



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2018 – 12:19 pm GMT

PDB ID : 3N2M  
Title : Crystal structure of Plasmodium falciparum orotidine 5'-monophosphate de-carboxylase complexed with 5-fluoro-6-amino-UMP  
Authors : Liu, Y.; Kotra, L.P.; Pai, E.F.  
Deposited on : 2010-05-18  
Resolution : 1.80 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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

**i**

## X-RAY DIFFRACTION

A.

Metric	Percentile Banks	Value
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Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	5253 (1.80-1.80)
Clashscore	122126	6077 (1.80-1.80)
Ramachandran outliers	120053	6011 (1.80-1.80)
Sidechain outliers	120020	6010 (1.80-1.80)
RSRZ outliers	108989	5157 (1.80-1.80)

Mol	Chain	Length	Quality of chain
1	A	342	<div> <div></div> <div>82%</div> <div>13%</div> <div>• •</div> </div>
1	B	342	<div> <div></div> <div>78%</div> <div>15%</div> <div>• 6%</div> </div>

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	EDO	B	326	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6040 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 Orotidine 5'-phosphate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	12	0
			2790	1792	455	526	17			
1	B	322	Total	C	N	O	S	0	13	0
			2757	1771	448	520	18			

There are 38 discrepancies between the modelled and reference sequences:

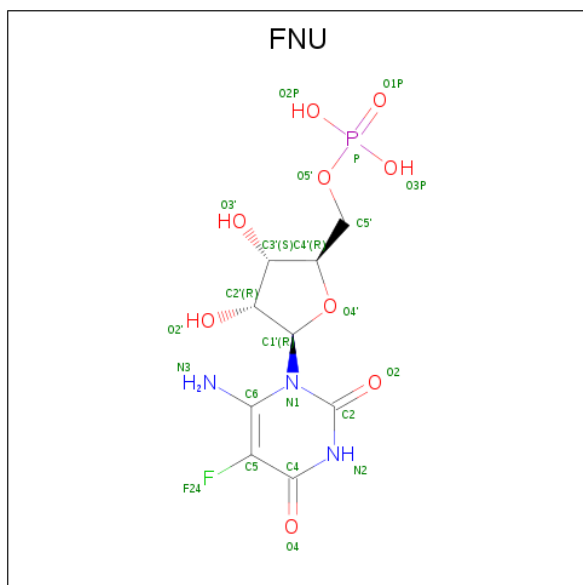
Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	EXPRESSION TAG	UNP Q8IJH3
A	-17	GLY	-	EXPRESSION TAG	UNP Q8IJH3
A	-16	SER	-	EXPRESSION TAG	UNP Q8IJH3
A	-15	SER	-	EXPRESSION TAG	UNP Q8IJH3
A	-14	HIS	-	EXPRESSION TAG	UNP Q8IJH3
A	-13	HIS	-	EXPRESSION TAG	UNP Q8IJH3
A	-12	HIS	-	EXPRESSION TAG	UNP Q8IJH3
A	-11	HIS	-	EXPRESSION TAG	UNP Q8IJH3
A	-10	HIS	-	EXPRESSION TAG	UNP Q8IJH3
A	-9	HIS	-	EXPRESSION TAG	UNP Q8IJH3
A	-8	SER	-	EXPRESSION TAG	UNP Q8IJH3
A	-7	SER	-	EXPRESSION TAG	UNP Q8IJH3
A	-6	GLY	-	EXPRESSION TAG	UNP Q8IJH3
A	-5	LEU	-	EXPRESSION TAG	UNP Q8IJH3
A	-4	VAL	-	EXPRESSION TAG	UNP Q8IJH3
A	-3	PRO	-	EXPRESSION TAG	UNP Q8IJH3
A	-2	ARG	-	EXPRESSION TAG	UNP Q8IJH3
A	-1	GLY	-	EXPRESSION TAG	UNP Q8IJH3
A	0	SER	-	EXPRESSION TAG	UNP Q8IJH3
B	-18	MET	-	EXPRESSION TAG	UNP Q8IJH3
B	-17	GLY	-	EXPRESSION TAG	UNP Q8IJH3
B	-16	SER	-	EXPRESSION TAG	UNP Q8IJH3
B	-15	SER	-	EXPRESSION TAG	UNP Q8IJH3
B	-14	HIS	-	EXPRESSION TAG	UNP Q8IJH3
B	-13	HIS	-	EXPRESSION TAG	UNP Q8IJH3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	EXPRESSION TAG	UNP Q8IJH3
B	-11	HIS	-	EXPRESSION TAG	UNP Q8IJH3
B	-10	HIS	-	EXPRESSION TAG	UNP Q8IJH3
B	-9	HIS	-	EXPRESSION TAG	UNP Q8IJH3
B	-8	SER	-	EXPRESSION TAG	UNP Q8IJH3
B	-7	SER	-	EXPRESSION TAG	UNP Q8IJH3
B	-6	GLY	-	EXPRESSION TAG	UNP Q8IJH3
B	-5	LEU	-	EXPRESSION TAG	UNP Q8IJH3
B	-4	VAL	-	EXPRESSION TAG	UNP Q8IJH3
B	-3	PRO	-	EXPRESSION TAG	UNP Q8IJH3
B	-2	ARG	-	EXPRESSION TAG	UNP Q8IJH3
B	-1	GLY	-	EXPRESSION TAG	UNP Q8IJH3
B	0	SER	-	EXPRESSION TAG	UNP Q8IJH3

