



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:39 PM GMT

PDB ID : 1Y64  
Title : Bni1p Formin Homology 2 Domain complexed with ATP-actin  
Authors : Otomo, T.; Tomchick, D.R.; Otomo, C.; Panchal, S.C.; Machius, M.; Rosen, M.K.  
Deposited on : 2004-12-03  
Resolution : 3.05 Å(reported)

This is a wwPDB X-ray Structure 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/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 (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

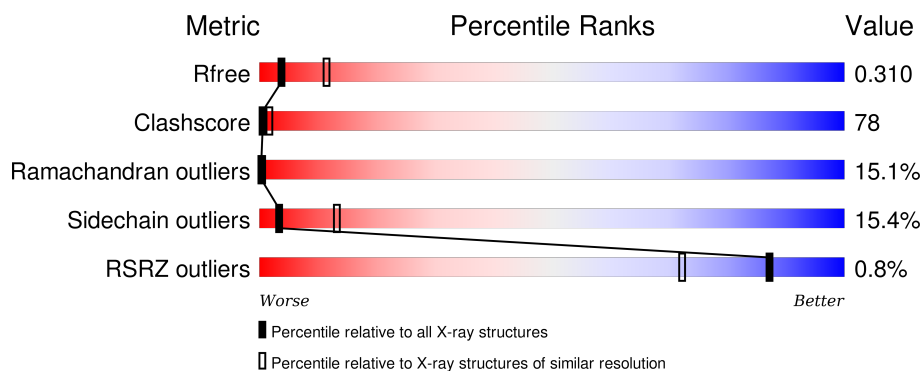
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.05 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	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)

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	375	<div> <div>17%</div> <div>53%</div> <div>21%</div> <div>• 5%</div> </div>
2	B	443	<div> <div>23%</div> <div>51%</div> <div>17%</div> <div>• 7%</div> </div>

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
3	CA	A	382	-	-	-	X
4	ATP	A	2000	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6162 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	0	0
			2795	1772	469	536	18			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	HIC	HIS	MODIFIED RESIDUE	UNP P68135

- Molecule 2 is a protein called BNI1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	411	Total	C	N	O	S	7	0	0
			3335	2124	560	641	10			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).

