



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 04:29 AM BST

PDB ID : 5D9Z  
Title : Structure of Colocasia Esculenta Agglutinin with mannose bound  
Authors : Chattopadhyaya, R.  
Deposited on : 2015-08-19  
Resolution : 1.85 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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

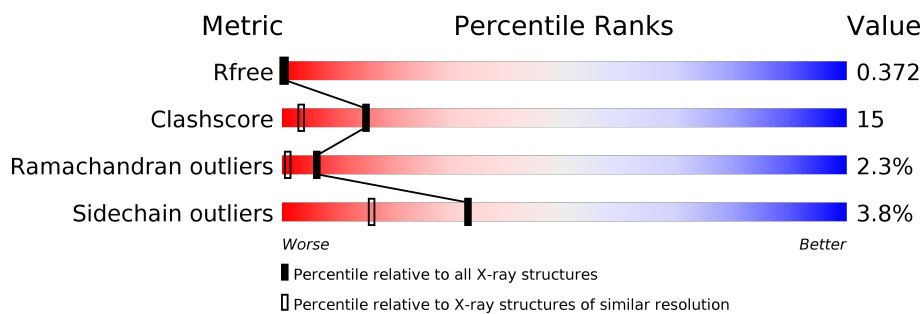
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)

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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	109	
2	B	112	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PO4	B	204	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 1814 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.

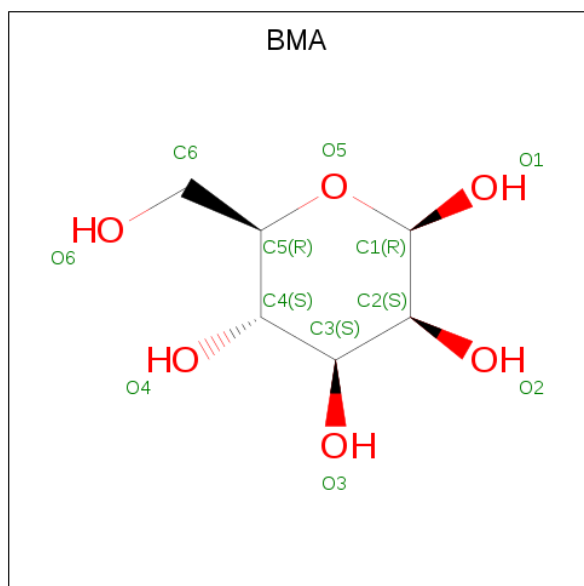
- Molecule 1 is a protein called Tuber agglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	109	Total	C	N	O	S	0	0	0
			836	524	147	162	3			

- Molecule 2 is a protein called Tuber agglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	112	Total	C	N	O	S	0	0	0
			880	559	152	166	3			

- Molecule 3 is beta-D-mannopyranose (three-letter code: BMA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



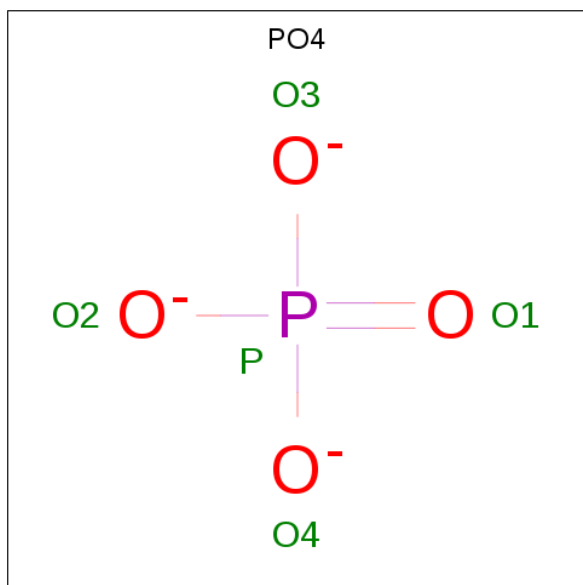
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	A	1	Total	C	O	0	0
			12	6	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		

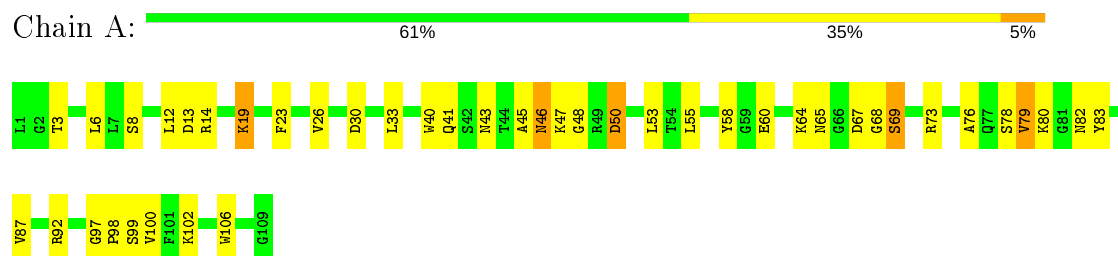
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total	O	0	0
			10	10		
5	B	23	Total	O	0	0
			23	23		

