



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:09 AM GMT

PDB ID : 1ZYD
Title : Crystal Structure of eIF2alpha Protein Kinase GCN2: Wild-Type Complexed with ATP.
Authors : Padyana, A.K.; Qiu, H.; Roll-Mecak, A.; Hinnebusch, A.G.; Burley, S.K.
Deposited on : 2005-06-09
Resolution : 2.75 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

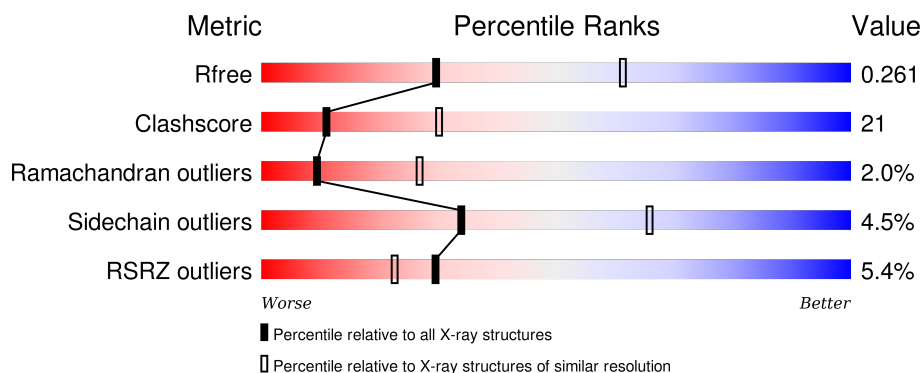
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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 $\leq 5\%$. 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	303	<div> <div>5%</div> <div>58%</div> <div>28%</div> <div>•</div> <div>11%</div> </div>
1	B	303	<div> <div>4%</div> <div>52%</div> <div>27%</div> <div>•</div> <div>17%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4446 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 GCN2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			2226	1429	386	402	9			
1	B	253	Total	C	N	O	S	0	0	0
			2086	1340	360	377	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	592	SER	-	CLONING ARTIFACT	UNP P15442
A	593	LEU	-	CLONING ARTIFACT	UNP P15442
B	592	SER	-	CLONING ARTIFACT	UNP P15442
B	593	LEU	-	CLONING ARTIFACT	UNP P15442

- 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	37	Total	O	0	0
			37	37		
4	B	31	Total	O	0	0
			31	31		

- Molecule 1: Serine/threonine-protein kinase GCN2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	82.11Å 175.21Å 47.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.59 – 2.75 47.59 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.7 (47.59-2.75) 98.8 (47.59-2.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 2.77Å)	Xtriage
Refinement program	CNX 2000.1	Depositor
R, R_{free}	0.208 , 0.270 0.205 , 0.261	Depositor DCC
R_{free} test set	762 reflections (4.34%)	DCC
Wilson B-factor (Å ²)	53.1	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 18323 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4446	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	0.32	0/2270	0.59	0/3053
1	B	0.33	0/2129	0.64	2/2868 (0.1%)
All	All	0.32	0/4399	0.61	2/5921 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	770	ASN	N-CA-C	6.82	129.40	111.00
1	B	897	ASP	N-CA-C	5.19	125.00	111.00

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	2226	0	2249	82	1
1	B	2086	0	2090	102	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	31	0	12	1	0
3	B	31	0	12	3	0
4	A	37	0	0	7	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	31	0	0	6	0
All	All	4446	0	4363	183	2

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 21.

