



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2017 – 04:15 AM EDT

PDB ID : 2RKU  
Title : Structure of PLK1 in complex with BI2536  
Authors : Ding, Y.-H.; Kothe, M.; Kohls, D.; Low, S.  
Deposited on : unknown  
Resolution : 1.95 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

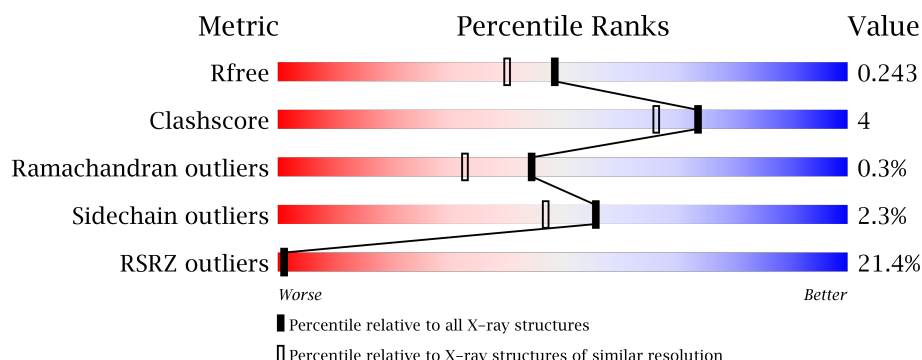
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2004 (1.96-1.96)
Clashscore	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)
RSRZ outliers	101464	2018 (1.96-1.96)

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	294	<div> <div>21%</div> <div> <div></div> <div>90%</div> <div>10%</div> </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
2	ZN	A	501	-	-	-	X
4	TLA	A	502	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SRT	A	505	X	-	-	-
5	SRT	A	507	X	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 2785 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 Serine/threonine-protein kinase PLK1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	5	0
			2411	1546	428	425	12			

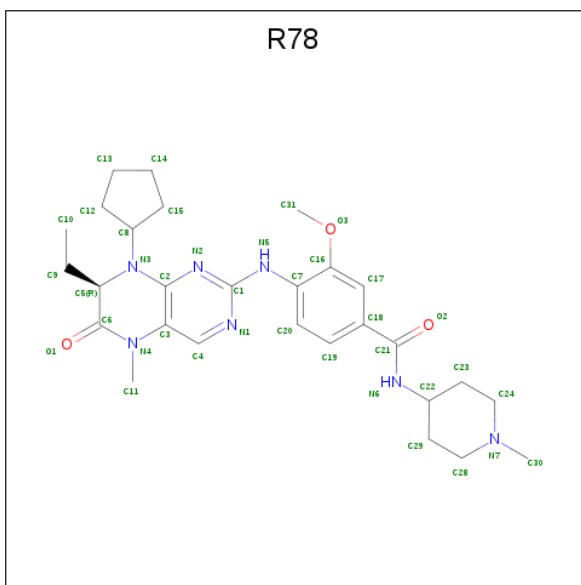
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	210	VAL	THR	ENGINEERED	UNP P53350

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

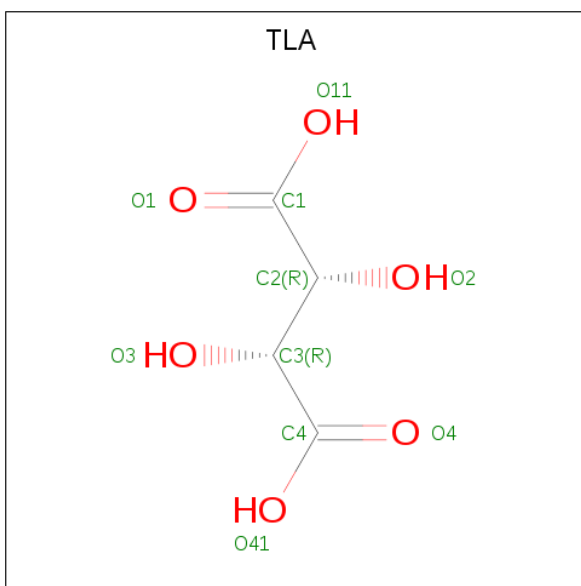
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 4-[(7R)-8-cyclopentyl-7-ethyl-5-methyl-6-oxo-5,6,7,8-tetrahydropteridin-2-yl]amino}-3-methoxy-N-(1-methylpiperidin-4-yl)benzamide (three-letter code: R78) (formula: C<sub>28</sub>H<sub>39</sub>N<sub>7</sub>O<sub>3</sub>).



