



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 10:41 pm BST

PDB ID : 3GCG  
Title : crystal structure of MAP and CDC42 complex  
Authors : Chai, J.; Huang, Z.; Feng, Y.; Wu, X.  
Deposited on : 2009-02-22  
Resolution : 2.30 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.

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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  
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

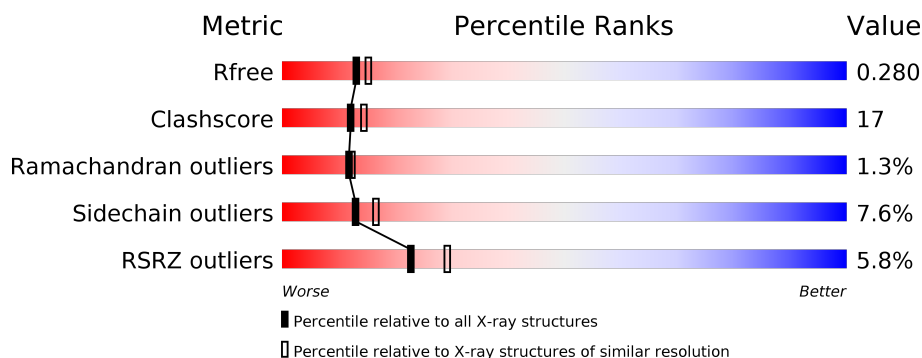
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	182	
2	B	172	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2767 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 division control protein 42 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	173	Total	C	N	O	S	0	0	0
			1348	865	215	262	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP P60953
A	-2	PRO	-	EXPRESSION TAG	UNP P60953
A	-1	LEU	-	EXPRESSION TAG	UNP P60953
A	0	GLY	-	EXPRESSION TAG	UNP P60953
A	1	SER	-	EXPRESSION TAG	UNP P60953
A	163	LYS	ARG	SEE REMARK 999	UNP P60953

- Molecule 2 is a protein called L0028 (Mitochondria associated protein).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	152	Total	C	N	O	S	0	0	0
			1233	765	226	238	4			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	32	GLY	-	EXPRESSION TAG	UNP Q9R8E4
B	33	PRO	-	EXPRESSION TAG	UNP Q9R8E4
B	34	LEU	-	EXPRESSION TAG	UNP Q9R8E4
B	35	GLY	-	EXPRESSION TAG	UNP Q9R8E4
B	36	SER	-	EXPRESSION TAG	UNP Q9R8E4

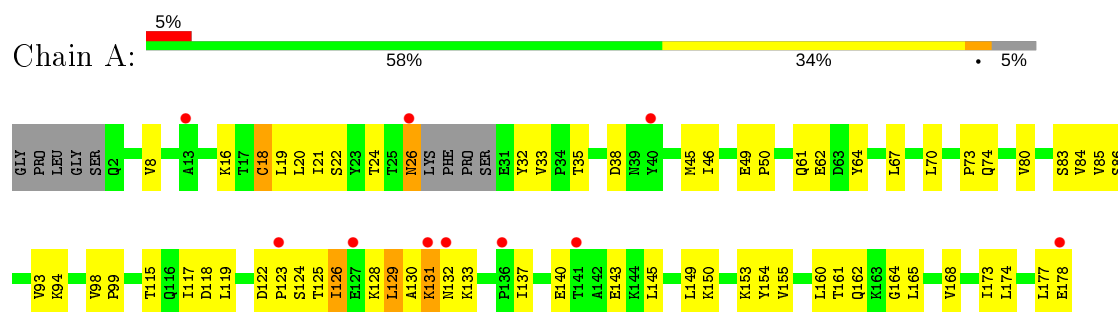
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	95	Total 95	O 95	0	0
3	B	91	Total 91	O 91	0	0

