



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:18 AM GMT

PDB ID : 3LMH  
Title : Crystal Structure of the Alpha-kinase Domain of Myosin Heavy Chain Kinase A Complex with ADP  
Authors : Ye, Q.; Jia, Z.  
Deposited on : 2010-01-30  
Resolution : 2.00 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 (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

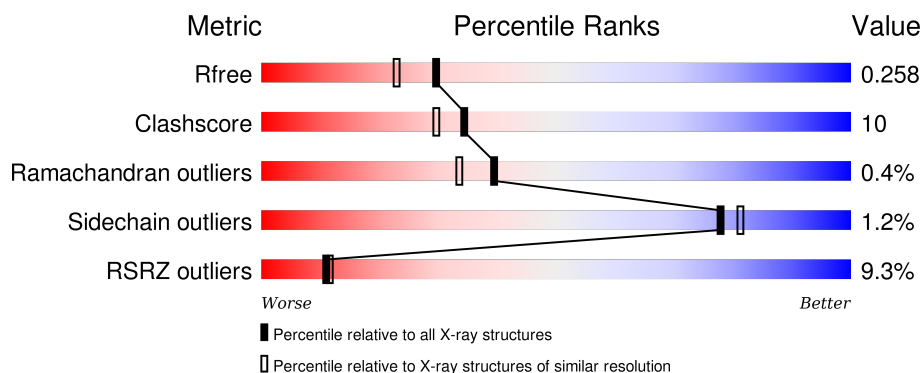
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	307	<div> <div>7%</div> <div>68%</div> <div>12%</div> <div>•</div> <div>19%</div> </div>
1	B	307	<div> <div>8%</div> <div>66%</div> <div>11%</div> <div>•</div> <div>22%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4327 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 Myosin heavy chain kinase A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	P	S	0	0	0
			1978	1270	329	366	1	12			
1	B	240	Total	C	N	O	P	S	0	0	0
			1915	1231	317	354	1	12			

There are 34 discrepancies between the modelled and reference sequences:

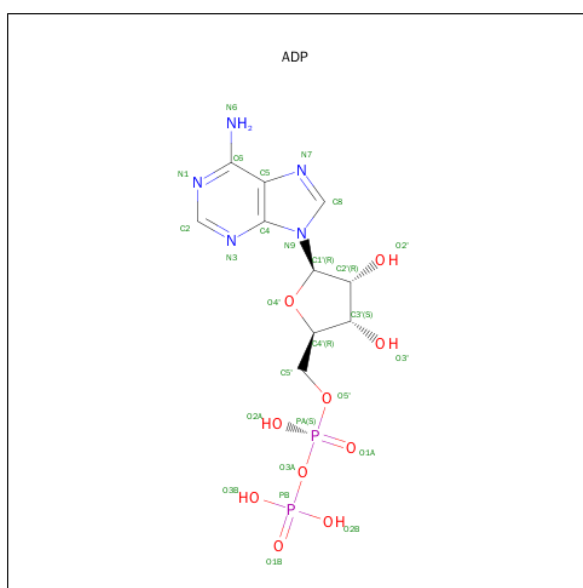
Chain	Residue	Modelled	Actual	Comment	Reference
A	535	MET	-	EXPRESSION TAG	UNP P42527
A	536	GLY	-	EXPRESSION TAG	UNP P42527
A	537	GLY	-	EXPRESSION TAG	UNP P42527
A	538	HIS	-	EXPRESSION TAG	UNP P42527
A	539	HIS	-	EXPRESSION TAG	UNP P42527
A	540	HIS	-	EXPRESSION TAG	UNP P42527
A	541	HIS	-	EXPRESSION TAG	UNP P42527
A	542	HIS	-	EXPRESSION TAG	UNP P42527
A	543	HIS	-	EXPRESSION TAG	UNP P42527
A	544	GLY	-	EXPRESSION TAG	UNP P42527
A	545	GLU	-	EXPRESSION TAG	UNP P42527
A	546	ASN	-	EXPRESSION TAG	UNP P42527
A	547	LEU	-	EXPRESSION TAG	UNP P42527
A	548	TYR	-	EXPRESSION TAG	UNP P42527
A	549	PHE	-	EXPRESSION TAG	UNP P42527
A	550	GLN	-	EXPRESSION TAG	UNP P42527
A	551	GLY	-	EXPRESSION TAG	UNP P42527
B	535	MET	-	EXPRESSION TAG	UNP P42527
B	536	GLY	-	EXPRESSION TAG	UNP P42527
B	537	GLY	-	EXPRESSION TAG	UNP P42527
B	538	HIS	-	EXPRESSION TAG	UNP P42527
B	539	HIS	-	EXPRESSION TAG	UNP P42527
B	540	HIS	-	EXPRESSION TAG	UNP P42527
B	541	HIS	-	EXPRESSION TAG	UNP P42527
B	542	HIS	-	EXPRESSION TAG	UNP P42527

