W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:18 AM GMT

PDB ID : 3LMI
Title : Crystal Structure of the Inactive Alpha-kinase Domain of Myosin Heavy Chain Kinase A (D766A) complex with ATP
Authors : Ye, Q.; Jia, Z.
Deposited on : 2010-01-30
Resolution : 2.20 Å(reported)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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.
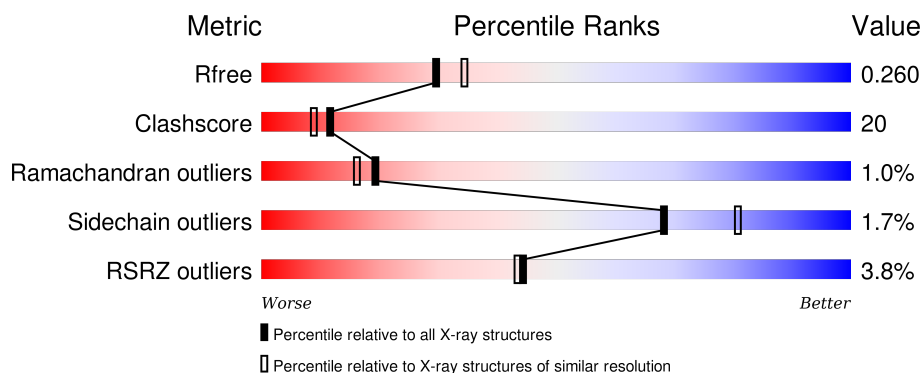
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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 >=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 <=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	2% 65% 15% 20%
1	B	307	3% 62% 19% • 17%
1	C	307	3% 62% 18% • 19%
1	D	307	5% 64% 18% • 18%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8689 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	246	Total	C	N	O	S	0	0	0
			1953	1256	329	356	12			
1	B	254	Total	C	N	O	S	0	0	0
			2012	1291	338	371	12			
1	C	250	Total	C	N	O	S	0	0	0
			1986	1276	334	364	12			
1	D	253	Total	C	N	O	S	0	0	0
			2005	1287	335	371	12			

There are 72 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
A	766	ALA	ASP	ENGINEERED	UNP P42527
B	535	MET	-	EXPRESSION TAG	UNP P42527
B	536	GLY	-	EXPRESSION TAG	UNP P42527
B	537	GLY	-	EXPRESSION TAG	UNP P42527

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
B	766	ALA	ASP	ENGINEERED	UNP P42527
C	535	MET	-	EXPRESSION TAG	UNP P42527
C	536	GLY	-	EXPRESSION TAG	UNP P42527
C	537	GLY	-	EXPRESSION TAG	UNP P42527
C	538	HIS	-	EXPRESSION TAG	UNP P42527
C	539	HIS	-	EXPRESSION TAG	UNP P42527
C	540	HIS	-	EXPRESSION TAG	UNP P42527
C	541	HIS	-	EXPRESSION TAG	UNP P42527
C	542	HIS	-	EXPRESSION TAG	UNP P42527
C	543	HIS	-	EXPRESSION TAG	UNP P42527
C	544	GLY	-	EXPRESSION TAG	UNP P42527
C	545	GLU	-	EXPRESSION TAG	UNP P42527
C	546	ASN	-	EXPRESSION TAG	UNP P42527
C	547	LEU	-	EXPRESSION TAG	UNP P42527
C	548	TYR	-	EXPRESSION TAG	UNP P42527
C	549	PHE	-	EXPRESSION TAG	UNP P42527
C	550	GLN	-	EXPRESSION TAG	UNP P42527
C	551	GLY	-	EXPRESSION TAG	UNP P42527
C	766	ALA	ASP	ENGINEERED	UNP P42527
D	535	MET	-	EXPRESSION TAG	UNP P42527
D	536	GLY	-	EXPRESSION TAG	UNP P42527
D	537	GLY	-	EXPRESSION TAG	UNP P42527
D	538	HIS	-	EXPRESSION TAG	UNP P42527
D	539	HIS	-	EXPRESSION TAG	UNP P42527
D	540	HIS	-	EXPRESSION TAG	UNP P42527
D	541	HIS	-	EXPRESSION TAG	UNP P42527
D	542	HIS	-	EXPRESSION TAG	UNP P42527
D	543	HIS	-	EXPRESSION TAG	UNP P42527

