



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 10:37 pm GMT

PDB ID : 2PNN  
Title : Crystal Structure of the Ankyrin Repeat Domain of Trpv1  
Authors : Jin, X.; Gaudet, R.  
Deposited on : 2007-04-24  
Resolution : 2.70 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 : trunk28620  
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) : recalc28949

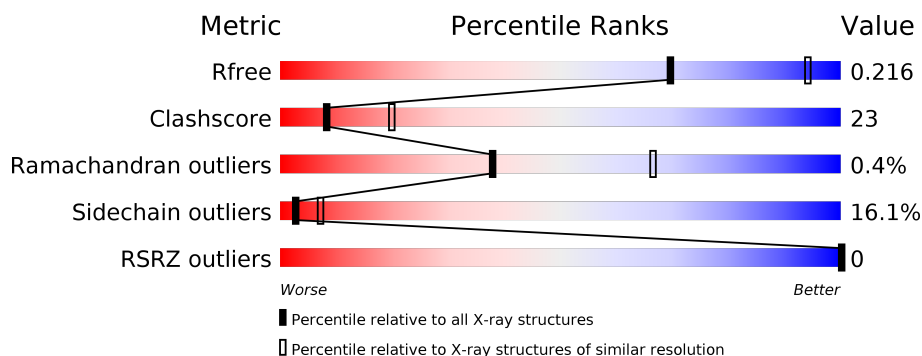
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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	273	<div> <div></div> <div>56%</div> <div>27%</div> <div>7%</div> <div>9%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2034 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 Transient receptor potential cation channel subfamily V member 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	Se	0	0	0
			1932	1225	335	366	3	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	162	MSE	MET	MODIFIED RESIDUE	UNP O35433
A	214	MSE	MET	MODIFIED RESIDUE	UNP O35433
A	308	MSE	MET	MODIFIED RESIDUE	UNP O35433
A	365	ALA	-	CLONING ARTIFACT	UNP O35433
A	366	ALA	-	CLONING ARTIFACT	UNP O35433
A	367	ALA	-	CLONING ARTIFACT	UNP O35433
A	368	HIS	-	CLONING ARTIFACT	UNP O35433
A	369	HIS	-	CLONING ARTIFACT	UNP O35433
A	370	HIS	-	CLONING ARTIFACT	UNP O35433
A	371	HIS	-	CLONING ARTIFACT	UNP O35433
A	372	HIS	-	CLONING ARTIFACT	UNP O35433
A	373	HIS	-	CLONING ARTIFACT	UNP O35433

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



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

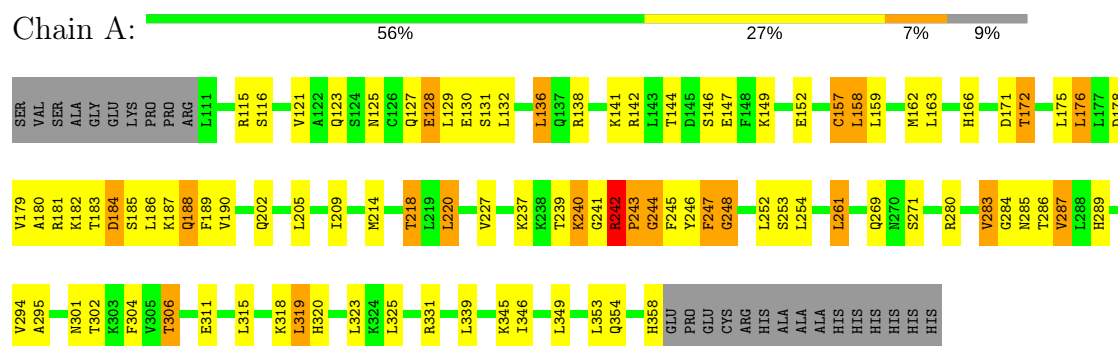
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	71	Total O 71 71	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: Transient receptor potential cation channel subfamily V member 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.47Å 99.47Å 106.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.70 28.71 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.7 (20.00-2.70) 92.6 (28.71-2.50)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.91 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.199 , 0.248 0.207 , 0.216	Depositor DCC
$R_{free}$ test set	496 reflections (5.16%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.8	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 13.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.087 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2034	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.45% 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: 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	0.54	0/1959	0.71	1/2647 (0.0%)

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	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	ASP	CB-CG-OD2	5.17	122.95	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	LYS	Peptide
1	A	242	ARG	Peptide
1	A	243	PRO	Peptide
1	A	244	GLY	Peptide
1	A	247	PHE	Peptide
1	A	248	GLY	Peptide

## 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	1932	0	1972	92	0
2	A	31	0	12	2	0
3	A	71	0	0	3	0
All	All	2034	0	1984	92	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 23.

