



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 09:41 PM GMT

PDB ID : 4ZAC  
Title : Structure of *S. cerevisiae* Fdc1 with the prenylated-flavin cofactor in the iminium form.  
Authors : White, M.D.; Leys, D.  
Deposited on : 2015-04-13  
Resolution : 1.65 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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-20026982

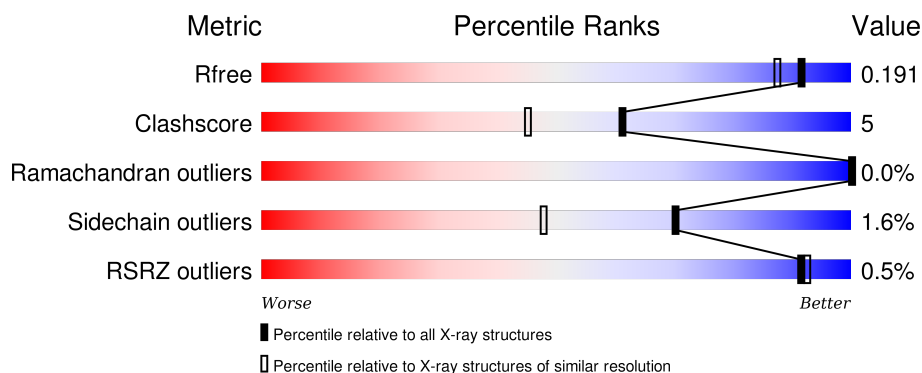
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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))
$R_{free}$	91344	1226 (1.66-1.66)
Clashscore	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)
RSRZ outliers	91569	1227 (1.66-1.66)

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	503	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">%</span> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>85%</span> <span>14%</span> </div> </div>
1	B	503	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>84%</span> <span>15%</span> </div> </div>
1	C	503	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>82%</span> <span>17%</span> </div> </div>
1	D	503	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">%</span> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>86%</span> <span>13%</span> </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
4	MN	A	603	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 17693 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	503	Total	C	N	O	S	0	14	0
			4052	2604	667	756	25			
1	B	503	Total	C	N	O	S	0	11	0
			4032	2594	659	755	24			
1	C	501	Total	C	N	O	S	0	9	0
			3975	2560	648	743	24			
1	D	503	Total	C	N	O	S	0	12	0
			4032	2593	658	755	26			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	A	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		

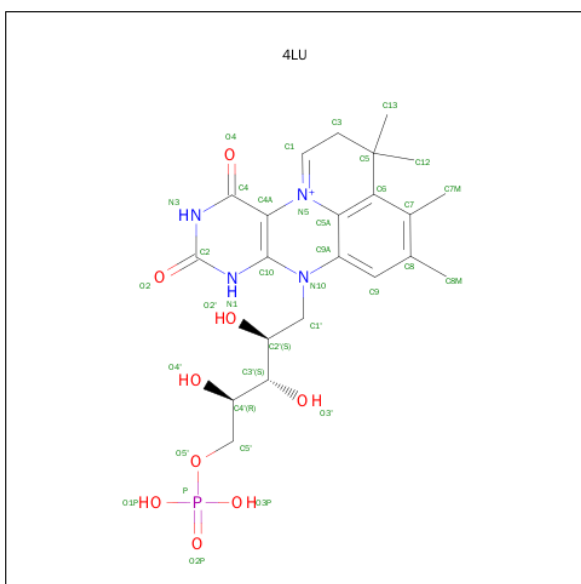
- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	K	0	0
			1	1		
3	A	1	Total	K	0	0
			1	1		
3	D	1	Total	K	0	0
			1	1		
3	C	1	Total	K	0	0
			1	1		

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mn 1 1	0	0
4	A	1	Total Mn 1 1	0	0
4	D	1	Total Mn 1 1	0	0
4	C	1	Total Mn 1 1	0	0

- Molecule 5 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-ribose (three-letter code: 4LU) (formula:  $C_{22}H_{30}N_4O_9P$ ).



