



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:27 PM GMT

PDB ID : 1KDS  
Title : X-ray crystal structure of AmpC beta-lactamase from E. coli in complex with the inhibitor 3-nitrophenylboronic acid  
Authors : Powers, R.A.; Shoichet, B.K.  
Deposited on : 2001-11-13  
Resolution : 2.15 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

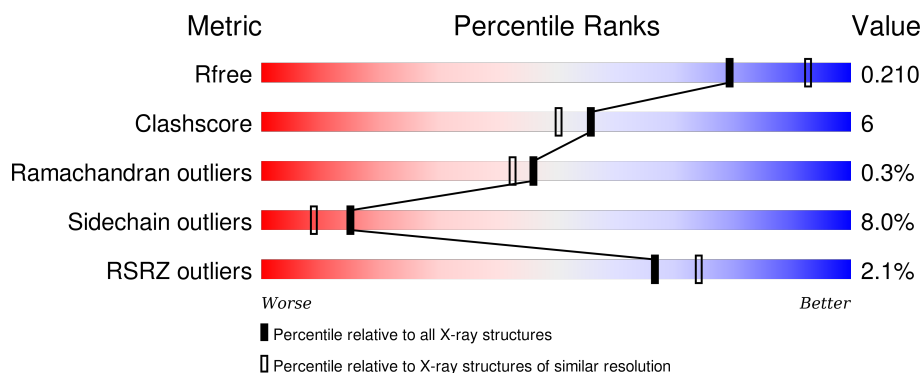
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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))
$R_{free}$	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	358	<div> <div>4%</div> <div>82%</div> <div>16%</div> <div>•</div> </div>
1	B	358	<div> <div>%</div> <div>82%</div> <div>17%</div> <div>•</div> </div>

## 2 Entry composition [i](#)

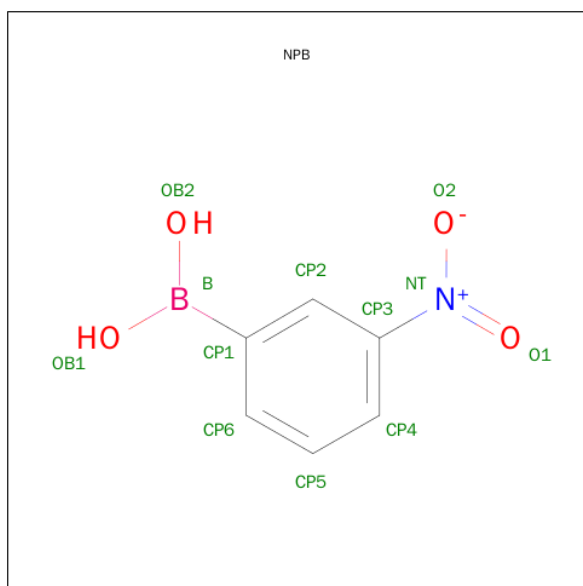
There are 3 unique types of molecules in this entry. The entry contains 5623 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BETA-LACTAMASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2732	1764	458	504	6			
1	B	358	Total	C	N	O	S	0	0	0
			2727	1764	456	501	6			

- Molecule 2 is 3-NITROPHENYLBORONIC ACID (three-letter code: NPB) (formula:  $C_6H_6BNO_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	B	C	N	O	0	0
			12	1	6	1	4		
2	B	1	Total	B	C	N	O	0	0
			12	1	6	1	4		

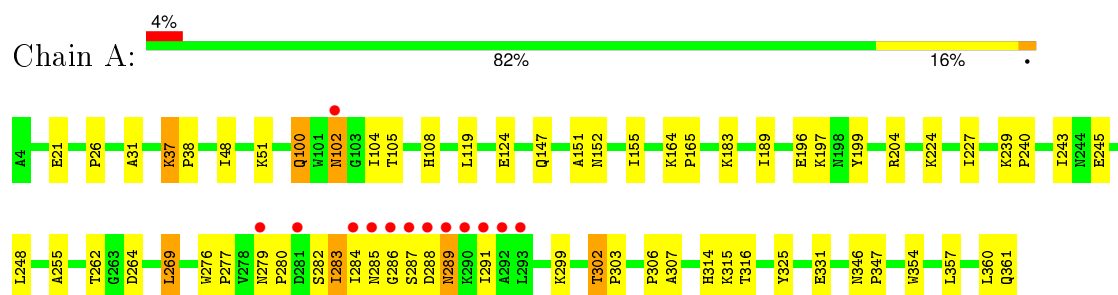
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	61	Total 61	O 61	0	0
3	B	79	Total 79	O 79	0	0