All (183) 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:809:ARG:HH21	1:B:950:LYS:NZ	1.45	1.15
1:B:809:ARG:CG	1:B:809:ARG:HH11	1.82	0.92
1:B:809:ARG:HH21	1:B:950:LYS:HZ1	1.15	0.88
1:B:809:ARG:NH2	1:B:950:LYS:NZ	2.25	0.85
1:A:953:VAL:HG12	4:A:62:HOH:O	1.75	0.85
1:B:809:ARG:NH2	1:B:950:LYS:HZ1	1.74	0.84
1:B:652:HIS:HD2	1:B:654:TYR:H	1.22	0.83
1:B:959:ARG:HD3	1:B:959:ARG:O	1.77	0.83
1:A:652:HIS:HD2	1:A:654:TYR:H	1.29	0.78
1:A:769:ARG:O	1:A:780:LYS:HE3	1.83	0.78
1:B:809:ARG:HH11	1:B:809:ARG:HG2	1.49	0.76
1:B:925:GLY:O	1:B:929:VAL:HG23	1.87	0.74
1:B:652:HIS:CD2	1:B:654:TYR:H	2.04	0.73
1:B:613:VAL:HB	3:B:304:ATP:H5'1	1.70	0.73
1:A:953:VAL:N	4:A:62:HOH:O	2.21	0.73
1:B:809:ARG:HG3	1:B:809:ARG:HH11	1.55	0.72
1:B:964:HIS:NE2	4:B:22:HOH:O	2.23	0.70
1:A:652:HIS:CD2	1:A:654:TYR:H	2.08	0.70
1:B:770:ASN:O	1:B:771:PHE:C	2.30	0.69
1:A:638:SER:HA	1:A:641:LEU:HG	1.73	0.69
1:B:809:ARG:HH21	1:B:950:LYS:HZ3	1.37	0.68
1:B:899:THR:C	1:B:901:HIS:H	1.97	0.68
1:A:613:VAL:HB	3:A:303:ATP:H5'1	1.78	0.66
1:A:953:VAL:CG1	4:A:62:HOH:O	2.39	0.65
1:B:768:ARG:HD3	1:B:771:PHE:HE1	1.61	0.65
1:B:953:VAL:HG13	1:B:954:GLU:OE1	1.96	0.65
1:A:838:PRO:HD3	1:A:914:ILE:HG12	1.79	0.65
1:A:618:ASN:HD21	1:A:620:LEU:HB2	1.62	0.64
1:B:951:MET:HB3	1:B:954:GLU:HG2	1.78	0.64
1:B:617:ARG:HD3	4:B:40:HOH:O	1.97	0.63
1:A:611:GLY:HA3	1:A:629:LYS:O	1.99	0.63
1:B:768:ARG:HD3	1:B:771:PHE:CE1	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:925:GLY:O	1:A:929:VAL:HG23	1.98	0.62
1:B:958:ILE:O	1:B:962:ILE:HG12	1.99	0.62
1:A:769:ARG:NH1	1:A:770:ASN:OD1	2.33	0.61
1:B:768:ARG:C	1:B:770:ASN:H	2.03	0.61
1:B:946:PHE:HE2	1:B:955:LYS:HB2	1.65	0.61
1:B:631:ARG:NH2	1:B:769:ARG:HG3	2.15	0.60
1:A:593:LEU:HD23	1:A:664:GLU:HG2	1.83	0.60
1:A:953:VAL:HG13	1:A:954:GLU:OE1	2.01	0.60
1:B:815:LEU:O	1:B:819:ILE:HG13	2.02	0.60
1:A:958:ILE:O	1:A:962:ILE:HG12	2.02	0.60
1:B:926:MET:HA	1:B:926:MET:CE	2.32	0.59
1:A:805:LEU:HA	1:A:808:GLN:HE21	1.67	0.59
1:B:641:LEU:O	1:B:645:MET:HG2	2.01	0.59
1:B:611:GLY:HA3	1:B:629:LYS:O	2.03	0.59
1:B:768:ARG:CD	1:B:771:PHE:HE1	2.16	0.58
1:A:858:LYS:NZ	1:A:891:VAL:HG13	2.18	0.58
1:A:779:LYS:HD3	1:A:779:LYS:C	2.24	0.57
1:B:817:ARG:O	1:B:821:GLU:HG2	2.04	0.57
1:A:939:SER:HB2	1:A:941:GLU:HG3	1.86	0.57
1:B:940:ILE:HD12	1:B:959:ARG:NH1	2.19	0.57
1:B:628:LYS:HE3	4:B:13:HOH:O	2.04	0.57
1:B:653:GLN:HG3	1:B:654:TYR:CD2	2.39	0.57
1:A:833:HIS:HD2	1:A:835:ASP:H	1.51	0.57
1:A:903:ASN:HB2	1:A:904:GLU:OE1	2.05	0.57
