



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:23 PM GMT

PDB ID : 3R3I  
Title : Crystal Structure of C-terminal truncation of UDP-glucose Pyrophosphorylase of Homo sapiens  
Authors : Zheng, X.; Yu, Q.  
Deposited on : 2011-03-15  
Resolution : 3.57 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

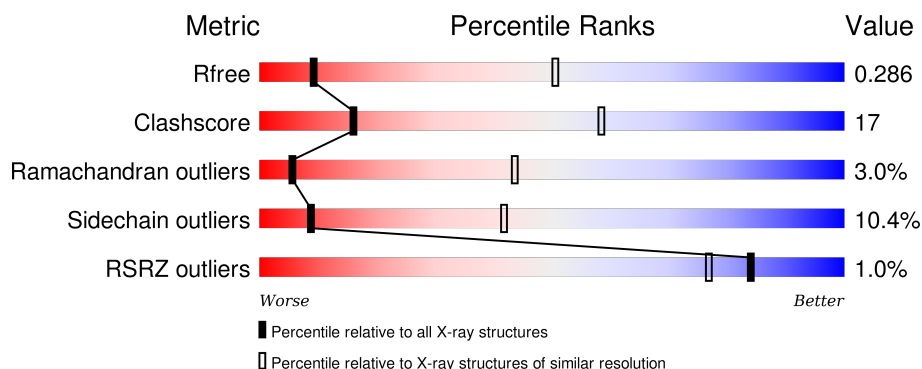
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.57 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	1261 (3.76-3.40)
Clashscore	102246	1026 (3.72-3.44)
Ramachandran outliers	100387	1028 (3.74-3.42)
Sidechain outliers	100360	1028 (3.74-3.42)
RSRZ outliers	91569	1268 (3.76-3.40)

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	528	<div> <div>55%</div> <div>27%</div> <div>•</div> <div>13%</div> </div>
1	B	528	<div> <div>52%</div> <div>30%</div> <div>5%</div> <div>12%</div> </div>
1	C	528	<div> <div>3%</div> <div>65%</div> <div>16%</div> <div>•</div> <div>17%</div> </div>
1	D	528	<div> <div>54%</div> <div>27%</div> <div>5%</div> <div>13%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13580 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 UTP--glucose-1-phosphate uridylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	0	0
			3435	2190	577	658	10			
1	B	463	Total	C	N	O	S	0	0	0
			3468	2208	587	662	11			
1	C	439	Total	C	N	O	S	0	0	0
			3191	2027	528	627	9			
1	D	460	Total	C	N	O	S	0	0	0
			3486	2225	589	661	11			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-30	MET	-	EXPRESSION TAG	UNP Q16851
A	-29	GLY	-	EXPRESSION TAG	UNP Q16851
A	-28	SER	-	EXPRESSION TAG	UNP Q16851
A	-27	SER	-	EXPRESSION TAG	UNP Q16851
A	-26	HIS	-	EXPRESSION TAG	UNP Q16851
A	-25	HIS	-	EXPRESSION TAG	UNP Q16851
A	-24	HIS	-	EXPRESSION TAG	UNP Q16851
A	-23	HIS	-	EXPRESSION TAG	UNP Q16851
A	-22	HIS	-	EXPRESSION TAG	UNP Q16851
A	-21	HIS	-	EXPRESSION TAG	UNP Q16851
A	-20	SER	-	EXPRESSION TAG	UNP Q16851
A	-19	SER	-	EXPRESSION TAG	UNP Q16851
A	-18	GLY	-	EXPRESSION TAG	UNP Q16851
A	-17	LEU	-	EXPRESSION TAG	UNP Q16851
A	-16	VAL	-	EXPRESSION TAG	UNP Q16851
A	-15	PRO	-	EXPRESSION TAG	UNP Q16851
A	-14	ARG	-	EXPRESSION TAG	UNP Q16851
A	-13	GLY	-	EXPRESSION TAG	UNP Q16851
A	-12	SER	-	EXPRESSION TAG	UNP Q16851
A	-11	HIS	-	EXPRESSION TAG	UNP Q16851
B	-30	MET	-	EXPRESSION TAG	UNP Q16851

