



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:08 AM GMT

PDB ID : 2AQX
Title : Crystal Structure of the Catalytic and CaM-Binding domains of Inositol 1,4,5-Trisphosphate 3-Kinase B
Authors : Chamberlain, P.P.; Sandberg, M.L.; Sauer, K.; Cooke, M.P.; Lesley, S.A.; Spraggon, G.
Deposited on : 2005-08-18
Resolution : 2.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

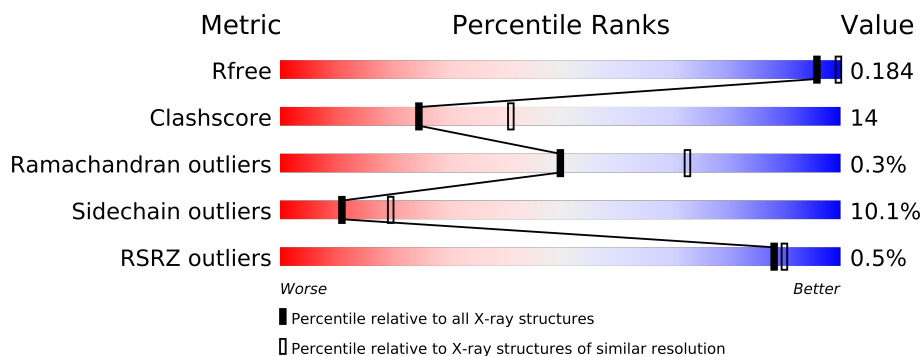
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.50 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	289	
1	B	289	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	A	600	-	X
2	MG	A	601	-	X
2	MG	B	1600	-	X
2	MG	B	1601	-	X

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 4837 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

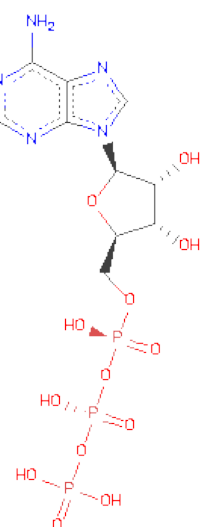
- Molecule 1 is a protein called PREDICTED: inositol 1,4,5-trisphosphate 3-kinase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2342	1479	411	436	16			
1	B	287	Total	C	N	O	S	5	0	0
			2330	1472	409	434	15			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 4 is water.

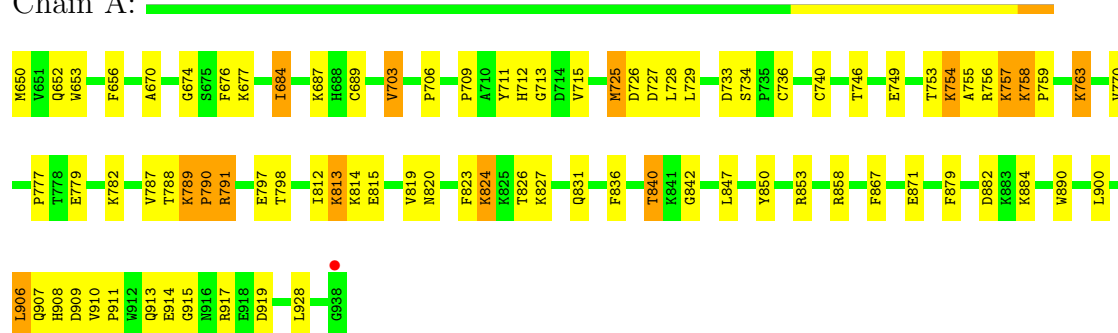
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	48	Total	O	0	0
			48	48		
4	B	51	Total	O	0	0
			51	51		

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.