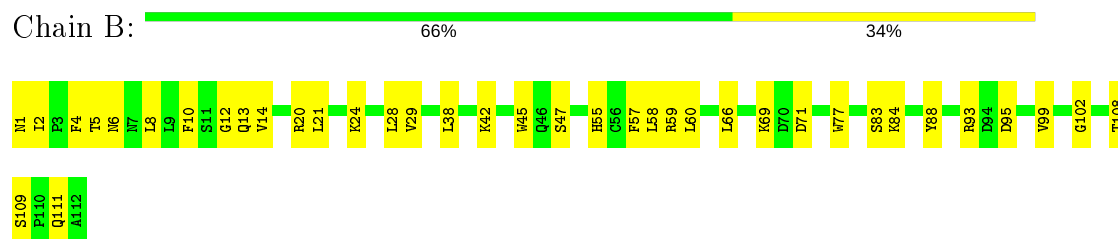
### 3 Residue-property plots [i](#)

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. 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. 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: Tuber agglutinin



#### • Molecule 2: Tuber agglutinin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.90 Å 75.90 Å 124.06 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.80 – 1.85 29.04 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.80-1.85) 85.5 (29.04-1.70)	Depositor EDS
$R_{merge}$	0.31	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 1.70 Å)	Xtriage
Refinement program	PHENIX 1.8.1 _1168	Depositor
R, $R_{free}$	0.316 , 0.369 0.326 , 0.372	Depositor DCC
$R_{free}$ test set	767 reflections (1.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.3	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 96.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	1814	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.21% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, BMA

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	0.53	0/854	0.70	0/1161
2	B	0.54	0/903	0.70	0/1222
All	All	0.53	0/1757	0.70	0/2383

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	836	0	799	27	0
2	B	880	0	838	30	0
3	A	24	0	24	0	0
3	B	36	0	36	1	0
4	B	5	0	0	5	0
5	A	10	0	0	2	0
5	B	23	0	0	2	0
All	All	1814	0	1697	53	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 15.

All (53) 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:8:SER:HA	1:A:55:LEU:HB3	1.74	0.70
2:B:4:PHE:HA	4:B:204:PO4:O1	1.94	0.67
2:B:55:HIS:HB2	2:B:71:ASP:HB2	1.78	0.65
1:A:78:SER:OG	1:A:79:VAL:N	2.32	0.62
2:B:2:ILE:HB	2:B:13:GLN:HE21	1.65	0.60
2:B:58:LEU:HD11	2:B:66:LEU:HG	1.81	0.60
2:B:47:SER:HB2	2:B:77:TRP:CD1	2.38	0.58
1:A:92:ARG:HD2	2:B:109:SER:O	2.03	0.58
1:A:65:ASN:HD21	1:A:67:ASP:HB2	1.71	0.55
1:A:82:ASN:O	1:A:98:PRO:HA	2.07	0.54
1:A:26:VAL:O	1:A:33:LEU:HD12	2.08	0.54
1:A:12:LEU:HB3	1:A:53:LEU:HB3	1.90	0.54
1:A:60:GLU:OE2	1:A:73:ARG:HB3	2.07	0.54
2:B:88:TYR:CD2	2:B:102:GLY:HA3	2.43	0.54
2:B:60:LEU:HA	2:B:66:LEU:HA	1.91	0.53
1:A:76:ALA:HB3	5:A:303:HOH:O	2.10	0.52
1:A:64:LYS:HA	1:A:69:SER:O	2.09	0.52
2:B:8:LEU:HB2	4:B:204:PO4:O2	2.11	0.50
1:A:40:TRP:CE2	2:B:108:THR:HG22	2.47	0.50
2:B:20:ARG:HB3	2:B:29:VAL:HG22	1.93	0.49
2:B:83:SER:OG	2:B:84:LYS:N	2.44	0.49
1:A:45:ALA:C	1:A:47:LYS:H	2.15	0.49
2:B:45:TRP:CH2	2:B:47:SER:HB3	2.48	0.49
1:A:41:GLN:HG3	1:A:43:ASN:HB2	1.95	0.48
2:B:28:LEU:HA	2:B:38:LEU:HA	1.95	0.48
2:B:1:ASN:HB2	3:B:203:BMA:O4	2.14	0.48
1:A:58:TYR:OH	1:A:80:LYS:HD2	2.14	0.47
2:B:4:PHE:CE2	2:B:6:ASN:HA	2.49	0.47
2:B:93:ARG:NH2	2:B:95:ASP:OD2	2.45	0.47
2:B:10:PHE:HD1	4:B:204:PO4:O4	1.98	0.47
2:B:5:THR:OG1	4:B:204:PO4:O3	2.14	0.47
1:A:45:ALA:O	1:A:47:LYS:N	2.47	0.46
2:B:12:GLY:N	5:B:304:HOH:O	2.48	0.46
2:B:57:PHE:CZ	2:B:69:LYS:HB2	2.51	0.46
1:A:83:TYR:CD2	1:A:97:GLY:HA3	2.51	0.46
1:A:30:ASP:HB2	1:A:46:ASN:H	1.82	0.45
1:A:106:TRP:HE3	2:B:42:LYS:HB2	1.81	0.45
1:A:19:LYS:HG2	1:A:23:PHE:O	2.16	0.44
2:B:13:GLN:NE2	4:B:204:PO4:O4	2.51	0.43
1:A:102:LYS:HG3	2:B:99:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:VAL:HG12	1:A:100:VAL:O	2.18	0.43
2:B:13:GLN:N	5:B:304:HOH:O	2.51	0.43
1:A:58:TYR:CZ	1:A:80:LYS:HD2	2.55	0.42
2:B:58:LEU:HD11	2:B:66:LEU:CG	2.48	0.42
1:A:102:LYS:NZ	5:A:302:HOH:O	2.47	0.41
2:B:14:VAL:HG22	2:B:59:ARG:HB2	2.03	0.41
1:A:6:LEU:HA	1:A:6:LEU:HD12	1.89	0.41
2:B:2:ILE:HB	2:B:13:GLN:NE2	2.33	0.41
1:A:46:ASN:C	1:A:48:GLY:H	2.23	0.40
1:A:14:ARG:NE	1:A:50:ASP:OD1	2.53	0.40
2:B:21:LEU:HA	2:B:21:LEU:HD23	1.62	0.40
2:B:6:ASN:N	2:B:6:ASN:OD1	2.55	0.40
1:A:8:SER:N	1:A:55:LEU:HD23	2.37	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	107/109 (98%)	87 (81%)	17 (16%)	3 (3%)	5	0
2	B	110/112 (98%)	98 (89%)	10 (9%)	2 (2%)	8	2
All	All	217/221 (98%)	185 (85%)	27 (12%)	5 (2%)	6	1

