



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:51 AM UTC

PDB ID : 6EVC / pdb\_00006evc  
Title : Structure of E282Q A. niger Fdc1 in complex with pentafluoro-cinnamic acid  
Authors : Bailey, S.S.; David, L.; Payne, K.A.P.  
Deposited on : 2017-11-01  
Resolution : 1.18 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.

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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

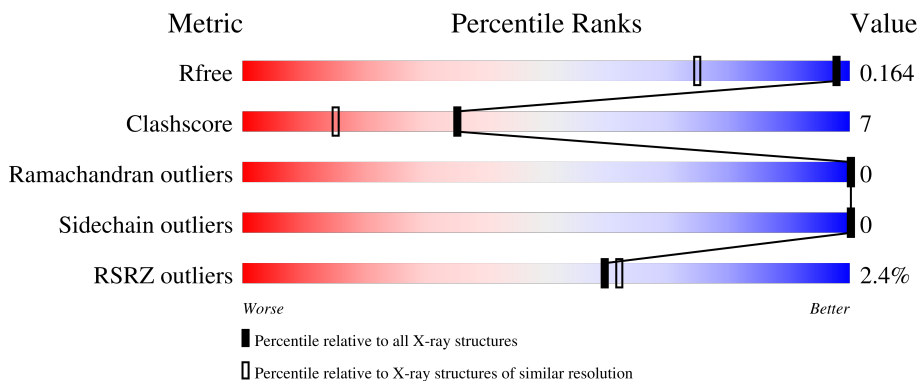
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


The reported resolution of this entry is 1.18 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))
$R_{free}$	180053	1789 (1.20-1.16)
Clashscore	190562	1845 (1.20-1.16)
Ramachandran outliers	187476	1789 (1.20-1.16)
Sidechain outliers	187428	1789 (1.20-1.16)
RSRZ outliers	180081	1787 (1.20-1.16)

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	508	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	F5C	A	605	-	X	-	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4884 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.

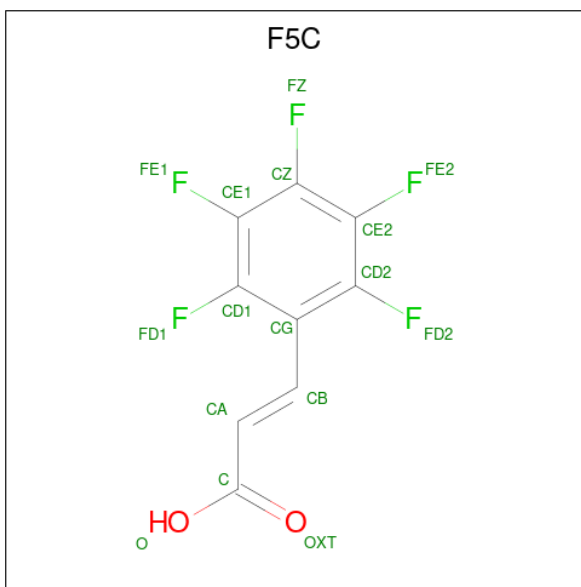
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	500	4100	2595	706	769	30	0	33	1

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	282	GLN	GLU	conflict	UNP A2QHE5
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 (CCD ID: 4LU) (formula: C<sub>22</sub>H<sub>30</sub>N<sub>4</sub>O<sub>9</sub>P).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	F	O		
5	A	1	16	9	5	2	0	0