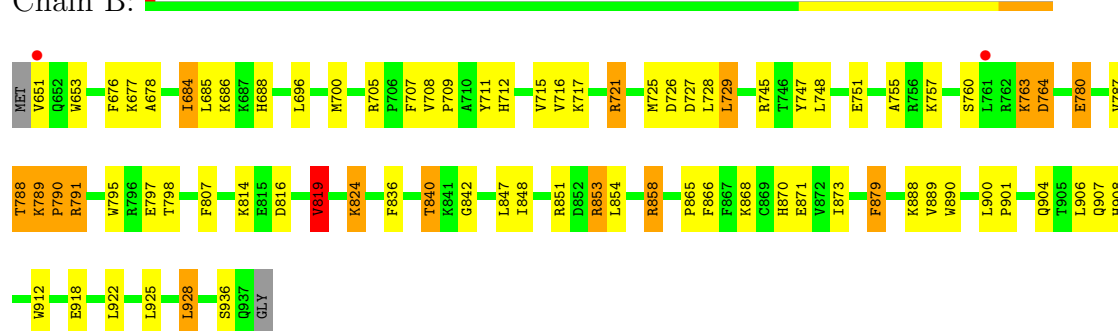
- Molecule 1: PREDICTED: inositol 1,4,5-trisphosphate 3-kinase B

Chain A:



- Molecule 1: PREDICTED: inositol 1,4,5-trisphosphate 3-kinase B

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.20Å 60.66Å 56.85Å 59.90° 72.74° 88.18°	Depositor
Resolution (Å)	50.00 – 2.50 46.52 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.4 (50.00-2.50) 95.4 (46.52-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.31 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.184 , 0.268 0.190 , 0.184	Depositor DCC
R_{free} test set	973 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 30.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 19206 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4837	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.69	2/2391 (0.1%)	0.77	1/3215 (0.0%)
1	B	0.67	2/2379 (0.1%)	0.73	1/3200 (0.0%)
All	All	0.68	4/4770 (0.1%)	0.75	2/6415 (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	1
1	B	1	1
All	All	1	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	780	GLU	CD-OE1	7.82	1.34	1.25
1	A	740	CYS	CB-SG	-6.36	1.71	1.82
1	A	689	CYS	CB-SG	-5.91	1.72	1.81
1	B	780	GLU	CD-OE2	5.09	1.31	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	819	VAL	CB-CA-C	-5.94	100.12	111.40
1	A	909	ASP	CB-CG-OD2	5.38	123.15	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	651	VAL	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	789	LYS	Peptide
1	B	789	LYS	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2342	0	2334	66	0
1	B	2330	0	2322	70	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	31	0	12	5	0
3	B	31	0	12	3	0
4	A	48	0	0	2	0
4	B	51	0	0	0	0
All	All	4837	0	4680	131	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (131) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:725:MET:CE	3:A:1462:ATP:HN61	1.83	0.91
1:A:763:LYS:H	1:A:763:LYS:HD3	1.33	0.90
1:B:707:PHE:HD2	1:B:853:ARG:NH1	1.69	0.90
1:B:788:THR:CG2	1:B:790:PRO:HB2	2.03	0.89
1:A:725:MET:HE2	3:A:1462:ATP:HN61	1.40	0.87
1:B:789:LYS:N	1:B:790:PRO:HD2	1.90	0.86
1:B:788:THR:HG23	1:B:790:PRO:HB2	1.58	0.83
1:B:789:LYS:H	1:B:790:PRO:HD2	1.46	0.81
1:A:840:THR:HG22	1:A:842:GLY:H	1.46	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:858:ARG:HE	1:B:922:LEU:HD22	1.47	0.79
1:A:763:LYS:H	1:A:763:LYS:CD	1.98	0.76
1:B:853:ARG:HH21	1:B:888:LYS:HE3	1.49	0.76
1:B:707:PHE:HD2	1:B:853:ARG:HH11	1.36	0.74
1:B:788:THR:HG22	1:B:791:ARG:H	1.53	0.73
1:B:763:LYS:H	1:B:763:LYS:HD3	1.56	0.70
1:B:788:THR:CG2	1:B:791:ARG:H	2.04	0.70
1:A:836:PHE:O	1:A:840:THR:HB	1.93	0.68
1:B:853:ARG:NH2	1:B:888:LYS:HE3	2.09	0.67
1:A:814:LYS:NZ	1:A:820:ASN:HD21	1.95	0.65
1:A:908:HIS:HD2	1:A:919:ASP:OD1	1.82	0.63
1:B:709:PRO:HG3	1:B:728:LEU:HD11	1.79	0.63
1:A:789:LYS:HB3	1:A:790:PRO:HD2	1.82	0.62
1:A:725:MET:HE1	3:A:1462:ATP:HN61	1.64	0.62
1:B:684:ILE:HD13	1:B:727:ASP:HB2	1.82	0.61
1:B:707:PHE:CD2	1:B:853:ARG:NH1	2.60	0.61
1:B:709:PRO:HB2	1:B:725:MET:HE2	1.82	0.61
1:A:757:LYS:O	1:A:759:PRO:HD3	2.01	0.61
1:A:753:THR:O	1:A:757:LYS:HE2	2.02	0.60
1:B:696:LEU:O	1:B:700:MET:HG2	2.01	0.59
1:B:788:THR:HG23	1:B:790:PRO:CB	2.31	0.58
1:B:712:HIS:HE1	1:B:726:ASP:OD1	1.87	0.58
1:B:789:LYS:N	1:B:790:PRO:CD	2.67	0.58
1:A:712:HIS:HE1	1:A:726:ASP:OD1	1.85	0.58
1:A:819:VAL:HG21	1:B:653:TRP:CG	2.40	0.57
1:A:725:MET:HE2	3:A:1462:ATP:N6	2.16	0.56
1:B:858:ARG:HH21	1:B:922:LEU:HD13	1.70	0.56
1:A:703:VAL:O	1:A:706:PRO:HD2	2.04	0.56
1:B:795:TRP:O	1:B:798:THR:HG22	2.06	0.56
1:A:812:ILE:HD12	1:A:823:PHE:CZ	2.41	0.56
1:B:788:THR:HG22	1:B:791:ARG:HB3	1.86	0.56
1:A:813:LYS:HB2	1:A:819:VAL:HG22	1.86	0.56
1:B:789:LYS:HB3	1:B:790:PRO:CD	2.36	0.56
1:A:840:THR:HG22	1:A:842:GLY:N	2.19	0.55
1:B:907:GLN:O	1:B:908:HIS:HB2	2.05	0.55
1:A:867:PHE:O	1:A:908:HIS:HE1	1.89	0.55
1:B:688:HIS:HB3	1:B:721:ARG:HB3	1.89	0.55
