



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2017 – 07:22 PM EDT

PDB ID : 1Z0M  
Title : the glycogen-binding domain of the AMP-activated protein kinase beta1 subunit  
Authors : Polekhina, G.; Gupta, A.; van Denderen, B.J.; Feil, S.C.; Kemp, B.E.; Stapleton, D.; Parker, M.W.  
Deposited on : unknown  
Resolution : 1.91 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

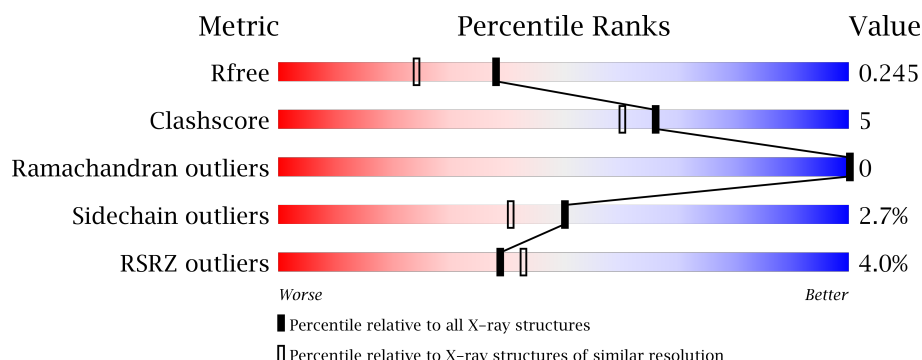
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.91 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))
$R_{free}$	100719	6276 (1.94-1.90)
Clashscore	112137	7025 (1.94-1.90)
Ramachandran outliers	110173	6947 (1.94-1.90)
Sidechain outliers	110143	6948 (1.94-1.90)
RSRZ outliers	101464	6332 (1.94-1.90)

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. 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	96	<div> <div>0.5%</div> <div>79%</div> <div>10%</div> <div>9%</div> </div>
1	B	96	<div> <div>5%</div> <div>71%</div> <div>14%</div> <div>16%</div> </div>
1	C	96	<div> <div>4%</div> <div>78%</div> <div>5%</div> <div>17%</div> </div>

## 2 Entry composition [i](#)

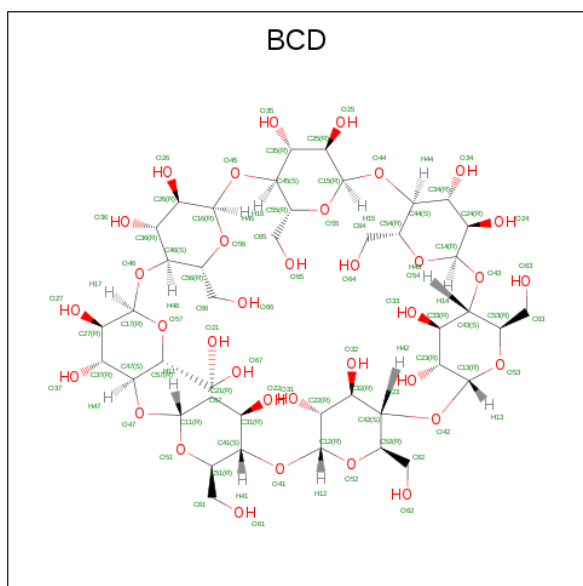
There are 3 unique types of molecules in this entry. The entry contains 2432 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 5'-AMP-activated protein kinase, beta-1 subunit.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
1	A	87	Total	C	N	O	0	0
			706	455	119	132		
1	B	81	Total	C	N	O	0	0
			652	418	113	121		
1	C	80	Total	C	N	O	0	0
			643	413	111	119		

- Molecule 2 is BETA-CYCLODEXTRIN (three-letter code: BCD) (formula:  $C_{42}H_{70}O_{35}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			77	42	35		
2	B	1	Total	C	O	0	0
			77	42	35		
2	C	1	Total	C	O	0	0
			77	42	35		

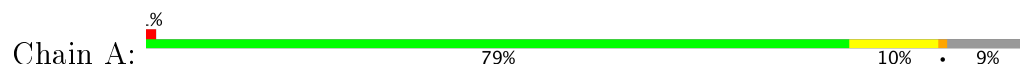
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	82	Total 82	O 82	0	0
3	B	58	Total 58	O 58	0	0
3	C	60	Total 60	O 60	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.