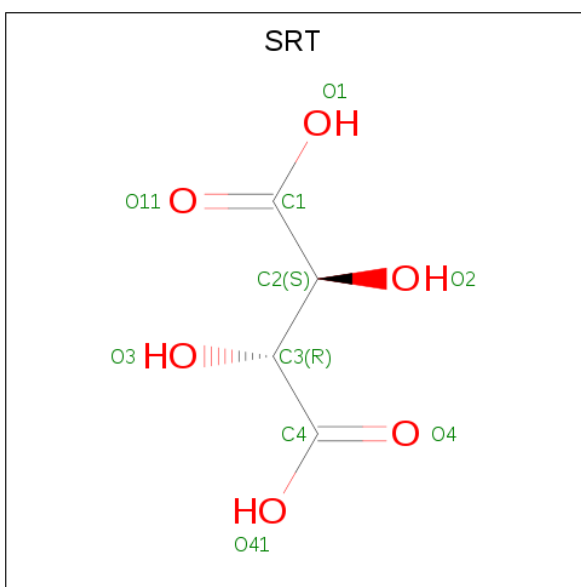
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			38	28	7	3		

- Molecule 4 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula:  $C_4H_6O_6$ ).



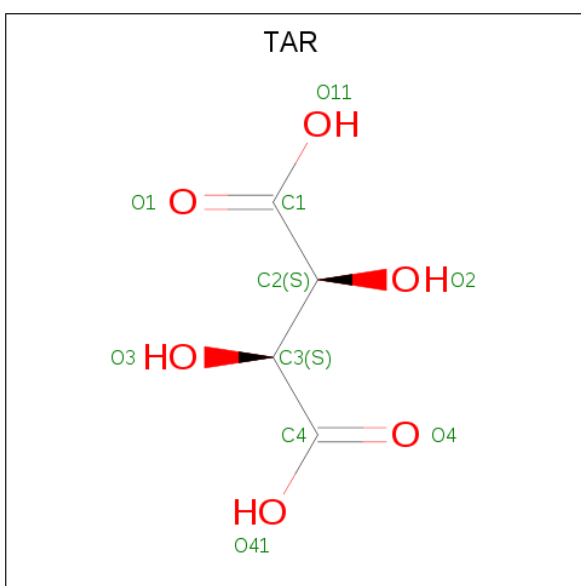
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	4	6		
4	A	1	Total	C	O	0	0
			10	4	6		

- Molecule 5 is S,R MESO-TARTARIC ACID (three-letter code: SRT) (formula:  $C_4H_6O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	4	6		
5	A	1	Total	C	O	0	0
			10	4	6		

- Molecule 6 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula:  $C_4H_6O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	4	6		

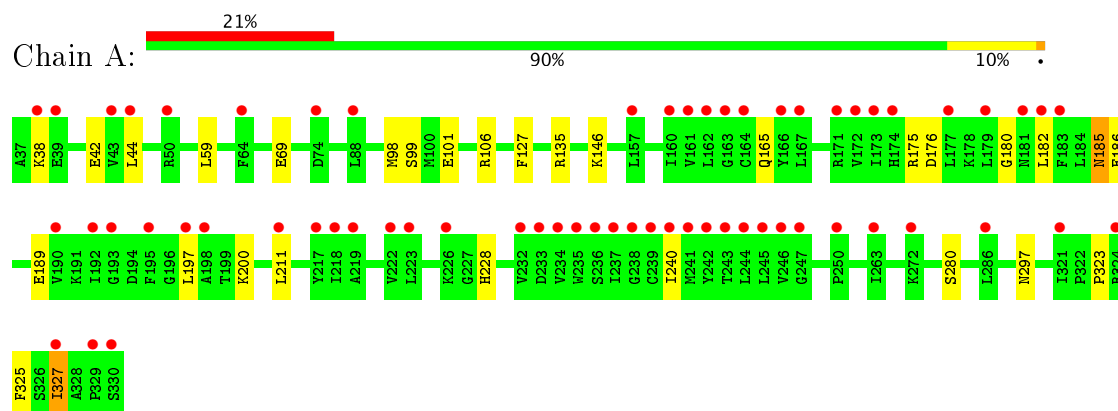
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	285	Total 285	O 285	0	0