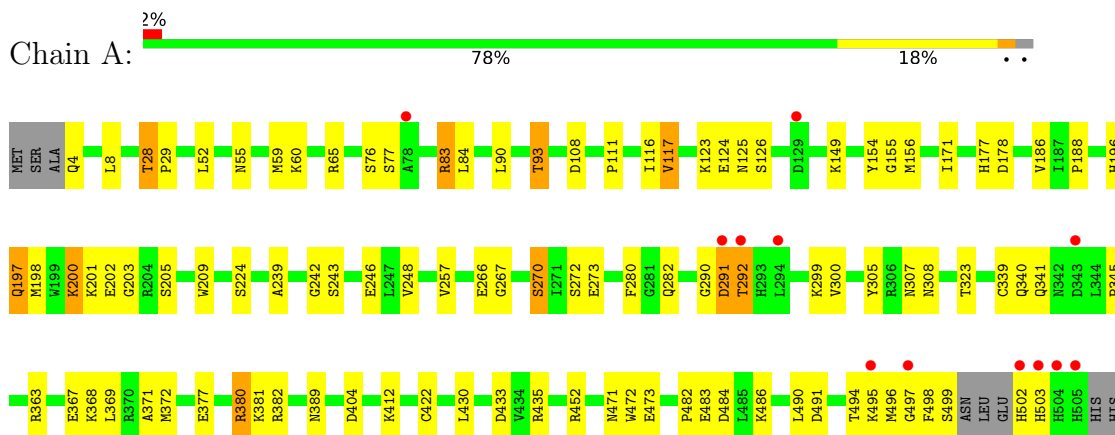
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	729	729	729	0	0

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

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Ferulic acid decarboxylase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.24Å 64.33Å 88.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.05 – 1.18 44.05 – 1.18	Depositor EDS
% Data completeness (in resolution range)	98.0 (44.05-1.18) 98.0 (44.05-1.18)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 1.18Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.141 , 0.158 (Not available) , 0.164	Depositor DCC
$R_{free}$ test set	8802 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.2	Xtrriage
Anisotropy	0.417	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 36.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4884	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MN, 4LU, K, F5C

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	1.83	71/4201 (1.7%)	1.39	25/5708 (0.4%)