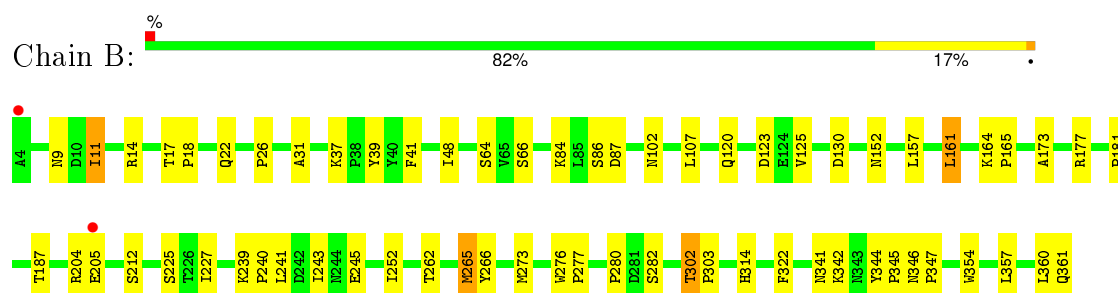
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $\text{RSRZ} > 2$ ). 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: BETA-LACTAMASE



#### • Molecule 1: BETA-LACTAMASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.11Å 77.73Å 99.01Å 90.00° 115.86° 90.00°	Depositor
Resolution (Å)	20.00 – 2.15 25.18 – 2.15	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.15) 97.8 (25.18-2.15)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.93 (at 2.15Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.174 , 0.211 0.173 , 0.210	Depositor DCC
$R_{free}$ test set	4330 reflections (11.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.0	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 58.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 43506 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5623	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.16% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NPB

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	0.37	0/2812	0.62	0/3857
1	B	0.36	0/2807	0.63	0/3850
All	All	0.37	0/5619	0.63	0/7707

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	2732	0	2633	34	0
1	B	2727	0	2635	32	0
2	A	12	0	6	2	0
2	B	12	0	6	2	0
3	A	61	0	0	0	0
3	B	79	0	0	1	0
All	All	5623	0	5280	67	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 6.

