.85 – 1.30	Depositor EDS
% Data completeness (in resolution range)	95.8 (64.85-1.30) 95.8 (64.85-1.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.173 , 0.197 0.173 , 0.197	Depositor DCC
$R_{free}$ test set	6290 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.2	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4932	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% 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: FZZ, K, MN, 4LU

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	1.13	11/4224 (0.3%)	1.18	32/5739 (0.6%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	377[A]	GLU	CD-OE1	7.49	1.33	1.25
1	A	377[B]	GLU	CD-OE1	7.49	1.33	1.25
1	A	473	GLU	CD-OE1	5.91	1.32	1.25
1	A	377[A]	GLU	CD-OE2	5.88	1.32	1.25
1	A	377[B]	GLU	CD-OE2	5.88	1.32	1.25
1	A	15[A]	GLU	CG-CD	5.32	1.59	1.51
1	A	15[B]	GLU	CG-CD	5.32	1.59	1.51
1	A	452	ARG	CZ-NH1	5.30	1.40	1.33
1	A	336	ARG	CZ-NH1	-5.08	1.26	1.33
1	A	254	ASP	CB-CG	5.06	1.62	1.51
1	A	355	SER	CB-OG	5.02	1.48	1.42

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	452	ARG	NE-CZ-NH2	-11.43	114.58	120.30
1	A	435	ARG	NE-CZ-NH2	-8.33	116.14	120.30
1	A	380	ARG	CG-CD-NE	8.26	129.14	111.80
1	A	398	ARG	NE-CZ-NH2	7.68	124.14	120.30
1	A	42[A]	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	A	42[B]	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	A	452	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	306	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	A	398	ARG	NE-CZ-NH1	-7.21	116.70	120.30
1	A	229	ASP	CB-CG-OD1	7.17	124.75	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	ARG	NE-CZ-NH1	-7.13	116.74	120.30
1	A	173	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	A	380	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	A	65	ARG	NE-CZ-NH2	6.82	123.71	120.30
1	A	484[A]	ASP	CB-CG-OD1	6.58	124.22	118.30
1	A	484[B]	ASP	CB-CG-OD1	6.58	124.22	118.30
1	A	306	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	A	377[A]	GLU	CG-CD-OE2	-6.40	105.50	118.30
1	A	377[B]	GLU	CG-CD-OE2	-6.40	105.50	118.30
1	A	423	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	254	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	A	291	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	A	380	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	A	128	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	A	491	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	A	413	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	20	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	173	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	286	TYR	CB-CG-CD1	5.11	124.07	121.00
1	A	65	ARG	NE-CZ-NH1	-5.07	117.76	120.30
1	A	31	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	A	254	ASP	CB-CG-OD1	5.02	122.82	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	4122	0	4001	42	0
2	A	36	0	28	4	0
3	A	1	0	0	0	0
4	A	2	0	0	0	0
5	A	36	0	26	5	0
6	A	735	0	0	31	3
All	All	4932	0	4055	47	3

