



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 01:14 am BST

PDB ID : 6ICP  
Title : Pseudomonas putida CBB5 NdmA QL mutant with caffeine  
Authors : Kim, J.H.; Kim, B.H.; Kang, S.Y.; Song, H.K.  
Deposited on : 2018-09-06  
Resolution : 2.20 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

<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  
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

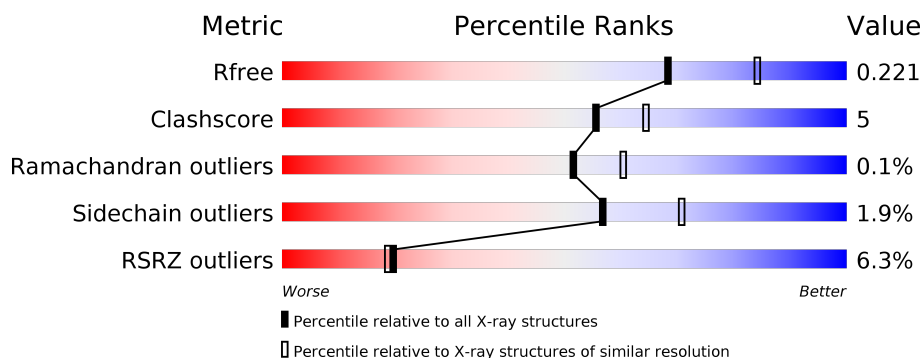
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	369	<div> <div>6%</div> <div> <div></div> <div>82%</div> <div>8%</div> <div>9%</div> </div> </div>
1	B	369	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>9%</div> </div> </div>
1	C	369	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>9%</div> <div>9%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8804 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 Methylxanthine N1-demethylase NdmA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2714	1730	465	507	12			
1	B	334	Total	C	N	O	S	0	0	0
			2707	1725	464	506	12			
1	C	334	Total	C	N	O	S	0	0	0
			2707	1725	464	506	12			

There are 60 discrepancies between the modelled and reference sequences:

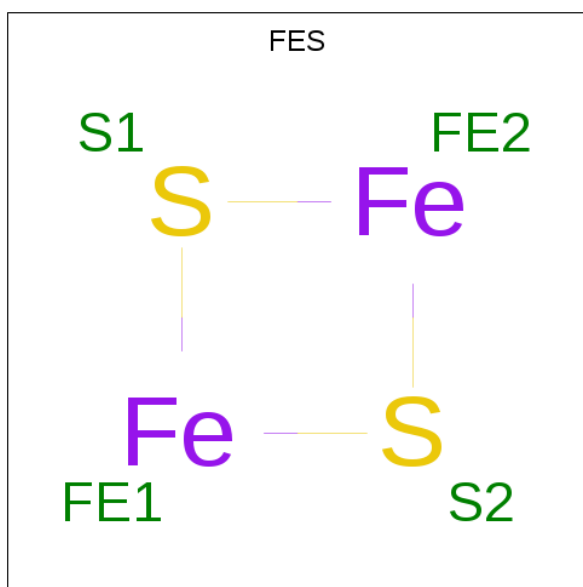
Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	expression tag	UNP H9N289
A	-16	GLY	-	expression tag	UNP H9N289
A	-15	SER	-	expression tag	UNP H9N289
A	-14	SER	-	expression tag	UNP H9N289
A	-13	HIS	-	expression tag	UNP H9N289
A	-12	HIS	-	expression tag	UNP H9N289
A	-11	HIS	-	expression tag	UNP H9N289
A	-10	HIS	-	expression tag	UNP H9N289
A	-9	HIS	-	expression tag	UNP H9N289
A	-8	HIS	-	expression tag	UNP H9N289
A	-7	GLU	-	expression tag	UNP H9N289
A	-6	ASN	-	expression tag	UNP H9N289
A	-5	LEU	-	expression tag	UNP H9N289
A	-4	TYR	-	expression tag	UNP H9N289
A	-3	PHE	-	expression tag	UNP H9N289
A	-2	GLN	-	expression tag	UNP H9N289
A	-1	GLY	-	expression tag	UNP H9N289
A	0	SER	-	expression tag	UNP H9N289
A	282	GLN	ASN	engineered mutation	UNP H9N289
A	286	LEU	PHE	engineered mutation	UNP H9N289
B	-17	MET	-	expression tag	UNP H9N289
B	-16	GLY	-	expression tag	UNP H9N289
B	-15	SER	-	expression tag	UNP H9N289