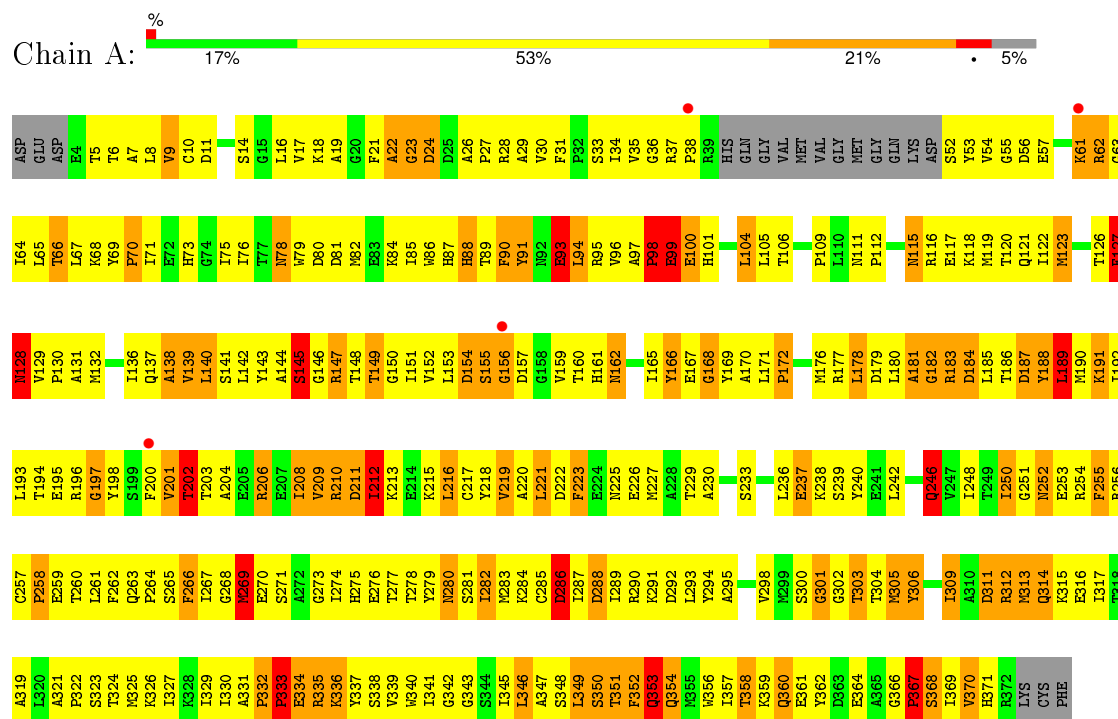


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

### 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: Actin, alpha skeletal muscle



K1584	D1648	E1710	F1652	L1591	E1718	S1720	K1723	F1724	A1725	K1726	I1727	S1728	F1729	F1730	K1731	K1732	F1733	F1736	I1737	Y1740	K1741	K1742	A1743	Q1746	M1747	E1751	E1752	R1755	L1756	Y1757	I1758	K1759	H1760	LYS	LYS	ILE	VAL	GLU	GLU	GLN	GLN	LYS
Q1585	C1649	S1711	L1653	L1590	H1714	D1719	K1723	F1724	A1725	K1726	I1727	S1728	F1729	F1730	K1731	K1732	F1733	F1736	I1737	Y1740	K1741	K1742	A1743	Q1746	M1747	E1751	E1752	R1755	L1756	Y1757	I1758	K1759	H1760	LYS	LYS	ILE	VAL	GLU	GLU	GLN	GLN	LYS
A1586		L1712	S1655	F1589	T1715	S1720	K1723	F1724	A1725	K1726	I1727	S1728	F1729	F1730	K1731	K1732	F1733	F1736	I1737	Y1740	K1741	K1742	A1743	Q1746	M1747	E1751	E1752	R1755	L1756	Y1757	I1758	K1759	H1760	LYS	LYS	ILE	VAL	GLU	GLU	GLN	GLN	LYS
		M1713	S1656	K1590		S1720	K1723	F1724	A1725	K1726	I1727	S1728	F1729	F1730	K1731	K1732	F1733	F1736	I1737	Y1740	K1741	K1742	A1743	Q1746	M1747	E1751	E1752	R1755	L1756	Y1757	I1758	K1759	H1760	LYS	LYS	ILE	VAL	GLU	GLU	GLN	GLN	LYS
			V1657	L1591	E1718	S1720	K1723	F1724	A1725	K1726	I1727	S1728	F1729	F1730	K1731	K1732	F1733	F1736	I1737	Y1740	K1741	K1742	A1743	Q1746	M1747	E1751	E1752	R1755	L1756	Y1757	I1758	K1759	H1760	LYS	LYS	ILE	VAL	GLU	GLU	GLN	GLN	LYS
				L1590	H1714	D1719	K1723	F1724	A1725	K1726	I1727	S1728	F1729	F1730	K1731	K1732	F1733	F1736	I1737	Y1740	K1741	K1742	A1743	Q1746	M1747	E1751	E1752	R1755	L1756	Y1757	I1758	K1759	H1760	LYS	LYS	ILE	VAL	GLU	GLU	GLN	GLN	LYS
						S1720	K1723	F1724	A1725	K1726	I1727	S1728	F1729	F1730	K1731	K1732	F1733	F1736	I1737	Y1740	K1741	K1742	A1743	Q1746	M1747	E1751	E1752	R1755	L1756	Y1757	I1758	K1759	H1760	LYS	LYS	ILE	VAL	GLU	GLU	GLN	GLN	LYS
						S1720	K1723	F1724	A1725	K1726	I1727	S1728	F1729	F1730	K1731	K1732	F1733	F1736	I1737	Y1740	K1741	K1742	A1743	Q1746	M1747	E1751	E1752	R1755	L1756	Y1757	I1758	K1759	H1760	LYS	LYS	ILE	VAL	GLU	GLU	GLN	GLN	LYS
						S1720	K1723	F1724	A1725	K1726	I1727	S1728	F1729	F1730	K1731	K1732	F1733	F1736	I1737	Y1740	K1741	K1742	A1743	Q1746	M1747	E1751	E1752	R1755	L1756	Y1757	I1758	K1759	H1760	LYS	LYS	ILE	VAL	GLU	GLU	GLN	GLN	LYS