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 (47) 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)
2:A:601[A]:4LU:H13	2:A:601[A]:4LU:H14	1.40	1.03
1:A:381:LYS:CD	6:A:703:HOH:O	2.16	0.93
2:A:601[A]:4LU:C12	2:A:601[A]:4LU:H14	2.05	0.86
1:A:381:LYS:HG3	6:A:722:HOH:O	1.81	0.79
1:A:381:LYS:HD3	6:A:703:HOH:O	1.79	0.79
1:A:480[B]:SER:HB2	1:A:481:TYR:CE2	2.24	0.72
1:A:59[A]:MET:SD	6:A:1009:HOH:O	2.47	0.72
1:A:124:GLU:OE1	6:A:701:HOH:O	2.09	0.71
1:A:59[A]:MET:CE	6:A:1009:HOH:O	2.44	0.66
1:A:255:LEU:HD21	6:A:710:HOH:O	1.98	0.61
2:A:601[A]:4LU:C4	6:A:705:HOH:O	2.49	0.59
1:A:381:LYS:HD2	6:A:703:HOH:O	1.94	0.58
1:A:196[B]:HIS:HE1	1:A:270:SER:O	1.87	0.57
1:A:377[B]:GLU:HG3	6:A:722:HOH:O	2.07	0.54
1:A:160:GLN:N	6:A:710:HOH:O	2.42	0.52
1:A:149[A]:LYS:HD3	6:A:1037:HOH:O	2.10	0.51
1:A:381:LYS:HE3	6:A:722:HOH:O	2.11	0.51
1:A:76[B]:SER:HB3	6:A:971:HOH:O	2.11	0.50
5:A:605[B]:FZZ:H20	5:A:605[B]:FZZ:N2	2.28	0.48
1:A:470:ARG:NE	6:A:712:HOH:O	2.45	0.48
1:A:153:THR:O	5:A:605[B]:FZZ:H12	2.14	0.48
1:A:381:LYS:CG	6:A:722:HOH:O	2.52	0.48
1:A:223:SER:O	5:A:605[B]:FZZ:O4	2.30	0.48
1:A:363:ARG:NH1	6:A:713:HOH:O	2.45	0.48
1:A:445:HIS:HE1	6:A:747:HOH:O	1.97	0.47
1:A:255:LEU:HG	6:A:1195:HOH:O	2.15	0.46
1:A:381:LYS:CD	6:A:722:HOH:O	2.64	0.46
1:A:170:SER:HB2	5:A:605[B]:FZZ:C22	2.46	0.46
1:A:307:ASN:N	6:A:701:HOH:O	2.49	0.45
1:A:430:LEU:HD12	6:A:1379:HOH:O	2.17	0.45
1:A:196[B]:HIS:CE1	1:A:270:SER:O	2.68	0.44
1:A:484[A]:ASP:CG	6:A:887:HOH:O	2.56	0.44
1:A:55:ASN:C	6:A:744:HOH:O	2.56	0.43
1:A:267:GLY:HA3	1:A:299:LYS:O	2.18	0.43
1:A:376:SER:O	1:A:380:ARG:HG3	2.19	0.43
1:A:170:SER:HB2	5:A:605[B]:FZZ:H27	2.00	0.43
1:A:377[B]:GLU:CG	6:A:722:HOH:O	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:HIS:HB3	6:A:717:HOH:O	2.19	0.42
1:A:228:PRO:HA	6:A:1230:HOH:O	2.19	0.42
1:A:53:PHE:HB3	6:A:744:HOH:O	2.18	0.42
1:A:27:ASN:N	6:A:723:HOH:O	2.49	0.41
1:A:56[B]:LEU:HD11	1:A:66:ILE:HD12	2.02	0.41
2:A:601[A]:4LU:C12	2:A:601[A]:4LU:C7M	2.87	0.41
1:A:280:PHE:O	1:A:282[A]:GLU:HG3	2.20	0.41
1:A:66:ILE:HA	1:A:311:MET:O	2.21	0.41
1:A:149[A]:LYS:CE	6:A:1063:HOH:O	2.68	0.41
1:A:381:LYS:HE2	6:A:1264:HOH:O	2.21	0.41

All (3) 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)
6:A:1334:HOH:O	6:A:1337:HOH:O[3_555]	0.79	1.41
6:A:1016:HOH:O	6:A:1016:HOH:O[2_655]	0.90	1.30
6:A:771:HOH:O	6:A:1169:HOH:O[2_555]	2.00	0.20

## 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	531/508 (104%)	515 (97%)	16 (3%)	0	<b>100</b> <b>100</b>

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	445/430 (104%)	443 (100%)	2 (0%)	91	76

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	217	PRO
1	A	452	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 5 ligands modelled in this entry, 3 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	4LU	A	601[A]	3,4	32,39,39	1.52	6 (18%)	41,62,62	2.62	13 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	FZZ	A	605[B]	3,4	31,39,39	3.44	9 (29%)	32,62,62	3.69	15 (46%)