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	3

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	ARG	CZ-NH1	-13.31	1.14	1.32
1	A	380	ARG	CA-CB	11.60	1.71	1.53
1	A	292	THR	N-CA	11.21	1.60	1.46
1	A	156	MET	CA-CB	11.07	1.68	1.53
1	A	126	SER	C-O	9.04	1.34	1.23
1	A	116	ILE	C-O	7.86	1.33	1.24
1	A	380	ARG	CA-C	-7.44	1.43	1.52
1	A	197	GLN	CD-OE1	-7.39	1.09	1.23
1	A	198	MET	C-O	7.22	1.32	1.24
1	A	60	LYS	N-CA	6.89	1.54	1.46
1	A	389	ASN	CG-ND2	-6.86	1.18	1.33
1	A	111	PRO	C-O	6.84	1.31	1.23
1	A	203	GLY	CA-C	-6.84	1.42	1.51
1	A	282	GLN	CA-CB	-6.83	1.43	1.53
1	A	123	LYS	C-O	6.83	1.33	1.24
1	A	201	LYS	C-O	6.37	1.31	1.24
1	A	93	THR	CA-CB	6.33	1.64	1.53
1	A	367	GLU	N-CA	6.29	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	323	THR	C-O	6.25	1.32	1.24
1	A	389	ASN	CA-C	-6.25	1.43	1.52
1	A	382	ARG	CD-NE	-6.22	1.37	1.46
1	A	186	VAL	C-O	6.22	1.30	1.24
1	A	90	LEU	C-N	6.16	1.39	1.33
1	A	282	GLN	CD-OE1	6.16	1.35	1.23
1	A	77	SER	N-CA	-6.02	1.38	1.46
1	A	246	GLU	C-O	5.97	1.31	1.24
1	A	482	PRO	CA-C	-5.88	1.45	1.52
1	A	345	PRO	CA-C	5.86	1.58	1.53
1	A	270	SER	C-N	5.79	1.40	1.34
1	A	28	THR	C-O	5.77	1.31	1.23
1	A	270	SER	CA-C	-5.74	1.45	1.52
1	A	209	TRP	CA-C	-5.72	1.45	1.52
1	A	473	GLU	CA-CB	5.72	1.66	1.53
1	A	239	ALA	CA-CB	-5.72	1.44	1.53
1	A	272	SER	CB-OG	-5.72	1.30	1.42
1	A	380	ARG	N-CA	5.68	1.53	1.46
1	A	482	PRO	N-CA	5.67	1.53	1.47
1	A	177	HIS	ND1-CE1	5.66	1.38	1.32
1	A	305	TYR	C-O	5.61	1.30	1.23
1	A	178	ASP	CA-C	-5.59	1.46	1.53
1	A	154	TYR	N-CA	5.58	1.51	1.46
1	A	117	VAL	C-N	5.58	1.41	1.34
1	A	300	VAL	C-O	5.56	1.30	1.24
1	A	368	LYS	C-N	5.54	1.41	1.33
1	A	29	PRO	CA-CB	5.53	1.60	1.53
1	A	52	LEU	C-O	5.50	1.30	1.24
1	A	498	PHE	C-O	5.50	1.30	1.23
1	A	472	TRP	CA-C	-5.47	1.45	1.52
1	A	124	GLU	C-O	5.44	1.30	1.24
1	A	200[A]	LYS	C-O	5.39	1.30	1.24
1	A	200[B]	LYS	C-O	5.39	1.30	1.24
1	A	371	ALA	N-CA	5.34	1.53	1.46
1	A	178	ASP	C-O	5.34	1.29	1.24
1	A	270	SER	N-CA	5.33	1.52	1.46