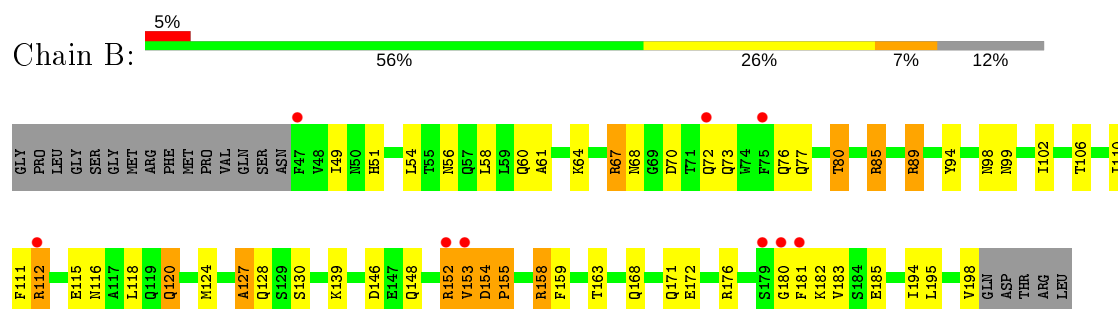
### 3 Residue-property plots [i](#)

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: Cell division control protein 42 homolog



- Molecule 2: L0028 (Mitochondria associated protein)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	41.63Å 83.03Å 99.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 63.75 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.1 (20.00-2.30) 99.4 (63.75-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.10 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.235 , 0.277 0.235 , 0.280	Depositor DCC
$R_{free}$ test set	774 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.4	Xtriage
Anisotropy	0.509	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 58.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	2767	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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](#)

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	0.44	1/1375 (0.1%)	0.67	0/1870
2	B	0.36	0/1252	0.58	1/1686 (0.1%)
All	All	0.40	1/2627 (0.0%)	0.63	1/3556 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	TYR	CD2-CE2	-5.39	1.31	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	154	ASP	N-CA-C	-6.74	92.80	111.00

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	1348	0	1358	51	0
2	B	1233	0	1210	40	0
3	A	95	0	0	4	0
3	B	91	0	0	4	0
All	All	2767	0	2568	88	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 17.