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	4LU	A	601[A]	3,4	-	2/18/30/30	0/3/4/4
5	FZZ	A	605[B]	3,4	-	7/16/29/29	0/3/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	605[B]	FZZ	C3-C17	13.70	1.52	1.38
5	A	605[B]	FZZ	C5-C4	-8.72	1.44	1.50
5	A	605[B]	FZZ	C15-C16	-4.36	1.38	1.43
5	A	605[B]	FZZ	C1-C3	4.07	1.48	1.41
2	A	601[A]	4LU	C2-N3	-3.90	1.30	1.38
2	A	601[A]	4LU	C9A-N10	3.84	1.43	1.38
5	A	605[B]	FZZ	C17-N2	3.74	1.41	1.35
5	A	605[B]	FZZ	O6-C22	-3.63	1.30	1.44
5	A	605[B]	FZZ	C1-N1	2.54	1.37	1.33
5	A	605[B]	FZZ	C19-C20	-2.53	1.48	1.53
2	A	601[A]	4LU	C6-C7	2.48	1.49	1.40
2	A	601[A]	4LU	C2'-C3'	-2.41	1.48	1.53
2	A	601[A]	4LU	C2-N1	-2.30	1.33	1.38
2	A	601[A]	4LU	O4-C4	-2.16	1.19	1.24
5	A	605[B]	FZZ	C14-C16	-2.01	1.36	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	605[B]	FZZ	C22-C21-C20	-13.02	87.05	112.20
5	A	605[B]	FZZ	C1-C3-C17	-11.14	112.58	119.95
2	A	601[A]	4LU	C4-N3-C2	9.63	123.27	115.14
2	A	601[A]	4LU	C4-C4A-C10	-8.45	114.36	119.95
5	A	605[B]	FZZ	P1-O6-C22	-4.78	105.14	118.30
5	A	605[B]	FZZ	C1-N1-C2	4.13	124.61	115.56
5	A	605[B]	FZZ	C3-C1-N1	-4.01	117.95	123.43
2	A	601[A]	4LU	C8M-C8-C7	-3.56	115.63	121.17

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*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	605[B]	FZZ	C21-C20-C19	3.55	120.75	113.36
2	A	601[A]	4LU	C4A-N5-C5A	-3.52	118.44	120.99
5	A	605[B]	FZZ	O7-P1-O6	-3.37	97.76	106.73
2	A	601[A]	4LU	C9A-N10-C10	-3.36	117.50	121.91
2	A	601[A]	4LU	C1'-N10-C9A	3.12	120.75	118.29
5	A	605[B]	FZZ	O9-P1-O6	-3.01	98.72	106.73
2	A	601[A]	4LU	C4A-C4-N3	-2.74	119.69	123.43
5	A	605[B]	FZZ	O9-P1-O7	2.72	118.04	107.64
2	A	601[A]	4LU	C4A-C10-N10	2.72	123.10	120.30
5	A	605[B]	FZZ	O3-C19-C20	-2.69	102.55	109.10
5	A	605[B]	FZZ	O5-C21-C20	2.64	115.52	109.10
2	A	601[A]	4LU	O3P-P-O5'	2.49	113.36	106.73
2	A	601[A]	4LU	C3-C5-C6	-2.40	101.91	107.38
2	A	601[A]	4LU	C7-C6-C5A	-2.31	116.76	119.06
5	A	605[B]	FZZ	O4-C20-C21	-2.28	103.30	108.81
5	A	605[B]	FZZ	O6-C22-C21	2.27	115.42	109.36
5	A	605[B]	FZZ	C12-C10-C9	-2.24	117.45	119.43
2	A	601[A]	4LU	O3'-C3'-C2'	-2.12	103.69	108.81
2	A	601[A]	4LU	O5'-P-O2P	-2.08	100.64	106.47
5	A	605[B]	FZZ	O6-P1-O8	2.04	112.21	106.47

There are no chirality outliers.