All (92) 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:243:PRO:HB2	1:A:244:GLY:HA3	1.30	1.06
1:A:239:THR:OG1	1:A:243:PRO:HB3	1.61	1.00
1:A:136:LEU:H	1:A:136:LEU:HD23	1.41	0.86
1:A:239:THR:CB	1:A:243:PRO:HB3	2.06	0.86
1:A:121:VAL:HG22	1:A:172:THR:HG21	1.58	0.84
1:A:127:GLN:O	1:A:130:GLU:HG3	1.78	0.84
1:A:243:PRO:HB2	1:A:244:GLY:CA	2.08	0.81
1:A:127:GLN:HG2	1:A:130:GLU:OE2	1.85	0.77
1:A:240:LYS:N	1:A:241:GLY:HA2	2.01	0.74
1:A:136:LEU:HB2	1:A:141:LYS:O	1.90	0.70
1:A:243:PRO:CB	1:A:244:GLY:HA3	2.15	0.70
1:A:158:LEU:HD21	1:A:162:MSE:HE2	1.73	0.69
1:A:302:THR:O	1:A:306:THR:HB	1.94	0.68
1:A:280:ARG:HG2	1:A:284:GLY:O	1.95	0.67
1:A:239:THR:HB	1:A:243:PRO:HB3	1.76	0.66
1:A:184:ASP:C	1:A:186:LEU:H	1.96	0.66
1:A:142:ARG:HD3	1:A:183:THR:HG21	1.78	0.64
1:A:158:LEU:HD21	1:A:162:MSE:CE	2.27	0.64
1:A:239:THR:HB	1:A:243:PRO:CB	2.29	0.63
1:A:158:LEU:HD22	1:A:158:LEU:O	1.99	0.63
1:A:214:MSE:HE3	1:A:218:THR:OG1	1.99	0.63
1:A:253:SER:HA	1:A:287:VAL:HG13	1.81	0.62
1:A:239:THR:CB	1:A:243:PRO:CB	2.75	0.62
1:A:142:ARG:CD	1:A:183:THR:HG21	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:GLN:HE21	1:A:188:GLN:H	1.46	0.61
1:A:320:HIS:HB3	1:A:323:LEU:HD23	1.82	0.61
1:A:142:ARG:NE	1:A:183:THR:CG2	2.64	0.60
1:A:358:HIS:HB2	3:A:42:HOH:O	2.02	0.59
1:A:125:ASN:ND2	1:A:128:GLU:HG2	2.18	0.58
1:A:246:TYR:CE1	1:A:248:GLY:CA	2.86	0.58
1:A:159:LEU:O	1:A:163:LEU:HD22	2.04	0.58
1:A:158:LEU:CD2	1:A:162:MSE:HE2	2.33	0.58
1:A:349:LEU:C	1:A:349:LEU:HD23	2.25	0.57
1:A:175:LEU:O	1:A:179:VAL:HG23	2.04	0.57
1:A:205:LEU:HA	1:A:220:LEU:HD23	1.86	0.56
1:A:247:PHE:CE1	1:A:254:LEU:HD13	2.40	0.56
1:A:246:TYR:CE1	1:A:248:GLY:HA3	2.41	0.56
1:A:285:ASN:HA	1:A:289:HIS:CD2	2.41	0.56
1:A:286:THR:H	1:A:289:HIS:CD2	2.24	0.55
1:A:157:CYS:HB2	1:A:176:LEU:HD21	1.89	0.55
1:A:184:ASP:C	1:A:186:LEU:N	2.59	0.55
1:A:349:LEU:CD2	1:A:353:LEU:HD12	2.36	0.55
1:A:121:VAL:HG22	1:A:172:THR:CG2	2.33	0.55
1:A:180:ALA:O	1:A:185:SER:N	2.39	0.55
1:A:240:LYS:HB3	1:A:242:ARG:HB2	1.89	0.54
1:A:239:THR:OG1	1:A:243:PRO:CB	2.45	0.54
1:A:214:MSE:CE	1:A:218:THR:OG1	2.56	0.54
1:A:349:LEU:HD23	1:A:353:LEU:HD12	1.88	0.54
1:A:202:GLN:HE22	2:A:374:ATP:N6	2.06	0.54
1:A:320:HIS:CB	1:A:323:LEU:HD23	2.37	0.53
1:A:286:THR:H	1:A:289:HIS:HD2	1.57	0.53
1:A:354:GLN:HE21	1:A:358:HIS:HE1	1.55	0.53
1:A:142:ARG:CZ	1:A:183:THR:HG22	2.39	0.52
1:A:354:GLN:HE21	1:A:358:HIS:CE1	2.27	0.51
1:A:178:ASP:O	1:A:182:LYS:HG2	2.11	0.51
1:A:240:LYS:N	1:A:241:GLY:CA	2.70	0.50
1:A:242:ARG:H	1:A:243:PRO:CA	2.24	0.50
1:A:158:LEU:HB2	1:A:189:PHE:CZ	2.47	0.50
1:A:136:LEU:CD2	1:A:136:LEU:H	2.19	0.50
1:A:319:LEU:HB3	1:A:320:HIS:CD2	2.47	0.50
1:A:181:ARG:C	1:A:184:ASP:H	2.15	0.50
1:A:142:ARG:CD	1:A:183:THR:CG2	2.91	0.49
1:A:247:PHE:CZ	1:A:254:LEU:HD13	2.47	0.48
1:A:127:GLN:HA	1:A:130:GLU:HG3	1.94	0.48
1:A:205:LEU:O	1:A:209:ILE:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ARG:H	1:A:243:PRO:HA	1.77	0.47
1:A:158:LEU:CD2	1:A:158:LEU:O	2.61	0.47
1:A:239:THR:HA	1:A:243:PRO:HA	1.97	0.47
1:A:129:LEU:HD22	1:A:132:LEU:HD22	1.97	0.46
1:A:239:THR:C	1:A:241:GLY:HA2	2.35	0.46
1:A:142:ARG:NE	1:A:183:THR:HG22	2.31	0.46
1:A:115:ARG:HD3	1:A:115:ARG:O	2.15	0.45
1:A:172:THR:O	1:A:176:LEU:HB2	2.15	0.45
1:A:261:LEU:HD21	1:A:311:GLU:HG2	2.00	0.44
1:A:158:LEU:C	1:A:158:LEU:HD22	2.38	0.43
1:A:269:GLN:HE22	1:A:318:LYS:NZ	2.17	0.43
1:A:237:LYS:HB2	1:A:237:LYS:HE3	1.67	0.43
1:A:283:VAL:O	1:A:331:ARG:HB2	2.19	0.43
1:A:295:ALA:HA	1:A:301:ASN:HD21	1.84	0.42
1:A:239:THR:OG1	1:A:241:GLY:HA2	2.19	0.42
1:A:142:ARG:C	1:A:144:THR:H	2.22	0.42
1:A:202:GLN:HE22	2:A:374:ATP:HN62	1.67	0.42
1:A:158:LEU:C	1:A:158:LEU:CD2	2.89	0.41
1:A:243:PRO:HG3	3:A:5:HOH:O	2.20	0.41
1:A:188:GLN:H	1:A:188:GLN:NE2	2.13	0.41
1:A:136:LEU:N	1:A:136:LEU:HD23	2.21	0.41
1:A:349:LEU:HD23	1:A:349:LEU:O	2.20	0.41
1:A:166:HIS:CG	1:A:166:HIS:O	2.74	0.41
1:A:180:ALA:O	1:A:184:ASP:N	2.54	0.41
1:A:295:ALA:HB3	1:A:345:LYS:HD2	2.03	0.40
1:A:243:PRO:HD3	3:A:5:HOH:O	2.21	0.40
1:A:146:SER:HA	1:A:149:LYS:HE2	2.04	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	246/273 (90%)	227 (92%)	18 (7%)	1 (0%)	38 66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	ARG

