



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2017 – 11:00 AM EDT

PDB ID : 5ML5  
Title : Human p38alpha MAPK in complex with imidazolyl pyridine inhibitor 11b  
Authors : Buehrmann, M.; Rauh, D.  
Deposited on : 2016-12-06  
Resolution : 1.90 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-20029077  
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-20029077

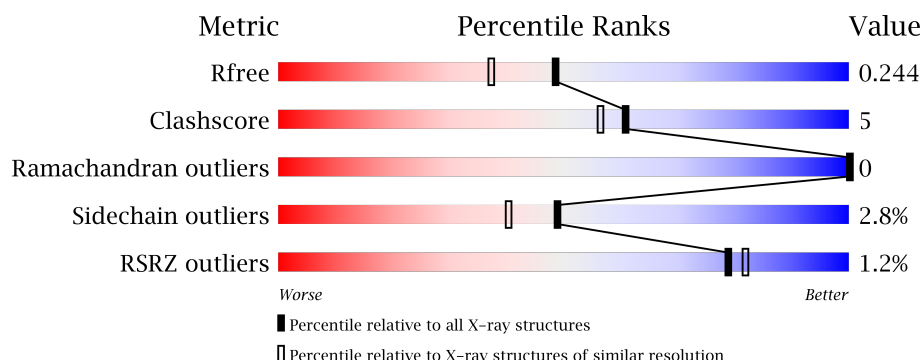
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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	360	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; right: 0; text-align: center;">%</div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 76%, yellow 76%, yellow 89%, grey 89%);"></div> <div style="position: absolute; bottom: -10px; left: 0; right: 0; text-align: center;">76% 13% 9%</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	BOG	A	403	-	-	-	X

## 2 Entry composition [i](#)

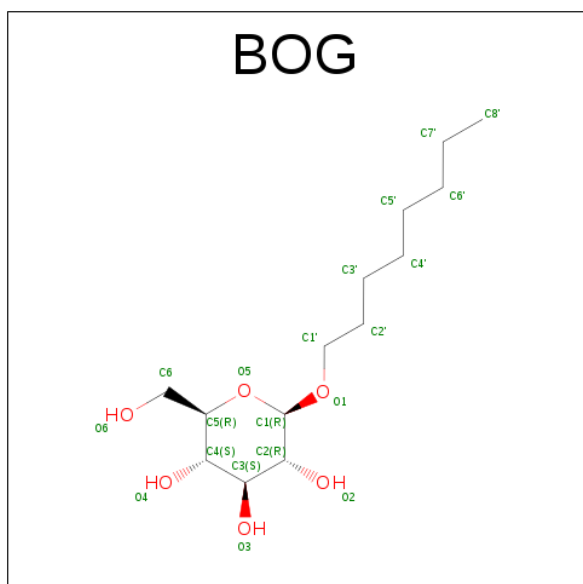
There are 4 unique types of molecules in this entry. The entry contains 2821 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Mitogen-activated protein kinase 14.

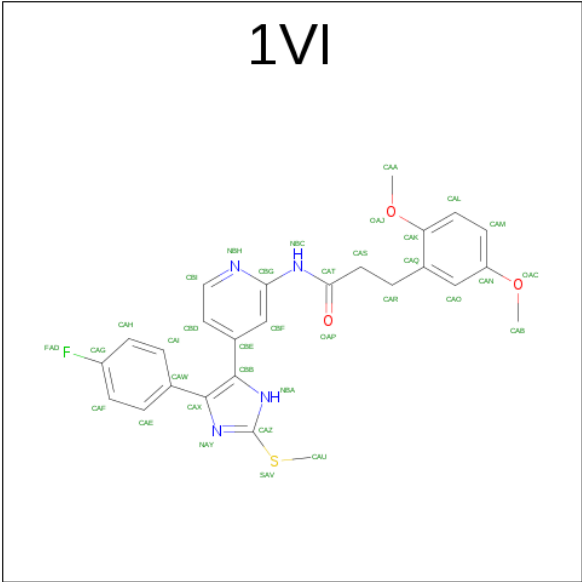
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2623	1686	445	482	10			

