



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2018 – 10:56 PM EST

PDB ID : 6EVC  
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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

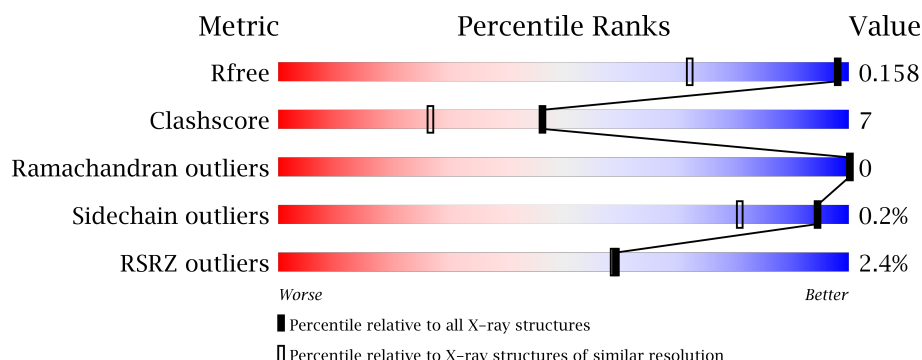
# 1 Overall quality at a glance

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))
$R_{free}$	100719	1232 (1.22-1.14)
Clashscore	112137	1309 (1.22-1.14)
Ramachandran outliers	110173	1257 (1.22-1.14)
Sidechain outliers	110143	1256 (1.22-1.14)
RSRZ outliers	101464	1235 (1.22-1.14)

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. 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	<div> <div>2%</div> <div>81%</div> <div>15%</div> <div>...</div> </div>

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.

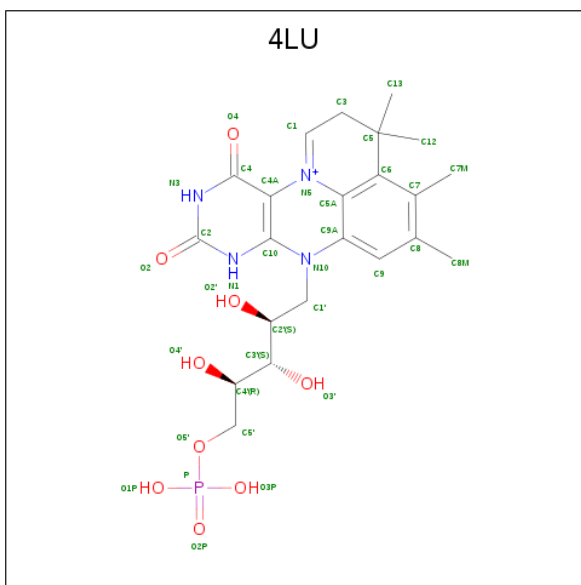
- Molecule 1 is a protein called Ferulic acid decarboxylase 1.

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

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 (three-letter code: 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
2	A	1	Total	C	N	O	P	0	0
			36	22	4	9	1		

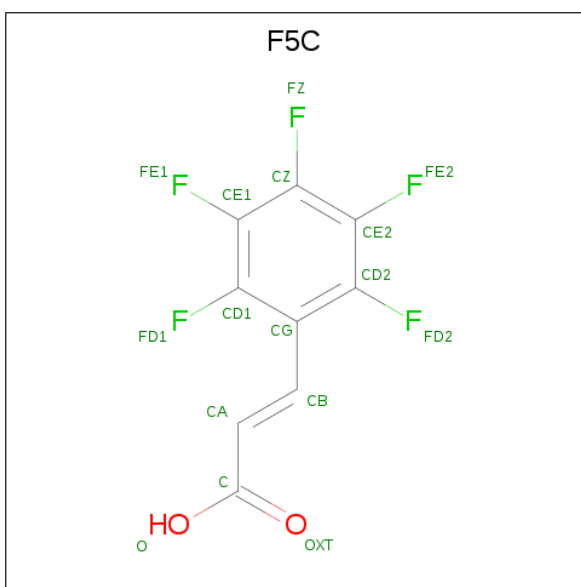
- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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 penta-fluorocinnamic acid (three-letter code: F5C) (formula:  $\text{C}_9\text{H}_3\text{F}_5\text{O}_2$ ).