### 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 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: Serine/threonine-protein kinase PLK1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.59Å 66.59Å 154.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.41 – 1.95 32.55 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.4 (33.41-1.95) 99.4 (32.55-1.95)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.17 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.190 , 0.241 0.205 , 0.243	Depositor DCC
$R_{free}$ test set	1494 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.9	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2785	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: R78, ZN, SRT, TLA, TAR

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	0.67	2/2466 (0.1%)	0.67	0/3327

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	42	GLU	CD-OE1	9.52	1.36	1.25
1	A	42	GLU	CG-CD	7.78	1.63	1.51

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2411	0	2465	17	1
2	A	1	0	0	0	0
3	A	38	0	39	2	0
4	A	20	0	8	0	0
5	A	20	0	8	1	0
6	A	10	0	4	1	0
7	A	285	0	0	3	0
All	All	2785	0	2524	19	1

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 4.

All (19) 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:176:ASP:OD2	7:A:513:HOH:O	2.03	0.74
1:A:186:GLU:HB2	7:A:664:HOH:O	2.05	0.55
1:A:175:ARG:HH11	1:A:228:HIS:HE1	1.55	0.53
1:A:180:GLY:N	6:A:503:TAR:O4	2.41	0.53
3:A:500:R78:N2	3:A:500:R78:H20	2.25	0.51
1:A:185:ASN:ND2	1:A:189:GLU:H	2.09	0.50
3:A:500:R78:H4	3:A:500:R78:H11	1.64	0.46
1:A:59:LEU:HD21	1:A:69:GLU:HG3	1.99	0.45
1:A:182:LEU:HD11	1:A:240:ILE:HD13	2.00	0.44
1:A:185:ASN:HD22	1:A:185:ASN:C	2.20	0.44
1:A:101:GLU:OE2	7:A:704:HOH:O	2.21	0.44
1:A:165:GLN:HG2	1:A:297:ASN:HD22	1.83	0.44
1:A:175:ARG:HH11	1:A:228:HIS:CE1	2.35	0.43
1:A:146:LYS:HD3	1:A:146:LYS:HA	1.81	0.42
1:A:197:LEU:HD13	1:A:211:LEU:HD21	2.02	0.42
1:A:165:GLN:HG2	1:A:297:ASN:ND2	2.35	0.41
1:A:44:LEU:HD22	1:A:127:PHE:CE2	2.55	0.41
1:A:135:ARG:NH2	5:A:507:SRT:O4	2.51	0.41
1:A:323:PRO:HG2	1:A:325:PHE:CE1	2.55	0.41

All (1) 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)
1:A:99[B]:SER:OG	1:A:327:ILE:O[2_564]	2.09	0.11

## 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	297/294 (101%)	286 (96%)	10 (3%)	1 (0%)	44 33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	LYS

### 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	268/263 (102%)	262 (98%)	6 (2%)	57 49

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

Mol	Chain	Res	Type
1	A	98	MET
1	A	106	ARG
1	A	185	ASN
1	A	200	LYS
1	A	280	SER
1	A	327	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	123	ASN
1	A	165	GLN
1	A	185	ASN
1	A	228	HIS
1	A	297	ASN

### 5.3.3 RNA ⓘ

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](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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$
3	R78	A	500	-	40,42,42	0.87	2 (5%)	44,60,60	2.12	12 (27%)
4	TLA	A	502	2	3,9,9	0.66	0	6,12,12	0.75	0
6	TAR	A	503	-	3,9,9	0.72	0	6,12,12	1.64	1 (16%)
4	TLA	A	504	-	3,9,9	0.88	0	6,12,12	0.67	0
5	SRT	A	505	-	3,9,9	0.49	0	6,12,12	0.67	0
5	SRT	A	507	-	3,9,9	0.44	0	6,12,12	1.02	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	R78	A	500	-	-	0/20/57/57	0/5/5/5
4	TLA	A	502	2	-	0/4/12/12	0/0/0/0
6	TAR	A	503	-	-	0/4/12/12	0/0/0/0
4	TLA	A	504	-	-	0/4/12/12	0/0/0/0
5	SRT	A	505	-	2/2/4/4	0/4/12/12	0/0/0/0
5	SRT	A	507	-	2/2/4/4	0/4/12/12	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	R78	C5-C6	-2.10	1.48	1.51
3	A	500	R78	O1-C6	2.10	1.26	1.22