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Chain	Residue	Modelled	Actual	Comment	Reference
B	543	HIS	-	EXPRESSION TAG	UNP P42527
B	544	GLY	-	EXPRESSION TAG	UNP P42527
B	545	GLU	-	EXPRESSION TAG	UNP P42527
B	546	ASN	-	EXPRESSION TAG	UNP P42527
B	547	LEU	-	EXPRESSION TAG	UNP P42527
B	548	TYR	-	EXPRESSION TAG	UNP P42527
B	549	PHE	-	EXPRESSION TAG	UNP P42527
B	550	GLN	-	EXPRESSION TAG	UNP P42527
B	551	GLY	-	EXPRESSION TAG	UNP P42527

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

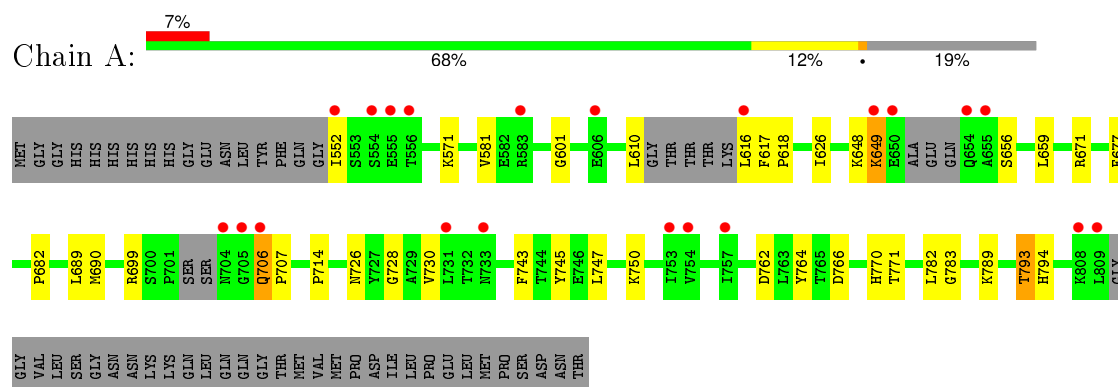
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	204	Total	O	0	0
			204	204		
5	B	164	Total	O	0	0
			164	164		

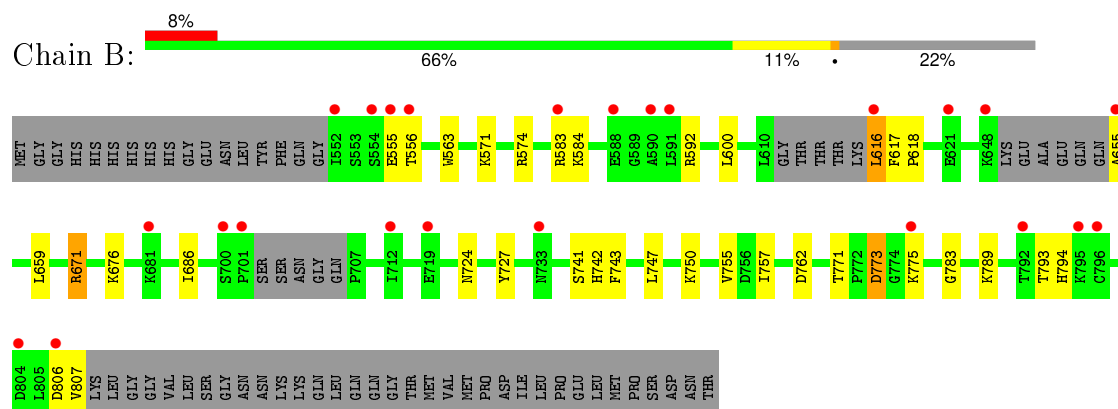
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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: Myosin heavy chain kinase A