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	24	LYS
1	A	3	THR
2	B	111	GLN
1	A	46	ASN
1	A	68	GLY

### 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	90/92 (98%)	83 (92%)	7 (8%)	12	2
2	B	95/95 (100%)	95 (100%)	0	100	100
All	All	185/187 (99%)	178 (96%)	7 (4%)	33	16

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASP
1	A	19	LYS
1	A	50	ASP
1	A	69	SER
1	A	79	VAL
1	A	87	VAL
1	A	99	SER

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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

6 ligands 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	BMA	B	202	-	12,12,12	0.67	0	17,17,17	1.64	4 (23%)
3	BMA	B	201	-	12,12,12	0.79	0	17,17,17	1.27	2 (11%)
3	BMA	A	201	-	12,12,12	0.47	0	17,17,17	1.16	2 (11%)
3	BMA	A	202	-	12,12,12	0.59	0	17,17,17	1.11	1 (5%)
3	BMA	B	203	-	12,12,12	0.68	0	17,17,17	1.39	2 (11%)
4	PO4	B	204	-	4,4,4	1.09	0	6,6,6	1.28	0

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	BMA	B	202	-	-	2/2/22/22	0/1/1/1
3	BMA	B	203	-	-	2/2/22/22	0/1/1/1
3	BMA	B	201	-	-	1/2/22/22	0/1/1/1
3	BMA	A	202	-	-	0/2/22/22	0/1/1/1
3	BMA	A	201	-	-	2/2/22/22	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	203	BMA	C1-O5-C5	-4.30	105.54	113.66
3	B	202	BMA	C4-C3-C2	3.70	117.28	110.82
3	B	202	BMA	C3-C4-C5	3.37	116.24	110.24
3	A	201	BMA	C1-C2-C3	-2.69	104.74	110.31
3	B	201	BMA	O2-C2-C3	-2.54	104.47	110.35
3	B	203	BMA	O5-C5-C6	2.43	112.47	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	202	BMA	C1-C2-C3	-2.37	105.39	110.31
3	A	201	BMA	O5-C1-C2	-2.33	106.13	110.28
3	B	202	BMA	O5-C5-C6	2.23	111.98	106.44
3	B	201	BMA	O3-C3-C2	-2.14	105.41	110.35
3	B	202	BMA	C1-C2-C3	2.09	114.65	110.31

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	BMA	O5-C5-C6-O6
3	B	203	BMA	O5-C5-C6-O6
3	A	201	BMA	C4-C5-C6-O6
3	B	203	BMA	C4-C5-C6-O6
3	B	201	BMA	O5-C5-C6-O6
3	B	202	BMA	C4-C5-C6-O6
3	B	202	BMA	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	203	BMA	1	0
4	B	204	PO4	5	0

## 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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.