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	SER	-	expression tag	UNP H9N289
B	-13	HIS	-	expression tag	UNP H9N289
B	-12	HIS	-	expression tag	UNP H9N289
B	-11	HIS	-	expression tag	UNP H9N289
B	-10	HIS	-	expression tag	UNP H9N289
B	-9	HIS	-	expression tag	UNP H9N289
B	-8	HIS	-	expression tag	UNP H9N289
B	-7	GLU	-	expression tag	UNP H9N289
B	-6	ASN	-	expression tag	UNP H9N289
B	-5	LEU	-	expression tag	UNP H9N289
B	-4	TYR	-	expression tag	UNP H9N289
B	-3	PHE	-	expression tag	UNP H9N289
B	-2	GLN	-	expression tag	UNP H9N289
B	-1	GLY	-	expression tag	UNP H9N289
B	0	SER	-	expression tag	UNP H9N289
B	282	GLN	ASN	engineered mutation	UNP H9N289
B	286	LEU	PHE	engineered mutation	UNP H9N289
C	-17	MET	-	expression tag	UNP H9N289
C	-16	GLY	-	expression tag	UNP H9N289
C	-15	SER	-	expression tag	UNP H9N289
C	-14	SER	-	expression tag	UNP H9N289
C	-13	HIS	-	expression tag	UNP H9N289
C	-12	HIS	-	expression tag	UNP H9N289
C	-11	HIS	-	expression tag	UNP H9N289
C	-10	HIS	-	expression tag	UNP H9N289
C	-9	HIS	-	expression tag	UNP H9N289
C	-8	HIS	-	expression tag	UNP H9N289
C	-7	GLU	-	expression tag	UNP H9N289
C	-6	ASN	-	expression tag	UNP H9N289
C	-5	LEU	-	expression tag	UNP H9N289
C	-4	TYR	-	expression tag	UNP H9N289
C	-3	PHE	-	expression tag	UNP H9N289
C	-2	GLN	-	expression tag	UNP H9N289
C	-1	GLY	-	expression tag	UNP H9N289
C	0	SER	-	expression tag	UNP H9N289
C	282	GLN	ASN	engineered mutation	UNP H9N289
C	286	LEU	PHE	engineered mutation	UNP H9N289

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).

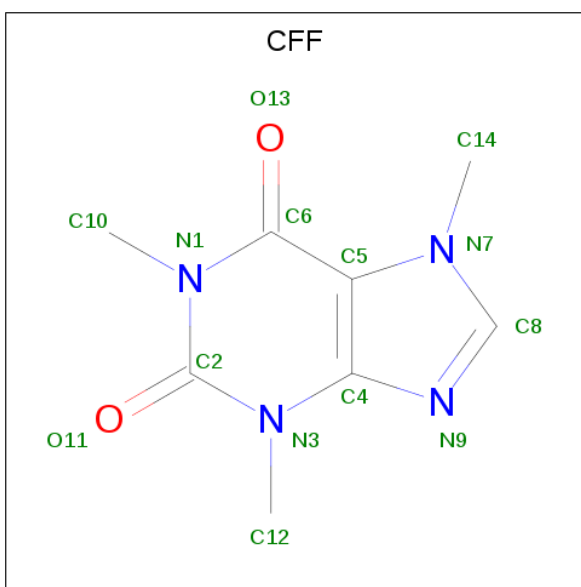


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		
2	C	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 4 is CAFFEINE (three-letter code: CFF) (formula: C<sub>8</sub>H<sub>10</sub>N<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	4	2		
4	B	1	Total	C	N	O	0	0
			14	8	4	2		
4	C	1	Total	C	N	O	0	0
			14	8	4	2		