- Molecule 2 is 6-amino-5-fluorouridine 5'-(dihydrogen phosphate) (three-letter code: FNU) (formula:  $C_9H_{13}FN_3O_9P$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	P	0	0
			23	9	1	3	9	1		
2	B	1	Total	C	F	N	O	P	0	0
			23	9	1	3	9	1		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



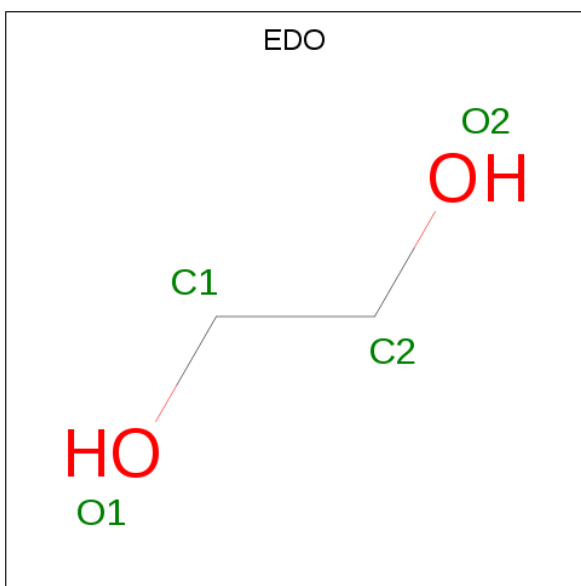
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is water.

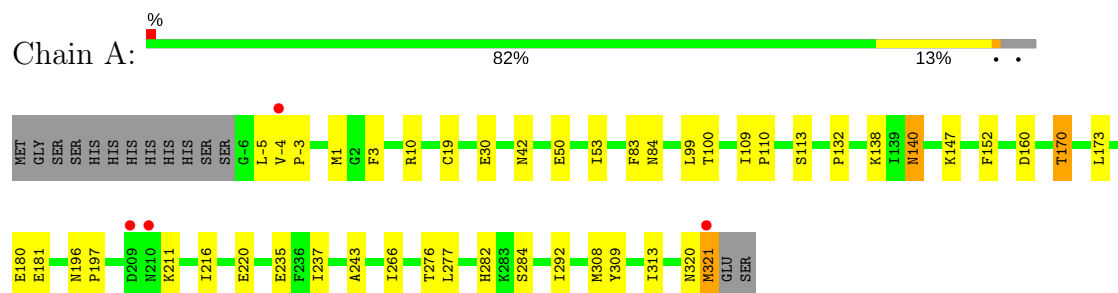
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	218	Total 218	O 218	0	0
7	B	205	Total 205	O 205	0	0



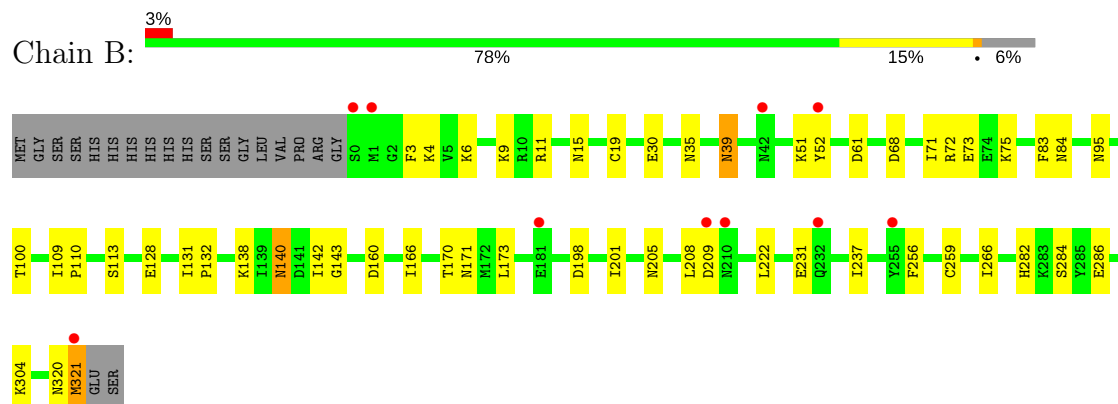
### 3 Residue-property plots [i](#)

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: Orotidine 5'-phosphate decarboxylase



- Molecule 1: Orotidine 5'-phosphate decarboxylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.64Å 83.35Å 89.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 30.55 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-1.80) 99.7 (30.55-1.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.54 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.155 , 0.189 0.155 , 0.190	Depositor DCC
$R_{free}$ test set	2872 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.0	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 54.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6040	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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: TRS, FNU, PEG, EDO, SO4

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	0.51	0/2848	0.73	0/3839
1	B	0.48	0/2813	0.75	0/3789
All	All	0.49	0/5661	0.74	0/7628

There are no bond length outliers.

