



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:50 PM UTC

PDB ID : 2PC5 / pdb\_00002pc5  
Title : Native crystal structure analysis on Arabidopsis dUTPase  
Authors : Moriyama, H.; Bajaj, M.  
Deposited on : 2007-03-29  
Resolution : 2.20 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

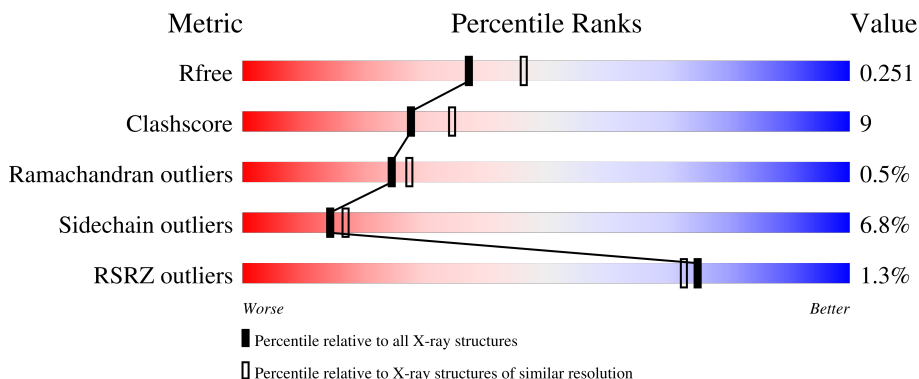
# 1 Overall quality at a glance

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))
$R_{free}$	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 of 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	169	 2% 62% 10% 2% 25%
1	B	169	 2% 51% 18% 2% 25%
1	C	169	 59% 13% 2% 25%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3078 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 DUTP pyrophosphatase-like protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	127	958	614	161	183	0	0	0
1	B	126	949	609	160	180	0	0	0
1	C	127	958	614	161	183	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q9STG6
A	-1	SER	-	expression tag	UNP Q9STG6
A	0	HIS	-	expression tag	UNP Q9STG6
B	-2	GLY	-	expression tag	UNP Q9STG6
B	-1	SER	-	expression tag	UNP Q9STG6
B	0	HIS	-	expression tag	UNP Q9STG6
C	-2	GLY	-	expression tag	UNP Q9STG6
C	-1	SER	-	expression tag	UNP Q9STG6
C	0	HIS	-	expression tag	UNP Q9STG6

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	62	Total	O	0	0
			62	62		

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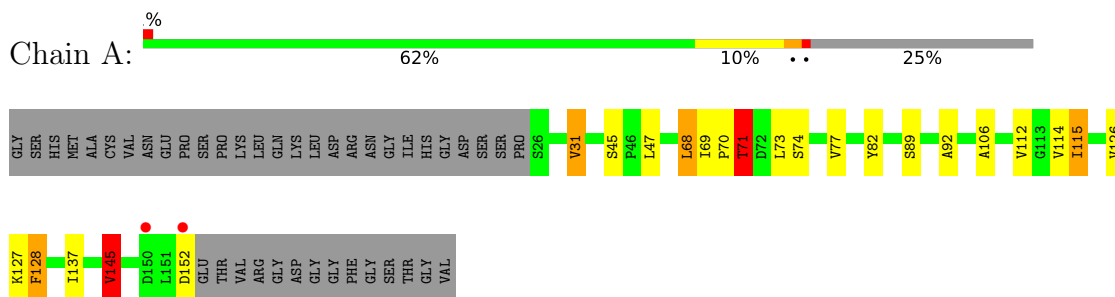
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	B	70	Total	O	0	0
			70	70		
3	C	80	Total	O	0	0
			80	80		