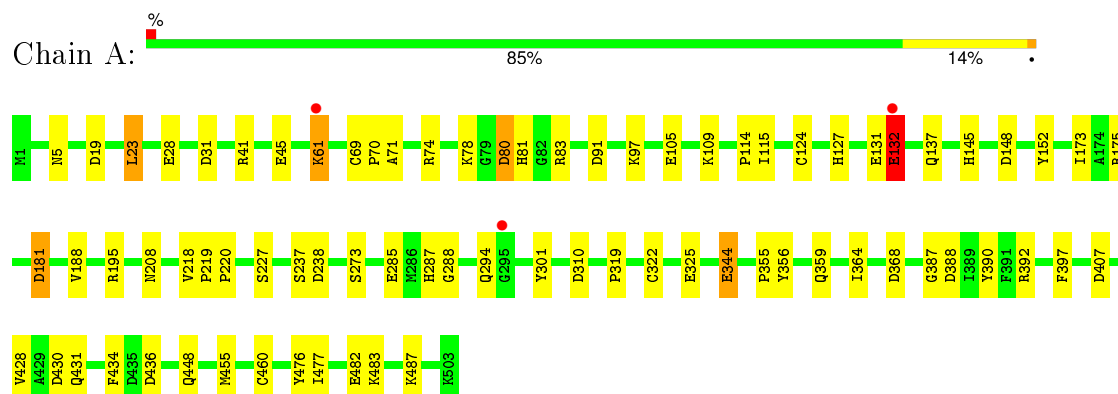
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	358	Total 358	O 358	0	0
6	C	275	Total 275	O 275	0	0
6	D	377	Total 377	O 377	0	0

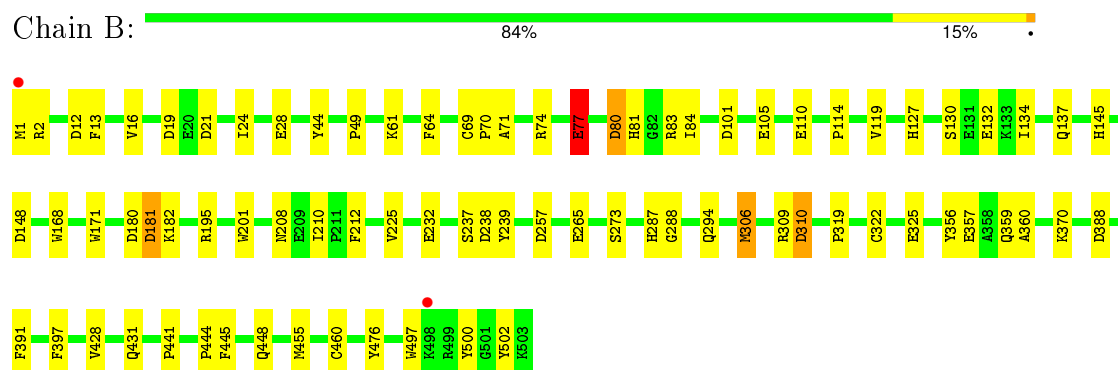
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

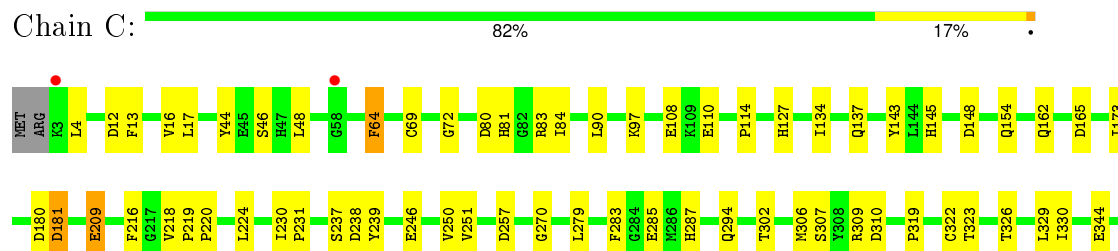
#### • Molecule 1: Ferulic acid decarboxylase 1



