



# Full wwPDB X-ray Structure Validation Report

May 13, 2020 – 03:33 am BST

PDB ID : 4BL0  
Title : Crystal structure of yeast Bub3-Bub1 bound to phospho-Spc105  
Authors : Primorac, I.; Weir, J.R.; Musacchio, A.  
Deposited on : 2013-04-30  
Resolution : 1.95 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 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

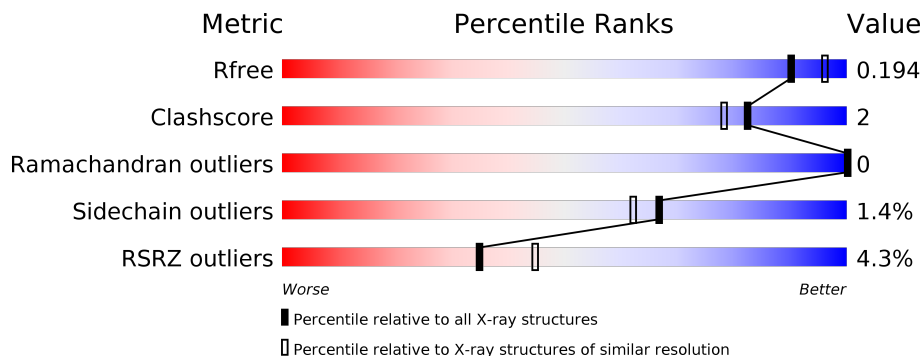
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	341	
1	D	341	
2	B	75	
2	E	75	
3	C	19	
3	F	19	

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 6408 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 CELL CYCLE ARREST PROTEIN BUB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	331	2569	1636	433	486	14	0	2	0
1	D	331	2575	1642	430	490	13	0	2	0

- Molecule 2 is a protein called CHECKPOINT SERINE/THREONINE-PROTEIN KINASE BUB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	44	348	232	54	61	1	0	0	0
2	E	45	373	244	60	68	1	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	285	PRO	-	expression tag	UNP P41695
B	286	LEU	-	expression tag	UNP P41695
B	287	GLY	-	expression tag	UNP P41695
B	288	SER	-	expression tag	UNP P41695
E	285	PRO	-	expression tag	UNP P41695
E	286	LEU	-	expression tag	UNP P41695
E	287	GLY	-	expression tag	UNP P41695
E	288	SER	-	expression tag	UNP P41695

- Molecule 3 is a protein called SPINDLE POLE BODY COMPONENT SPC105.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
3	C	12	94	57	12	22	1	2	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	P				S
3	F	12	91	56	12	20	1	2	0	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

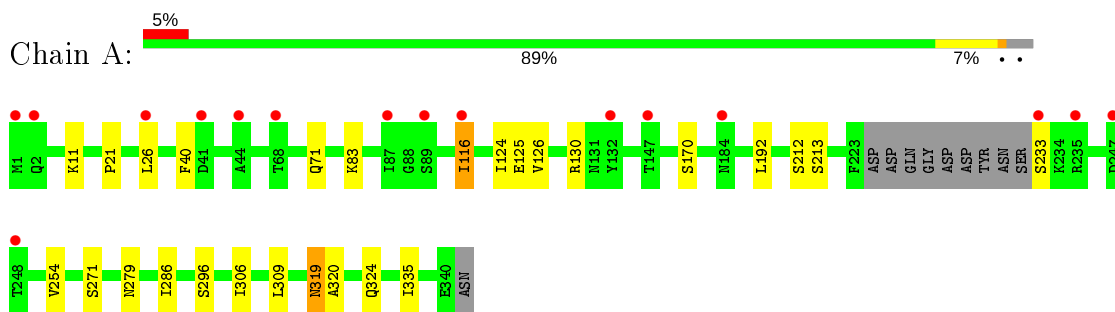
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	153	Total	O	0	0
			153	153		
5	B	10	Total	O	0	0
			10	10		
5	C	4	Total	O	0	0
			4	4		
5	D	163	Total	O	0	0
			163	163		
5	E	20	Total	O	0	0
			20	20		
5	F	6	Total	O	0	0
			6	6		