All (9) torsion outliers are listed below:

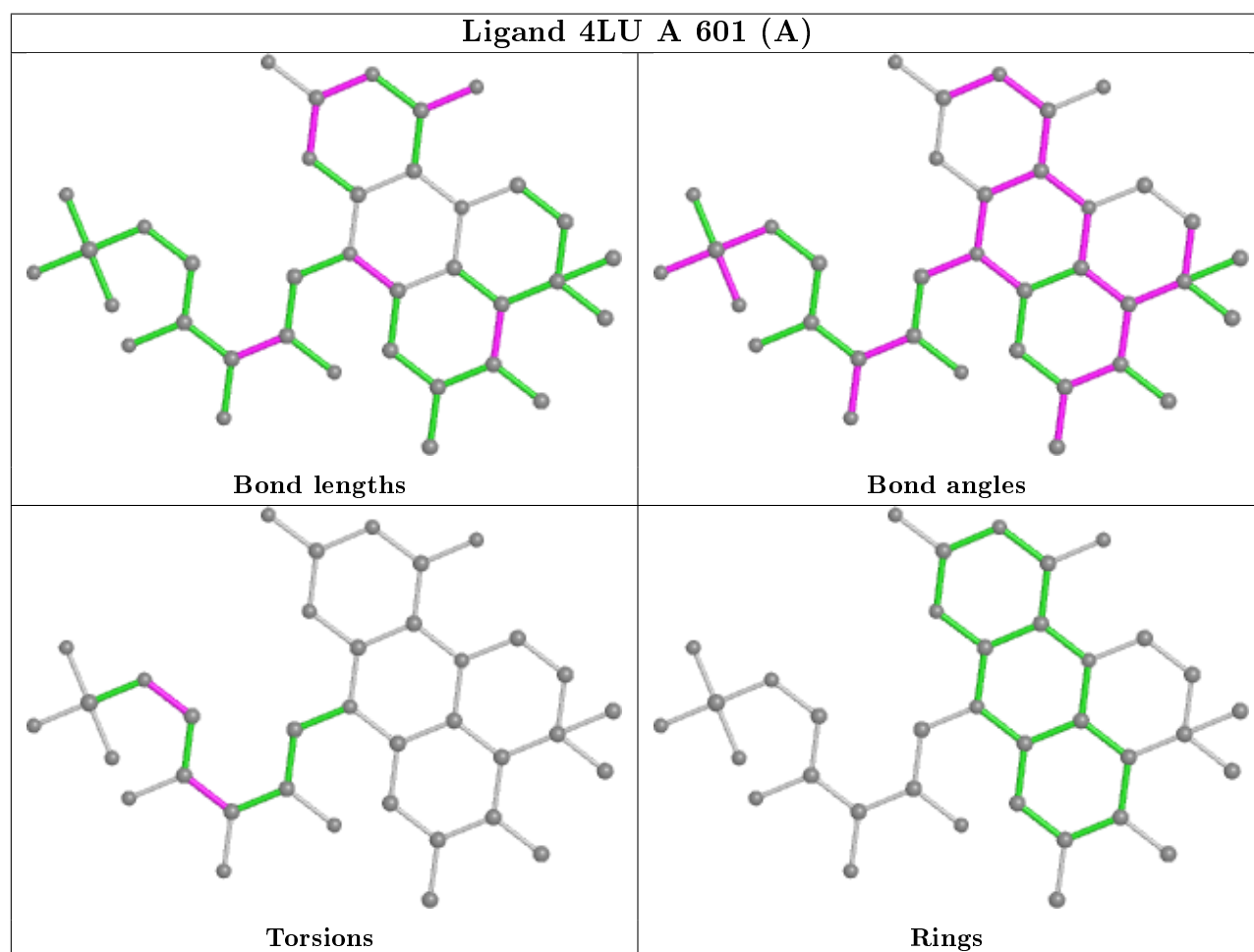
Mol	Chain	Res	Type	Atoms
5	A	605[B]	FZZ	C18-C19-C20-C21
5	A	605[B]	FZZ	C22-O6-P1-O7
5	A	605[B]	FZZ	C22-O6-P1-O8
5	A	605[B]	FZZ	C22-O6-P1-O9
5	A	605[B]	FZZ	O3-C19-C20-C21
5	A	605[B]	FZZ	C21-C22-O6-P1
2	A	601[A]	4LU	C2'-C3'-C4'-C5'
5	A	605[B]	FZZ	O3-C19-C20-O4
2	A	601[A]	4LU	C4'-C5'-O5'-P