- Molecule 2 is B-OCTYLGLUCOSIDE (three-letter code: BOG) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			20	14	6		

- Molecule 3 is 3-(2,5-dimethoxyphenyl)- {N}-[4-[4-(4-fluorophenyl)-2-methylsulfanyl-1 {H}-imidazol-5-yl]pyridin-2-yl]propanamide (three-letter code: 1VI) (formula: C<sub>26</sub>H<sub>25</sub>FN<sub>4</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	S		
3	A	1	35	26	1	4	3	1	0	0

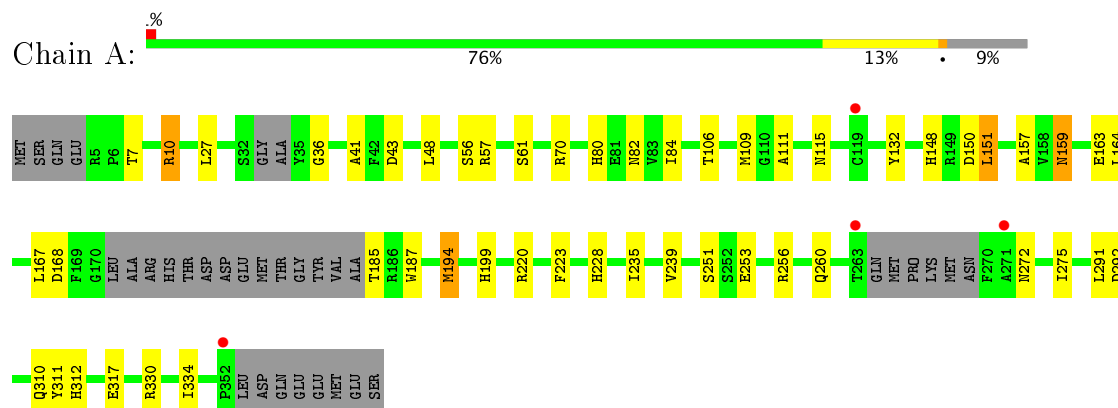
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	103	Total	O	0	0
			103	103		

### 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: Mitogen-activated protein kinase 14



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.50Å 69.39Å 74.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.01 – 1.90 48.01 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.01-1.90) 100.0 (48.01-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.13 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.193 , 0.240 0.202 , 0.244	Depositor DCC
$R_{free}$ test set	1384 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.0	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2821	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% 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: 1VI, BOG

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	0.94	1/2683 (0.0%)	0.96	9/3645 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	TYR	CE1-CZ	-6.13	1.30	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	MET	CG-SD-CE	-7.28	88.55	100.20
1	A	10	ARG	NE-CZ-NH2	5.93	123.27	120.30
1	A	168	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	151	LEU	CB-CG-CD2	5.60	120.53	111.00
1	A	43	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	292	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	A	194	MET	CA-CB-CG	-5.34	104.22	113.30
1	A	70	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	151	LEU	CA-CB-CG	5.01	126.81	115.30

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	2623	0	2601	28	0
2	A	60	0	82	1	0
3	A	35	0	0	0	0
4	A	103	0	0	0	0
All	All	2821	0	2683	28	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 5.