#### • Molecule 1: Myosin heavy chain kinase A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.82Å 110.05Å 78.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.70 – 2.00 19.70 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.70-2.00) 99.7 (19.70-2.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.63 (at 2.01Å)	Xtriage
Refinement program	REFMAC 6.1.0	Depositor
R, $R_{free}$	0.216 , 0.259 0.215 , 0.258	Depositor DCC
$R_{free}$ test set	2484 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.5	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 52.2	EDS
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 49114 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4327	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.70% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PO4, ADP, PHD

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	0.50	0/2006	0.61	0/2701
1	B	0.48	0/1943	0.60	1/2618 (0.0%)
All	All	0.49	0/3949	0.61	1/5319 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	671	ARG	NE-CZ-NH2	-5.24	117.68	120.30

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	1978	0	1993	41	0
1	B	1915	0	1929	39	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	204	0	0	10	0
5	B	164	0	0	9	0
All	All	4327	0	3946	79	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 10.

All (79) 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:B:743:PHE:CZ	1:B:747:LEU:HD12	2.00	0.95
1:B:659:LEU:HD11	5:B:94:HOH:O	1.73	0.87
1:B:743:PHE:CZ	1:B:747:LEU:CD1	2.61	0.83
1:A:770:HIS:HD2	1:A:782:LEU:H	1.28	0.81
1:A:770:HIS:CD2	1:A:782:LEU:H	1.99	0.80
1:A:671:ARG:NE	5:A:281:HOH:O	2.13	0.75
1:A:730:VAL:HG23	1:A:793:THR:CG2	2.19	0.73
1:A:706:GLN:HB3	1:A:707:PRO:HD2	1.74	0.70
1:A:728:GLY:O	1:A:793:THR:HG21	1.95	0.66
1:A:671:ARG:NH1	5:A:25:HOH:O	2.28	0.66
1:A:743:PHE:CZ	1:A:747:LEU:HD22	2.33	0.63
1:B:773:ASP:HB2	5:B:81:HOH:O	1.98	0.63
1:A:771:THR:O	1:A:783:GLY:HA2	1.98	0.63
1:A:706:GLN:CB	1:A:707:PRO:HD2	2.29	0.62
1:A:648:LYS:O	1:A:649:LYS:HB2	1.99	0.62
1:A:766:PHD:P	5:A:283:HOH:O	2.57	0.61
1:B:743:PHE:CE2	1:B:747:LEU:HD12	2.36	0.60
1:B:743:PHE:CE1	1:B:747:LEU:CD1	2.84	0.60
1:A:671:ARG:NH1	1:A:690:MET:HG2	2.16	0.60
1:A:581:VAL:HG11	1:A:699:ARG:NH2	2.17	0.59
1:A:552:ILE:HG22	1:A:601:GLY:HA3	1.85	0.58
1:B:741:SER:OG	1:B:757:ILE:CD1	2.51	0.58
1:B:592:ARG:NH1	5:B:282:HOH:O	2.35	0.58
1:B:743:PHE:CE1	1:B:747:LEU:HD12	2.40	0.55
1:A:728:GLY:HA3	1:A:789:LYS:HG3	1.89	0.54
1:B:616:LEU:N	1:B:618:PRO:O	2.41	0.54
1:A:730:VAL:HG23	1:A:793:THR:HG21	1.90	0.54