1:B:788:THR:HG21	1:B:790:PRO:HB2	1.88	0.55
1:A:907:GLN:O	1:A:908:HIS:HB2	2.07	0.54
1:B:684:ILE:CD1	1:B:727:ASP:HB2	2.37	0.54
1:A:736:CYS:SG	1:A:815:GLU:HG2	2.47	0.54
1:A:814:LYS:HZ3	1:A:820:ASN:HD21	1.56	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:789:LYS:CB	1:B:790:PRO:CD	2.86	0.54
1:B:836:PHE:O	1:B:840:THR:HB	2.07	0.53
1:A:709:PRO:HG2	1:A:725:MET:HE2	1.91	0.53
1:B:763:LYS:H	1:B:763:LYS:CD	2.22	0.53
1:B:715:VAL:HG22	1:B:716:VAL:N	2.23	0.53
1:A:913:GLN:O	1:A:914:GLU:C	2.46	0.52
1:A:787:VAL:HG12	1:A:788:THR:N	2.25	0.52
1:A:826:THR:HG23	1:A:831:GLN:HB3	1.91	0.52
1:B:700:MET:HA	1:B:705:ARG:HG3	1.92	0.52
1:B:763:LYS:HG2	1:B:764:ASP:H	1.74	0.51
1:A:824:LYS:HA	4:A:98:HOH:O	2.09	0.51
1:A:746:THR:N	1:A:797:GLU:OE1	2.33	0.51
1:A:900:LEU:HD11	1:A:906:LEU:HD22	1.92	0.51
1:A:827:LYS:NZ	1:A:827:LYS:HB3	2.25	0.51
1:A:910:VAL:HB	1:A:911:PRO:HD2	1.93	0.51
1:A:758:LYS:O	1:A:758:LYS:CG	2.58	0.50
1:B:745:ARG:NH1	1:B:918:GLU:O	2.43	0.50
1:B:900:LEU:HD11	1:B:906:LEU:HG	1.94	0.49
1:A:733:ASP:O	1:A:882:ASP:HB2	2.11	0.49
1:B:727:ASP:OD1	1:B:729:LEU:HB2	2.12	0.49
1:B:854:LEU:HD21	1:B:889:VAL:HG11	1.94	0.49
1:B:755:ALA:HB1	1:B:789:LYS:HG2	1.93	0.48
1:A:725:MET:HE1	3:A:1462:ATP:N7	2.28	0.48
1:B:745:ARG:NH1	1:B:912:TRP:CD1	2.81	0.48
1:B:901:PRO:HD2	1:B:904:GLN:HE21	1.78	0.48
1:A:653:TRP:CD1	1:B:819:VAL:HG22	2.48	0.48
1:B:748:LEU:HB2	1:B:751:GLU:HG3	1.96	0.48
1:A:674:GLY:O	1:A:687:LYS:HD3	2.14	0.48
1:A:787:VAL:CG1	1:A:791:ARG:HD2	2.43	0.48
1:A:709:PRO:HG3	1:A:728:LEU:HD11	1.95	0.47
1:B:865:PRO:HA	1:B:868:LYS:HE2	1.96	0.47
1:B:906:LEU:HD22	1:B:918:GLU:CD	2.34	0.47
1:A:840:THR:CG2	1:A:842:GLY:H	2.23	0.47
1:B:807:PHE:CE2	1:B:928:LEU:HD13	2.50	0.47
1:B:866:PHE:CE1	1:B:870:HIS:CE1	3.03	0.46
1:B:840:THR:HG22	1:B:842:GLY:H	1.80	0.46
1:A:670:ALA:HB1	4:A:6:HOH:O	2.15	0.46
1:B:676:PHE:HA	1:B:685:LEU:O	2.16	0.45
1:B:871:GLU:HG2	1:B:873:ILE:HG12	1.98	0.45
1:A:787:VAL:HG11	1:A:791:ARG:HD2	1.98	0.45
1:A:755:ALA:HB1	1:A:790:PRO:CD	2.46	0.45
1:B:814:LYS:HE2	1:B:814:LYS:HB2	1.65	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:840:THR:CG2	1:A:842:GLY:N	2.79	0.45
1:A:656:PHE:CD1	1:B:678:ALA:HB2	2.52	0.45
1:A:777:PRO:HG2	1:A:782:LYS:HE3	1.97	0.45
1:B:858:ARG:HB2	1:B:925:LEU:HD21	1.99	0.44
1:B:685:LEU:HD22	1:B:715:VAL:HG11	2.00	0.44
1:B:789:LYS:HB3	1:B:790:PRO:HD3	1.98	0.44
1:A:711:TYR:CZ	1:A:713:GLY:HA2	2.53	0.43
1:B:824:LYS:HB2	1:B:824:LYS:HE3	1.58	0.43
1:B:676:PHE:CE1	3:B:2462:ATP:H5'1	2.53	0.43
1:A:879:PHE:CD2	1:A:879:PHE:N	2.86	0.43
1:A:728:LEU:HD22	1:A:890:TRP:CE2	2.53	0.43
1:A:755:ALA:HB1	1:A:790:PRO:HD2	1.99	0.43
1:B:879:PHE:N	1:B:879:PHE:CD2	2.86	0.43
1:B:728:LEU:HD22	1:B:890:TRP:CE2	2.54	0.43
1:B:676:PHE:CZ	1:B:686:LYS:HD2	2.53	0.43
1:A:684:ILE:HG22	1:A:725:MET:HG2	2.00	0.43
1:B:745:ARG:HD2	1:B:747:TYR:CE1	2.54	0.42
1:A:867:PHE:O	1:A:908:HIS:CE1	2.72	0.42
1:B:848:ILE:HG13	1:B:936:SER:HB2	2.01	0.42
1:A:676:PHE:O	1:A:677:LYS:HD2	2.18	0.42
1:A:756:ARG:NH2	1:A:914:GLU:OE1	2.53	0.42
1:B:696:LEU:HB3	1:B:711:TYR:CG	2.54	0.42
1:A:684:ILE:HD13	1:A:727:ASP:HB2	2.02	0.42
1:A:910:VAL:HA	1:A:911:PRO:HD3	1.85	0.42
1:A:653:TRP:HD1	1:B:819:VAL:HG22	1.85	0.42
1:B:712:HIS:CE1	1:B:726:ASP:OD1	2.72	0.42
1:A:819:VAL:HG21	1:B:653:TRP:CD1	2.55	0.42
1:A:754:LYS:O	1:A:757:LYS:HB2	2.20	0.41
1:B:686:LYS:NZ	3:B:2462:ATP:O1A	2.40	0.41
1:A:749:GLU:OE2	1:A:915:GLY:N	2.54	0.41
1:A:871:GLU:OE1	1:A:917:ARG:NE	2.48	0.41
1:A:712:HIS:CE1	1:A:726:ASP:OD1	2.71	0.41
1:A:727:ASP:OD1	1:A:729:LEU:HB2	2.21	0.41
1:A:814:LYS:HB2	1:A:814:LYS:HE2	1.54	0.41
1:A:814:LYS:HZ2	1:A:820:ASN:HD21	1.69	0.40
1:A:755:ALA:CB	1:A:790:PRO:HD3	2.51	0.40
1:B:858:ARG:O	1:B:858:ARG:HG3	2.22	0.40
1:B:676:PHE:HE1	3:B:2462:ATP:H5'1	1.84	0.40