All (28) 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:253:GLU:OE2	1:A:256:ARG:NH1	2.00	0.94
1:A:148:HIS:HD2	1:A:150:ASP:H	1.35	0.75
1:A:272:ASN:O	1:A:275:ILE:HG12	1.92	0.70
1:A:194:MET:O	1:A:228:HIS:HE1	1.76	0.69
1:A:159:ASN:HD22	1:A:159:ASN:C	1.95	0.69
1:A:239:VAL:HG21	1:A:291:LEU:HD13	1.73	0.69
1:A:111:ALA:HA	1:A:115:ASN:HD22	1.62	0.65
1:A:36:GLY:HA2	1:A:56:SER:HB2	1.77	0.64
1:A:80:HIS:CD2	1:A:82:ASN:H	2.15	0.64
1:A:80:HIS:HD2	1:A:82:ASN:H	1.50	0.59
1:A:251:SER:O	1:A:256:ARG:NH2	2.37	0.58
1:A:194:MET:O	1:A:228:HIS:CE1	2.57	0.57
1:A:312:HIS:HD2	1:A:317:GLU:OE1	1.91	0.54
1:A:61:SER:HA	1:A:334:ILE:HD11	1.92	0.51
1:A:310:GLN:HG3	1:A:311:TYR:CD1	2.46	0.50
1:A:310:GLN:HG3	1:A:311:TYR:CE1	2.47	0.49
1:A:27:LEU:HD23	1:A:41:ALA:HB2	1.92	0.49
1:A:111:ALA:HA	1:A:115:ASN:ND2	2.28	0.47
1:A:84:ILE:HD11	1:A:106:THR:OG1	2.15	0.46
1:A:256:ARG:O	1:A:260:GLN:HG3	2.17	0.45
1:A:148:HIS:HE1	1:A:167:LEU:O	1.99	0.45
1:A:185:THR:HG22	1:A:187:TRP:H	1.83	0.44
1:A:157:ALA:O	1:A:164:LEU:HA	2.18	0.43
1:A:159:ASN:ND2	1:A:159:ASN:C	2.67	0.42
1:A:159:ASN:HD21	1:A:163:GLU:H	1.66	0.41
1:A:223:PHE:CE2	1:A:235:ILE:HA	2.55	0.41
1:A:199:HIS:O	2:A:401:BOG:H62	2.20	0.41
1:A:57:ARG:HH21	1:A:57:ARG:HG2	1.85	0.41

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	318/360 (88%)	311 (98%)	7 (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	287/320 (90%)	279 (97%)	8 (3%)	49	40

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	10	ARG
1	A	48	LEU
1	A	109	MET
1	A	151	LEU
1	A	159	ASN
1	A	220	ARG
1	A	330	ARG

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	14	ASN
1	A	80	HIS
1	A	100	ASN
1	A	115	ASN
1	A	148	HIS
1	A	159	ASN
1	A	201	ASN
1	A	202	GLN
1	A	228	HIS
1	A	260	GLN
1	A	310	GLN
1	A	312	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](#)

4 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	BOG	A	401	-	20,20,20	1.10	1 (5%)	25,25,25	1.71	5 (20%)
2	BOG	A	402	-	20,20,20	0.92	2 (10%)	25,25,25	1.86	6 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	BOG	A	403	-	20,20,20	2.48	5 (25%)	25,25,25	2.86	11 (44%)
3	1VI	A	404	-	38,38,38	2.68	9 (23%)	43,52,52	2.06	15 (34%)

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	BOG	A	401	-	-	0/11/31/31	0/1/1/1
2	BOG	A	402	-	-	0/11/31/31	0/1/1/1
2	BOG	A	403	-	-	0/11/31/31	0/1/1/1
3	1VI	A	404	-	-	0/21/23/23	0/4/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	404	1VI	CAW-CAX	-9.80	1.38	1.49
3	A	404	1VI	CBE-CBB	-9.46	1.38	1.49
2	A	403	BOG	O2-C2	-7.17	1.26	1.43
2	A	403	BOG	O3-C3	-4.33	1.33	1.43
3	A	404	1VI	CAR-CAQ	-3.24	1.46	1.51
3	A	404	1VI	CAZ-NBA	-2.74	1.30	1.34
2	A	402	BOG	O2-C2	-2.60	1.37	1.43
2	A	403	BOG	C4-C3	-2.59	1.45	1.52
2	A	403	BOG	C4-C5	-2.43	1.47	1.53
3	A	404	1VI	CAX-CBB	-2.33	1.38	1.43
3	A	404	1VI	CBG-NBC	-2.30	1.35	1.40
2	A	402	BOG	C4-C3	-2.26	1.46	1.52
3	A	404	1VI	CAM-CAN	2.00	1.42	1.38
3	A	404	1VI	OAC-CAB	2.30	1.49	1.42
2	A	401	BOG	O4-C4	3.39	1.50	1.43
3	A	404	1VI	CBI-NBH	3.59	1.42	1.34
2	A	403	BOG	O1-C1	5.48	1.49	1.40