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Chain	Residue	Modelled	Actual	Comment	Reference
D	544	GLY	-	EXPRESSION TAG	UNP P42527
D	545	GLU	-	EXPRESSION TAG	UNP P42527
D	546	ASN	-	EXPRESSION TAG	UNP P42527
D	547	LEU	-	EXPRESSION TAG	UNP P42527
D	548	TYR	-	EXPRESSION TAG	UNP P42527
D	549	PHE	-	EXPRESSION TAG	UNP P42527
D	550	GLN	-	EXPRESSION TAG	UNP P42527
D	551	GLY	-	EXPRESSION TAG	UNP P42527
D	766	ALA	ASP	ENGINEERED	UNP P42527

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
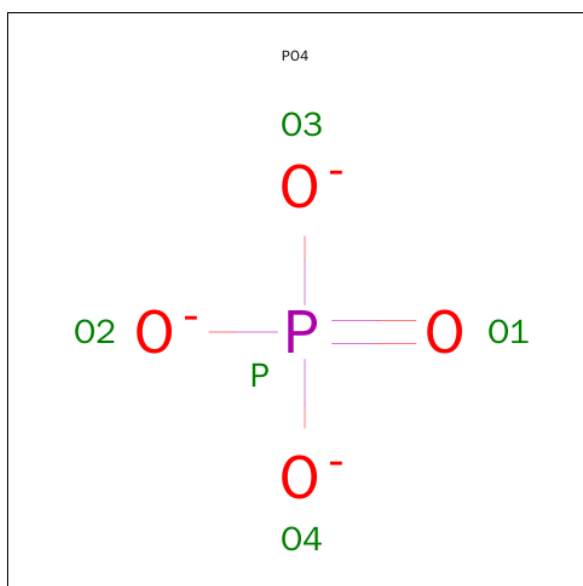
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	P 1	0	0
2	B	1	Total 5	O 4	P 1	0	0
2	B	1	Total 5	O 4	P 1	0	0
2	C	1	Total 5	O 4	P 1	0	0
2	D	1	Total 5	O 4	P 1	0	0
2	D	1	Total 5	O 4	P 1	0	0

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

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Mg 1	0	0
4	A	1	Total 1	Mg 1	0	0
4	D	1	Total 1	Mg 1	0	0
4	C	1	Total 1	Mg 1	0	0

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).
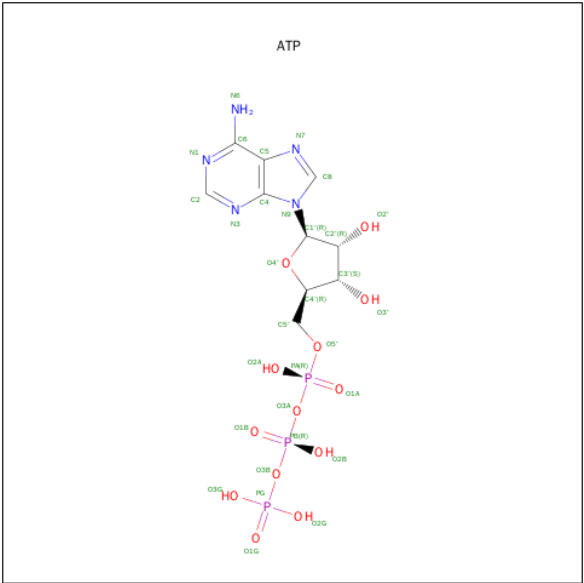
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	31	10	5	13	3	0	0

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	130	Total	O	0	0
			130	130		
6	B	153	Total	O	0	0
			153	153		
6	C	138	Total	O	0	0
			138	138		
6	D	150	Total	O	0	0
			150	150		