There are no bond angle outliers.

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	2790	0	2751	54	0
1	B	2757	0	2722	49	0
2	A	23	0	11	5	0
2	B	23	0	11	2	0
3	A	8	0	12	2	0
4	A	7	0	10	1	0
5	B	5	0	0	0	0
6	B	4	0	6	11	0
7	A	218	0	0	9	0
7	B	205	0	0	12	0
All	All	6040	0	5523	99	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 9.

The worst 5 of 99 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:143:GLY:H	6:B:326:EDO:H12	1.28	0.94
1:B:6[A]:LYS:HE3	7:B:472:HOH:O	1.75	0.86
1:A:138[A]:LYS:NZ	2:A:324:FNU:N3	2.24	0.86
1:A:113:SER:HB2	1:B:113:SER:HB2	1.58	0.85
1:B:320:ASN:O	1:B:321:MET:HB2	1.79	0.82

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	338/342 (99%)	333 (98%)	5 (2%)	0	100	100
1	B	333/342 (97%)	326 (98%)	7 (2%)	0	100	100
All	All	671/684 (98%)	659 (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	309/311 (99%)	302 (98%)	7 (2%)	53	40
1	B	306/311 (98%)	299 (98%)	7 (2%)	53	40
All	All	615/622 (99%)	601 (98%)	14 (2%)	58	40

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	321	MET
1	B	39[A]	ASN
1	B	84	ASN
1	A	170[B]	THR
1	B	83	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	279	ASN
1	B	270	ASN
1	B	183	ASN
1	A	223	ASN
1	A	319	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 ⓘ

6 ligands are modelled in this entry.

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	FNU	A	324	-	20,24,24	1.26	2 (10%)	22,37,37	1.31	4 (18%)
3	TRS	A	325	-	7,7,7	0.25	0	9,9,9	1.07	1 (11%)
4	PEG	A	326	-	6,6,6	0.47	0	5,5,5	1.01	0
2	FNU	B	324	-	20,24,24	1.14	1 (5%)	22,37,37	1.29	1 (4%)
5	SO4	B	325	-	4,4,4	0.23	0	6,6,6	0.46	0
6	EDO	B	326	-	3,3,3	0.43	0	2,2,2	1.23	0

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	FNU	A	324	-	-	0/6/26/26	0/2/2/2
3	TRS	A	325	-	-	0/9/9/9	0/0/0/0
4	PEG	A	326	-	-	0/4/4/4	0/0/0/0
2	FNU	B	324	-	-	0/6/26/26	0/2/2/2
5	SO4	B	325	-	-	0/0/0/0	0/0/0/0
6	EDO	B	326	-	-	0/1/1/1	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	324	FNU	O4'-C1'	2.92	1.45	1.41
2	B	324	FNU	O4-C4	3.18	1.32	1.24
2	A	324	FNU	O4-C4	3.71	1.33	1.24

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	324	FNU	O3P-P-O2P	2.01	115.53	107.59
3	A	325	TRS	O3-C3-C	2.24	116.97	110.47
2	A	324	FNU	O4'-C1'-N1	2.32	111.64	108.31
2	A	324	FNU	P-O5'-C5'	2.41	124.93	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	324	FNU	F24-C5-C6	2.88	121.91	119.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	324	FNU	5	0
3	A	325	TRS	2	0
4	A	326	PEG	1	0
2	B	324	FNU	2	0
6	B	326	EDO	11	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	328/342 (95%)	-0.38	4 (1%) 79 76	8, 15, 28, 50	0
1	B	322/342 (94%)	-0.15	10 (3%) 49 43	9, 16, 30, 48	0
All	All	650/684 (95%)	-0.27	14 (2%) 62 57	8, 15, 29, 50	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	0	SER	5.2
1	B	210	ASN	4.3
1	B	255	TYR	3.7
1	A	210	ASN	3.4
1	B	321	MET	3.1

### 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
3	TRS	A	325	8/8	0.71	0.23	32,33,33,35	0
4	PEG	A	326	7/7	0.72	0.17	31,37,40,40	1
6	EDO	B	326	4/4	0.93	0.14	19,24,24,25	0
5	SO4	B	325	5/5	0.96	0.15	30,35,38,39	0
2	FNU	A	324	23/23	0.97	0.08	12,14,17,20	0
2	FNU	B	324	23/23	0.98	0.08	9,13,16,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.