1:B:959:ARG:C	1:B:959:ARG:HD3	2.25	0.57
1:A:904:GLU:CD	1:A:904:GLU:H	2.06	0.57
1:A:811:GLU:HG2	1:A:847:ARG:HH12	1.69	0.57
1:B:946:PHE:CE2	1:B:955:LYS:HD2	2.41	0.56
1:A:770:ASN:O	1:A:772:VAL:HG22	2.06	0.56
1:B:922:PHE:CD2	1:B:928:ARG:HG3	2.41	0.56
1:B:899:THR:O	1:B:901:HIS:N	2.33	0.56
1:B:637:LEU:HD13	1:B:663:LEU:HD21	1.87	0.56
1:B:917:GLU:OE1	1:B:928:ARG:NH1	2.38	0.56
1:A:772:VAL:O	4:A:73:HOH:O	2.18	0.55
1:B:922:PHE:CG	1:B:928:ARG:HG3	2.42	0.55
1:B:806:ASN:ND2	1:B:921:PRO:HB3	2.21	0.55
1:B:892:ALA:HA	1:B:909:TYR:CD2	2.42	0.54
1:A:837:LYS:HA	1:A:914:ILE:HD11	1.90	0.54
1:B:947:ASP:OD2	1:B:950:LYS:HD3	2.07	0.54
1:A:815:LEU:O	1:A:819:ILE:HG13	2.08	0.54
1:B:661:ALA:HA	1:B:785:PHE:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:894:GLU:O	1:A:898:GLY:HA3	2.08	0.53
1:B:894:GLU:OE2	1:B:969:ARG:NH2	2.42	0.53
1:A:927:GLU:O	1:A:931:ILE:HG13	2.09	0.53
1:B:809:ARG:CG	1:B:809:ARG:NH1	2.52	0.53
1:A:809:ARG:NH2	1:A:950:LYS:HE2	2.23	0.52
1:B:809:ARG:HG3	1:B:809:ARG:NH1	2.17	0.52
1:A:809:ARG:HG3	1:A:809:ARG:HH11	1.73	0.52
1:B:656:VAL:HG13	1:B:789:GLU:HB3	1.92	0.52
1:A:963:ASP:O	1:A:969:ARG:NH1	2.41	0.51
1:A:811:GLU:CG	1:A:847:ARG:HH12	2.24	0.51
1:B:805:LEU:HD22	1:B:812:TYR:HB3	1.91	0.51
1:B:768:ARG:NE	1:B:771:PHE:HE1	2.08	0.51
1:B:817:ARG:HH12	1:B:981:LEU:HB2	1.75	0.51
1:A:809:ARG:HA	1:A:812:TYR:CE2	2.45	0.51
1:A:635:GLU:HA	4:A:55:HOH:O	2.11	0.51
1:A:954:GLU:OE1	4:A:62:HOH:O	2.19	0.50
1:B:768:ARG:CZ	1:B:771:PHE:HE1	2.24	0.50
1:A:896:LEU:HD11	1:A:936:ARG:HH22	1.76	0.50
1:B:833:HIS:HD2	1:B:835:ASP:H	1.59	0.50
1:B:793:ASN:C	1:B:793:ASN:HD22	2.15	0.50
1:A:894:GLU:OE2	1:A:969:ARG:NH2	2.45	0.50
3:B:304:ATP:H3'	3:B:304:ATP:O3A	2.13	0.49
1:A:894:GLU:CD	1:A:969:ARG:HH22	2.16	0.49
1:A:809:ARG:HH22	1:A:950:LYS:HE2	1.77	0.49
1:B:768:ARG:CZ	1:B:771:PHE:CE1	2.96	0.48
1:A:805:LEU:O	1:A:805:LEU:HD22	2.13	0.48
1:A:951:MET:HB3	1:A:954:GLU:HG2	1.95	0.48
1:B:837:LYS:HA	1:B:914:ILE:HD11	1.96	0.48
1:B:653:GLN:HG3	1:B:654:TYR:CE2	2.49	0.48
1:B:965:ASP:HB3	1:B:968:LYS:HG3	1.95	0.48
1:A:769:ARG:C	1:A:771:PHE:H	2.17	0.48
1:B:809:ARG:HG2	1:B:812:TYR:CZ	2.48	0.48
1:A:845:GLU:C	1:A:847:ARG:H	2.17	0.48
1:A:924:THR:O	1:A:927:GLU:HB3	2.14	0.48
1:A:934:LYS:HD2	1:A:941:GLU:HB2	1.96	0.47
1:A:961:LEU:O	1:A:969:ARG:HD2	2.14	0.47
1:B:903:ASN:OD1	1:B:905:LYS:HB2	2.14	0.47
1:B:946:PHE:CD2	1:B:955:LYS:HD2	2.49	0.47
1:A:661:ALA:HA	1:A:785:PHE:O	2.15	0.47
1:A:629:LYS:HE2	1:A:785:PHE:HE2	1.80	0.47