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-29	GLY	-	EXPRESSION TAG	UNP Q16851
B	-28	SER	-	EXPRESSION TAG	UNP Q16851
B	-27	SER	-	EXPRESSION TAG	UNP Q16851
B	-26	HIS	-	EXPRESSION TAG	UNP Q16851
B	-25	HIS	-	EXPRESSION TAG	UNP Q16851
B	-24	HIS	-	EXPRESSION TAG	UNP Q16851
B	-23	HIS	-	EXPRESSION TAG	UNP Q16851
B	-22	HIS	-	EXPRESSION TAG	UNP Q16851
B	-21	HIS	-	EXPRESSION TAG	UNP Q16851
B	-20	SER	-	EXPRESSION TAG	UNP Q16851
B	-19	SER	-	EXPRESSION TAG	UNP Q16851
B	-18	GLY	-	EXPRESSION TAG	UNP Q16851
B	-17	LEU	-	EXPRESSION TAG	UNP Q16851
B	-16	VAL	-	EXPRESSION TAG	UNP Q16851
B	-15	PRO	-	EXPRESSION TAG	UNP Q16851
B	-14	ARG	-	EXPRESSION TAG	UNP Q16851
B	-13	GLY	-	EXPRESSION TAG	UNP Q16851
B	-12	SER	-	EXPRESSION TAG	UNP Q16851
B	-11	HIS	-	EXPRESSION TAG	UNP Q16851
C	-30	MET	-	EXPRESSION TAG	UNP Q16851
C	-29	GLY	-	EXPRESSION TAG	UNP Q16851
C	-28	SER	-	EXPRESSION TAG	UNP Q16851
C	-27	SER	-	EXPRESSION TAG	UNP Q16851
C	-26	HIS	-	EXPRESSION TAG	UNP Q16851
C	-25	HIS	-	EXPRESSION TAG	UNP Q16851
C	-24	HIS	-	EXPRESSION TAG	UNP Q16851
C	-23	HIS	-	EXPRESSION TAG	UNP Q16851
C	-22	HIS	-	EXPRESSION TAG	UNP Q16851
C	-21	HIS	-	EXPRESSION TAG	UNP Q16851
C	-20	SER	-	EXPRESSION TAG	UNP Q16851
C	-19	SER	-	EXPRESSION TAG	UNP Q16851
C	-18	GLY	-	EXPRESSION TAG	UNP Q16851
C	-17	LEU	-	EXPRESSION TAG	UNP Q16851
C	-16	VAL	-	EXPRESSION TAG	UNP Q16851
C	-15	PRO	-	EXPRESSION TAG	UNP Q16851
C	-14	ARG	-	EXPRESSION TAG	UNP Q16851
C	-13	GLY	-	EXPRESSION TAG	UNP Q16851
C	-12	SER	-	EXPRESSION TAG	UNP Q16851
C	-11	HIS	-	EXPRESSION TAG	UNP Q16851
D	-30	MET	-	EXPRESSION TAG	UNP Q16851
D	-29	GLY	-	EXPRESSION TAG	UNP Q16851
D	-28	SER	-	EXPRESSION TAG	UNP Q16851

