



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 10:55 AM GMT

PDB ID : 1H26  
Title : CDK2/CYCLIN A IN COMPLEX WITH AN 11-RESIDUE RECRUITMENT PEPTIDE FROM P53  
Authors : Tews, I.; Cheng, K.Y.; Lowe, E.D.; Noble, M.E.M.; Brown, N.R.; Gul, S.; Gamblin, S.; Johnson, L.N.  
Deposited on : 2002-07-31  
Resolution : 2.24 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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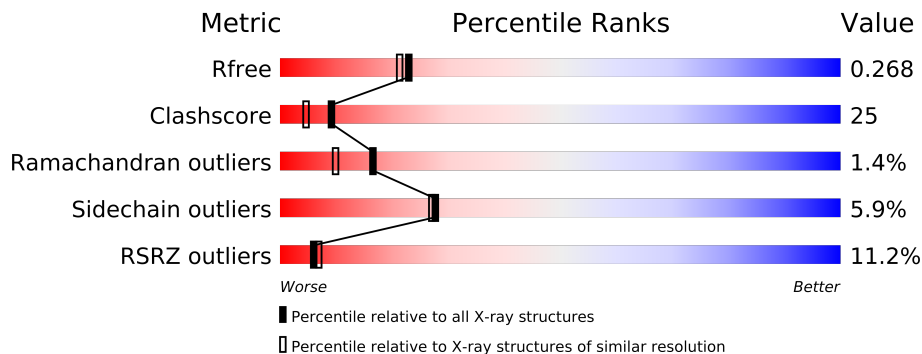
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance


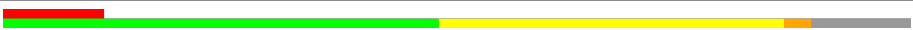

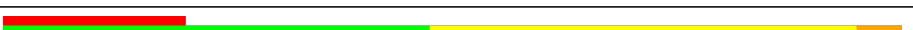
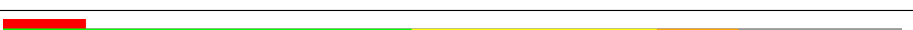
The reported resolution of this entry is 2.24 Å.

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))
$R_{free}$	66092	1112 (2.26-2.22)
Clashscore	79885	1317 (2.26-2.22)
Ramachandran outliers	78287	1282 (2.26-2.22)
Sidechain outliers	78261	1282 (2.26-2.22)
RSRZ outliers	66119	1112 (2.26-2.22)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	303	
1	C	303	
2	B	259	
2	D	259	
3	E	11	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8981 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	P	S	9	0	1
			2389	1550	405	425	1	8			
1	C	269	Total	C	N	O	P	S	0	0	1
			2149	1392	367	382	1	7			

- Molecule 2 is a protein called CYCLIN A2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S		0	0	0
			2084	1350	339	384	11				
2	D	258	Total	C	N	O	S		0	0	0
			2084	1350	339	384	11				

- Molecule 3 is a protein called CELLULAR TUMOR ANTIGEN P53.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	9	Total	C	N	O	S		0	0	0
			82	53	17	11	1				

- Molecule 4 is water.