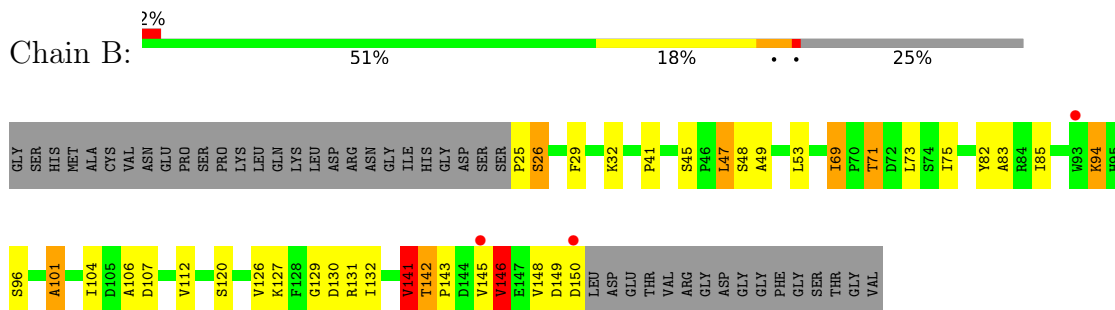
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

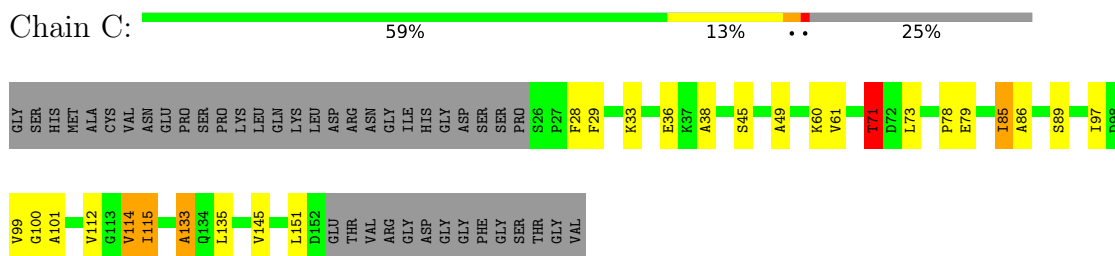
- Molecule 1: DUTP pyrophosphatase-like protein



- Molecule 1: DUTP pyrophosphatase-like protein



- Molecule 1: DUTP pyrophosphatase-like protein



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.90Å 70.86Å 75.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.46 – 2.20 21.46 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (21.46-2.20) 99.1 (21.46-2.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	52.61 (at 2.19Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.182 , 0.251 0.182 , 0.251	Depositor DCC
$R_{free}$ test set	992 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.2	Xtrriage
Anisotropy	0.062	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 39.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.014 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3078	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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: MG

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	1.37	5/978 (0.5%)	1.32	8/1330 (0.6%)
1	B	1.39	3/970 (0.3%)	1.34	10/1319 (0.8%)
1	C	1.35	4/978 (0.4%)	1.25	7/1330 (0.5%)
All	All	1.37	12/2926 (0.4%)	1.30	25/3979 (0.6%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	70	PRO	C-N	-13.43	1.14	1.33
1	C	60	LYS	C-N	-9.40	1.24	1.33
1	C	133	ALA	CA-CB	6.26	1.63	1.53
1	A	77	VAL	CA-CB	6.02	1.60	1.55
1	A	115	ILE	CA-CB	6.02	1.61	1.54
1	B	101	ALA	CA-C	5.75	1.58	1.53
1	C	115	ILE	CA-CB	5.40	1.60	1.54
1	A	92	ALA	CA-CB	5.25	1.61	1.53
1	C	86	ALA	CA-CB	-5.23	1.47	1.53
1	B	75	ILE	CA-CB	5.16	1.62	1.54
1	A	137	ILE	CA-CB	5.12	1.59	1.53
1	B	69	ILE	CA-C	5.00	1.57	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	61	VAL	CB-CA-C	11.75	122.24	111.08
1	A	145	VAL	CB-CA-C	-9.05	97.50	111.26
1	A	69	ILE	CA-C-N	8.46	128.22	119.76
1	A	69	ILE	C-N-CA	8.46	128.22	119.76
1	C	71	THR	N-CA-C	-6.94	105.43	114.04
1	B	141	VAL	CB-CA-C	6.64	121.05	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	130	ASP	N-CA-C	6.28	119.78	110.48
1	A	115	ILE	N-CA-CB	6.14	117.41	110.72
1	A	128	PHE	CB-CA-C	6.02	118.87	109.84
1	A	71	THR	N-CA-CB	-5.91	101.84	110.53
1	C	71	THR	N-CA-CB	-5.81	102.21	110.81
1	B	146	VAL	N-CA-C	5.68	121.16	109.34
1	A	114	VAL	CA-C-N	-5.63	115.11	122.37
1	A	114	VAL	C-N-CA	-5.63	115.11	122.37
1	C	115	ILE	N-CA-CB	5.41	117.17	111.00
1	B	41	PRO	CA-C-N	-5.38	114.14	122.59
1	B	41	PRO	C-N-CA	-5.38	114.14	122.59
1	B	106	ALA	CA-C-N	5.36	131.37	121.52
1	B	106	ALA	C-N-CA	5.36	131.37	121.52
1	C	115	ILE	CA-CB-CG2	5.36	119.61	110.50
1	B	129	GLY	CA-C-N	-5.35	112.51	121.39
1	B	129	GLY	C-N-CA	-5.35	112.51	121.39
1	C	114	VAL	CA-C-N	-5.10	116.00	122.37
1	C	114	VAL	C-N-CA	-5.10	116.00	122.37
1	B	94	LYS	CB-CA-C	5.05	120.55	109.99