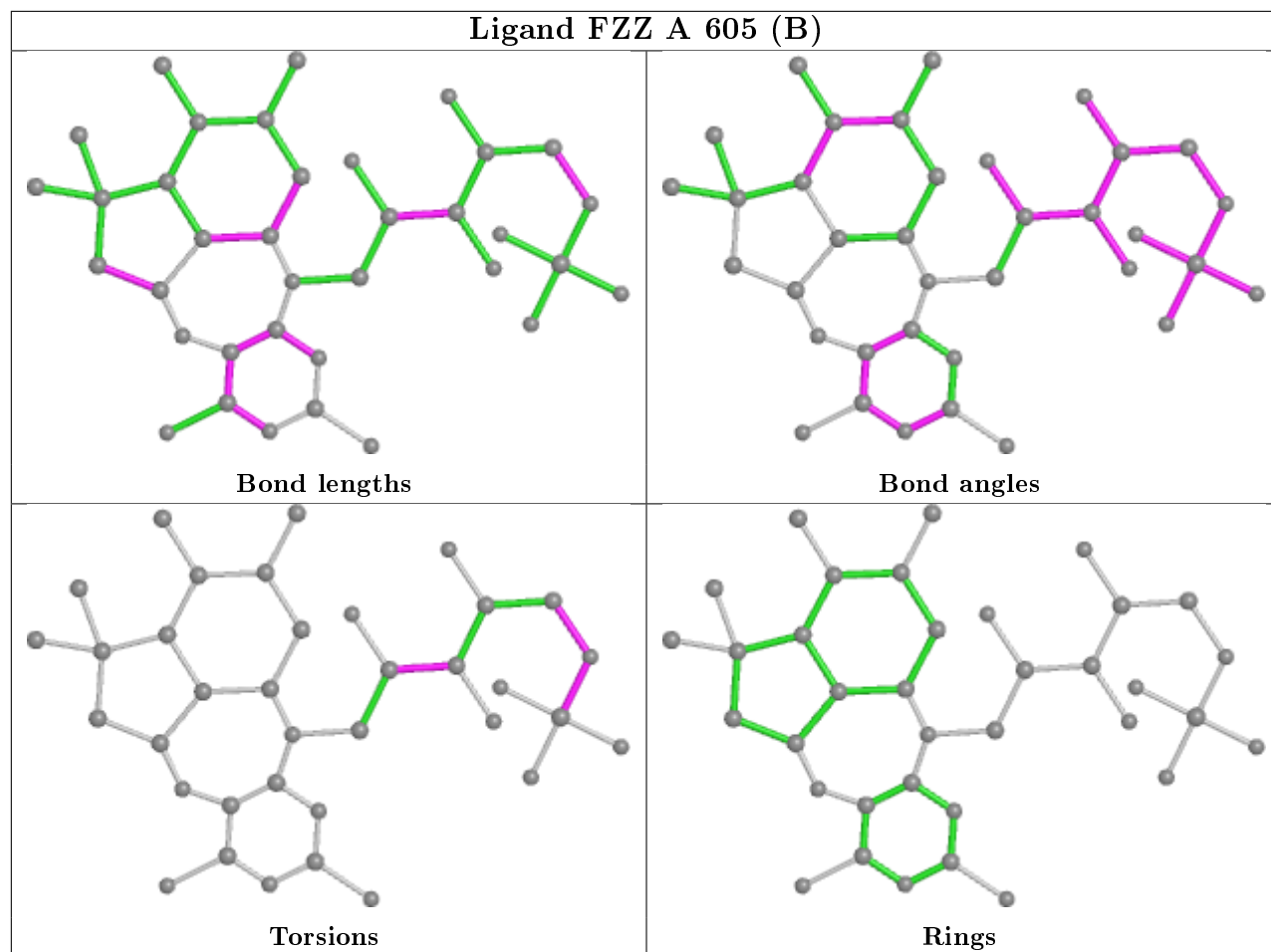
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601[A]	4LU	4	0
5	A	605[B]	FZZ	5	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 [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, 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	500/508 (98%)	-0.63	1 (0%) 95 94	9, 12, 22, 59	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	503	HIS	3.4

### 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 carbohydrates 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.