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	287/289 (99%)	271 (94%)	15 (5%)	1 (0%)	50	73
1	B	285/289 (99%)	269 (94%)	15 (5%)	1 (0%)	43	66
All	All	572/578 (99%)	540 (94%)	30 (5%)	2 (0%)	50	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	790	PRO
1	B	790	PRO

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	254/254 (100%)	229 (90%)	25 (10%)	12	21
1	B	253/254 (100%)	227 (90%)	26 (10%)	10	19
All	All	507/508 (100%)	456 (90%)	51 (10%)	11	20

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	650	MET
1	A	652	GLN
1	A	684	ILE
1	A	703	VAL
1	A	715	VAL
1	A	725	MET
1	A	734	SER

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Mol	Chain	Res	Type
1	A	754	LYS
1	A	757	LYS
1	A	758	LYS
1	A	763	LYS
1	A	770	VAL
1	A	779	GLU
1	A	791	ARG
1	A	798	THR
1	A	813	LYS
1	A	824	LYS
1	A	840	THR
1	A	847	LEU
1	A	850	TYR
1	A	853	ARG
1	A	858	ARG
1	A	884	LYS
1	A	906	LEU
1	A	928	LEU
1	B	651	VAL
1	B	677	LYS
1	B	684	ILE
1	B	708	VAL
1	B	717	LYS
1	B	721	ARG
1	B	729	LEU
1	B	757	LYS
1	B	760	SER
1	B	763	LYS
1	B	764	ASP
1	B	780	GLU
1	B	787	VAL
1	B	788	THR
1	B	791	ARG
1	B	797	GLU
1	B	816	ASP
1	B	819	VAL
1	B	824	LYS
1	B	840	THR
1	B	847	LEU
1	B	851	ARG
1	B	853	ARG
1	B	858	ARG