1:B:727:TYR:CE1	1:B:789:LYS:HG3	2.42	0.53
1:A:656:SER:OG	1:A:659:LEU:HD13	2.08	0.53
1:B:743:PHE:CE1	1:B:747:LEU:HD11	2.44	0.53
1:B:655:ALA:HA	1:B:659:LEU:HD23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:755:VAL:HA	1:B:757:ILE:HD12	1.91	0.52
1:A:571:LYS:HE3	5:A:143:HOH:O	2.09	0.52
1:B:773:ASP:OD2	1:B:775:LYS:HB2	2.10	0.51
1:A:552:ILE:N	5:A:255:HOH:O	2.42	0.51
1:B:727:TYR:CZ	1:B:789:LYS:HG3	2.45	0.51
1:A:745:TYR:CZ	1:A:750:LYS:HG2	2.45	0.51
1:B:671:ARG:NH1	5:B:42:HOH:O	2.43	0.51
1:B:741:SER:OG	1:B:757:ILE:HD13	2.12	0.49
1:B:771:THR:O	1:B:783:GLY:HA2	2.12	0.49
1:B:659:LEU:HB2	5:B:296:HOH:O	2.12	0.49
1:A:689:LEU:HB3	1:A:714:PRO:HD2	1.95	0.48
1:A:581:VAL:HG11	1:A:699:ARG:HH22	1.78	0.48
1:B:676:LYS:HE3	1:B:747:LEU:HD13	1.95	0.47
1:A:706:GLN:N	1:A:706:GLN:OE1	2.47	0.47
1:A:745:TYR:CE1	1:A:750:LYS:HG2	2.50	0.47
1:A:726:ASN:O	1:A:770:HIS:CE1	2.68	0.47
1:A:706:GLN:CB	1:A:707:PRO:CD	2.92	0.47
1:B:755:VAL:HA	1:B:757:ILE:CD1	2.44	0.47
1:A:610:LEU:HD22	1:A:616:LEU:HD11	1.96	0.47
1:B:773:ASP:HB3	1:B:775:LYS:H	1.80	0.46
1:A:766:PHD:P	5:A:12:HOH:O	2.72	0.46
1:A:766:PHD:OP1	5:A:12:HOH:O	2.20	0.46
1:B:741:SER:OG	1:B:757:ILE:HD11	2.15	0.46
1:B:794:HIS:HD2	5:B:30:HOH:O	1.98	0.45
1:A:617:PHE:HA	1:A:618:PRO:C	2.37	0.45
1:A:671:ARG:HH12	1:A:690:MET:HG2	1.80	0.45
1:A:581:VAL:HG12	5:A:15:HOH:O	2.16	0.45
1:A:677:PHE:CE2	1:A:682:PRO:HG3	2.52	0.45
1:B:583:ARG:NH1	1:B:584:LYS:HE3	2.32	0.44
1:B:671:ARG:NH2	5:B:42:HOH:O	2.50	0.44
1:A:682:PRO:HB2	5:A:20:HOH:O	2.16	0.44
1:B:583:ARG:HH12	1:B:584:LYS:HE3	1.83	0.43
1:B:743:PHE:CZ	1:B:747:LEU:HD11	2.48	0.43
1:B:741:SER:HG	1:B:757:ILE:HD11	1.82	0.43
1:A:730:VAL:HG23	1:A:793:THR:HG22	2.01	0.43
1:A:730:VAL:CG2	1:A:793:THR:CG2	2.93	0.43
1:B:617:PHE:CG	1:B:618:PRO:HA	2.54	0.42
1:A:762:ASP:OD1	1:A:764:TYR:OH	2.20	0.42
1:B:563:TRP:CH2	1:B:574:ARG:HD2	2.55	0.42
1:A:626:ILE:HD13	1:B:750:LYS:HD2	2.01	0.42
1:B:806:ASP:O	1:B:807:VAL:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:742:HIS:HE1	5:B:66:HOH:O	2.03	0.41
1:A:706:GLN:HB3	1:A:707:PRO:CD	2.47	0.41
1:A:794:HIS:HD2	5:A:51:HOH:O	2.04	0.41
1:B:555:GLU:HB2	1:B:600:LEU:CD2	2.51	0.41
1:B:571:LYS:HE3	5:B:106:HOH:O	2.21	0.40
1:B:686:ILE:HG22	1:B:762:ASP:HB3	2.03	0.40
1:B:724:ASN:HD21	1:B:757:ILE:HD13	1.85	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	239/307 (78%)	234 (98%)	3 (1%)	2 (1%)	24	15
1	B	231/307 (75%)	226 (98%)	5 (2%)	0	100	100
All	All	470/614 (76%)	460 (98%)	8 (2%)	2 (0%)	39	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	649	LYS
1	A	706	GLN