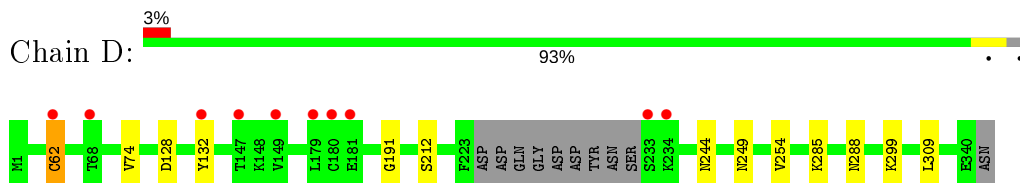
### 3 Residue-property plots [i](#)

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.

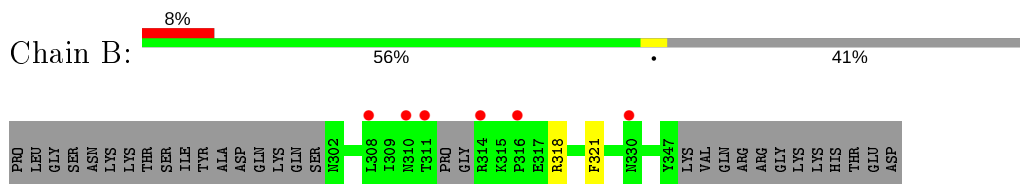
- Molecule 1: CELL CYCLE ARREST PROTEIN BUB3



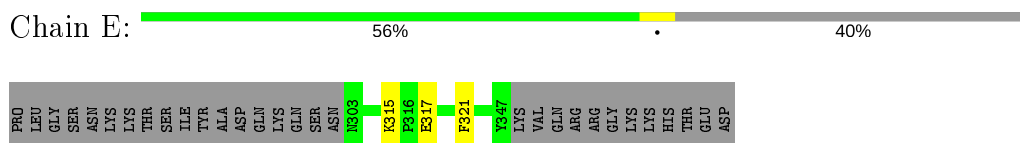
- Molecule 1: CELL CYCLE ARREST PROTEIN BUB3



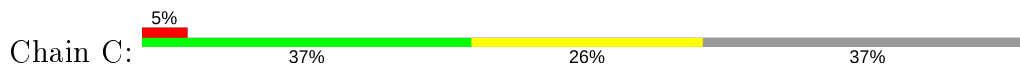
- Molecule 2: CHECKPOINT SERINE/THREONINE-PROTEIN KINASE BUB1

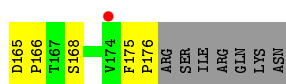


- Molecule 2: CHECKPOINT SERINE/THREONINE-PROTEIN KINASE BUB1



- Molecule 3: SPINDLE POLE BODY COMPONENT SPC105





- Molecule 3: SPINDLE POLE BODY COMPONENT SPC105



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.74Å 57.90Å 118.67Å 90.00° 102.53° 90.00°	Depositor
Resolution (Å)	46.88 – 1.95 46.88 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.7 (46.88-1.95) 98.7 (46.88-1.95)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.88 (at 1.95Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.1_1168)	Depositor
R, $R_{free}$	0.179 , 0.192 0.181 , 0.194	Depositor DCC
$R_{free}$ test set	3361 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.2	Xtrriage
Anisotropy	0.046	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 54.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6408	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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: TPO, 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	0.50	2/2614 (0.1%)	0.52	1/3548 (0.0%)
1	D	0.33	0/2620	0.49	0/3554
2	B	0.48	0/355	0.53	1/481 (0.2%)
2	E	0.25	0/382	0.40	0/518
3	C	1.08	0/84	0.75	0/112
3	F	0.26	0/81	0.42	0/107
All	All	0.43	2/6136 (0.0%)	0.51	2/8320 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	116	ILE	C-N	-6.99	1.18	1.34
1	A	319	ASN	CG-ND2	-5.25	1.19	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	ILE	O-C-N	-6.89	111.67	122.70
2	B	318	ARG	NE-CZ-NH1	5.08	122.84	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	2569	0	2528	19	0
1	D	2575	0	2533	7	0
2	B	348	0	335	0	0
2	E	373	0	369	2	0
3	C	94	0	78	3	0
3	F	91	0	77	2	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	A	153	0	0	3	0
5	B	10	0	0	0	0
5	C	4	0	0	0	0
5	D	163	0	0	0	0
5	E	20	0	0	0	0
5	F	6	0	0	1	0
All	All	6408	0	5920	30	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 2.