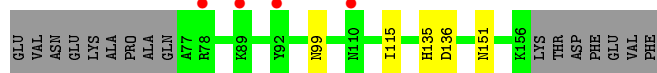
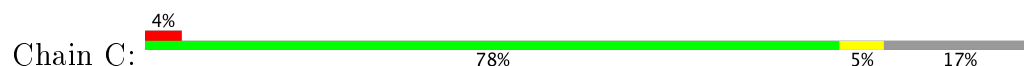
- Molecule 1: 5'-AMP-activated protein kinase, beta-1 subunit



- Molecule 1: 5'-AMP-activated protein kinase, beta-1 subunit



- Molecule 1: 5'-AMP-activated protein kinase, beta-1 subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	43.73Å 44.89Å 50.34Å 70.72° 68.77° 65.79°	Depositor
Resolution (Å)	30.00 – 1.91 24.17 – 1.91	Depositor EDS
% Data completeness (in resolution range)	95.6 (30.00-1.91) 89.3 (24.17-1.91)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	9.61 (at 1.90Å)	Xtriage
Refinement program	CNS, REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.191 , 0.243 0.192 , 0.245	Depositor DCC
$R_{free}$ test set	1208 reflections (5.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.3	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	2432	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.23% 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: BCD

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	0.77	0/727	0.43	0/988
1	B	0.78	0/671	0.42	0/914
1	C	0.65	0/662	0.42	0/902
All	All	0.74	0/2060	0.42	0/2804

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	706	0	677	7	0
1	B	652	0	628	9	0
1	C	643	0	620	5	0
2	A	77	0	70	0	0
2	B	77	0	70	0	1
2	C	77	0	70	0	0
3	A	82	0	0	1	2
3	B	58	0	0	2	1
3	C	60	0	0	2	0
All	All	2432	0	2135	20	2

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 5.

All (20) 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:136:ASP:H	1:B:151:ASN:HD21	1.17	0.88
1:C:136:ASP:H	1:C:151:ASN:HD21	0.88	0.88
1:C:136:ASP:H	1:C:151:ASN:ND2	1.73	0.85
1:C:136:ASP:N	1:C:151:ASN:HD21	1.74	0.84
1:B:105:LEU:HD22	1:B:114:ALA:HB2	1.66	0.75
1:C:135:HIS:CE1	3:C:242:HOH:O	2.49	0.64
1:B:136:ASP:N	1:B:151:ASN:HD21	1.93	0.64
1:B:136:ASP:H	1:B:151:ASN:ND2	1.97	0.59
1:C:135:HIS:HE1	3:C:242:HOH:O	1.88	0.55
1:B:120:GLU:HG2	1:B:156:LYS:HA	1.94	0.50
1:A:81:VAL:HG22	1:A:115:ILE:HG12	1.94	0.50
1:A:126:LYS:HE2	1:A:133:TRP:HB3	1.94	0.49
1:A:109:GLN:O	1:A:110:ASN:HB2	2.12	0.48
1:B:83:ARG:HG3	1:B:113:VAL:HG22	1.95	0.48
1:A:81:VAL:HG21	1:B:81:VAL:HG21	1.99	0.45
1:B:145:GLN:HG2	3:B:215:HOH:O	2.16	0.45
1:A:91:VAL:HG13	1:A:129:VAL:HG22	2.00	0.44
1:A:78:ARG:HD2	1:A:156:LYS:O	2.17	0.43
1:B:109:GLN:HB2	3:B:231:HOH:O	2.18	0.43
1:A:126:LYS:NZ	3:A:226:HOH:O	2.52	0.41

All (2) 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	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:BCD:O35	3:A:254:HOH:O[1_465]	2.06	0.14
3:A:235:HOH:O	3:B:233:HOH:O[1_545]	2.19	0.01

## 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	85/96 (88%)	83 (98%)	2 (2%)	0	100	100
1	B	79/96 (82%)	79 (100%)	0	0	100	100
1	C	78/96 (81%)	76 (97%)	2 (3%)	0	100	100
All	All	242/288 (84%)	238 (98%)	4 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	78/85 (92%)	76 (97%)	2 (3%)	51	42
1	B	72/85 (85%)	70 (97%)	2 (3%)	49	39
1	C	71/85 (84%)	69 (97%)	2 (3%)	49	39
All	All	221/255 (87%)	215 (97%)	6 (3%)	50	41

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ARG
1	A	109	GLN
1	B	76	GLN
1	B	143	THR
1	C	99	ASN
1	C	115	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	GLN

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Mol	Chain	Res	Type
1	B	151	ASN
1	C	151	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

3 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	$\# Z  > 2$
2	BCD	A	201	-	84,84,84	0.61	0	126,126,126	2.24	51 (40%)
2	BCD	B	202	-	84,84,84	0.62	0	126,126,126	2.20	54 (42%)
2	BCD	C	203	-	84,84,84	0.66	0	126,126,126	2.23	50 (39%)

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
2	BCD	A	201	-	-	0/42/182/182	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BCD	B	202	-	-	0/42/182/182	0/0/8/8
2	BCD	C	203	-	-	0/42/182/182	0/0/8/8

There are no bond length outliers.