1	A	116	ILE	C-N	-5.32	1.27	1.33
1	A	242	GLY	C-O	5.27	1.30	1.24
1	A	116	ILE	CA-C	-5.27	1.46	1.52
1	A	280	PHE	C-O	5.26	1.29	1.23
1	A	341	GLN	C-O	5.21	1.30	1.24
1	A	242	GLY	CA-C	-5.20	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	340	GLN	C-O	5.20	1.30	1.24
1	A	430	LEU	C-O	5.19	1.30	1.23
1	A	404	ASP	CA-CB	5.18	1.62	1.53
1	A	483	GLU	CA-CB	5.16	1.61	1.53
1	A	404	ASP	CA-C	-5.15	1.45	1.52
1	A	490	LEU	CA-C	5.13	1.59	1.52
1	A	83	ARG	CA-C	-5.12	1.46	1.52
1	A	486	LYS	C-O	-5.09	1.18	1.24
1	A	155	GLY	N-CA	5.09	1.50	1.44
1	A	372	MET	N-CA	-5.07	1.39	1.46
1	A	339	CYS	C-O	5.01	1.29	1.24

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	496	MET	CA-C-O	-8.03	110.73	119.97
1	A	382	ARG	CG-CD-NE	-7.42	95.68	112.00
1	A	257	VAL	O-C-N	-6.98	115.60	121.40
1	A	495	LYS	N-CA-CB	6.79	120.06	109.94
1	A	188	PRO	O-C-N	-6.53	118.08	121.15
1	A	65	ARG	NE-CZ-NH1	-6.43	115.07	121.50
1	A	497	GLY	N-CA-C	6.41	123.99	114.95
1	A	380	ARG	CG-CD-NE	6.26	125.78	112.00
1	A	494	THR	CA-C-N	6.12	128.80	120.54
1	A	494	THR	C-N-CA	6.12	128.80	120.54
1	A	496	MET	CA-C-N	6.08	131.96	122.30
1	A	496	MET	C-N-CA	6.08	131.96	122.30
1	A	452	ARG	NE-CZ-NH2	-5.97	113.83	119.20
1	A	490	LEU	O-C-N	5.88	128.35	122.12
1	A	435	ARG	NE-CZ-NH2	-5.87	113.92	119.20
1	A	498	PHE	CA-C-O	-5.79	114.81	121.82
1	A	156	MET	N-CA-CB	-5.77	101.48	110.55
1	A	291	ASP	N-CA-CB	-5.74	102.08	110.86
1	A	266	GLU	CA-C-O	-5.49	114.77	120.70
1	A	178	ASP	O-C-N	-5.32	116.61	122.72
1	A	369	LEU	O-C-N	5.18	127.41	122.07
1	A	291	ASP	CB-CA-C	-5.11	104.34	111.85
1	A	125	ASN	O-C-N	-5.08	117.38	123.27
1	A	486	LYS	CA-C-O	5.07	126.32	120.90
1	A	125	ASN	OD1-CG-ND2	-5.02	117.58	122.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	243	SER	Mainchain
1	A	380	ARG	Sidechain
1	A	83	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4100	0	3983	56	0
2	A	36	0	28	5	0
3	A	1	0	0	0	0
4	A	2	0	0	0	0
5	A	16	0	2	1	0
6	A	729	0	0	48	8
All	All	4884	0	4013	61	8