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	958	0	972	13	0
1	B	949	0	966	28	0
1	C	958	0	973	21	0
2	A	1	0	0	0	0
3	A	62	0	0	0	0
3	B	70	0	0	2	0
3	C	80	0	0	0	0
All	All	3078	0	2911	52	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.

All (52) 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:85:ILE:HD11	1:B:104:ILE:HD11	1.49	0.91
1:B:45:SER:O	1:B:48:SER:HB2	1.74	0.88
1:A:71:THR:CG2	1:A:73:LEU:HB2	2.16	0.76
1:B:25:PRO:HA	1:B:26:SER:O	1.89	0.71
1:B:69:ILE:HG21	1:B:132:ILE:HD13	1.72	0.70
1:B:145:VAL:HG12	1:B:145:VAL:O	1.90	0.70
1:B:141:VAL:HG13	1:B:143:PRO:HD3	1.74	0.70
1:C:33:LYS:HE3	1:C:38:ALA:O	1.91	0.69
1:A:145:VAL:HG13	1:B:29:PHE:CD2	2.28	0.68
1:B:71:THR:HB	1:B:112:VAL:O	1.94	0.68
1:C:85:ILE:HD12	1:C:133:ALA:HB1	1.74	0.68
1:C:85:ILE:HD13	1:C:114:VAL:HG22	1.76	0.67
1:A:31:VAL:HG13	1:C:145:VAL:HG13	1.77	0.66
1:A:71:THR:HB	1:A:112:VAL:O	1.95	0.66
1:B:69:ILE:CG2	1:B:132:ILE:HD13	2.29	0.63
1:B:142:THR:O	1:B:142:THR:HG23	1.99	0.62
1:C:85:ILE:HD12	1:C:133:ALA:CB	2.31	0.60
1:A:71:THR:HG22	1:A:73:LEU:H	1.67	0.59
1:B:82:TYR:HB3	1:C:49:ALA:HB2	1.84	0.58
1:A:47:LEU:HD22	1:C:79:GLU:HG3	1.85	0.58
1:C:85:ILE:HG13	1:C:85:ILE:O	2.03	0.58
1:C:85:ILE:HD11	1:C:114:VAL:HG13	1.86	0.57
1:B:148:VAL:HG23	1:B:150:ASP:H	1.69	0.56
1:B:45:SER:O	1:B:48:SER:CB	2.51	0.55
1:B:101:ALA:HB2	1:C:89:SER:HA	1.89	0.54
1:B:107:ASP:OD2	1:C:45:SER:HB3	2.08	0.53
1:B:32:LYS:NZ	3:B:221:HOH:O	2.35	0.53
1:B:71:THR:HG22	1:B:73:LEU:H	1.73	0.53
1:B:85:ILE:CD1	1:B:104:ILE:HD11	2.32	0.52
1:C:85:ILE:HG13	1:C:99:VAL:HG11	1.92	0.51
1:B:25:PRO:HA	1:B:26:SER:C	2.34	0.50
1:B:146:VAL:HG12	1:B:146:VAL:O	2.12	0.50
1:B:83:ALA:HB3	1:B:104:ILE:HB	1.93	0.50
1:B:142:THR:HG22	3:B:231:HOH:O	2.12	0.49
1:C:100:GLY:O	1:C:101:ALA:C	2.57	0.48
1:B:96:SER:HB2	1:B:120:SER:HB3	1.97	0.47
1:C:71:THR:HG23	1:C:73:LEU:HG	1.96	0.47
1:C:71:THR:HG22	1:C:73:LEU:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:SER:HA	1:C:101:ALA:HB2	1.96	0.47
1:C:28:PHE:O	1:C:78:PRO:HD3	2.15	0.47
1:B:142:THR:O	1:B:142:THR:CG2	2.63	0.45
1:A:106:ALA:HB3	1:B:47:LEU:HB3	1.99	0.45
1:C:85:ILE:CD1	1:C:133:ALA:CB	2.95	0.45
1:A:127:LYS:O	1:A:128:PHE:C	2.57	0.45
1:A:74:SER:HB3	1:C:151:LEU:HD11	1.99	0.44
1:B:71:THR:CG2	1:B:73:LEU:HB2	2.48	0.43
1:C:29:PHE:CZ	1:C:135:LEU:HD23	2.54	0.43
1:A:71:THR:HG23	1:A:73:LEU:CG	2.49	0.43
1:A:68:LEU:C	1:A:68:LEU:HD13	2.44	0.42
1:A:82:TYR:HB3	1:B:49:ALA:HB2	2.03	0.41
1:B:53:LEU:O	1:B:131:ARG:HA	2.20	0.41
1:C:71:THR:HB	1:C:112:VAL:O	2.21	0.40