### 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	211/228 (92%)	177 (84%)	34 (16%)	3 7

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	SER
1	A	123	GLN
1	A	128	GLU
1	A	131	SER
1	A	136	LEU
1	A	138	ARG
1	A	147	GLU
1	A	152	GLU
1	A	157	CYS
1	A	158	LEU
1	A	171	ASP
1	A	172	THR
1	A	176	LEU
1	A	187	LYS
1	A	188	GLN
1	A	190	VAL
1	A	218	THR
1	A	220	LEU
1	A	227	VAL
1	A	242	ARG

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Mol	Chain	Res	Type
1	A	245	PHE
1	A	252	LEU
1	A	261	LEU
1	A	271	SER
1	A	283	VAL
1	A	287	VAL
1	A	294	VAL
1	A	304	PHE
1	A	306	THR
1	A	315	LEU
1	A	319	LEU
1	A	325	LEU
1	A	339	LEU
1	A	346	ILE

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	125	ASN
1	A	188	GLN
1	A	269	GLN
1	A	289	HIS
1	A	358	HIS

### 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](#)

1 ligand 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	$\# Z  > 2$
2	ATP	A	374	-	27,33,33	1.09	2 (7%)	25,52,52	1.58	2 (8%)

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	ATP	A	374	-	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	374	ATP	C2-N3	2.04	1.35	1.32
2	A	374	ATP	C5-C4	3.40	1.48	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	374	ATP	N3-C2-N1	-5.67	123.92	128.86
2	A	374	ATP	C1'-N9-C4	-2.20	122.84	126.64

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
2	A	374	ATP	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	245/273 (89%)	-0.75	0 100 100	29, 37, 43, 49	0

There are no RSRZ outliers to report.

### 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(Å <sup>2</sup> )	Q<0.9
2	ATP	A	374	31/31	0.97	0.10	-1.06	50,53,58,59	2

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

There are no such residues in this entry.