#### • Molecule 1: Ferulic acid decarboxylase 1

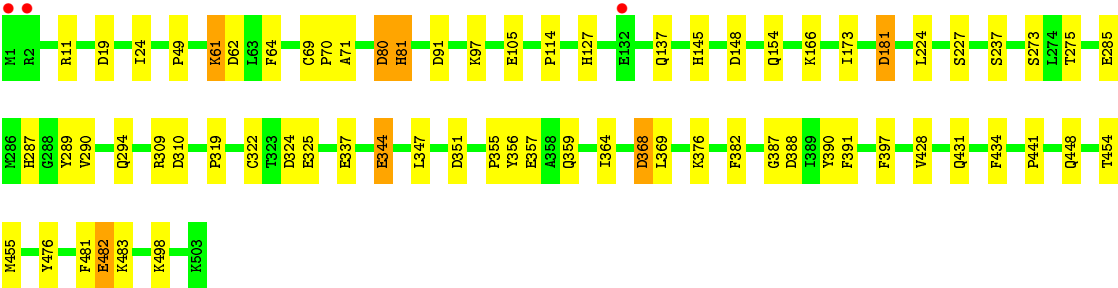
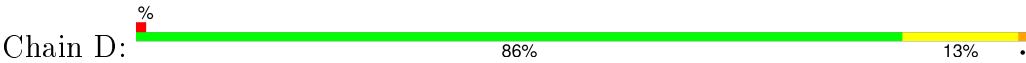


#### • Molecule 1: Ferulic acid decarboxylase 1





● Molecule 1: Ferulic acid decarboxylase 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.41Å 96.18Å 116.64Å 90.00° 96.58° 90.00°	Depositor
Resolution (Å)	54.19 – 1.65 54.19 – 1.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (54.19-1.65) 98.7 (54.19-1.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.163 , 0.192 0.161 , 0.191	Depositor DCC
$R_{free}$ test set	15010 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.4	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.0	EDS
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 297244 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	17693	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage'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, 0.375 respectively for untwinned datasets, and 0.333, 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: NA, 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	1.49	15/4152 (0.4%)	1.32	21/5637 (0.4%)
1	B	1.46	20/4133 (0.5%)	1.30	25/5612 (0.4%)
1	C	1.49	19/4078 (0.5%)	1.29	19/5542 (0.3%)
1	D	1.43	15/4132 (0.4%)	1.26	21/5611 (0.4%)
All	All	1.47	69/16495 (0.4%)	1.29	86/22402 (0.4%)

The worst 5 of 69 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	482	GLU	CG-CD	9.18	1.65	1.51
1	C	69	CYS	CB-SG	-8.50	1.67	1.82
1	A	301	TYR	CD2-CE2	7.54	1.50	1.39
1	A	344	GLU	CG-CD	7.47	1.63	1.51
1	A	482	GLU	CB-CG	7.44	1.66	1.52

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	83	ARG	NE-CZ-NH2	-12.17	114.22	120.30
1	D	91	ASP	CB-CG-OD1	11.08	128.27	118.30
1	B	238	ASP	CB-CG-OD1	10.83	128.05	118.30
1	A	83	ARG	NE-CZ-NH2	-10.26	115.17	120.30
1	B	74	ARG	NE-CZ-NH2	-9.54	115.53	120.30

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	4052	0	4048	45	0
1	B	4032	0	4021	38	0
1	C	3975	0	3963	44	0
1	D	4032	0	4026	38	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	36	0	28	4	0
5	B	36	0	28	4	0
5	C	36	0	27	4	0
5	D	36	0	28	3	0
6	A	437	0	0	23	1
6	B	358	0	0	12	1
6	C	275	0	0	6	0
6	D	377	0	0	13	0
All	All	17693	0	16169	178	1

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 5.

The worst 5 of 178 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:430:ASP:CG	6:A:701:HOH:O	1.69	1.31
1:B:28[B]:GLU:OE2	6:B:701:HOH:O	1.56	1.22
1:D:368:ASP:CG	6:D:701:HOH:O	1.77	1.22
5:C:603:4LU:H14	5:C:603:4LU:H5	1.34	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:604:4LU:H5	5:A:604:4LU:H14	1.34	1.04

All (1) 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:878:HOH:O	6:B:978:HOH:O[2_646]	2.15	0.05

## 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	515/503 (102%)	506 (98%)	9 (2%)	0	100	100
1	B	512/503 (102%)	497 (97%)	14 (3%)	1 (0%)	52	30
1	C	508/503 (101%)	495 (97%)	13 (3%)	0	100	100
1	D	513/503 (102%)	503 (98%)	10 (2%)	0	100	100
All	All	2048/2012 (102%)	2001 (98%)	46 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2	ARG