						S1720	K1723	F1724	A1725	K1726	I1727	S1728	F1729	F1730	K1731	K1732	F1733	F1736	I1737	Y1740	K1741	K1742	A1743	Q1746	M1747	E1751	E1752	R1755	L1756	Y1757	I1758	K1759	H1760	LYS	LYS	ILE	VAL	GLU	GLU	GLN	GLN	LYS
						S1720	K1723	F1724	A1725	K1726	I1727	S1728	F1729	F1730	K1731	K1732	F1733	F1736	I1737	Y1740	K1741	K1742	A1743	Q1746	M1747	E1751	E1752	R1755	L1756	Y1757	I1758	K1759	H1760	LYS	LYS	ILE	VAL	GLU	GLU	GLN	GLN	LYS
						S1720	K1723	F1724	A1725	K1726	I1727	S1728	F1729	F1730	K1731	K1732	F1733	F1736	I1737	Y1740	K1741	K1742	A1743	Q1746	M1747	E1751	E1752	R1755	L1756	Y1757	I1758	K1759	H1760	LYS	LYS	ILE	VAL	GLU	GLU	GLN	GLN	LYS
						S1720	K1723	F1724	A1725	K1726	I1727	S1728	F1729	F1730	K1731	K1732	F1733	F1736	I1737	Y1740	K1741	K1742	A1743	Q1746	M1747	E1751	E1752	R1755	L1756	Y1757	I1758	K1759	H1760	LYS	LYS	ILE	VAL	GLU	GLU	GLN	GLN	LYS
						S1720	K1723	F1724	A1725	K1726	I1727	S1728	F1729	F1730	K1731	K1732	F1733	F1736	I1737	Y1740	K1741	K1742	A1743	Q1746	M1747	E1751	E1752	R1755	L1756	Y1757	I1758	K1759	H1760	LYS	LYS	ILE	VAL	GLU	GLU	GLN	GLN	LYS
						S1720	K1723	F1724	A1725	K1726	I1727	S1728	F1729	F1730	K1731	K1732	F1733	F1736	I1737	Y1740	K1741	K1742	A1743	Q1746	M1747	E1751	E1752	R1755	L1756	Y1757	I1758	K1759	H1760	LYS	LYS	ILE	VAL	GLU	GLU	GLN	GLN	LYS
						S1720	K1723	F1724	A1725	K1726	I1727	S1728	F1729	F1730	K1731	K1732	F1733	F1736	I1737	Y1740	K1741	K1742	A1743	Q1746	M1747	E1751	E1752	R1755	L1756	Y1757	I1758	K1759	H1760	LYS	LYS	ILE	VAL	GLU	GLU	GLN	GLN	LYS
						S1720	K1723	F1724	A1725	K1726	I1727	S1728	F1729	F1730	K1731	K1732	F1733	F1736	I1737	Y1740	K1741	K1742	A1743	Q1746	M1747	E1751	E1752	R1755	L1756	Y1757	I1758	K1759	H1760	LYS	LYS	ILE	VAL	GLU	GLU	GLN	GLN	LYS
						S1720	K1723	F1724	A1725	K1726	I1727	S1728	F1729	F1730	K1731	K1732	F1733	F1736	I1737	Y1740	K1741	K1742	A1743	Q1746	M1747	E1751	E1752	R1755	L1756	Y1757	I1758	K1759	H1760	LYS	LYS	ILE	VAL	GLU	GLU	GLN	GLN	LYS
						S1720	K1723	F1724	A1725	K1726	I1727	S1728	F1729	F1730	K1731	K1732	F1733	F1736	I1737	Y1740	K1741	K1742	A1743	Q1746	M1747	E1751	E1752	R1755	L1756	Y1757	I1758	K1759	H1760	LYS	LYS	ILE	VAL	GLU	GLU	GLN	GLN	LYS