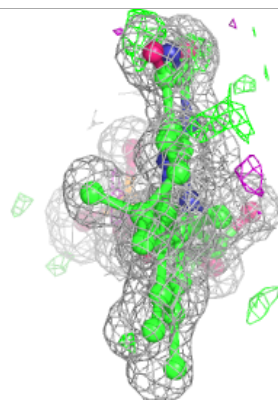
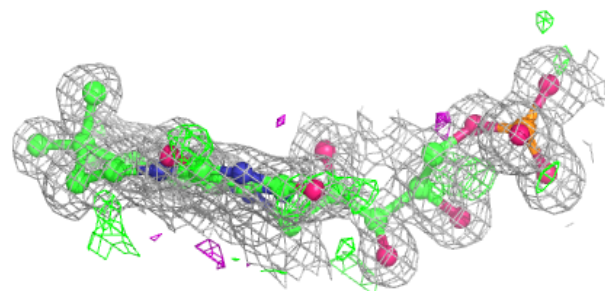
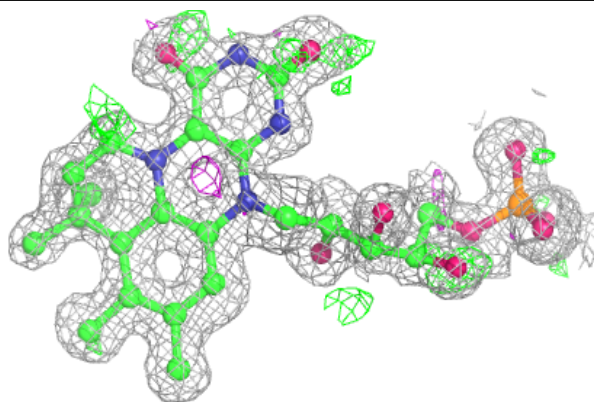
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	4LU	A	601[A]	36/36	0.97	0.08	6,8,10,12	36
5	FZZ	A	605[B]	36/36	0.97	0.09	7,12,14,15	36
4	K	A	604	1/1	1.00	0.03	9,9,9,9	0
3	MN	A	602	1/1	1.00	0.03	10,10,10,10	0
4	K	A	603	1/1	1.00	0.04	10,10,10,10	0

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.

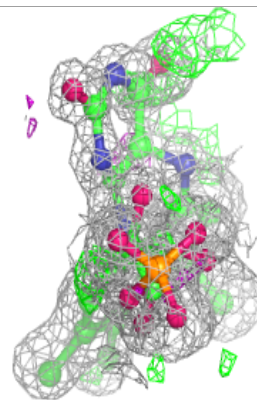
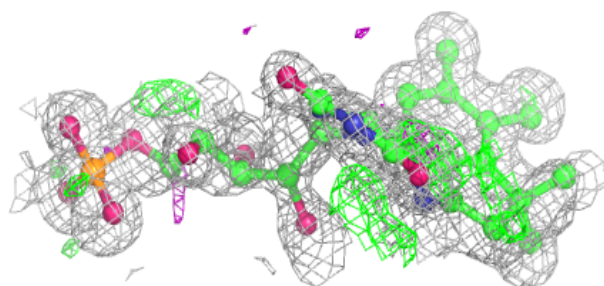
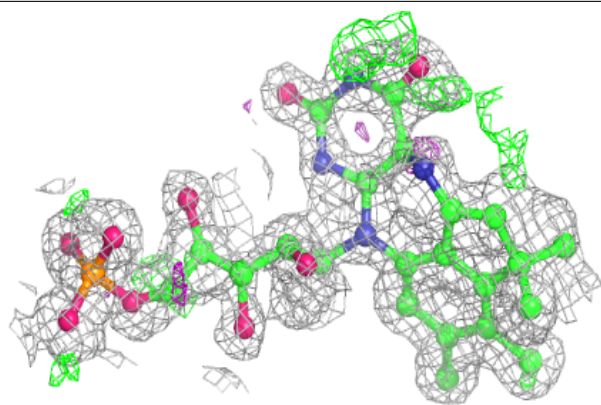
**Electron density around 4LU A 601 (A):**

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



**Electron density around FZZ A 605 (B):**

$2mF_o-DF_c$  (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.