All (30) 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:26:LEU:CD1	1:A:335:ILE:HD11	2.25	0.67
1:A:319:ASN:OD1	1:A:324:GLN:NE2	2.30	0.65
1:A:320:ALA:HB3	1:A:324:GLN:OE1	1.97	0.65
1:A:21:PRO:O	5:A:2029:HOH:O	2.16	0.61
1:A:26:LEU:HG	1:A:40:PHE:HD2	1.69	0.58
1:A:116:ILE:HD11	1:A:124:ILE:HG22	1.89	0.55
1:D:212:SER:HB2	1:D:254:VAL:HB	1.90	0.54
1:A:116:ILE:HD12	1:A:125:GLU:O	2.09	0.53
1:A:26:LEU:HG	1:A:40:PHE:CD2	2.43	0.53
1:A:212:SER:HB2	1:A:254:VAL:HB	1.91	0.52
3:F:167:THR:HG22	5:F:2001:HOH:O	2.09	0.51
1:A:11:LYS:NZ	5:A:2016:HOH:O	2.41	0.51
1:A:26:LEU:HD11	1:A:335:ILE:HD11	1.93	0.51
1:A:26:LEU:HD11	1:A:335:ILE:CD1	2.41	0.51
1:D:62:CYS:HB2	1:D:74:VAL:HG12	1.94	0.50
1:D:249:ASN:HB2	2:E:317:GLU:HG2	1.93	0.49
1:A:26:LEU:HD21	1:A:306:ILE:HD11	1.95	0.48
1:A:192:LEU:HD13	1:A:213:SER:HB3	1.96	0.48
3:C:165:ASP:N	3:C:166:PRO:HD2	2.29	0.47
1:D:285:LYS:NZ	1:D:288:ASN:HD21	2.12	0.47

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:175:PHE:HA	3:C:176:PRO:HD3	1.75	0.46
1:A:271:SER:HA	1:A:296[A]:SER:HB3	1.98	0.45
1:A:71:GLN:OE1	1:A:83:LYS:HE3	2.17	0.45
1:A:116:ILE:HD13	1:A:126:VAL:HG22	1.99	0.44
1:A:233:SER:N	5:A:2107:HOH:O	2.51	0.43
1:D:191:GLY:HA2	3:F:175:PHE:O	2.18	0.43
1:D:128:ASP:HB3	1:D:132:TYR:HD2	1.84	0.42
3:C:165:ASP:HB3	3:C:166:PRO:CD	2.49	0.42
1:D:244:ASN:OD1	2:E:315:LYS:NZ	2.50	0.41
1:A:279:ASN:HB2	1:A:286:ILE:HD11	2.02	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	329/341 (96%)	322 (98%)	7 (2%)	0	100	100
1	D	329/341 (96%)	319 (97%)	10 (3%)	0	100	100
2	B	40/75 (53%)	36 (90%)	4 (10%)	0	100	100
2	E	43/75 (57%)	40 (93%)	3 (7%)	0	100	100
3	C	9/19 (47%)	9 (100%)	0	0	100	100
3	F	9/19 (47%)	9 (100%)	0	0	100	100
All	All	759/870 (87%)	735 (97%)	24 (3%)	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	281/305 (92%)	278 (99%)	3 (1%)	73	71
1	D	281/305 (92%)	278 (99%)	3 (1%)	73	71
2	B	35/69 (51%)	34 (97%)	1 (3%)	42	31
2	E	41/69 (59%)	40 (98%)	1 (2%)	49	40
3	C	10/18 (56%)	9 (90%)	1 (10%)	7	2
3	F	9/18 (50%)	9 (100%)	0	100	100
All	All	657/784 (84%)	648 (99%)	9 (1%)	67	62