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 7.

All (61) 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:290[A]:GLY:HA2	6:A:709:HOH:O	1.35	1.23
1:A:292:THR:HA	6:A:703:HOH:O	1.50	1.10
1:A:202:GLU:OE1	6:A:702:HOH:O	1.81	0.99
1:A:290[A]:GLY:CA	6:A:709:HOH:O	1.99	0.97
1:A:503:HIS:N	6:A:705:HOH:O	2.00	0.92
1:A:381:LYS:HG3	6:A:739:HOH:O	1.72	0.90
1:A:499:SER:CA	6:A:963:HOH:O	2.21	0.89
1:A:291:ASP:O	6:A:703:HOH:O	1.91	0.88
1:A:290[A]:GLY:C	6:A:709:HOH:O	2.14	0.87
1:A:197:GLN:HG2	6:A:708:HOH:O	1.73	0.86
1:A:28:THR:O	6:A:704:HOH:O	1.93	0.85
1:A:412[B]:LYS:CD	6:A:1374:HOH:O	2.29	0.80
2:A:601:4LU:H5	2:A:601:4LU:H14	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ASP:OD2	6:A:707:HOH:O	2.02	0.78
1:A:76[B]:SER:HB3	6:A:977:HOH:O	1.84	0.77
1:A:197:GLN:OE1	6:A:708:HOH:O	2.09	0.70
1:A:59[A]:MET:CE	6:A:1040:HOH:O	2.44	0.66
1:A:422:CYS:SG	6:A:741:HOH:O	2.54	0.66
1:A:308:ASN:N	6:A:720:HOH:O	2.29	0.65
1:A:381:LYS:HE2	6:A:1278:HOH:O	1.99	0.63
1:A:381:LYS:HE3	6:A:739:HOH:O	1.98	0.62
1:A:196[B]:HIS:HE1	1:A:270:SER:O	1.81	0.62
1:A:290[A]:GLY:O	6:A:709:HOH:O	2.14	0.62
1:A:8:LEU:O	6:A:710:HOH:O	2.16	0.62
1:A:149[A]:LYS:CE	6:A:1194:HOH:O	2.49	0.60
1:A:308:ASN:ND2	6:A:722:HOH:O	2.35	0.60
2:A:601:4LU:O4	2:A:601:4LU:H6	2.02	0.58
1:A:93:THR:OG1	6:A:711:HOH:O	2.18	0.56
1:A:197:GLN:CG	6:A:708:HOH:O	2.44	0.55
1:A:149[A]:LYS:HE2	6:A:1194:HOH:O	2.05	0.55
2:A:601:4LU:H14	2:A:601:4LU:C13	2.36	0.54
2:A:601:4LU:C2	5:A:605:F5C:CD1	2.86	0.54
1:A:381:LYS:CG	6:A:739:HOH:O	2.43	0.53
1:A:502:HIS:ND1	6:A:706:HOH:O	2.00	0.53
1:A:84[B]:LEU:HD12	1:A:84[B]:LEU:N	2.25	0.52
1:A:307:ASN:OD1	6:A:712:HOH:O	2.19	0.51
1:A:273:GLU:HG3	6:A:1296:HOH:O	2.10	0.51
1:A:108[A]:ASP:OD1	1:A:108[A]:ASP:C	2.50	0.51
1:A:363:ARG:NH1	6:A:726:HOH:O	2.44	0.50
1:A:149[A]:LYS:CD	6:A:1092:HOH:O	2.61	0.49
1:A:377[B]:GLU:HG3	6:A:739:HOH:O	2.12	0.49
1:A:433:ASP:HB2	6:A:1267:HOH:O	2.13	0.48
1:A:205[A]:SER:HB2	6:A:1209:HOH:O	2.14	0.48
1:A:171:ILE:HD12	1:A:224[A]:SER:OG	2.14	0.48
1:A:149[A]:LYS:HD3	6:A:1092:HOH:O	2.13	0.48
1:A:117:VAL:O	6:A:713:HOH:O	2.21	0.47
1:A:55:ASN:O	6:A:704:HOH:O	2.21	0.46
1:A:196[B]:HIS:CE1	1:A:270:SER:O	2.67	0.45
1:A:197:GLN:CD	6:A:708:HOH:O	2.55	0.45
1:A:484[A]:ASP:OD1	6:A:714:HOH:O	2.21	0.44
1:A:4:GLN:HG3	6:A:1226:HOH:O	2.17	0.44
2:A:601:4LU:C13	2:A:601:4LU:C7M	2.96	0.43
1:A:149[A]:LYS:NZ	6:A:724:HOH:O	2.38	0.42
1:A:267:GLY:HA3	1:A:299:LYS:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200[A]:LYS:HE2	6:A:1263:HOH:O	2.18	0.42
1:A:59[A]:MET:SD	6:A:1040:HOH:O	2.61	0.42
1:A:471:ASN:ND2	6:A:728:HOH:O	2.49	0.41
1:A:491:ASP:C	6:A:715:HOH:O	2.62	0.41
1:A:117:VAL:HG23	1:A:248[B]:VAL:HG22	2.03	0.41
1:A:196[A]:HIS:HE1	1:A:270:SER:O	2.04	0.40
1:A:381:LYS:CE	6:A:739:HOH:O	2.64	0.40