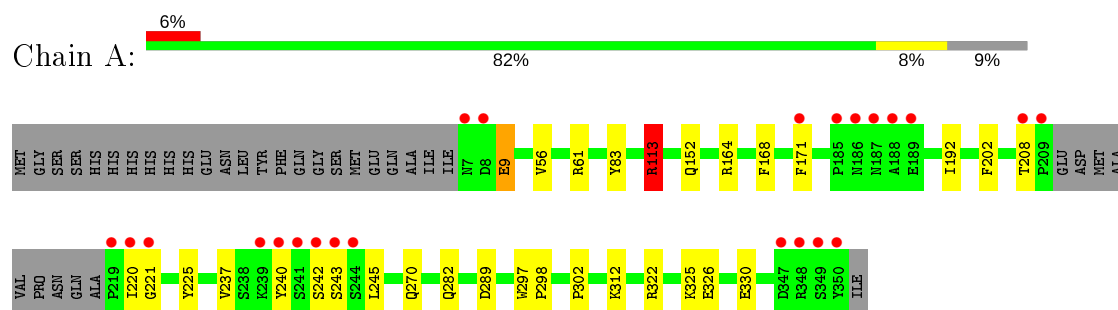
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	205	Total	O	0	0
			205	205		
5	B	200	Total	O	0	0
			200	200		
5	C	214	Total	O	0	0
			214	214		

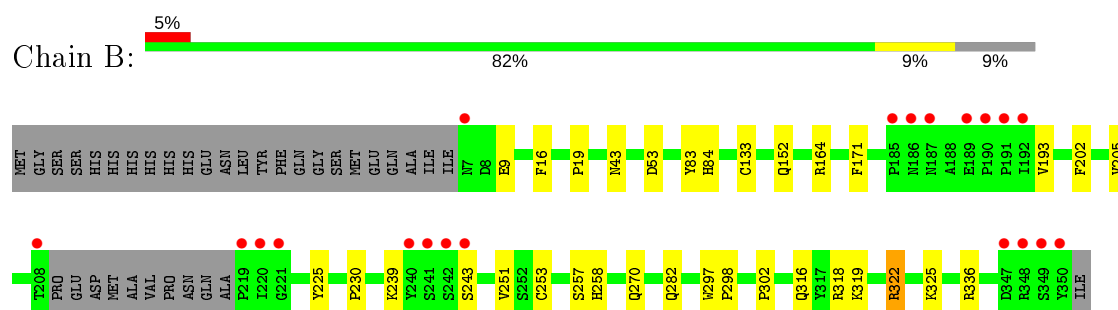
### 3 Residue-property plots [i](#)

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.

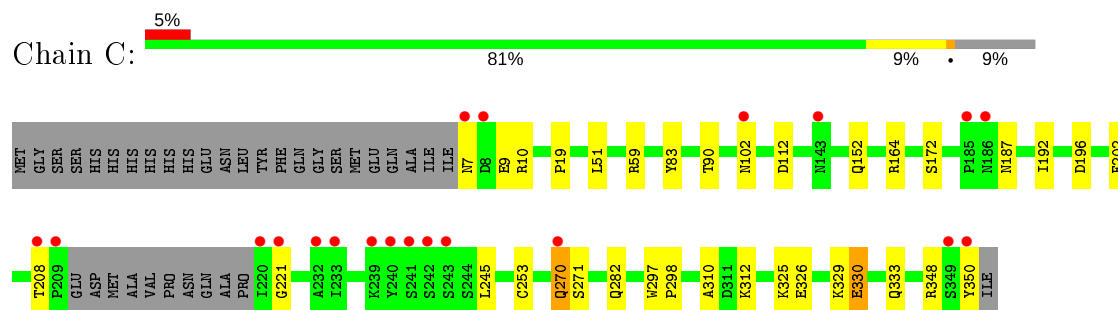
- Molecule 1: Methylxanthine N1-demethylase NdmA



- Molecule 1: Methylxanthine N1-demethylase NdmA



- Molecule 1: Methylxanthine N1-demethylase NdmA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.24Å 136.24Å 154.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.67 – 2.20 33.67 – 2.19	Depositor EDS
% Data completeness (in resolution range)	93.8 (33.67-2.20) 93.8 (33.67-2.19)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.93 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.179 , 0.221 0.178 , 0.221	Depositor DCC
$R_{free}$ test set	2010 reflections (2.52%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.9	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8804	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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: CFF, FE, FES

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.47	0/2796	0.61	1/3807 (0.0%)
1	B	0.48	0/2788	0.60	0/3795
1	C	0.49	0/2788	0.60	0/3796
All	All	0.48	0/8372	0.60	1/11398 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	ARG	NE-CZ-NH1	5.25	122.93	120.30

There are no chirality outliers.

There are no planarity outliers.