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	403	BOG	C1'-O1-C1	-4.99	105.29	113.87
2	A	403	BOG	O2-C2-C3	-4.88	99.74	110.36
2	A	402	BOG	C1'-O1-C1	-4.31	106.46	113.87
2	A	403	BOG	O4-C4-C5	-4.24	98.61	109.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	402	BOG	O2-C2-C3	-3.66	102.40	110.36
3	A	404	1VI	CAH-CAG-CAF	-3.60	117.85	122.86
2	A	402	BOG	O3-C3-C2	-3.55	102.64	110.36
2	A	401	BOG	C6-C5-C4	-3.33	105.22	113.00
2	A	401	BOG	O6-C6-C5	-3.30	100.22	111.34
3	A	404	1VI	CBD-CBI-NBH	-3.24	120.18	123.92
2	A	403	BOG	O3-C3-C2	-3.11	103.59	110.36
3	A	404	1VI	CAX-CBB-NBA	-2.85	106.08	113.76
2	A	403	BOG	O3-C3-C4	-2.79	104.29	110.36
2	A	401	BOG	O2-C2-C3	-2.73	104.42	110.36
3	A	404	1VI	CBB-CAX-NAY	-2.56	106.86	113.76
2	A	403	BOG	O5-C1-C2	-2.53	105.42	110.30
3	A	404	1VI	CAO-CAQ-CAK	-2.53	115.55	118.30
3	A	404	1VI	CAS-CAR-CAQ	-2.46	106.45	112.35
2	A	403	BOG	C1-C2-C3	-2.36	105.60	109.98
3	A	404	1VI	OAJ-CAK-CAL	-2.22	120.63	124.37
3	A	404	1VI	CAR-CAQ-CAO	-2.16	114.97	119.40
2	A	402	BOG	C4'-C3'-C2'	-2.09	103.67	114.45
3	A	404	1VI	CBD-CBE-CBF	-2.02	115.55	118.16
3	A	404	1VI	OAJ-CAK-CAQ	2.04	118.44	115.86
3	A	404	1VI	CAE-CAW-CAX	2.37	124.33	120.59
2	A	403	BOG	O6-C6-C5	2.46	119.61	111.34
3	A	404	1VI	CBE-CBF-CBG	2.48	122.08	118.90
2	A	402	BOG	O1-C1-C2	2.55	112.40	108.23
3	A	404	1VI	CAN-CAO-CAQ	2.79	124.54	120.53
2	A	403	BOG	O5-C5-C4	2.86	114.93	109.66
2	A	401	BOG	O1-C1-C2	3.05	113.21	108.23
2	A	401	BOG	C1-O5-C5	3.42	120.15	113.72
2	A	402	BOG	O5-C1-O1	3.76	118.95	110.02
3	A	404	1VI	CAI-CAH-CAG	4.64	123.24	118.35
3	A	404	1VI	CAR-CAQ-CAK	5.33	129.45	121.18
2	A	403	BOG	O1-C1-C2	5.98	117.99	108.23
2	A	403	BOG	O5-C1-O1	7.03	126.71	110.02

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	A	401	BOG	1	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	326/360 (90%)	-0.24	4 (1%) 79 82	14, 24, 45, 65	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	119	CYS	3.9
1	A	271	ALA	2.8
1	A	352	PRO	2.4
1	A	263	THR	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(Å <sup>2</sup> )	Q<0.9
2	BOG	A	403	20/20	0.75	0.19	4.13	40,60,75,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	1VI	A	404	35/35	0.96	0.12	0.70	15,20,75,78	0
2	BOG	A	401	20/20	0.95	0.10	0.38	16,20,27,29	0
2	BOG	A	402	20/20	0.96	0.10	-0.02	21,27,40,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.