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

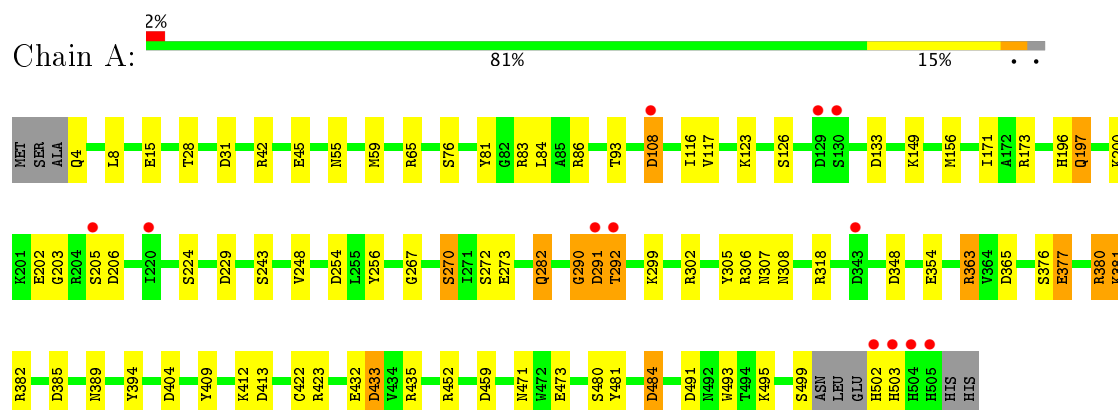
- Molecule 6 is water.

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

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

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

- Molecule 1: 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)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.141 , 0.158 0.141 , 0.158	Depositor DCC
$R_{free}$ test set	8802 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	10.2	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4884	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage'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: K, MN, F5C, 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	1.52	37/4201 (0.9%)	1.41	51/5708 (0.9%)

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 (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	ARG	CZ-NH1	-14.56	1.14	1.33
1	A	272	SER	CB-OG	-8.87	1.30	1.42
1	A	473	GLU	CD-OE1	8.01	1.34	1.25
1	A	377[A]	GLU	CD-OE1	7.99	1.34	1.25
1	A	377[B]	GLU	CD-OE1	7.99	1.34	1.25
1	A	256	TYR	CE1-CZ	-7.95	1.28	1.38
1	A	380	ARG	CA-CB	7.93	1.71	1.53
1	A	354	GLU	CD-OE2	7.39	1.33	1.25
1	A	292	THR	N-CA	7.10	1.60	1.46
1	A	493	TRP	CG-CD1	-6.95	1.27	1.36
1	A	377[A]	GLU	CD-OE2	6.93	1.33	1.25
1	A	377[B]	GLU	CD-OE2	6.93	1.33	1.25
1	A	156	MET	CA-CB	6.67	1.68	1.53
1	A	197	GLN	CD-OE1	-6.57	1.09	1.24
1	A	432	GLU	CD-OE1	-6.34	1.18	1.25
1	A	290[A]	GLY	N-CA	-6.32	1.36	1.46
1	A	290[B]	GLY	N-CA	-6.32	1.36	1.46
1	A	203	GLY	CA-C	-6.10	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	SER	C-O	6.05	1.34	1.23
1	A	376	SER	CB-OG	5.89	1.50	1.42
1	A	473	GLU	CA-CB	5.87	1.66	1.53
1	A	81	TYR	CZ-OH	5.80	1.47	1.37
1	A	126	SER	CA-CB	-5.68	1.44	1.52
1	A	389	ASN	CG-ND2	-5.61	1.18	1.32
1	A	480[A]	SER	CB-OG	5.50	1.49	1.42
1	A	480[B]	SER	CB-OG	5.50	1.49	1.42
1	A	116	ILE	C-O	5.39	1.33	1.23
1	A	394	TYR	CE1-CZ	-5.33	1.31	1.38
1	A	45	GLU	CD-OE1	5.27	1.31	1.25
1	A	382	ARG	CD-NE	-5.24	1.37	1.46
1	A	305	TYR	CD2-CE2	5.22	1.47	1.39
1	A	291	ASP	CB-CG	-5.15	1.41	1.51
1	A	123	LYS	C-O	5.14	1.33	1.23
1	A	282	GLN	CD-OE1	5.14	1.35	1.24
1	A	256	TYR	CZ-OH	5.11	1.46	1.37
1	A	270	SER	CB-OG	5.02	1.48	1.42
1	A	481	TYR	CE1-CZ	-5.01	1.32	1.38