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	202	BCD	O42-C13-O53	-3.37	102.51	110.70
2	C	203	BCD	O41-C12-O52	-3.36	102.55	110.70
2	B	202	BCD	O43-C14-O54	-3.20	102.94	110.70
2	A	201	BCD	O44-C15-O55	-3.14	103.08	110.70
2	B	202	BCD	O41-C12-O52	-3.09	103.18	110.70
2	C	203	BCD	O47-C11-O51	-3.04	103.31	110.70
2	A	201	BCD	O47-C11-O51	-2.99	103.44	110.70
2	B	202	BCD	O47-C11-O51	-2.79	103.91	110.70
2	C	203	BCD	O45-C16-C26	-2.78	101.86	108.11
2	B	202	BCD	O45-C16-O56	-2.72	104.10	110.70
2	C	203	BCD	O46-C17-O57	-2.71	104.11	110.70
2	A	201	BCD	O41-C12-O52	-2.71	104.11	110.70
2	C	203	BCD	O42-C13-O53	-2.70	104.13	110.70
2	A	201	BCD	O45-C16-O56	-2.70	104.14	110.70
2	C	203	BCD	C17-O46-C46	-2.68	111.47	118.00
2	A	201	BCD	O43-C14-O54	-2.60	104.37	110.70
2	C	203	BCD	O45-C16-O56	-2.60	104.38	110.70
2	B	202	BCD	O46-C17-O57	-2.55	104.50	110.70
2	B	202	BCD	O44-C15-O55	-2.52	104.58	110.70
2	A	201	BCD	O42-C13-O53	-2.51	104.61	110.70
2	A	201	BCD	O46-C17-O57	-2.39	104.90	110.70
2	A	201	BCD	C11-O47-C47	-2.38	112.21	118.00
2	C	203	BCD	O44-C15-O55	-2.29	105.14	110.70
2	B	202	BCD	C16-O45-C45	-2.23	112.57	118.00
2	C	203	BCD	O43-C14-O54	-2.19	105.39	110.70
2	B	202	BCD	C12-O41-C41	-2.16	112.72	118.00
2	B	202	BCD	C11-O47-C47	-2.04	113.01	118.00
2	B	202	BCD	C17-O46-C46	-2.03	113.05	118.00
2	A	201	BCD	O57-C57-C67	2.01	111.24	106.41
2	C	203	BCD	O31-C31-C21	2.06	114.83	110.36
2	A	201	BCD	C31-C41-C51	2.10	115.32	110.88
2	C	203	BCD	C31-C41-C51	2.12	115.38	110.88
2	B	202	BCD	O43-C43-C53	2.14	114.61	109.34
2	B	202	BCD	O53-C53-C63	2.15	111.55	106.41
2	B	202	BCD	C14-O54-C54	2.18	117.82	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	202	BCD	C32-C42-C52	2.41	115.99	110.88
2	A	201	BCD	C34-C44-C54	2.44	116.05	110.88
2	B	202	BCD	C35-C45-C55	2.44	116.05	110.88
2	B	202	BCD	C36-C46-C56	2.47	116.12	110.88
2	B	202	BCD	O53-C13-C23	2.55	115.22	110.30
2	B	202	BCD	C15-C25-C35	2.55	114.73	109.98
2	A	201	BCD	C35-C45-C55	2.56	116.32	110.88
2	C	203	BCD	C37-C47-C57	2.60	116.39	110.88
2	B	202	BCD	C31-C41-C51	2.60	116.39	110.88
2	B	202	BCD	O54-C54-C64	2.60	112.64	106.41
2	A	201	BCD	O53-C53-C63	2.61	112.66	106.41
2	A	201	BCD	C21-C31-C41	2.61	115.03	109.61
2	A	201	BCD	C36-C46-C56	2.65	116.51	110.88
2	B	202	BCD	C11-C21-C31	2.65	114.91	109.98
2	C	203	BCD	C35-C45-C55	2.66	116.51	110.88
2	A	201	BCD	C24-C34-C44	2.66	115.12	109.61
2	A	201	BCD	O52-C12-C22	2.67	115.45	110.30
2	A	201	BCD	C22-C32-C42	2.69	115.19	109.61
2	C	203	BCD	C36-C46-C56	2.72	116.64	110.88
2	B	202	BCD	C12-C22-C32	2.74	115.07	109.98
2	B	202	BCD	O55-C15-C25	2.74	115.59	110.30
2	C	203	BCD	O52-C12-C22	2.76	115.61	110.30
2	C	203	BCD	C25-C35-C45	2.77	115.34	109.61
2	C	203	BCD	C26-C36-C46	2.78	115.37	109.61