All (67) 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:240:PRO:HA	1:A:243:ILE:HD13	1.56	0.87
1:A:286:GLY:HA2	1:A:291:ILE:HD13	1.60	0.81
1:B:240:PRO:HA	1:B:243:ILE:HD12	1.64	0.78
1:A:164:LYS:HB2	1:A:165:PRO:HD3	1.75	0.67
1:A:26:PRO:HB3	1:A:48:ILE:HD11	1.77	0.66
1:A:255:ALA:HA	1:A:269:LEU:HB2	1.78	0.66
1:A:280:PRO:O	1:A:284:ILE:HG13	1.96	0.65
1:B:11:ILE:HD11	1:B:360:LEU:HD21	1.77	0.65
1:B:181:PRO:HB3	1:B:245:GLU:HG3	1.84	0.59
1:A:280:PRO:HG3	1:A:354:TRP:CE2	2.38	0.58
1:B:18:PRO:O	1:B:22:GLN:HG2	2.03	0.58
1:B:360:LEU:O	1:B:361:GLN:CB	2.52	0.57
1:B:26:PRO:HB3	1:B:48:ILE:HD11	1.88	0.55
1:B:164:LYS:HB2	1:B:165:PRO:HD3	1.87	0.55
1:A:105:THR:H	1:A:108:HIS:CD2	2.26	0.54
1:A:280:PRO:HG3	1:A:354:TRP:CZ2	2.42	0.54
1:B:280:PRO:HG3	1:B:354:TRP:CZ2	2.43	0.53
1:B:14:ARG:O	1:B:18:PRO:HG2	2.09	0.53
1:B:276:TRP:CD2	1:B:277:PRO:HA	2.44	0.52
1:A:285:ASN:O	1:A:291:ILE:HG21	2.09	0.52
1:A:287:SER:O	1:A:288:ASP:C	2.48	0.51
1:B:9:ASN:HD22	1:B:41:PHE:HE2	1.57	0.51
1:B:262:THR:O	1:B:262:THR:HG23	2.12	0.50
1:B:17:THR:HB	1:B:18:PRO:HD3	1.93	0.50
1:B:243:ILE:HD13	1:B:252:ILE:HD12	1.94	0.49
1:A:360:LEU:O	1:A:361:GLN:CB	2.60	0.49
2:B:364:NPB:CP6	2:B:364:NPB:OB2	2.59	0.49
1:A:303:PRO:HD3	1:B:107:LEU:HD22	1.95	0.48
1:B:346:ASN:HB2	1:B:347:PRO:HD3	1.95	0.48
1:A:37:LYS:HE3	1:A:38:PRO:O	2.12	0.48
1:B:265:MET:HG2	1:B:266:TYR:N	2.29	0.48
1:A:240:PRO:HA	1:A:243:ILE:CD1	2.36	0.48
1:A:316:THR:HG22	1:A:325:TYR:CD1	2.49	0.47
1:A:279:ASN:O	1:A:282:SER:HB2	2.14	0.47
1:A:276:TRP:CD2	1:A:277:PRO:HA	2.49	0.47
1:A:100:GLN:HG3	1:A:100:GLN:H	1.37	0.47
1:A:287:SER:HB2	1:A:346:ASN:HB3	1.96	0.47
1:B:120:GLN:HG2	3:B:457:HOH:O	2.14	0.46
1:B:31:ALA:HB2	1:B:227:ILE:HG13	1.96	0.45
1:A:245:GLU:HB2	1:A:248:LEU:HB3	1.98	0.45
1:B:164:LYS:HA	1:B:164:LYS:HD2	1.80	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:TYR:HB2	1:B:345:PRO:HD2	1.99	0.45
1:A:105:THR:H	1:A:108:HIS:HD2	1.64	0.44
1:A:31:ALA:HB2	1:A:227:ILE:HG13	1.99	0.44
1:B:84:LYS:HB2	1:B:87:ASP:OD1	2.18	0.44
1:A:119:LEU:HA	1:A:151:ALA:HA	2.00	0.43
1:A:104:ILE:HA	1:A:108:HIS:HD2	1.83	0.43
1:A:283:ILE:HG12	1:A:283:ILE:H	1.52	0.43
1:A:243:ILE:HD12	1:A:243:ILE:N	2.33	0.43
1:B:322:PHE:CD2	1:B:341:ASN:HA	2.53	0.43
1:B:187:THR:HG23	1:B:225:SER:HB2	2.01	0.43
1:B:173:ALA:O	1:B:177:ARG:HB2	2.19	0.43
1:B:11:ILE:HD11	1:B:360:LEU:CD2	2.44	0.42
1:A:286:GLY:HA2	1:A:291:ILE:CD1	2.40	0.42
1:A:346:ASN:N	1:A:347:PRO:CD	2.83	0.42
1:B:152:ASN:HD21	2:B:364:NPB:CP4	2.32	0.42
1:A:276:TRP:HA	1:A:277:PRO:C	2.39	0.42
1:B:125:VAL:HG13	1:B:130:ASP:HB3	2.02	0.41
1:B:64:SER:C	1:B:66:SER:N	2.73	0.41
1:B:302:THR:HA	1:B:303:PRO:HA	1.74	0.41
2:A:364:NPB:OB2	2:A:364:NPB:CP6	2.65	0.41
1:B:157:LEU:HG	1:B:161:LEU:HD22	2.03	0.41
1:A:306:PRO:O	1:A:307:ALA:C	2.58	0.41
1:B:37:LYS:HE3	1:B:39:TYR:CZ	2.56	0.41
1:A:119:LEU:O	1:A:152:ASN:HB2	2.20	0.40
1:A:152:ASN:HD21	2:A:364:NPB:CP4	2.35	0.40
1:A:302:THR:HA	1:A:303:PRO:HA	1.86	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	356/358 (99%)	345 (97%)	9 (2%)	2 (1%)	30	21
1	B	356/358 (99%)	351 (99%)	5 (1%)	0	100	100
All	All	712/716 (99%)	696 (98%)	14 (2%)	2 (0%)	46	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	289	ASN