						S1720	K1723	F1724	A1725	K1726	I1727	S1728	F1729	F1730	K1731	K1732	F1733	F1736	I1737	Y1740	K1741	K1742	A1743	Q1746	M1747	E1751	E1752	R1755	L1756	Y1757	I1758	K1759	H1760	LYS	LYS	ILE	VAL	GLU	GLU	GLN	GLN	LYS
						S1720	K1723	F1724	A1725	K1726	I1727	S1728	F1729	F1730	K1731	K1732	F1733	F1736	I1737	Y1740	K1741	K1742	A1743	Q1746	M1747	E1751	E1752	R1755	L1756	Y1757	I1758	K1759	H1760	LYS	LYS	ILE	VAL	GLU	GLU	GLN	GLN	LYS
						S1720	K1723	F1724	A1725	K1726	I1727	S1728	F1729	F1730	K1731	K1732	F1733	F1736	I1737	Y1740	K1741	K1742	A1743	Q1746	M1747	E1751	E1752	R1755	L1756	Y1757	I1758	K1759	H1760	LYS	LYS	ILE	VAL	GLU	GLU	GLN	GLN	LYS
						S1720	K1723	F1724	A1725	K1726	I1727	S1728	F1729	F1730	K1731	K1732	F1733	F1736	I1737	Y1740	K1741	K1742	A1743	Q1746	M1747	E1751	E1752	R1755	L1756	Y1757	I1758	K1759	H1760	LYS	LYS	ILE	VAL	GLU	GLU	GLN	GLN	LYS
						S1720	K1723	F1724	A1725	K1726	I1727	S1728	F1729	F1730	K1731	K1732	F1733	F1736	I1737	Y1740	K1741	K1742	A1743	Q1746	M1747	E1751	E1752	R1755	L1756	Y1757	I1758	K1759	H1760	LYS	LYS	ILE	VAL	GLU	GLU	GLN	GLN	LYS
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						S1720	K1723	F1724	A1725	K1726	I1727	S1728	F1729	F1730	K1731	K1732	F1733	F1736	I1737	Y1740	K1741	K1742	A1743	Q1746	M1747	E1751	E1752	R1755	L1756	Y1757	I1758	K1759	H1760	LYS	LYS	ILE	VAL	GLU	GLU	GLN	GLN	LYS
						S1720	K1723	F1724	A1725	K1726	I1727	S1728	F1729	F1730	K1731	K1732	F1733	F1736	I1737	Y1740	K1741	K1742	A1743	Q1746	M1747	E1751	E1752	R1755	L1756	Y1757	I1758	K1759	H1760	LYS	LYS	ILE	VAL	GLU	GLU	GLN	GLN	LYS
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						S1720	K1723	F1724	A1725	K1726	I1727	S1728	F1729	F1730	K1731	K1732	F1733	F1736	I1737	Y1740	K1741	K1742	A1743	Q1746	M1747	E1751	E1752	R1755	L1756	Y1757	I1758	K1759	H1760	LYS	LYS	ILE	VAL	GLU	GLU	GLN	GLN	LYS
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						S1720	K1723	F1724	A1725	K1726	I1727	S1728	F1729	F1730	K1731	K1732	F1733	F1736	I1737	Y1740	K1741	K1742	A1743	Q1746	M1747	E1751	E1752	R1755	L1756	Y1757	I1758	K1759	H1760	LYS	LYS	ILE	VAL	GLU	GLU	GLN	GLN	LYS
						S1720	K1723	F1724	A1725	K1726	I1727	S1728	F1729	F1730	K1731	K1732	F1733	F1736	I1737	Y1740	K1741	K1742	A1743	Q1746	M1747	E1751																