2	A	201	BCD	C13-C23-C33	2.78	115.15	109.98
2	C	203	BCD	C12-C22-C32	2.83	115.23	109.98
2	A	201	BCD	C12-C22-C32	2.83	115.24	109.98
2	A	201	BCD	C25-C35-C45	2.85	115.52	109.61
2	C	203	BCD	O51-C11-C21	2.85	115.80	110.30
2	C	203	BCD	C21-C31-C41	2.87	115.55	109.61
2	C	203	BCD	O53-C13-C23	2.88	115.86	110.30
2	C	203	BCD	C27-C37-C47	2.89	115.61	109.61
2	B	202	BCD	C14-C24-C34	2.90	115.37	109.98
2	C	203	BCD	C34-C44-C54	2.97	117.17	110.88
2	A	201	BCD	O54-C14-C24	2.97	116.03	110.30
2	B	202	BCD	C26-C36-C46	2.97	115.77	109.61
2	A	201	BCD	C37-C47-C57	2.97	117.19	110.88
2	C	203	BCD	C16-C26-C36	2.98	115.51	109.98
2	B	202	BCD	O53-C53-C43	3.00	115.89	109.75
2	C	203	BCD	C22-C32-C42	3.00	115.83	109.61
2	C	203	BCD	C24-C34-C44	3.00	115.83	109.61
2	C	203	BCD	O54-C14-C24	3.02	116.11	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	BCD	O55-C15-C25	3.03	116.14	110.30
2	A	201	BCD	O53-C13-C23	3.03	116.14	110.30
2	B	202	BCD	C22-C32-C42	3.06	115.95	109.61
2	B	202	BCD	C16-C26-C36	3.13	115.80	109.98
2	A	201	BCD	C23-C33-C43	3.13	116.10	109.61
2	B	202	BCD	C24-C34-C44	3.13	116.10	109.61
2	B	202	BCD	O54-C14-C24	3.15	116.37	110.30
2	A	201	BCD	O51-C11-C21	3.16	116.38	110.30
2	C	203	BCD	C13-O53-C53	3.16	119.66	113.72
2	C	203	BCD	C13-C23-C33	3.16	115.85	109.98
2	C	203	BCD	C17-C27-C37	3.18	115.89	109.98
2	C	203	BCD	C11-C21-C31	3.19	115.91	109.98
2	B	202	BCD	O52-C52-C42	3.20	116.29	109.75
2	B	202	BCD	O33-C33-C23	3.21	117.34	110.36
2	C	203	BCD	O55-C15-C25	3.22	116.51	110.30
2	B	202	BCD	O55-C55-C45	3.23	116.35	109.75
2	A	201	BCD	O33-C33-C23	3.23	117.39	110.36
2	A	201	BCD	C26-C36-C46	3.25	116.34	109.61
2	A	201	BCD	C11-O51-C51	3.25	119.84	113.72
2	B	202	BCD	C12-O52-C52	3.27	119.88	113.72
2	C	203	BCD	C16-O56-C56	3.31	119.95	113.72
2	C	203	BCD	O56-C56-C46	3.32	116.54	109.75
2	A	201	BCD	O56-C16-C26	3.33	116.71	110.30
2	B	202	BCD	C25-C35-C45	3.33	116.51	109.61
2	A	201	BCD	C13-O53-C53	3.34	120.02	113.72
2	B	202	BCD	C16-O56-C56	3.39	120.09	113.72
2	A	201	BCD	C15-O55-C55	3.42	120.15	113.72
2	B	202	BCD	O51-C51-C41	3.42	116.76	109.75
2	B	202	BCD	C13-O53-C53	3.47	120.26	113.72
2	C	203	BCD	O52-C52-C42	3.48	116.87	109.75
2	C	203	BCD	O56-C16-C26	3.48	117.01	110.30
2	A	201	BCD	C16-C26-C36	3.48	116.45	109.98
2	B	202	BCD	O56-C16-C26	3.49	117.02	110.30
2	A	201	BCD	C27-C37-C47	3.49	116.83	109.61
2	B	202	BCD	C27-C37-C47	3.49	116.84	109.61
2	A	201	BCD	C11-C21-C31	3.50	116.49	109.98
2	B	202	BCD	C21-C31-C41	3.53	116.92	109.61
2	C	203	BCD	O57-C57-C47	3.54	116.99	109.75
2	B	202	BCD	O52-C12-C22	3.55	117.14	110.30
2	B	202	BCD	C37-C47-C57	3.59	118.50	110.88
2	C	203	BCD	O57-C17-C27	3.60	117.24	110.30
2	B	202	BCD	O56-C56-C46	3.63	117.18	109.75