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.
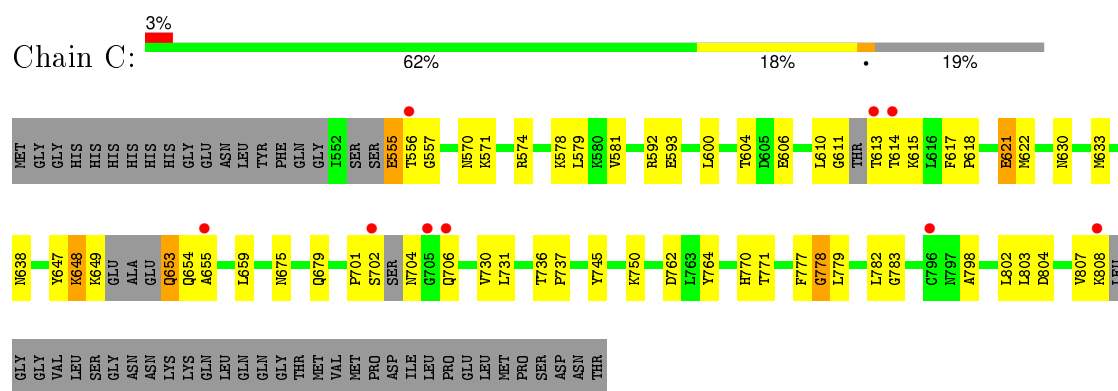
• Molecule 1: Myosin heavy chain kinase A
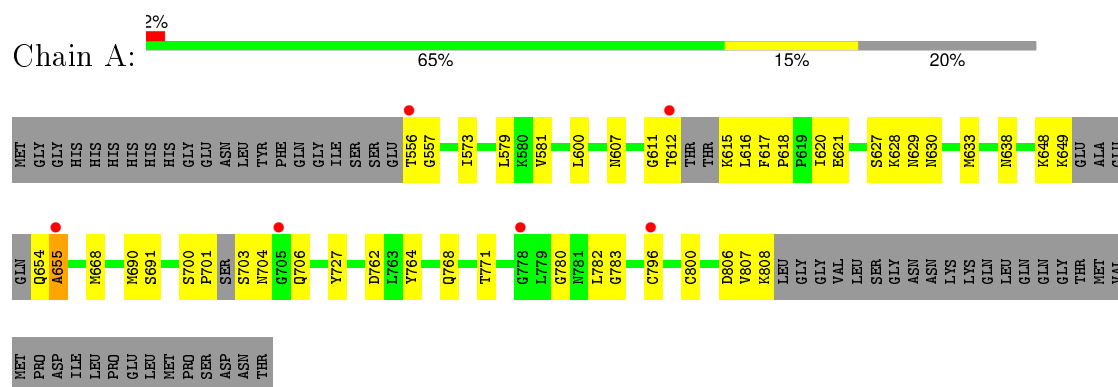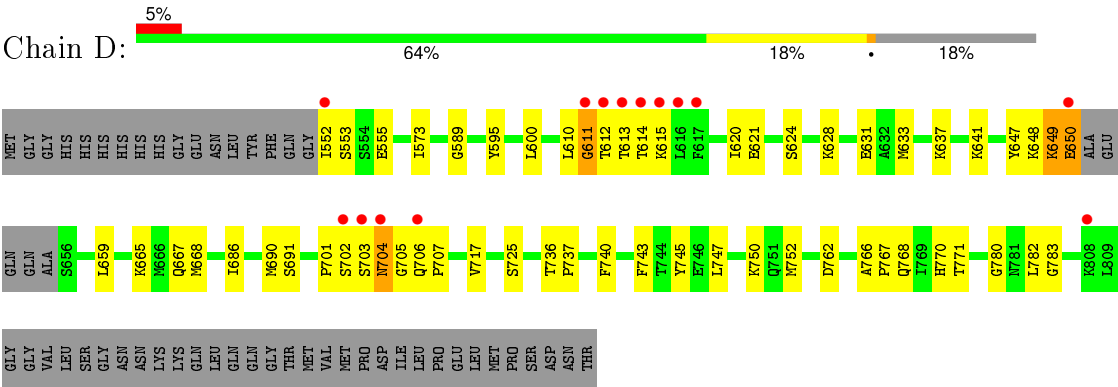
Chain A:

• Molecule 1: Myosin heavy chain kinase A
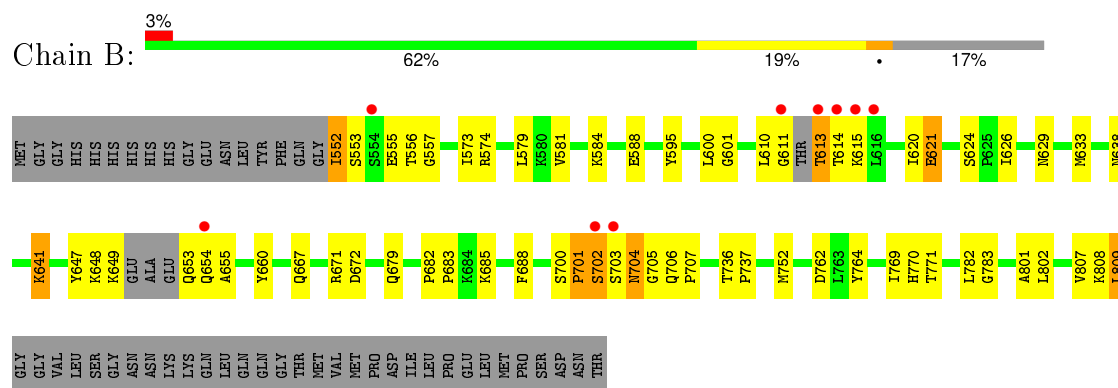
Chain B:

• Molecule 1: Myosin heavy chain kinase A

Chain C:

• Molecule 1: Myosin heavy chain kinase A

Chain D:

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	81.19Å 81.19Å 187.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.17 – 2.20 29.17 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.2 (29.17-2.20) 92.2 (29.17-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.24 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.199 , 0.269 0.196 , 0.260	Depositor DCC
R_{free} test set	2863 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	20.7	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 33.9	EDS
Estimated twinning fraction	0.477 for h,-k,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 56524 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8689	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.31% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: PO4, MG, ZN, 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	0.48	0/1994	0.56	0/2687
1	B	0.51	0/2054	0.57	0/2770
1	C	0.48	0/2026	0.55	0/2729
1	D	0.53	0/2048	0.59	0/2764
All	All	0.50	0/8122	0.57	0/10950

There are no bond length outliers.

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	1953	0	1982	57	1
1	B	2012	0	2040	95	1
1	C	1986	0	2013	103	0
1	D	2005	0	2033	71	0
2	A	5	0	0	0	0
2	B	10	0	0	1	0
2	C	5	0	0	0	0
2	D	10	0	0	1	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	31	0	12	0	0
5	B	31	0	12	2	0
5	C	31	0	12	2	0
5	D	31	0	12	3	0
6	A	130	0	0	21	0
6	B	153	0	0	29	0
6	C	138	0	0	12	0
6	D	150	0	0	23	0
All	All	8689	0	8116	330	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 20.

The worst 5 of 330 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:649:LYS:CD	1:B:653:GLN:N	1.76	1.48
1:D:631:GLU:HG3	1:D:690:MET:CE	1.57	1.34
1:B:613:THR:CG2	1:B:614:THR:H	1.37	1.34
1:B:660:TYR:CD1	6:B:344:HOH:O	1.79	1.34
1:B:648:LYS:O	1:B:649:LYS:HG2	1.18	1.29

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:615:LYS:NZ	1:B:801:ALA:CB[4_554]	1.09	1.11

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	238/307 (78%)	231 (97%)	5 (2%)	2 (1%)	24	22
1	B	248/307 (81%)	238 (96%)	7 (3%)	3 (1%)	16	12
1	C	241/307 (78%)	231 (96%)	9 (4%)	1 (0%)	39	42
1	D	249/307 (81%)	233 (94%)	12 (5%)	4 (2%)	12	8
All	All	976/1228 (80%)	933 (96%)	33 (3%)	10 (1%)	19	16

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	702	SER
1	D	611	GLY
1	D	704	ASN
1	D	649	LYS
1	A	655	ALA

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	217/269 (81%)	217 (100%)	0	100	100
1	B	225/269 (84%)	217 (96%)	8 (4%)	42	52
1	C	221/269 (82%)	217 (98%)	4 (2%)	66	79
1	D	225/269 (84%)	222 (99%)	3 (1%)	76	87
All	All	888/1076 (82%)	873 (98%)	15 (2%)	68	81

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	701	PRO
1	B	809	LEU
1	D	637	LYS
1	B	667	GLN
1	C	653	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	770	HIS
1	C	607	ASN
1	D	638	ASN
1	B	638	ASN
1	D	607	ASN

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)