### 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	451/438 (103%)	444 (98%)	7 (2%)	70	48
1	B	447/438 (102%)	439 (98%)	8 (2%)	66	43
1	C	441/438 (101%)	433 (98%)	8 (2%)	66	43
1	D	449/438 (102%)	443 (99%)	6 (1%)	76	57
All	All	1788/1752 (102%)	1759 (98%)	29 (2%)	70	48

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	370	LYS
1	C	108	GLU
1	D	154	GLN
1	B	460	CYS
1	C	137	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	431	GLN
1	C	127	HIS
1	D	359	GLN
1	C	81	HIS
1	C	137	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 15 ligands modelled in this entry, 11 are monoatomic - leaving 4 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	4LU	A	604	3,4	32,39,39	2.75	11 (34%)	33,62,62	2.58	12 (36%)
5	4LU	B	604	3,4	32,39,39	3.16	7 (21%)	33,62,62	2.62	14 (42%)
5	4LU	C	603	3,4	32,39,39	3.48	9 (28%)	33,62,62	2.45	10 (30%)
5	4LU	D	603	3,4	32,39,39	1.61	4 (12%)	33,62,62	2.15	7 (21%)

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	4LU	A	604	3,4	-	0/18/30/30	0/3/4/4
5	4LU	B	604	3,4	-	0/18/30/30	0/3/4/4
5	4LU	C	603	3,4	-	0/18/30/30	0/3/4/4
5	4LU	D	603	3,4	-	0/18/30/30	0/3/4/4

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	604	4LU	C5-C6	-14.11	1.42	1.54
5	C	603	4LU	C5-C6	-11.80	1.44	1.54
5	A	604	4LU	C5-C6	-11.45	1.44	1.54
5	C	603	4LU	C2'-C3'	-6.44	1.40	1.53
5	C	603	4LU	C4'-C3'	-5.07	1.43	1.53

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	603	4LU	C4-C4A-C10	-6.16	116.00	119.94
5	A	604	4LU	C4-C4A-C10	-5.89	116.17	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	603	4LU	C5A-C9A-N10	-5.85	115.86	120.47
5	B	604	4LU	N3-C2-N1	-5.40	118.59	127.69
5	D	603	4LU	N3-C2-N1	-5.26	118.83	127.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	604	4LU	4	0
5	B	604	4LU	4	0
5	C	603	4LU	4	0
5	D	603	4LU	3	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	503/503 (100%)	-0.45	3 (0%) 90 90	13, 20, 33, 46	0
1	B	503/503 (100%)	-0.48	2 (0%) 93 93	14, 22, 38, 62	0
1	C	501/503 (99%)	-0.37	2 (0%) 93 93	17, 26, 40, 57	0
1	D	503/503 (100%)	-0.38	3 (0%) 90 90	15, 22, 36, 66	0
All	All	2010/2012 (99%)	-0.42	10 (0%) 91 92	13, 22, 38, 66	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	6.5
1	B	1	MET	4.4
1	C	3	LYS	3.4
1	D	2	ARG	3.1
1	C	58	GLY	2.7

### 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( $\text{\AA}^2$ )	Q<0.9
4	MN	A	603	1/1	1.00	0.07	2.18	16,16,16,16	1
3	K	D	602	1/1	1.00	0.08	1.64	18,18,18,18	0
5	4LU	C	603	36/36	0.98	0.08	0.15	17,21,28,30	0
3	K	A	602	1/1	1.00	0.07	0.11	15,15,15,15	0
5	4LU	D	603	36/36	0.98	0.07	-0.04	15,18,24,27	0
5	4LU	B	604	36/36	0.98	0.07	-0.05	13,17,24,26	0
5	4LU	A	604	36/36	0.98	0.07	-0.16	13,15,24,28	0
3	K	C	602	1/1	0.98	0.08	-0.20	21,21,21,21	0
3	K	B	602	1/1	1.00	0.07	-0.57	16,16,16,16	0
4	MN	C	601	1/1	0.98	0.06	-1.10	21,21,21,21	1
4	MN	D	601	1/1	1.00	0.05	-1.38	20,20,20,20	1
4	MN	B	603	1/1	1.00	0.05	-1.49	17,17,17,17	1
2	NA	B	601	1/1	0.97	0.05	-	22,22,22,22	0
2	NA	C	604	1/1	0.93	0.08	-	38,38,38,38	0
2	NA	A	601	1/1	0.94	0.05	-	27,27,27,27	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.