### 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	274/292 (94%)	247 (90%)	27 (10%)	10	5
1	B	273/292 (94%)	256 (94%)	17 (6%)	23	17
All	All	547/584 (94%)	503 (92%)	44 (8%)	15	9

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLU
1	A	37	LYS
1	A	51	LYS
1	A	100	GLN
1	A	102	ASN
1	A	124	GLU
1	A	147	GLN
1	A	155	ILE
1	A	183	LYS
1	A	189	ILE
1	A	196	GLU
1	A	197	LYS
1	A	199	TYR
1	A	204	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	224	LYS
1	A	239	LYS
1	A	262	THR
1	A	264	ASP
1	A	269	LEU
1	A	283	ILE
1	A	289	ASN
1	A	299	LYS
1	A	302	THR
1	A	314	HIS
1	A	315	LYS
1	A	331	GLU
1	A	357	LEU
1	B	11	ILE
1	B	86	SER
1	B	102	ASN
1	B	123	ASP
1	B	161	LEU
1	B	204	ARG
1	B	205	GLU
1	B	212	SER
1	B	239	LYS
1	B	241	LEU
1	B	265	MET
1	B	273	MET
1	B	282	SER
1	B	302	THR
1	B	314	HIS
1	B	342	LYS
1	B	357	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	23	GLN
1	A	108	HIS
1	A	235	GLN
1	A	289	ASN
1	B	9	ASN
1	B	23	GLN
1	B	139	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	190	ASN
1	B	261	GLN
1	B	285	ASN
1	B	289	ASN

### 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](#)

2 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	NPB	A	364	1	10,12,12	3.29	5 (50%)	13,16,16	2.40	3 (23%)
2	NPB	B	364	1	10,12,12	3.21	4 (40%)	13,16,16	2.41	3 (23%)

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	NPB	A	364	1	-	0/8/8/8	0/1/1/1
2	NPB	B	364	1	-	0/8/8/8	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	364	NPB	CP6-CP1	-3.29	1.35	1.40
2	A	364	NPB	CP2-CP1	-3.03	1.36	1.40
2	A	364	NPB	CP6-CP1	-2.74	1.36	1.40
2	B	364	NPB	CP2-CP1	-2.37	1.37	1.40
2	A	364	NPB	O1-NT	-2.24	1.18	1.22
2	B	364	NPB	B-OB2	3.67	1.42	1.36
2	A	364	NPB	B-OB2	3.87	1.42	1.36
2	B	364	NPB	B-OB1	8.17	1.49	1.36
2	A	364	NPB	B-OB1	8.22	1.50	1.36

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	364	NPB	OB1-B-CP1	-5.67	102.27	119.58
2	B	364	NPB	OB2-B-CP1	-5.60	102.47	119.58
2	A	364	NPB	OB2-B-CP1	-5.37	103.19	119.58
2	B	364	NPB	OB1-B-CP1	-5.31	103.36	119.58
2	A	364	NPB	CP2-CP3-NT	2.01	120.56	118.80
2	B	364	NPB	CP2-CP3-NT	2.99	121.42	118.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	364	NPB	2	0
2	B	364	NPB	2	0

## 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 [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	358/358 (100%)	-0.01	13 (3%) 46 57	9, 19, 48, 92	0
1	B	358/358 (100%)	-0.30	2 (0%) 90 92	10, 19, 36, 50	0
All	All	716/716 (100%)	-0.16	15 (2%) 67 74	9, 19, 41, 92	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	291	ILE	8.8
1	A	293	LEU	8.4
1	A	285	ASN	8.4
1	A	287	SER	6.9
1	A	290	LYS	6.1
1	A	284	ILE	5.5
1	A	292	ALA	5.3
1	A	288	ASP	3.6
1	A	102	ASN	3.3
1	A	289	ASN	3.3
1	A	279	ASN	2.9
1	A	286	GLY	2.6
1	B	4	ALA	2.6
1	B	205	GLU	2.6
1	A	281	ASP	2.2

### 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	NPB	A	364	12/12	0.85	0.14	1.77	14,29,46,48	0
2	NPB	B	364	12/12	0.93	0.11	0.29	13,25,35,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.