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	ARG
1	A	170	SER
1	A	309	LEU
2	B	321	PHE
3	C	168	SER
1	D	62	CYS
1	D	299	LYS
1	D	309	LEU
2	E	321	PHE

Some 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](#)

2 non-standard protein/DNA/RNA residues 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
3	TPO	F	172	3	8,10,11	1.06	0	10,14,16	1.66	2 (20%)
3	TPO	C	172	3	8,10,11	0.97	0	10,14,16	1.69	2 (20%)

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
3	TPO	F	172	3	-	4/9/11/13	-
3	TPO	C	172	3	-	4/9/11/13	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	172	TPO	P-OG1-CB	-4.06	110.95	123.21
3	F	172	TPO	P-OG1-CB	-4.03	111.04	123.21
3	C	172	TPO	CG2-CB-CA	-2.69	107.85	113.16
3	F	172	TPO	CG2-CB-CA	-2.45	108.33	113.16

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	172	TPO	N-CA-CB-OG1
3	F	172	TPO	CB-OG1-P-O1P
3	C	172	TPO	N-CA-CB-OG1
3	C	172	TPO	CB-OG1-P-O1P
3	F	172	TPO	CB-OG1-P-O2P
3	C	172	TPO	CB-OG1-P-O2P
3	F	172	TPO	O-C-CA-CB
3	C	172	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are 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	116:ILE	C	117:ALA	N	1.18

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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	331/341 (97%)	0.15	16 (4%) 30 40	17, 32, 66, 93	11 (3%)
1	D	331/341 (97%)	0.04	10 (3%) 50 59	15, 28, 65, 98	12 (3%)
2	B	44/75 (58%)	0.67	6 (13%) 3 4	19, 35, 88, 94	1 (2%)
2	E	45/75 (60%)	-0.02	0 100 100	17, 29, 50, 69	4 (8%)
3	C	11/19 (57%)	0.35	1 (9%) 9 15	36, 42, 51, 76	0
3	F	11/19 (57%)	-0.14	0 100 100	30, 36, 60, 67	1 (9%)
All	All	773/870 (88%)	0.12	33 (4%) 35 45	15, 31, 71, 98	29 (3%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	233	SER	6.0
1	D	147	THR	4.9
1	A	87	ILE	4.7
2	B	311	THR	4.6
1	D	233	SER	3.9
1	A	26	LEU	3.7
1	A	147	THR	3.5
2	B	314	ARG	3.3
1	D	62	CYS	3.2
1	A	247	ASP	3.0
1	A	1	MET	3.0
1	A	132	TYR	2.9
1	D	132	TYR	2.9
1	D	179	LEU	2.9
2	B	308	LEU	2.8
2	B	330	ASN	2.8
1	A	89	SER	2.8
1	D	234	LYS	2.7
1	D	149	VAL	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	310	ASN	2.6
3	C	174	VAL	2.5
1	A	2	GLN	2.4
2	B	316	PRO	2.3
1	A	248	THR	2.3
1	A	116	ILE	2.3
1	A	235	ARG	2.2
1	D	180	CYS	2.2
1	A	68	THR	2.2
1	A	44	ALA	2.2
1	A	41	ASP	2.1
1	D	68	THR	2.1
1	D	181	GLU	2.1
1	A	184	ASN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
3	TPO	C	172	11/12	0.96	0.08	31,35,48,53	0
3	TPO	F	172	11/12	0.98	0.11	23,28,33,34	0

## 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(Å <sup>2</sup> )	Q<0.9
4	MG	A	1341	1/1	0.99	0.10	22,22,22,22	0
4	MG	D	1341	1/1	0.99	0.13	17,17,17,17	0

## 6.5 Other polymers

There are no such residues in this entry.