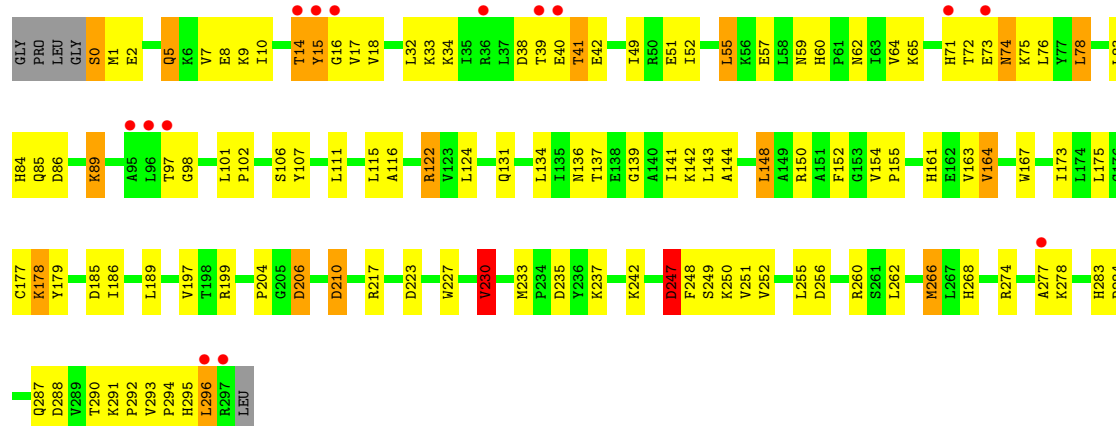
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	87	Total	O	0	0
			87	87		
4	B	66	Total	O	0	0
			66	66		
4	C	19	Total	O	0	0
			19	19		
4	D	21	Total	O	0	0
			21	21		

### 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 ( $RSRZ > 2$ ). 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.

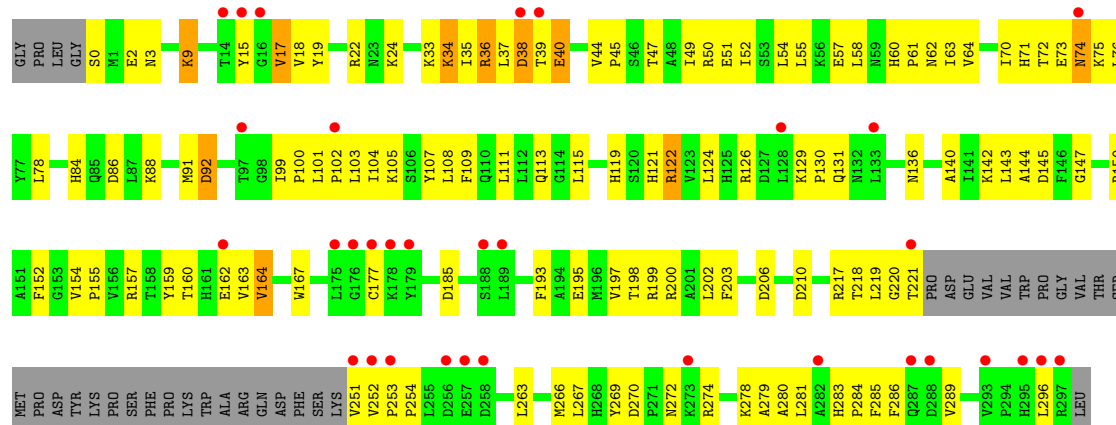
#### • Molecule 1: CELL DIVISION PROTEIN KINASE 2

Chain A: 



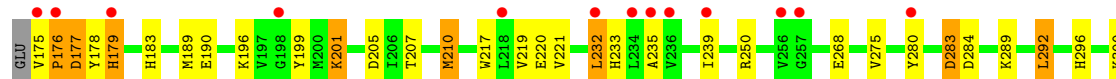
#### • Molecule 1: CELL DIVISION PROTEIN KINASE 2

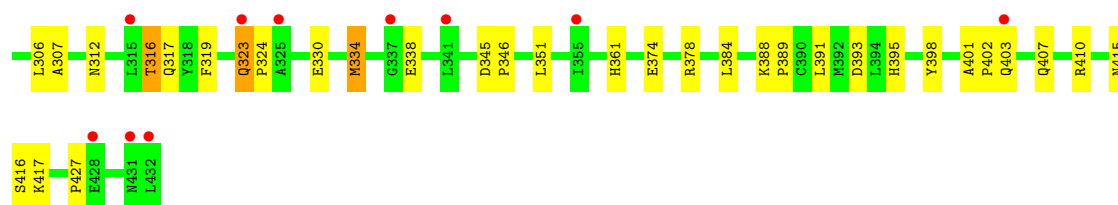
Chain C: 