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	125/169 (74%)	124 (99%)	1 (1%)	0	100	100
1	B	124/169 (73%)	114 (92%)	8 (6%)	2 (2%)	7	6
1	C	125/169 (74%)	123 (98%)	2 (2%)	0	100	100
All	All	374/507 (74%)	361 (96%)	11 (3%)	2 (0%)	24	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	146	VAL
1	B	26	SER

### 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	104/137 (76%)	96 (92%)	8 (8%)	12	13
1	B	103/137 (75%)	95 (92%)	8 (8%)	11	13
1	C	104/137 (76%)	99 (95%)	5 (5%)	23	30
All	All	311/411 (76%)	290 (93%)	21 (7%)	14	17

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	VAL
1	A	45	SER
1	A	68	LEU
1	A	71	THR
1	A	115	ILE
1	A	126	VAL
1	A	145	VAL
1	A	152	ASP
1	B	47	LEU
1	B	71	THR
1	B	94	LYS
1	B	126	VAL
1	B	127	LYS
1	B	141	VAL
1	B	142	THR
1	B	149	ASP
1	C	36	GLU
1	C	71	THR
1	C	85	ILE
1	C	97	ILE
1	C	115	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	70:PRO	C	71:THR	N	1.14

## 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	127/169 (75%)	-0.53	2 (1%) 70 67	10, 17, 31, 55	0
1	B	126/169 (74%)	-0.40	3 (2%) 59 56	10, 17, 41, 51	0
1	C	127/169 (75%)	-0.42	0 100 100	12, 20, 33, 45	0
All	All	380/507 (74%)	-0.45	5 (1%) 75 73	10, 18, 37, 55	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	152	ASP	3.2
1	A	150	ASP	3.2
1	B	145	VAL	2.3
1	B	150	ASP	2.2
1	B	93	TRP	2.1

### 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 oligosaccharides 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
2	MG	A	167	1/1	0.86	0.08	8,8,8,8	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.