All (88) 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)
2:B:61:ALA:HA	2:B:64:LYS:HE3	1.46	0.97
1:A:26:ASN:C	1:A:26:ASN:HD22	1.77	0.87
1:A:125:THR:O	1:A:129:LEU:HB2	1.78	0.82
1:A:153:LYS:HG2	1:A:154:TYR:H	1.45	0.78
2:B:146:ASP:OD1	2:B:158:ARG:NH1	2.17	0.78
1:A:61:GLN:HG3	3:A:244:HOH:O	1.85	0.77
1:A:70:LEU:HD12	2:B:130:SER:HB2	1.71	0.73
1:A:153:LYS:HG2	1:A:154:TYR:N	2.03	0.72
2:B:171:GLN:HG3	2:B:183:VAL:HG21	1.70	0.72
3:A:244:HOH:O	2:B:128:GLN:HB2	1.89	0.72
2:B:153:VAL:O	2:B:153:VAL:HG12	1.90	0.69
2:B:163:THR:HG22	3:B:2:HOH:O	1.93	0.68
1:A:35:THR:HG21	3:B:1:HOH:O	1.93	0.68
2:B:85:ARG:HB2	2:B:127:ALA:HA	1.74	0.67
1:A:94:LYS:HG2	1:A:149:LEU:HD21	1.77	0.65
2:B:168:GLN:O	2:B:172:GLU:HG3	1.98	0.63
1:A:8:VAL:HG21	1:A:20:LEU:HD11	1.81	0.61
1:A:26:ASN:C	1:A:26:ASN:ND2	2.51	0.61
1:A:153:LYS:HB2	1:A:153:LYS:NZ	2.18	0.59
1:A:80:VAL:HG11	1:A:93:VAL:HG13	1.84	0.59
2:B:76:GLN:O	2:B:80:THR:HG23	2.03	0.58
2:B:172:GLU:O	2:B:176:ARG:HG3	2.04	0.58
1:A:38:ASP:OD2	2:B:89:ARG:NH2	2.37	0.57
1:A:18:CYS:HA	1:A:21:ILE:HG22	1.86	0.57
1:A:83:SER:HB3	1:A:86:SER:HB3	1.87	0.57
2:B:68:ASN:ND2	2:B:70:ASP:HB2	2.19	0.57
1:A:84:VAL:HG21	1:A:117:ILE:HA	1.87	0.56
1:A:153:LYS:CG	1:A:154:TYR:H	2.17	0.56
1:A:123:PRO:HA	1:A:126:ILE:HG13	1.88	0.55
2:B:159:PHE:O	2:B:163:THR:HG23	2.06	0.55
1:A:125:THR:HG22	1:A:129:LEU:HD12	1.90	0.54
1:A:137:ILE:N	1:A:137:ILE:HD12	2.22	0.53
2:B:67:ARG:HG3	2:B:68:ASN:N	2.22	0.53
1:A:124:SER:O	1:A:128:LYS:HG2	2.09	0.52
2:B:110:ILE:HD11	2:B:198:VAL:HG23	1.92	0.52
1:A:70:LEU:HD12	2:B:130:SER:CB	2.38	0.51
1:A:177:LEU:C	1:A:178:GLU:OE2	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:HIS:HE1	2:B:172:GLU:OE1	1.93	0.51
1:A:153:LYS:CG	1:A:154:TYR:N	2.74	0.51
1:A:64:TYR:HB3	1:A:67:LEU:HD22	1.94	0.50
2:B:102:ILE:HG13	2:B:106:THR:HB	1.93	0.50
1:A:80:VAL:CG1	1:A:93:VAL:HG13	2.42	0.49
2:B:115:GLU:HG3	2:B:120:GLN:O	2.12	0.49
1:A:21:ILE:HD11	3:A:228:HOH:O	2.11	0.49
1:A:46:ILE:HD12	1:A:173:ILE:HG21	1.95	0.49
2:B:56:ASN:O	2:B:60:GLN:HG3	2.13	0.49
1:A:94:LYS:HB2	1:A:145:LEU:HD11	1.95	0.49
2:B:152:ARG:O	2:B:153:VAL:HG23	2.13	0.49
2:B:153:VAL:O	2:B:153:VAL:CG1	2.61	0.48
1:A:21:ILE:HG23	1:A:22:SER:N	2.28	0.48
1:A:161:THR:O	1:A:162:GLN:HB2	2.14	0.48
2:B:49:ILE:HD13	2:B:54:LEU:HD11	1.96	0.48
2:B:73:GLN:O	2:B:77:GLN:HG3	2.14	0.48
1:A:164:GLY:O	1:A:168:VAL:HG23	2.14	0.47
2:B:180:GLY:O	2:B:181:PHE:CD2	2.68	0.47
2:B:154:ASP:O	2:B:155:PRO:C	2.52	0.47
2:B:112:ARG:NH1	2:B:116:ASN:OD1	2.49	0.46
2:B:51:HIS:CE1	2:B:172:GLU:OE1	2.69	0.46
2:B:182:LYS:HB2	2:B:185:GLU:HG3	1.96	0.45
1:A:140:GLU:CD	1:A:140:GLU:H	2.20	0.45
1:A:155:VAL:HB	3:A:179:HOH:O	2.16	0.45
1:A:131:LYS:C	1:A:133:LYS:H	2.20	0.45
1:A:24:THR:C	1:A:26:ASN:H	2.21	0.45
1:A:122:ASP:O	1:A:126:ILE:CG1	2.65	0.45
2:B:194:ILE:O	2:B:198:VAL:HB	2.16	0.45
2:B:111:PHE:CE2	2:B:124:MET:HA	2.52	0.44
1:A:84:VAL:HG22	1:A:115:THR:O	2.18	0.44
1:A:149:LEU:O	1:A:150:LYS:HB2	2.17	0.44
1:A:98:VAL:HB	1:A:99:PRO:HD3	1.98	0.44
1:A:84:VAL:HG11	1:A:117:ILE:HG22	2.00	0.44
2:B:68:ASN:HD21	2:B:70:ASP:HB2	1.83	0.43
2:B:139:LYS:HG3	3:B:22:HOH:O	2.18	0.43
2:B:94:TYR:O	2:B:98:ASN:ND2	2.48	0.43
1:A:73:PRO:O	1:A:74:GLN:HB2	2.18	0.43
1:A:98:VAL:HG21	1:A:149:LEU:HD13	2.01	0.43
1:A:16:LYS:O	1:A:19:LEU:HB3	2.18	0.43
2:B:98:ASN:O	2:B:99:ASN:HB2	2.19	0.43
1:A:153:LYS:HB2	1:A:153:LYS:HZ2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:MET:CE	1:A:50:PRO:HB3	2.49	0.42
2:B:49:ILE:CD1	2:B:54:LEU:HD11	2.48	0.42
1:A:122:ASP:O	1:A:126:ILE:HG13	2.20	0.41
1:A:84:VAL:HG23	1:A:85:VAL:HG13	2.01	0.41
1:A:33:VAL:HG13	1:A:33:VAL:O	2.20	0.41
2:B:163:THR:HG21	3:B:3:HOH:O	2.21	0.41
1:A:118:ASP:OD2	1:A:119:LEU:HD13	2.21	0.41
2:B:70:ASP:OD2	2:B:72:GLN:HG3	2.19	0.41
1:A:126:ILE:O	1:A:130:ALA:HB2	2.21	0.41
2:B:118:LEU:HD22	2:B:181:PHE:CD2	2.57	0.40