All (8) 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:868:HOH:O	6:A:868:HOH:O[2_655]	1.03	1.17
6:A:785:HOH:O	6:A:981:HOH:O[2_655]	1.66	0.54
6:A:899:HOH:O	6:A:917:HOH:O[2_555]	1.69	0.51
6:A:954:HOH:O	6:A:1137:HOH:O[3_545]	1.71	0.49
6:A:1130:HOH:O	6:A:1203:HOH:O[2_655]	1.85	0.35
6:A:705:HOH:O	6:A:1019:HOH:O[3_545]	1.98	0.22
6:A:907:HOH:O	6:A:954:HOH:O[3_555]	2.00	0.20
6:A:967:HOH:O	6:A:1207:HOH:O[3_545]	2.13	0.07

## 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	529/508 (104%)	517 (98%)	12 (2%)	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	241/430 (56%)	241 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	160	GLN
1	A	197	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
5	F5C	A	605	-	16,16,16	4.92	9 (56%)	23,23,23	2.72	14 (60%)
2	4LU	A	601	3,4	35,39,39	1.55	6 (17%)	44,62,62	1.99	10 (22%)

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
5	F5C	A	605	-	-	0/5/5/5	0/1/1/1
2	4LU	A	601	3,4	-	3/18/30/30	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	605	F5C	FD2-CD2	-13.02	1.16	1.34
5	A	605	F5C	FZ-CZ	-7.56	1.24	1.34
5	A	605	F5C	OXT-C	6.64	1.39	1.23
5	A	605	F5C	CG-CB	-5.71	1.35	1.47
5	A	605	F5C	O-C	-5.34	1.16	1.30
2	A	601	4LU	O4-C4	4.66	1.32	1.23
5	A	605	F5C	FD1-CD1	3.91	1.40	1.34
5	A	605	F5C	CG-CD2	-3.51	1.34	1.39
2	A	601	4LU	C4A-C4	-3.34	1.33	1.43
5	A	605	F5C	CA-C	3.25	1.56	1.48
2	A	601	4LU	C2-N3	3.22	1.42	1.37
5	A	605	F5C	CA-CB	2.87	1.40	1.33
2	A	601	4LU	C3-C5	-2.82	1.50	1.54
2	A	601	4LU	C2'-C3'	-2.47	1.49	1.53
2	A	601	4LU	O4'-C4'	2.08	1.47	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	4LU	O4-C4-N3	-6.60	107.71	120.11
5	A	605	F5C	CD2-CG-CB	-5.42	102.79	122.59
2	A	601	4LU	O2-C2-N3	-4.81	113.32	121.86
5	A	605	F5C	CD1-CG-CB	4.37	138.55	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	605	F5C	CB-CA-C	-4.31	111.13	122.32
2	A	601	4LU	C5-C6-C5A	-4.29	116.79	121.48
5	A	605	F5C	O-C-CA	-4.02	101.39	116.16
5	A	605	F5C	O-C-OXT	3.59	130.01	122.70
5	A	605	F5C	CZ-CE2-CD2	3.51	123.08	119.53
2	A	601	4LU	C4-N3-C2	-3.50	121.55	126.37
2	A	601	4LU	C4A-C4-N3	3.33	118.72	111.84
2	A	601	4LU	C13-C5-C6	2.90	120.67	112.06
5	A	605	F5C	CD2-CG-CD1	2.88	118.66	115.12
5	A	605	F5C	CE2-CZ-CE1	-2.88	116.62	119.53
5	A	605	F5C	CG-CB-CA	2.65	134.50	128.50
2	A	601	4LU	C13-C5-C3	-2.62	105.47	109.50
5	A	605	F5C	FD1-CD1-CE1	-2.55	114.19	119.27
2	A	601	4LU	O4-C4-C4A	2.39	133.36	128.01
5	A	605	F5C	OXT-C-CA	2.39	128.38	121.06
5	A	605	F5C	CG-CD2-CE2	-2.38	119.89	122.61
2	A	601	4LU	C9-C8-C7	2.34	121.46	119.10
5	A	605	F5C	FD1-CD1-CG	2.15	122.88	119.74
2	A	601	4LU	C9-C9A-N10	-2.10	119.02	121.85
5	A	605	F5C	FZ-CZ-CE2	2.10	123.43	119.27

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	4LU	C5'-O5'-P-O2P
2	A	601	4LU	C2'-C3'-C4'-C5'
2	A	601	4LU	C4'-C5'-O5'-P