#### • Molecule 2: CYCLIN A2

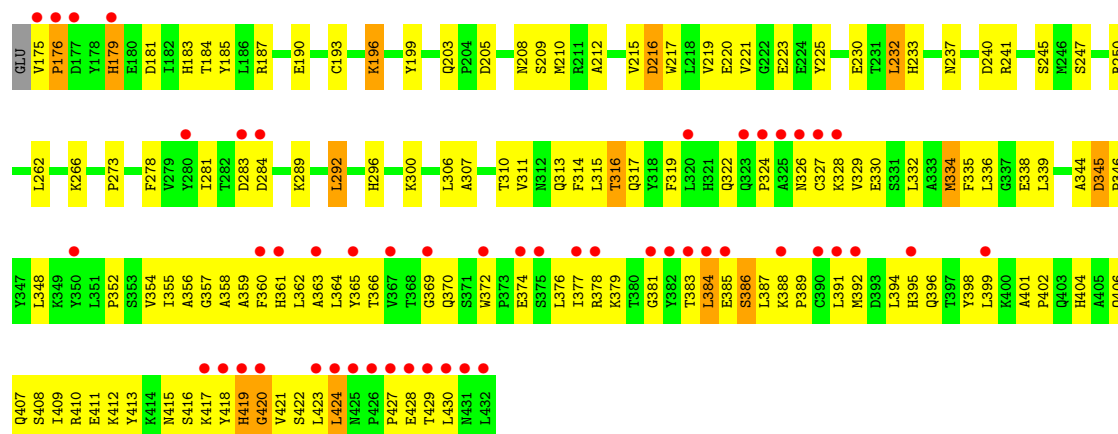
Chain B: 





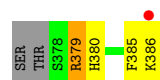
• Molecule 2: CYCLIN A2

Chain D:



• Molecule 3: CELLULAR TUMOR ANTIGEN P53

Chain E:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.67Å 134.03Å 147.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 2.24 29.87 – 2.24	Depositor EDS
% Data completeness (in resolution range)	96.5 (29.88-2.24) 96.5 (29.87-2.24)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 2.24Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.216 , 0.268 0.232 , 0.268	Depositor DCC
$R_{free}$ test set	3460 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.7	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 33.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 68281 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8981	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO

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	1.08	3/2439 (0.1%)	1.06	15/3310 (0.5%)
1	C	0.80	0/2186	0.90	5/2961 (0.2%)
2	B	0.98	4/2134 (0.2%)	0.88	8/2897 (0.3%)
2	D	0.86	0/2134	0.93	8/2897 (0.3%)
3	E	0.78	0/83	0.74	0/104
All	All	0.94	7/8976 (0.1%)	0.95	36/12169 (0.3%)

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	A	0	1
1	C	0	3
All	All	0	4

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	266	MET	SD-CE	-10.93	1.16	1.77
1	A	89	LYS	C-N	-8.29	1.15	1.34
1	A	116	ALA	CA-CB	5.64	1.64	1.52
2	B	210	MET	SD-CE	-5.60	1.46	1.77
2	B	268	GLU	CD-OE2	-5.53	1.19	1.25

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	LYS	C-N-CA	9.83	146.27	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	LYS	O-C-N	-8.60	108.93	122.70
2	B	378	ARG	NE-CZ-NH2	7.77	124.19	120.30
1	A	122	ARG	NE-CZ-NH1	7.43	124.01	120.30
2	D	181	ASP	CB-CG-OD2	7.18	124.76	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	0	SER	Peptide
1	C	160	TPO	Mainchain
1	C	37	LEU	Peptide
1	C	70	ILE	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2389	0	2428	137	1
1	C	2149	0	2203	150	0
2	B	2084	0	2107	72	1
2	D	2084	0	2107	131	0
3	E	82	0	92	9	0
4	A	87	0	0	10	0
4	B	66	0	0	8	0
4	C	19	0	0	1	0
4	D	21	0	0	2	0
All	All	8981	0	8937	443	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 25.