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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
5	ATP	A	1760	4	24,33,33	0.97	1 (4%)	31,52,52	1.82	5 (16%)
2	PO4	A	5955	-	4,4,4	0.42	0	6,6,6	0.29	0
5	ATP	B	1761	4	24,33,33	0.92	1 (4%)	31,52,52	2.41	8 (25%)
2	PO4	B	5956	-	4,4,4	0.55	0	6,6,6	0.28	0
2	PO4	B	5959	-	4,4,4	0.45	0	6,6,6	0.27	0
5	ATP	C	1762	4	24,33,33	0.99	1 (4%)	31,52,52	2.38	4 (12%)
2	PO4	C	5957	-	4,4,4	0.38	0	6,6,6	0.28	0
5	ATP	D	1763	4	24,33,33	0.97	2 (8%)	31,52,52	2.48	6 (19%)
2	PO4	D	5958	-	4,4,4	0.57	0	6,6,6	0.27	0
2	PO4	D	5960	-	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
5	ATP	A	1760	4	-	0/18/38/38	0/3/3/3
2	PO4	A	5955	-	-	0/0/0/0	0/0/0/0
5	ATP	B	1761	4	-	0/18/38/38	0/3/3/3
2	PO4	B	5956	-	-	0/0/0/0	0/0/0/0
2	PO4	B	5959	-	-	0/0/0/0	0/0/0/0
5	ATP	C	1762	4	-	0/18/38/38	0/3/3/3
2	PO4	C	5957	-	-	0/0/0/0	0/0/0/0
5	ATP	D	1763	4	-	0/18/38/38	0/3/3/3
2	PO4	D	5958	-	-	0/0/0/0	0/0/0/0
2	PO4	D	5960	-	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1763	ATP	O4'-C1'	2.56	1.44	1.41
5	D	1763	ATP	C5-C4	2.65	1.46	1.40
5	B	1761	ATP	C5-C4	2.82	1.46	1.40
5	C	1762	ATP	C5-C4	3.08	1.47	1.40
5	A	1760	ATP	C5-C4	3.13	1.47	1.40

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1761	ATP	N3-C2-N1	-8.82	122.14	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	1763	ATP	N3-C2-N1	-8.42	122.44	128.89
5	C	1762	ATP	PA-O3A-PB	-8.05	110.12	132.73
5	D	1763	ATP	PA-O3A-PB	-7.99	110.30	132.73
5	A	1760	ATP	N3-C2-N1	-7.78	122.94	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1761	ATP	2	0
2	B	5959	PO4	1	0
5	C	1762	ATP	2	0
5	D	1763	ATP	3	0
2	D	5960	PO4	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, 95th 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^2)	Q<0.9
1	A	246/307 (80%)	-0.29	6 (2%)	62	61	9, 20, 40, 50	0
1	B	254/307 (82%)	-0.31	9 (3%)	48	46	6, 16, 43, 55	0
1	C	250/307 (81%)	-0.26	9 (3%)	46	45	9, 20, 42, 57	0
1	D	253/307 (82%)	-0.30	14 (5%)	29	28	7, 16, 42, 50	0
All	All	1003/1228 (81%)	-0.29	38 (3%)	44	43	6, 18, 42, 57	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	612	THR	5.2
1	C	614	THR	4.9
1	B	702	SER	4.7
1	A	655	ALA	4.5
1	D	703	SER	3.9

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, 95th 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(Å²)	Q<0.9
2	PO4	D	5960	5/5	0.88	0.26	1.94	87,87,87,87	0
2	PO4	B	5959	5/5	0.80	0.24	1.80	89,89,89,89	0
3	ZN	D	1004	1/1	1.00	0.09	0.90	14,14,14,14	0
2	PO4	C	5957	5/5	0.98	0.09	0.78	18,19,20,20	0
5	ATP	B	1761	31/31	0.94	0.11	0.53	7,16,42,43	0
5	ATP	D	1763	31/31	0.93	0.13	0.41	8,17,43,44	0
5	ATP	C	1762	31/31	0.94	0.12	0.26	12,16,41,42	0
2	PO4	A	5955	5/5	0.98	0.08	0.01	14,17,18,19	0
5	ATP	A	1760	31/31	0.95	0.12	0.00	9,19,42,43	0
3	ZN	A	1001	1/1	0.99	0.10	-0.55	17,17,17,17	0
2	PO4	B	5956	5/5	0.99	0.08	-0.69	17,18,19,20	0
2	PO4	D	5958	5/5	0.98	0.09	-0.96	20,21,22,23	0
3	ZN	C	1003	1/1	0.99	0.08	-1.14	18,18,18,18	0
3	ZN	B	1002	1/1	1.00	0.08	-1.39	13,13,13,13	0
4	MG	A	1006	1/1	0.98	0.08	-	21,21,21,21	0
4	MG	B	1005	1/1	0.96	0.14	-	22,22,22,22	0
4	MG	D	1008	1/1	0.95	0.09	-	21,21,21,21	0
4	MG	C	1007	1/1	0.89	0.13	-	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.