There are no symmetry-related clashes.

## 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	169/182 (93%)	150 (89%)	18 (11%)	1 (1%)	25	31
2	B	150/172 (87%)	140 (93%)	7 (5%)	3 (2%)	7	6
All	All	319/354 (90%)	290 (91%)	25 (8%)	4 (1%)	12	12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	ASN
2	B	153	VAL
2	B	127	ALA
2	B	155	PRO

### 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	153/160 (96%)	142 (93%)	11 (7%)	14	18
2	B	138/155 (89%)	127 (92%)	11 (8%)	12	15
All	All	291/315 (92%)	269 (92%)	22 (8%)	13	16

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	CYS
1	A	26	ASN
1	A	49	GLU
1	A	62	GLU
1	A	126	ILE
1	A	129	LEU
1	A	131	LYS
1	A	143	GLU
1	A	160	LEU
1	A	165	LEU
1	A	174	LEU
2	B	58	LEU
2	B	67	ARG
2	B	80	THR
2	B	85	ARG
2	B	89	ARG
2	B	112	ARG
2	B	120	GLN
2	B	148	GLN
2	B	152	ARG
2	B	158	ARG
2	B	195	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
2	B	51	HIS
2	B	125	ASN
2	B	128	GLN
2	B	148	GLN

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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	173/182 (95%)	0.29	10 (5%)	23 29	11, 30, 64, 72	0
2	B	152/172 (88%)	0.30	9 (5%)	22 28	15, 29, 51, 60	0
All	All	325/354 (91%)	0.30	19 (5%)	23 29	11, 29, 58, 72	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	180	GLY	11.2
1	A	26	ASN	5.7
2	B	153	VAL	5.5
2	B	179	SER	4.2
1	A	136	PRO	3.2
2	B	152	ARG	3.2
1	A	131	LYS	3.0
1	A	178	GLU	2.8
2	B	181	PHE	2.7
1	A	123	PRO	2.5
1	A	127	GLU	2.4
1	A	141	THR	2.2
2	B	72	GLN	2.2
2	B	47	PHE	2.1
1	A	13	ALA	2.1
1	A	132	ASN	2.1
2	B	75	PHE	2.0
2	B	112	ARG	2.0
1	A	40	TYR	2.0

### 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.