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	452	ARG	NE-CZ-NH2	-12.95	113.83	120.30
1	A	435	ARG	NE-CZ-NH2	-12.77	113.92	120.30
1	A	291	ASP	CB-CG-OD2	-10.80	108.58	118.30
1	A	380	ARG	NE-CZ-NH1	10.71	125.65	120.30
1	A	65	ARG	NE-CZ-NH1	-10.46	115.07	120.30
1	A	491	ASP	CB-CG-OD2	-10.01	109.29	118.30
1	A	423	ARG	NE-CZ-NH2	-9.93	115.34	120.30
1	A	206	ASP	CB-CG-OD2	-9.84	109.44	118.30
1	A	377[A]	GLU	CG-CD-OE2	-9.69	98.93	118.30
1	A	377[B]	GLU	CG-CD-OE2	-9.69	98.93	118.30
1	A	173	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	A	435	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	A	385	ASP	CB-CG-OD1	8.15	125.64	118.30
1	A	31	ASP	CB-CG-OD1	8.03	125.53	118.30
1	A	254	ASP	CB-CG-OD2	-7.83	111.25	118.30
1	A	108[A]	ASP	CB-CG-OD1	-7.76	111.31	118.30
1	A	108[B]	ASP	CB-CG-OD1	-7.76	111.31	118.30
1	A	413	ASP	CB-CG-OD1	7.68	125.21	118.30
1	A	382	ARG	CG-CD-NE	-7.67	95.68	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	404	ASP	CB-CG-OD2	7.52	125.07	118.30
1	A	15[A]	GLU	OE1-CD-OE2	-7.47	114.33	123.30
1	A	15[B]	GLU	OE1-CD-OE2	-7.47	114.33	123.30
1	A	433	ASP	CB-CG-OD2	-7.35	111.68	118.30
1	A	229	ASP	CB-CG-OD1	6.97	124.57	118.30
1	A	133	ASP	CB-CG-OD1	6.92	124.52	118.30
1	A	377[A]	GLU	CG-CD-OE1	6.89	132.09	118.30
1	A	377[B]	GLU	CG-CD-OE1	6.89	132.09	118.30
1	A	380	ARG	CG-CD-NE	6.66	125.78	111.80
1	A	348	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	A	409	TYR	CB-CG-CD2	6.41	124.84	121.00
1	A	381	LYS	CD-CE-NZ	-6.30	97.22	111.70
1	A	363	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	A	459	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	306	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	31	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	A	452	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	302	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	A	173	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	A	484[A]	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	484[B]	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	254	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	81	TYR	CG-CD1-CE1	5.47	125.67	121.30
1	A	318	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	A	365	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	A	495	LYS	N-CA-CB	5.25	120.06	110.60
1	A	42[A]	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	A	42[B]	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	A	86	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	156	MET	N-CA-CB	-5.06	101.48	110.60
1	A	382	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	81	TYR	CD1-CE1-CZ	-5.00	115.30	119.80

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 ⓘ

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	55	0
2	A	36	0	28	4	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	47	8
All	All	4884	0	4013	59	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 (59) 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
2:A:601:4LU:H14	2:A:601:4LU:H5	1.50	0.94
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: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:290[A]:GLY:C	6:A:709:HOH:O	2.14	0.81
1:A:412[B]:LYS:CD	6:A:1374:HOH:O	2.29	0.80
2:A:601:4LU:H14	2:A:601:4LU:C13	2.13	0.78
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:422:CYS:SG	6:A:741:HOH:O	2.54	0.66
1:A:59[A]:MET:CE	6:A:1040:HOH:O	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:363:ARG:NH1	6:A:726:HOH:O	2.44	0.50
1:A:108[A]:ASP:C	1:A:108[A]:ASP:OD1	2.50	0.49
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:59[A]:MET:HE3	6:A:1040:HOH:O	2.14	0.44
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
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
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: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	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	442/430 (103%)	441 (100%)	1 (0%)	94	81