The worst 5 of 443 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:15:TYR:HE2	1:C:47:THR:OG1	1.16	1.29

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:17:VAL:HG11	1:C:19:TYR:CZ	1.70	1.25
1:A:266:MET:CE	1:A:266:MET:SD	1.16	1.25
1:A:266:MET:CG	1:A:266:MET:CE	2.21	1.18
1:C:39:THR:O	2:D:292:LEU:CD2	1.90	1.18

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	Distance(Å)	Clash(Å)
1:A:199:ARG:NH2	2:B:374:GLU:OE2[4_466]	1.97	0.23

## 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	295/303 (97%)	273 (92%)	19 (6%)	3 (1%)	22	17
1	C	264/303 (87%)	236 (89%)	23 (9%)	5 (2%)	12	5
2	B	256/259 (99%)	252 (98%)	3 (1%)	1 (0%)	43	46
2	D	256/259 (99%)	228 (89%)	22 (9%)	6 (2%)	10	3
3	E	7/11 (64%)	6 (86%)	1 (14%)	0	100	100
All	All	1078/1135 (95%)	995 (92%)	68 (6%)	15 (1%)	16	10

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	17	VAL
1	C	38	ASP
2	D	420	GLY
2	D	424	LEU
1	A	1	MET

### 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	261/265 (98%)	239 (92%)	22 (8%)	16	12
1	C	234/265 (88%)	220 (94%)	14 (6%)	27	26
2	B	232/233 (100%)	223 (96%)	9 (4%)	43	51
2	D	232/233 (100%)	221 (95%)	11 (5%)	36	40
3	E	9/11 (82%)	8 (89%)	1 (11%)	9	5
All	All	968/1007 (96%)	911 (94%)	57 (6%)	28	27

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	292	LEU
1	C	0	SER
2	D	348	LEU
2	B	316	THR
2	B	334	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	60	HIS
1	C	119	HIS
2	D	431	ASN
1	C	84	HIS
1	C	85	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	$\# Z  > 2$
1	TPO	A	160	1	10,10,11	14.51	5 (50%)	12,14,16	3.08	6 (50%)
1	TPO	C	160	1	10,10,11	14.58	5 (50%)	12,14,16	3.30	6 (50%)

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
1	TPO	A	160	1	-	0/9/11/13	0/0/0/0
1	TPO	C	160	1	-	0/9/11/13	0/0/0/0

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	TPO	O-C	45.31	1.42	1.11
1	A	160	TPO	O-C	45.29	1.42	1.11
1	C	160	TPO	P-O1P	5.35	1.69	1.51
1	C	160	TPO	P-O2P	4.20	1.70	1.54
1	A	160	TPO	P-O1P	4.06	1.64	1.51

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	TPO	O2P-P-OG1	-8.41	82.87	107.09
1	A	160	TPO	O2P-P-OG1	7.20	127.83	107.09
1	C	160	TPO	O2P-P-O1P	3.86	123.06	110.44
1	A	160	TPO	O3P-P-O2P	-3.85	92.63	107.61
1	C	160	TPO	CG2-CB-CA	-3.67	105.67	113.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

### 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	297/303 (98%)	0.03	14 (4%) 30 32	20, 29, 74, 105	0
1	C	269/303 (88%)	0.58	33 (12%) 5 6	27, 49, 86, 103	0
2	B	258/259 (99%)	0.43	23 (8%) 10 11	25, 40, 67, 96	0
2	D	258/259 (99%)	0.77	51 (19%) 2 1	26, 43, 73, 103	0
3	E	9/11 (81%)	1.23	1 (11%) 6 7	42, 55, 86, 87	0
All	All	1091/1135 (96%)	0.45	122 (11%) 6 7	20, 41, 79, 105	0

The worst 5 of 122 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	432	LEU	7.8
1	A	297	ARG	7.4
2	D	176	PRO	6.4
1	A	96	LEU	5.9
1	C	253	PRO	5.6

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	TPO	A	160	11/12	0.10	-0.36	21,30,35,38	0
1	TPO	C	160	11/12	0.09	-1.22	39,43,44,47	0

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

### 6.5 Other polymers ⓘ

There are no such residues in this entry.