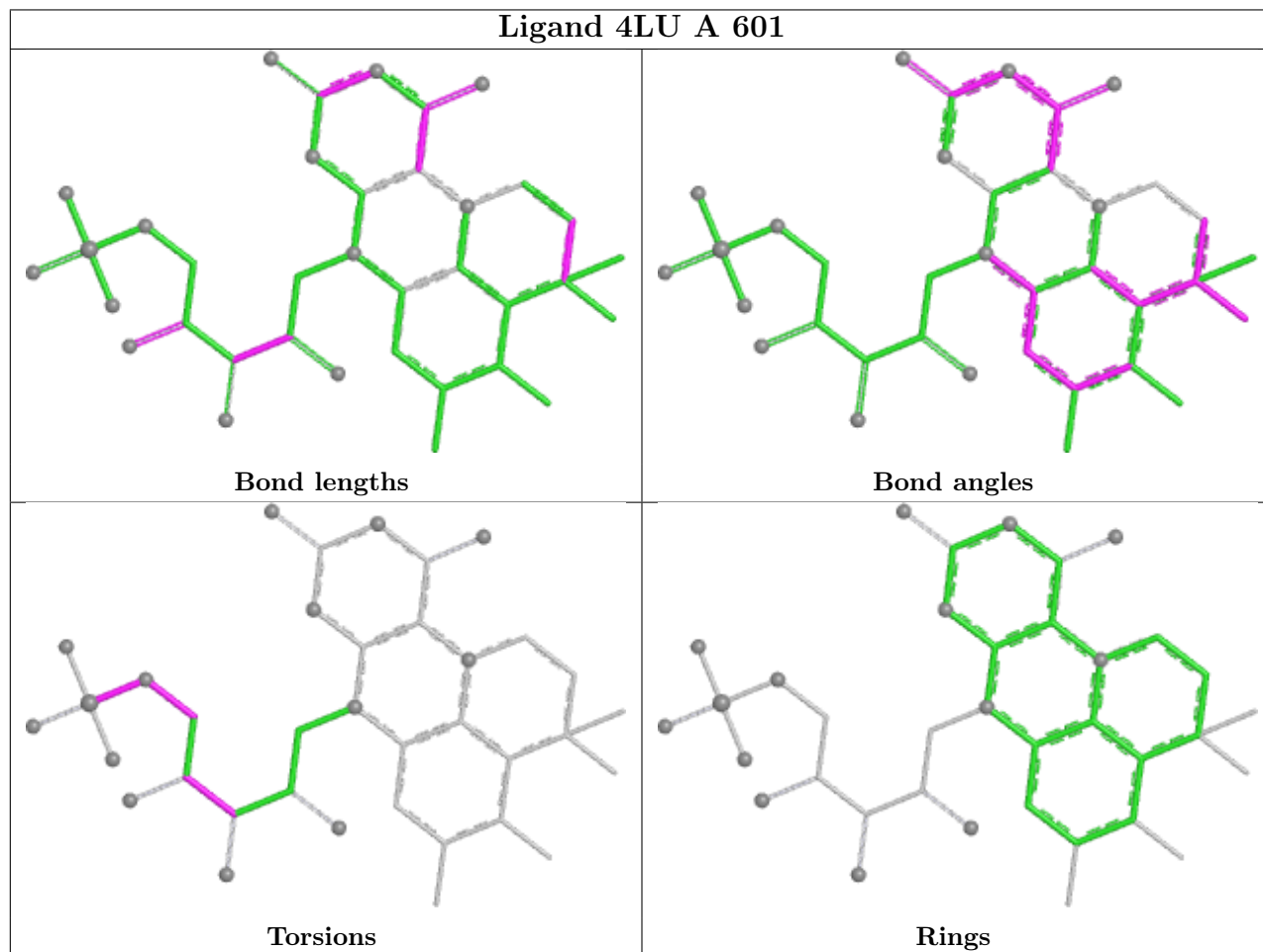
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	605	F5C	1	0
2	A	601	4LU	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%)	0.06	12 (2%) 59 62	4, 10, 20, 50	33 (6%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	505	HIS	5.8
1	A	503	HIS	4.7
1	A	292	THR	4.2
1	A	129[A]	ASP	3.9
1	A	502	HIS	3.7
1	A	291	ASP	3.5
1	A	504	HIS	3.4
1	A	497	GLY	2.8
1	A	495	LYS	2.4
1	A	343	ASP	2.2
1	A	78	ALA	2.0
1	A	294	LEU	2.0