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	282	GLN

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

Mol	Chain	Res	Type
1	A	197	GLN
1	A	282	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 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	3,4	33,39,39	1.80	11 (33%)	36,62,62	2.06	6 (16%)
5	F5C	A	605	-	13,16,16	4.33	5 (38%)	19,23,23	2.40	10 (52%)

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	3,4	-	0/16/30/30	0/3/4/4
5	F5C	A	605	-	-	0/3/5/5	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	605	F5C	FD2-CD2	-11.46	1.16	1.35
5	A	605	F5C	FZ-CZ	-6.68	1.24	1.35
5	A	605	F5C	CG-CB	-5.81	1.35	1.47
2	A	601	4LU	C4-C4A	-4.15	1.33	1.41
5	A	605	F5C	CG-CD2	-3.59	1.34	1.39
2	A	601	4LU	C3-C5	-2.81	1.50	1.54
2	A	601	4LU	C6-C5A	-2.74	1.38	1.43
2	A	601	4LU	C1'-N10	-2.51	1.45	1.48
2	A	601	4LU	C2'-C3'	-2.22	1.49	1.53
2	A	601	4LU	C5A-C9A	-2.14	1.37	1.40
2	A	601	4LU	C6-C7	2.23	1.45	1.40
2	A	601	4LU	C2-N3	2.33	1.42	1.38
2	A	601	4LU	C4-N3	3.11	1.38	1.33
2	A	601	4LU	O4-C4	3.13	1.32	1.24
5	A	605	F5C	FD1-CD1	3.38	1.40	1.35
2	A	601	4LU	C9A-N10	4.12	1.44	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	605	F5C	CD2-CG-CB	-5.19	102.79	122.58
2	A	601	4LU	C4A-C4-N3	-3.35	118.72	123.48
5	A	605	F5C	CE1-CZ-CE2	-2.58	116.62	119.53
5	A	605	F5C	CG-CD2-CE2	-2.52	119.89	122.68
5	A	605	F5C	FD1-CD1-CE1	-2.49	114.19	119.29
2	A	601	4LU	C13-C5-C3	-2.21	105.47	109.15
2	A	601	4LU	C12-C5-C6	-2.16	107.26	111.85
5	A	605	F5C	FD1-CD1-CG	2.00	122.88	119.75
5	A	605	F5C	FZ-CZ-CE2	2.02	123.43	119.29
5	A	605	F5C	CG-CB-CA	2.43	134.50	127.12
5	A	605	F5C	CZ-CE2-CD2	3.16	123.08	119.53
5	A	605	F5C	CD1-CG-CD2	3.31	118.66	115.09
2	A	601	4LU	C13-C5-C6	4.16	120.67	111.85
5	A	605	F5C	CD1-CG-CB	4.19	138.55	122.58
2	A	601	4LU	C1'-N10-C9A	6.19	124.02	118.35
2	A	601	4LU	C4-N3-C2	7.31	121.55	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	4LU	4	0
5	A	605	F5C	1	0

## 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%)	0.36	12 (2%) 59 59	7, 10, 20, 50	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	505	HIS	5.0
1	A	503	HIS	5.0
1	A	502	HIS	3.7
1	A	504	HIS	3.7
1	A	108[A]	ASP	3.2
1	A	130	SER	2.9
1	A	292	THR	2.8
1	A	291	ASP	2.8
1	A	129[A]	ASP	2.6
1	A	205[A]	SER	2.2
1	A	220	ILE	2.2
1	A	343	ASP	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 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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	F5C	A	605	16/16	0.85	0.32	16.82	11,18,23,24	16
2	4LU	A	601	36/36	0.98	0.10	0.33	6,8,15,18	0
3	MN	A	602	1/1	1.00	0.08	-0.04	6,6,6,6	0
4	K	A	603	1/1	1.00	0.08	-1.06	7,7,7,7	0
4	K	A	604	1/1	1.00	0.07	-1.17	8,8,8,8	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.