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	BCD	C14-O54-C54	3.66	120.62	113.72
2	C	203	BCD	O55-C55-C45	3.71	117.34	109.75
2	A	201	BCD	C15-C25-C35	3.73	116.92	109.98
2	C	203	BCD	C15-O55-C55	3.74	120.76	113.72
2	A	201	BCD	O52-C52-C42	3.74	117.41	109.75
2	B	202	BCD	C15-O55-C55	3.78	120.84	113.72
2	B	202	BCD	C23-C33-C43	3.79	117.46	109.61
2	C	203	BCD	C12-O52-C52	3.79	120.85	113.72
2	A	201	BCD	C12-O52-C52	3.79	120.85	113.72
2	C	203	BCD	C23-C33-C43	3.82	117.52	109.61
2	C	203	BCD	O51-C51-C41	3.85	117.63	109.75
2	C	203	BCD	C15-C25-C35	3.87	117.17	109.98
2	B	202	BCD	O57-C57-C47	3.92	117.78	109.75
2	B	202	BCD	C17-C27-C37	3.94	117.30	109.98
2	A	201	BCD	C14-C24-C34	3.94	117.30	109.98
2	A	201	BCD	O57-C17-C27	3.96	117.93	110.30
2	A	201	BCD	C17-O57-C57	3.97	121.19	113.72
2	A	201	BCD	C17-C27-C37	3.97	117.36	109.98
2	A	201	BCD	O56-C56-C46	3.98	117.89	109.75
2	B	202	BCD	O51-C11-C21	3.99	117.98	110.30
2	B	202	BCD	C11-O51-C51	4.00	121.25	113.72
2	A	201	BCD	O55-C55-C45	4.01	117.96	109.75
2	B	202	BCD	O54-C54-C44	4.03	117.99	109.75
2	A	201	BCD	O53-C53-C43	4.08	118.10	109.75
2	C	203	BCD	C17-O57-C57	4.11	121.45	113.72
2	A	201	BCD	O51-C51-C41	4.11	118.15	109.75
2	A	201	BCD	C16-O56-C56	4.13	121.49	113.72
2	B	202	BCD	C17-O57-C57	4.14	121.51	113.72
2	A	201	BCD	O54-C54-C44	4.17	118.28	109.75
2	B	202	BCD	O57-C17-C27	4.19	118.39	110.30
2	C	203	BCD	C11-O51-C51	4.20	121.63	113.72
2	C	203	BCD	O53-C53-C43	4.21	118.38	109.75
2	C	203	BCD	C14-C24-C34	4.26	117.90	109.98
2	A	201	BCD	O57-C57-C47	4.29	118.53	109.75
2	C	203	BCD	C14-O54-C54	4.39	121.99	113.72
2	C	203	BCD	O54-C54-C44	4.75	119.46	109.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	202	BCD	0	1

## 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	87/96 (90%)	-0.26	1 (1%) 80 83	17, 28, 47, 58	0
1	B	81/96 (84%)	-0.08	5 (6%) 21 25	17, 31, 57, 76	0
1	C	80/96 (83%)	0.13	4 (5%) 30 33	19, 39, 71, 78	0
All	All	248/288 (86%)	-0.07	10 (4%) 39 43	17, 31, 58, 78	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	76	GLN	3.6
1	C	110	ASN	3.4
1	C	78	ARG	3.2
1	B	156	LYS	2.8
1	B	77	ALA	2.7
1	B	78	ARG	2.6
1	C	92	TYR	2.6
1	C	89	LYS	2.4
1	A	110	ASN	2.1
1	B	110	ASN	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 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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BCD	B	202	77/77	0.90	0.10	0.11	20,33,46,53	0
2	BCD	A	201	77/77	0.90	0.10	0.05	22,34,46,51	0
2	BCD	C	203	77/77	0.90	0.11	-0.05	23,32,40,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.