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	232.00Å 56.23Å 100.94Å 90.00° 107.70° 90.00°	Depositor
Resolution (Å)	30.00 – 3.05 29.00 – 3.05	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.05) 99.2 (29.00-3.05)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.64 (at 3.05Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.289 , 0.313 0.283 , 0.310	Depositor DCC
$R_{free}$ test set	1145 reflections (4.79%)	DCC
Wilson B-factor (Å <sup>2</sup> )	89.0	Xtriage
Anisotropy	0.721	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 70.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	4 of 23883 reflections (0.017%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6162	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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: CA, HIC, ATP

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	0.51	0/2842	0.97	10/3852 (0.3%)
2	B	0.45	0/3395	0.81	3/4577 (0.1%)
All	All	0.48	0/6237	0.89	13/8429 (0.2%)

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

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	210	ARG	N-CA-C	-8.04	89.28	111.00
2	B	1429	PHE	N-CA-C	-7.39	91.03	111.00
1	A	127	PHE	O-C-N	-6.87	111.71	122.70
1	A	140	LEU	CA-CB-CG	6.57	130.40	115.30
1	A	306	TYR	N-CA-C	-6.14	94.43	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	PHE	Mainchain

## 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	2795	0	2765	557	0
2	B	3335	0	3349	424	0
3	A	1	0	0	0	0
4	A	31	0	12	13	0
All	All	6162	0	6126	958	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 78.

The worst 5 of 958 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:350:SER:OG	2:B:1411:ARG:HB3	1.39	1.21
1:A:350:SER:HB2	2:B:1411:ARG:HD3	1.27	1.15
1:A:259:GLU:HG3	1:A:263:GLN:HG3	1.29	1.11
2:B:1456:LEU:HD21	2:B:1532:LEU:HD23	1.25	1.10
1:A:196:ARG:HH22	1:A:251:GLY:HA3	1.15	1.09

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	352/375 (94%)	205 (58%)	91 (26%)	56 (16%)	<div>00</div>
2	B	409/443 (92%)	232 (57%)	118 (29%)	59 (14%)	<div>01</div>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	761/818 (93%)	437 (57%)	209 (28%)	115 (15%)	0 0

5 of 115 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	GLY
1	A	61	LYS
1	A	90	PHE
1	A	98	PRO
1	A	99	GLU

### 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	302/317 (95%)	249 (82%)	53 (18%)	2 9
2	B	374/404 (93%)	323 (86%)	51 (14%)	5 18
All	All	676/721 (94%)	572 (85%)	104 (15%)	3 13

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	352	PHE
2	B	1424	ASP
2	B	1686	PRO
1	A	353	GLN
1	A	370	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1457	GLN
2	B	1493	ASN
2	B	1675	HIS

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Mol	Chain	Res	Type
2	B	1476	ASN
2	B	1480	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	HIC	A	73	1	8,11,12	0.76	0	5,14,16	1.68	2 (40%)

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	HIC	A	73	1	-	0/4/6/8	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	HIC	O-C-CA	-2.27	119.57	125.49
1	A	73	HIC	CZ-NE2-CD2	2.31	134.86	126.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	73	HIC	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	$\# Z  > 2$
4	ATP	A	2000	3	24,33,33	1.79	3 (12%)	31,52,52	2.17	4 (12%)

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
4	ATP	A	2000	3	-	0/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2000	ATP	C5-N7	-2.07	1.32	1.39
4	A	2000	ATP	O4'-C1'	2.49	1.44	1.41
4	A	2000	ATP	C2-N1	7.02	1.47	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	A	2000	ATP	N3-C2-N1	-9.97	121.26	128.89
4	A	2000	ATP	PB-O3B-PG	-3.79	119.95	132.67
4	A	2000	ATP	C4-C5-N7	-2.55	107.13	109.48
4	A	2000	ATP	N6-C6-N1	2.20	123.92	119.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2000	ATP	13	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](#)

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	356/375 (94%)	-0.22	4 (1%)	82 63	41, 99, 154, 190	0
2	B	411/443 (92%)	-0.46	2 (0%)	91 81	57, 109, 159, 207	2 (0%)
All	All	767/818 (93%)	-0.35	6 (0%)	87 72	41, 103, 157, 207	2 (0%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	38	PRO	3.4
2	B	1757	TYR	2.6
1	A	156	GLY	2.6
1	A	200	PHE	2.3
1	A	61	LYS	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
1	HIC	A	73	11/12	0.95	0.15	-	57,67,67,67	0

### 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(Å <sup>2</sup> )	Q<0.9
3	CA	A	382	1/1	0.94	0.78	5.95	97,97,97,97	0
4	ATP	A	2000	31/31	0.86	0.34	1.25	97,97,97,97	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.