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	R78	N1-C1-N2	-6.51	120.42	126.68
3	A	500	R78	C9-C5-C6	-3.94	101.46	111.20
6	A	503	TAR	C1-C2-C3	-3.10	106.44	113.11
3	A	500	R78	C23-C22-N6	-3.01	105.10	110.53
3	A	500	R78	C30-N7-C24	-2.81	106.44	110.67
3	A	500	R78	C29-C22-N6	-2.78	105.52	110.53
3	A	500	R78	C22-N6-C21	-2.71	119.08	122.61
3	A	500	R78	C20-C19-C18	-2.40	118.11	120.79
3	A	500	R78	C4-C3-N4	-2.06	120.18	122.51
3	A	500	R78	C10-C9-C5	2.13	117.88	113.06
3	A	500	R78	O3-C16-C7	2.98	118.69	114.81
3	A	500	R78	C4-N1-C1	3.67	121.96	115.88
3	A	500	R78	C31-O3-C16	4.86	124.53	117.54

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	505	SRT	C2
5	A	505	SRT	C3
5	A	507	SRT	C2
5	A	507	SRT	C3

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	R78	2	0
6	A	503	TAR	1	0
5	A	507	SRT	1	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	294/294 (100%)	1.15	63 (21%) <b>1</b> <b>1</b>	24, 46, 56, 65	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	329	PRO	6.0
1	A	330	SER	5.6
1	A	177	LEU	5.5
1	A	240	ILE	5.3
1	A	237	ILE	4.6
1	A	226	LYS	4.4
1	A	244	LEU	4.3
1	A	218	ILE	4.2
1	A	239	CYS	4.1
1	A	160	ILE	4.0
1	A	182	LEU	3.8
1	A	192	ILE	3.7
1	A	245	LEU	3.5
1	A	286	LEU	3.5
1	A	64	PHE	3.4
1	A	167	LEU	3.4
1	A	50	ARG	3.3
1	A	246	VAL	3.2
1	A	222	VAL	3.2
1	A	164	CYS	3.2
1	A	172	VAL	3.2
1	A	190	VAL	3.1
1	A	217	TYR	3.1
1	A	234	VAL	3.0
1	A	324	ARG	3.0
1	A	235	TRP	3.0
1	A	211	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	44	LEU	2.9
1	A	157	LEU	2.9
1	A	243	THR	2.8
1	A	174	HIS	2.8
1	A	173	ILE	2.8
1	A	272	LYS	2.8
1	A	39	GLU	2.8
1	A	163	GLY	2.8
1	A	179	LEU	2.8
1	A	197	LEU	2.8
1	A	232	VAL	2.8
1	A	219	ALA	2.7
1	A	166	TYR	2.7
1	A	242	TYR	2.7
1	A	162	LEU	2.7
1	A	327	ILE	2.6
1	A	247	GLY	2.6
1	A	161	VAL	2.6
1	A	74	ASP	2.6
1	A	195	PHE	2.4
1	A	43	VAL	2.4
1	A	183	PHE	2.3
1	A	263	ILE	2.3
1	A	250	PRO	2.3
1	A	321	ILE	2.3
1	A	181[A]	ASN	2.3
1	A	238	GLY	2.2
1	A	193	GLY	2.2
1	A	236	SER	2.2
1	A	223	LEU	2.2
1	A	171	ARG	2.1
1	A	241	MET	2.1
1	A	198	ALA	2.1
1	A	88	LEU	2.1
1	A	233	ASP	2.1
1	A	38	LYS	2.0

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

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
5	SRT	A	507	10/10	0.83	0.42	8.20	78,81,82,82	0
2	ZN	A	501	1/1	0.77	0.26	3.87	34,34,34,34	0
4	TLA	A	502	10/10	0.77	0.23	3.14	35,39,43,44	0
6	TAR	A	503	10/10	0.68	0.24	0.64	56,65,68,69	0
3	R78	A	500	38/38	0.91	0.13	-0.19	24,28,47,49	0
4	TLA	A	504	10/10	0.65	0.20	-	56,57,58,58	0
5	SRT	A	505	10/10	0.72	0.31	-	86,87,88,88	0

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

There are no such residues in this entry.