### 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	2714	0	2585	30	0
1	B	2707	0	2578	27	0
1	C	2707	0	2577	24	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	14	0	10	5	0
4	B	14	0	10	4	0
4	C	14	0	10	3	0
5	A	205	0	0	9	0
5	B	200	0	0	3	0
5	C	214	0	0	6	0
All	All	8804	0	7770	81	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 81 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:GLU:OE2	1:B:325:LYS:NZ	1.73	1.21
1:A:113:ARG:NH2	5:A:501:HOH:O	1.99	0.94
1:C:333:GLN:NE2	5:C:502:HOH:O	2.03	0.90
1:A:113:ARG:NE	5:A:501:HOH:O	1.67	0.88
1:C:245:LEU:O	5:C:501:HOH:O	1.94	0.85

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	331/369 (90%)	316 (96%)	15 (4%)	0	100	100
1	B	330/369 (89%)	319 (97%)	11 (3%)	0	100	100
1	C	330/369 (89%)	322 (98%)	7 (2%)	1 (0%)	41	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	991/1107 (90%)	957 (97%)	33 (3%)	1 (0%)	51 60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	187	ASN

### 5.3.2 Protein sidechains ⓘ

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	299/328 (91%)	294 (98%)	5 (2%)	60 74
1	B	298/328 (91%)	293 (98%)	5 (2%)	60 74
1	C	298/328 (91%)	291 (98%)	7 (2%)	50 63
All	All	895/984 (91%)	878 (98%)	17 (2%)	57 71

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	164	ARG
1	B	202	PHE
1	C	270	GLN
1	B	83	TYR
1	C	271	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	ASN
1	B	187	ASN
1	B	258	HIS
1	B	316	GLN
1	C	270	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 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	FES	C	400	1	0,4,4	0.00	-	-		
4	CFF	B	402	-	8,15,15	1.81	2 (25%)	8,23,23	1.38	1 (12%)
4	CFF	C	402	-	8,15,15	1.73	2 (25%)	8,23,23	1.05	1 (12%)
4	CFF	A	402	-	8,15,15	1.80	2 (25%)	8,23,23	1.07	1 (12%)
2	FES	B	400	1	0,4,4	0.00	-	-		
2	FES	A	400	1	0,4,4	0.00	-	-		

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	FES	C	400	1	-	-	0/1/1/1
4	CFF	B	402	-	-	-	0/2/2/2
4	CFF	C	402	-	-	-	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CFF	A	402	-	-	-	0/2/2/2
2	FES	B	400	1	-	-	0/1/1/1
2	FES	A	400	1	-	-	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	402	CFF	C5-C4	-3.56	1.34	1.39
4	A	402	CFF	C5-C4	-3.30	1.35	1.39
4	C	402	CFF	C5-C4	-3.27	1.35	1.39
4	A	402	CFF	C6-N1	-2.84	1.34	1.38
4	B	402	CFF	C6-N1	-2.44	1.34	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	402	CFF	C14-N7-C8	-2.46	113.61	125.43
4	C	402	CFF	C14-N7-C8	-2.29	114.42	125.43
4	A	402	CFF	C14-N7-C8	-2.25	114.58	125.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	402	CFF	4	0
4	C	402	CFF	3	0
4	A	402	CFF	5	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	335/369 (90%)	-0.15	23 (6%) 16 15	21, 31, 72, 100	0
1	B	334/369 (90%)	-0.17	20 (5%) 21 20	20, 30, 70, 98	0
1	C	334/369 (90%)	-0.09	20 (5%) 21 20	19, 29, 69, 100	0
All	All	1003/1107 (90%)	-0.14	63 (6%) 20 19	19, 30, 70, 100	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	240	TYR	9.3
1	C	240	TYR	9.1
1	C	241	SER	8.6
1	B	219	PRO	7.3
1	A	219	PRO	6.7

### 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. 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( $\text{\AA}^2$ )	Q<0.9
4	CFF	B	402	14/14	0.89	0.13	38,43,47,48	0
4	CFF	A	402	14/14	0.94	0.09	38,42,45,45	0
4	CFF	C	402	14/14	0.95	0.12	36,41,44,44	0
3	FE	A	401	1/1	0.99	0.11	28,28,28,28	0
2	FES	C	400	4/4	0.99	0.10	21,22,23,23	0
3	FE	C	401	1/1	0.99	0.09	26,26,26,26	0
3	FE	B	401	1/1	0.99	0.10	28,28,28,28	0
2	FES	B	400	4/4	1.00	0.10	21,22,22,24	0
2	FES	A	400	4/4	1.00	0.10	21,21,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.