### 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 oligosaccharides in this entry.

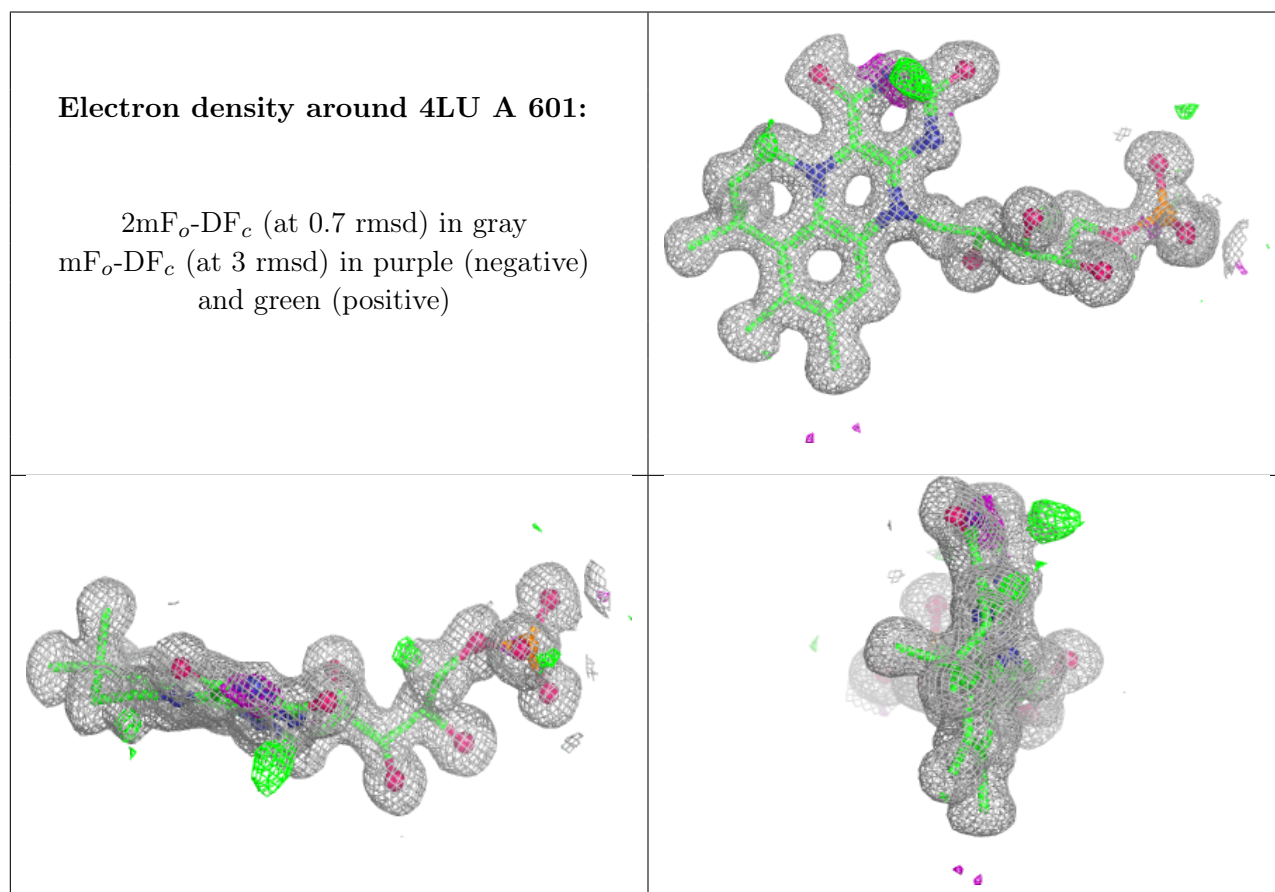
### 6.4 Ligands [i](#)

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
5	F5C	A	605	16/16	0.87	0.19	11,18,23,24	16
2	4LU	A	601	36/36	0.99	0.05	6,8,15,18	0
4	K	A	603	1/1	1.00	0.01	7,7,7,7	0
4	K	A	604	1/1	1.00	0.02	8,8,8,8	0
3	MN	A	602	1/1	1.00	0.01	6,6,6,6	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.