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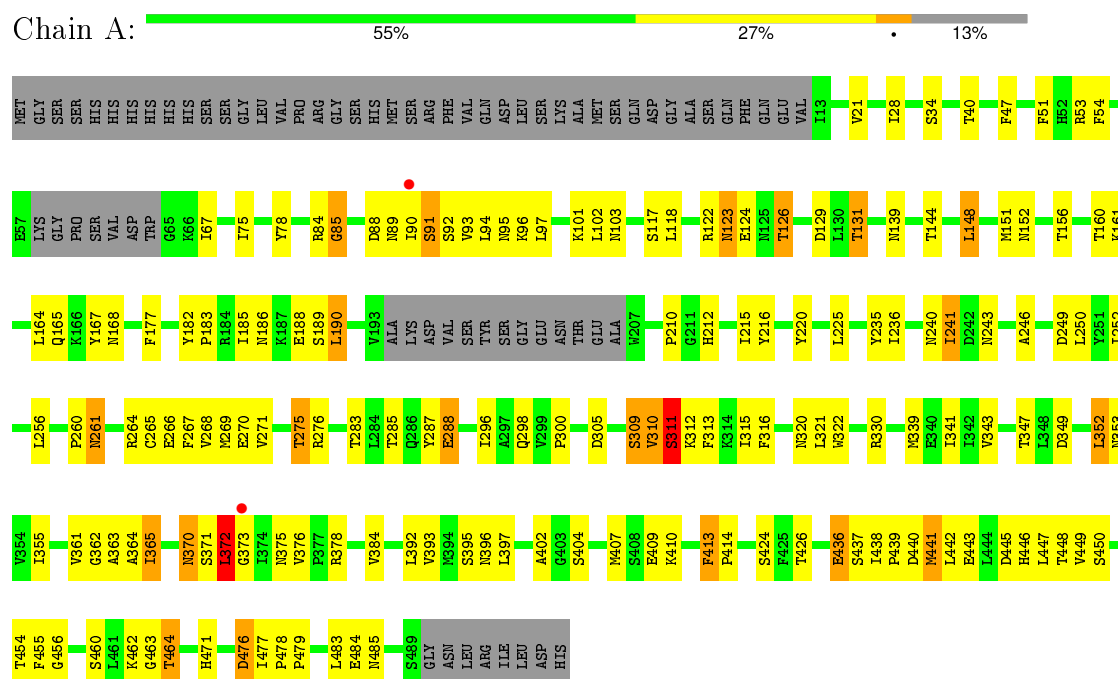
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-27	SER	-	EXPRESSION TAG	UNP Q16851
D	-26	HIS	-	EXPRESSION TAG	UNP Q16851
D	-25	HIS	-	EXPRESSION TAG	UNP Q16851
D	-24	HIS	-	EXPRESSION TAG	UNP Q16851
D	-23	HIS	-	EXPRESSION TAG	UNP Q16851
D	-22	HIS	-	EXPRESSION TAG	UNP Q16851
D	-21	HIS	-	EXPRESSION TAG	UNP Q16851
D	-20	SER	-	EXPRESSION TAG	UNP Q16851
D	-19	SER	-	EXPRESSION TAG	UNP Q16851
D	-18	GLY	-	EXPRESSION TAG	UNP Q16851
D	-17	LEU	-	EXPRESSION TAG	UNP Q16851
D	-16	VAL	-	EXPRESSION TAG	UNP Q16851
D	-15	PRO	-	EXPRESSION TAG	UNP Q16851
D	-14	ARG	-	EXPRESSION TAG	UNP Q16851
D	-13	GLY	-	EXPRESSION TAG	UNP Q16851
D	-12	SER	-	EXPRESSION TAG	UNP Q16851
D	-11	HIS	-	EXPRESSION TAG	UNP Q16851

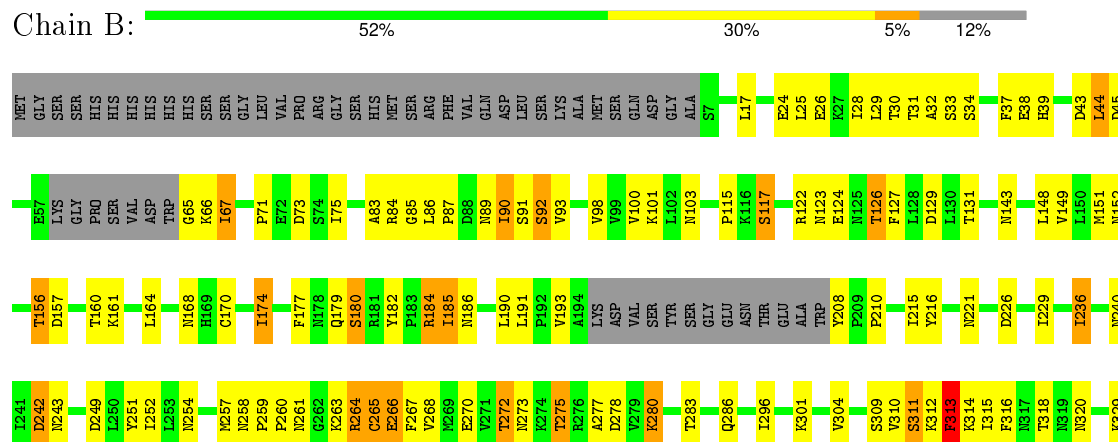
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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: UTP--glucose-1-phosphate uridylyltransferase