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Mol	Chain	Res	Type
1	B	879	PHE
1	B	928	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	712	HIS
1	A	784	GLN
1	A	820	ASN
1	A	908	HIS
1	B	693	GLN
1	B	712	HIS
1	B	784	GLN
1	B	820	ASN
1	B	886	GLN
1	B	904	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	ATP	A	1462	2	33,33,33	1.15	4 (12%)	52,52,52	1.93	11 (21%)
3	ATP	B	2462	2	33,33,33	1.20	3 (9%)	52,52,52	1.90	10 (19%)

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	ATP	A	1462	2	-	0/22/38/38	0/1/3/3
3	ATP	B	2462	2	-	0/22/38/38	0/1/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2462	ATP	C5-C4	3.53	1.48	1.40
3	A	1462	ATP	C5-C4	2.92	1.47	1.40
3	A	1462	ATP	C4-N9	-2.73	1.33	1.37
3	B	2462	ATP	PG-O3B	2.54	1.64	1.60
3	A	1462	ATP	PA-O3A	2.41	1.64	1.59
3	A	1462	ATP	PB-O3A	2.34	1.64	1.59
3	B	2462	ATP	C2'-C1'	-2.05	1.50	1.53

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1462	ATP	N3-C2-N1	-7.74	122.24	128.71
3	B	2462	ATP	O4'-C1'-N9	-6.95	101.97	108.44
3	A	1462	ATP	N3-C4-N9	5.19	134.81	125.43
3	B	2462	ATP	N3-C4-N9	5.18	134.79	125.43
3	B	2462	ATP	N3-C2-N1	-3.74	125.58	128.71
3	A	1462	ATP	O4'-C1'-N9	-3.59	105.11	108.44
3	B	2462	ATP	C4-C5-N7	-3.38	106.62	109.52
3	B	2462	ATP	PB-O3B-PG	-3.10	122.59	131.68
3	B	2462	ATP	C5-C4-N3	-2.96	119.25	125.70
3	A	1462	ATP	C8-N9-C4	2.91	109.12	106.90
3	A	1462	ATP	C5-C4-N3	-2.84	119.52	125.70
3	A	1462	ATP	C2-N3-C4	2.70	121.70	114.01
3	A	1462	ATP	C4-C5-N7	-2.51	107.37	109.52
3	A	1462	ATP	O2'-C2'-C1'	-2.40	103.96	111.23
3	B	2462	ATP	O2'-C2'-C1'	-2.39	104.00	111.23
3	B	2462	ATP	C8-N9-C4	2.38	108.72	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2462	ATP	PA-O3A-PB	-2.33	124.86	131.68
3	A	1462	ATP	O3'-C3'-C4'	-2.21	104.56	111.08
3	B	2462	ATP	C3'-C2'-C1'	2.16	104.28	100.91
3	A	1462	ATP	O3G-PG-O2G	2.12	115.86	107.61
3	A	1462	ATP	C3'-C2'-C1'	2.03	104.08	100.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	289/289 (100%)	-0.40	1 (0%) 91 93	19, 32, 53, 57	0
1	B	287/289 (99%)	-0.29	2 (0%) 84 86	18, 36, 52, 57	1 (0%)
All	All	576/578 (99%)	-0.35	3 (0%) 88 90	18, 34, 53, 57	1 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	651	VAL	3.7
1	A	938	GLY	3.2
1	B	761	LEU	2.2

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	A	600	1/1	0.19	5.62	17,17,17,17	0
2	MG	B	1601	1/1	0.15	5.34	20,20,20,20	0
2	MG	A	601	1/1	0.30	4.57	26,26,26,26	0
2	MG	B	1600	1/1	0.18	3.01	33,33,33,33	0
3	ATP	B	2462	31/31	0.11	-0.31	15,17,21,22	0
3	ATP	A	1462	31/31	0.10	-0.48	10,20,23,23	0

6.5 Other polymers ⓘ

There are no such residues in this entry.