### 5.3.2 Protein sidechains [i](#)

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	219/269 (81%)	218 (100%)	1 (0%)	92	94
1	B	213/269 (79%)	209 (98%)	4 (2%)	65	67
All	All	432/538 (80%)	427 (99%)	5 (1%)	78	81

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	793	THR
1	B	556	THR
1	B	616	LEU
1	B	773	ASP
1	B	793	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	607	ASN
1	A	629	ASN
1	A	675	ASN
1	A	770	HIS
1	A	794	HIS
1	B	607	ASN
1	B	629	ASN
1	B	742	HIS
1	B	794	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	PHD	A	766	1	8,11,12	0.57	0	9,15,17	1.57	3 (33%)
1	PHD	B	766	1	8,11,12	0.59	0	9,15,17	1.42	1 (11%)

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	PHD	A	766	1	-	0/7/11/13	0/0/0/0
1	PHD	B	766	1	-	0/7/11/13	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	766	PHD	OD2-CG-CB	-3.32	117.06	124.69
1	B	766	PHD	OD2-CG-CB	-2.68	118.53	124.69
1	A	766	PHD	O-C-CA	-2.05	120.16	125.49
1	A	766	PHD	OP2-P-OP1	2.14	117.48	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	766	PHD	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
2	ADP	A	1511	-	22,29,29	1.16	2 (9%)	27,45,45	1.81	4 (14%)
4	PO4	A	842	-	4,4,4	0.66	0	6,6,6	0.33	0
2	ADP	B	1512	-	22,29,29	1.00	1 (4%)	27,45,45	1.72	3 (11%)
4	PO4	B	842	-	4,4,4	0.46	0	6,6,6	0.27	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
2	ADP	A	1511	-	-	0/12/32/32	0/3/3/3
4	PO4	A	842	-	-	0/0/0/0	0/0/0/0
2	ADP	B	1512	-	-	0/12/32/32	0/3/3/3
4	PO4	B	842	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1511	ADP	O4'-C1'	2.83	1.44	1.41
2	B	1512	ADP	C5-C4	3.24	1.47	1.40
2	A	1511	ADP	C5-C4	3.36	1.48	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1511	ADP	N3-C2-N1	-6.96	123.56	128.89
2	B	1512	ADP	N3-C2-N1	-6.61	123.83	128.89
2	B	1512	ADP	C4-C5-N7	-3.40	106.35	109.48
2	A	1511	ADP	C4-C5-N7	-2.78	106.92	109.48
2	B	1512	ADP	PA-O3A-PB	-2.43	124.52	132.67
2	A	1511	ADP	PA-O3A-PB	-2.15	125.47	132.67
2	A	1511	ADP	O3A-PA-O5'	2.30	109.04	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	247/307 (80%)	0.42	21 (8%) 13 14	15, 28, 45, 57	0
1	B	239/307 (77%)	0.61	24 (10%) 9 10	19, 33, 46, 63	0
All	All	486/614 (79%)	0.51	45 (9%) 11 11	15, 30, 46, 63	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	554	SER	8.6
1	A	705	GLY	6.2
1	B	796	CYS	5.8
1	B	655	ALA	5.4
1	B	590	ALA	5.1
1	B	616	LEU	4.6
1	B	556	THR	4.5
1	A	654	GLN	4.2
1	B	583	ARG	4.0
1	A	556	THR	3.9
1	B	552	ILE	3.8
1	A	583	ARG	3.6
1	A	555	GLU	3.5
1	A	704	ASN	3.5
1	A	649	LYS	3.4
1	B	700	SER	3.4
1	B	701	PRO	3.4
1	A	554	SER	3.2
1	A	706	GLN	3.2
1	A	650	GLU	3.2
1	B	555	GLU	3.0
1	A	616	LEU	3.0
1	B	591	LEU	2.9
1	B	804	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	552	ILE	2.8
1	B	792	THR	2.7
1	A	809	LEU	2.6
1	A	655	ALA	2.6
1	B	648	LYS	2.5
1	A	753	ILE	2.5
1	B	719	GLU	2.3
1	B	806	ASP	2.3
1	B	775	LYS	2.3
1	B	795	LYS	2.3
1	B	621	GLU	2.3
1	B	733	ASN	2.2
1	B	681	LYS	2.1
1	A	808	LYS	2.1
1	A	757	ILE	2.1
1	A	733	ASN	2.1
1	B	588	GLU	2.1
1	B	712	ILE	2.1
1	A	731	LEU	2.1
1	A	606	GLU	2.0
1	A	754	VAL	2.0

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

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	PHD	B	766	12/13	0.84	0.19	-	26,34,46,46	0
1	PHD	A	766	12/13	0.86	0.14	-	19,27,38,40	0

## 6.3 Carbohydrates

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	ADP	A	1511	27/27	0.90	0.13	-0.10	27,38,55,55	0
2	ADP	B	1512	27/27	0.92	0.13	-0.55	30,42,60,61	0
4	PO4	A	842	5/5	0.95	0.11	-0.91	35,35,37,38	0
4	PO4	B	842	5/5	0.96	0.11	-1.12	42,42,46,47	0
3	ZN	B	2	1/1	0.99	0.06	-1.39	27,27,27,27	0
3	ZN	A	1	1/1	0.98	0.07	-1.61	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.