- Molecule 1: UTP--glucose-1-phosphate uridylyltransferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.27Å 140.27Å 315.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.98 – 3.57 19.98 – 3.57	Depositor EDS
% Data completeness (in resolution range)	98.7 (19.98-3.57) 98.7 (19.98-3.57)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 3.52Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.233 , 0.286 0.229 , 0.286	Depositor DCC
$R_{free}$ test set	2158 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	122.2	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 98.6	EDS
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 42839 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13580	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	175.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.56	0/3496	0.71	3/4759 (0.1%)
1	B	0.64	1/3530 (0.0%)	0.81	1/4812 (0.0%)
1	C	0.47	0/3242	0.61	0/4429
1	D	0.69	0/3549	0.86	2/4831 (0.0%)
All	All	0.60	1/13817 (0.0%)	0.76	6/18831 (0.0%)

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	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	424	SER	CB-OG	7.02	1.51	1.42

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	LEU	CA-CB-CG	5.85	128.76	115.30
1	D	123	ASN	N-CA-C	5.45	125.70	111.00
1	D	405	LEU	CA-CB-CG	5.33	127.57	115.30
1	A	372	LEU	CA-CB-CG	5.25	127.37	115.30
1	A	123	ASN	N-CA-C	5.19	125.02	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	89	ASN	Peptide

## 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	3435	0	3332	114	0
1	B	3468	0	3341	143	0
1	C	3191	0	2963	70	0
1	D	3486	0	3410	127	1
All	All	13580	0	13046	450	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 17.

The worst 5 of 450 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:C:265:CYS:CA	1:C:266:GLU:HB2	1.74	1.16
1:B:310:VAL:HB	1:B:312:LYS:HG3	1.26	1.12
1:C:265:CYS:HA	1:C:266:GLU:CB	1.80	1.11
1:A:413:PHE:CD2	1:A:414:PRO:HD2	1.91	1.04
1:A:264:ARG:NH1	1:A:372:LEU:HG	1.75	1.00

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)
1:D:309:SER:OG	1:D:412:GLU:OE2[4_555]	2.12	0.08

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	451/528 (85%)	386 (86%)	49 (11%)	16 (4%)	4	40
1	B	457/528 (87%)	380 (83%)	64 (14%)	13 (3%)	6	45
1	C	425/528 (80%)	376 (88%)	39 (9%)	10 (2%)	7	49
1	D	454/528 (86%)	393 (87%)	46 (10%)	15 (3%)	5	41
All	All	1787/2112 (85%)	1535 (86%)	198 (11%)	54 (3%)	5	43

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	SER
1	B	266	GLU
1	B	415	THR
1	C	266	GLU
1	C	418	LEU

### 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	365/470 (78%)	321 (88%)	44 (12%)	6	33
1	B	368/470 (78%)	319 (87%)	49 (13%)	5	29
1	C	328/470 (70%)	313 (95%)	15 (5%)	33	73
1	D	375/470 (80%)	334 (89%)	41 (11%)	8	39
All	All	1436/1880 (76%)	1287 (90%)	149 (10%)	9	42

5 of 149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	313	PHE
1	B	404	SER
1	D	393	VAL
1	B	318	THR
1	B	347	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	332	GLN
1	C	143	ASN
1	D	458	ASN
1	C	133	GLN
1	C	179	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 ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	457/528 (86%)	-0.44	2 (0%) 93 90	111, 166, 262, 329	0
1	B	463/528 (87%)	-0.55	0 100 100	118, 155, 259, 321	0
1	C	439/528 (83%)	-0.14	17 (3%) 43 34	112, 243, 336, 404	0
1	D	460/528 (87%)	-0.62	0 100 100	102, 130, 188, 244	0
All	All	1819/2112 (86%)	-0.44	19 (1%) 84 77	102, 158, 293, 404	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	258	ASN	7.2
1	C	288	GLU	5.3
1	C	16	GLU	3.3
1	C	265	CYS	3.0
1	C	349	ASP	2.8

### 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.