1:B:981:LEU:CD1	1:B:981:LEU:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:833:HIS:HE1	1:B:852:GLY:O	1.97	0.47
1:A:641:LEU:O	1:A:645:MET:HG2	2.15	0.47
1:B:809:ARG:HG2	1:B:812:TYR:OH	2.14	0.46
1:B:643:GLU:O	1:B:647:LEU:HB2	2.15	0.46
1:A:952:LYS:N	4:A:62:HOH:O	2.49	0.46
1:A:994:LEU:C	1:A:996:SER:H	2.19	0.46
1:A:811:GLU:HG2	1:A:847:ARG:NH1	2.29	0.46
1:A:799:LEU:HA	1:A:803:GLU:HB2	1.97	0.46
1:A:904:GLU:CD	1:A:904:GLU:N	2.69	0.46
1:A:645:MET:HE2	1:B:784:LEU:HD11	1.98	0.46
1:B:896:LEU:HD11	1:B:936:ARG:NH2	2.31	0.45
1:A:618:ASN:ND2	1:A:620:LEU:HB2	2.28	0.45
1:A:805:LEU:HA	1:A:808:GLN:NE2	2.31	0.45
1:B:957:ILE:HG23	1:B:975:LEU:HD21	1.98	0.45
1:A:956:LYS:NZ	1:A:956:LYS:HB2	2.32	0.45
1:A:946:PHE:HE2	1:A:955:LYS:HB2	1.81	0.45
1:A:645:MET:CE	1:B:784:LEU:HD11	2.46	0.45
1:B:811:GLU:OE2	1:B:811:GLU:HA	2.17	0.45
1:B:940:ILE:HD12	1:B:959:ARG:CZ	2.46	0.45
1:B:946:PHE:CE2	1:B:955:LYS:HB2	2.47	0.44
1:B:814:ARG:O	1:B:818:GLN:HG3	2.17	0.44
1:B:941:GLU:OE2	4:B:67:HOH:O	2.20	0.44
1:A:769:ARG:O	1:A:771:PHE:N	2.51	0.44
1:A:780:LYS:HG2	1:A:781:LYS:N	2.33	0.44
1:A:613:VAL:HG22	1:A:628:LYS:HG3	1.99	0.44
1:A:929:VAL:O	1:A:929:VAL:HG12	2.17	0.44
1:A:897:ASP:OD1	1:A:898:GLY:N	2.51	0.44
1:A:770:ASN:O	1:A:771:PHE:C	2.55	0.44
1:B:950:LYS:CB	1:B:950:LYS:HZ2	2.29	0.43
1:A:951:MET:HB3	1:A:954:GLU:CG	2.47	0.43
1:B:837:LYS:HE2	1:B:840:ASN:ND2	2.34	0.43
1:A:886:GLY:C	1:A:888:ALA:N	2.71	0.43
1:B:950:LYS:CB	1:B:950:LYS:NZ	2.81	0.43
1:A:652:HIS:HD2	1:A:654:TYR:N	2.07	0.43
1:A:909:TYR:CD1	1:A:962:ILE:HA	2.54	0.43
1:B:981:LEU:HD12	1:B:981:LEU:N	2.34	0.43
1:A:806:ASN:ND2	1:A:921:PRO:HB3	2.34	0.43
1:A:922:PHE:CD1	1:A:928:ARG:HB2	2.54	0.43
1:B:951:MET:HB3	1:B:954:GLU:CG	2.44	0.43
1:B:899:THR:C	1:B:901:HIS:N	2.64	0.43
1:B:950:LYS:HB3	1:B:950:LYS:NZ	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:812:TYR:CE2	1:B:919:ILE:HG22	2.54	0.42
1:A:811:GLU:HA	1:A:811:GLU:OE2	2.19	0.42
1:A:954:GLU:O	1:A:958:ILE:HG13	2.19	0.42
1:B:946:PHE:O	1:B:948:ASP:OD1	2.38	0.42
1:B:922:PHE:CD1	1:B:928:ARG:HG3	2.55	0.42
1:B:633:THR:OG1	1:B:636:LYS:HD3	2.19	0.42
1:B:895:VAL:O	1:B:897:ASP:N	2.52	0.42
1:B:922:PHE:CE2	1:B:928:ARG:HG3	2.55	0.42
1:B:636:LYS:N	1:B:636:LYS:HD2	2.35	0.42
1:B:936:ARG:HA	4:B:22:HOH:O	2.20	0.41
1:B:664:GLU:HB2	1:B:785:PHE:HE1	1.86	0.41
1:B:655:VAL:HG22	1:B:822:ALA:HB1	2.02	0.41
1:B:624:TYR:N	1:B:624:TYR:CD1	2.89	0.41
1:A:833:HIS:O	1:A:834:ARG:HB2	2.20	0.41
1:A:833:HIS:HE1	1:A:852:GLY:O	2.03	0.41
1:B:806:ASN:OD1	1:B:807:GLN:HG3	2.21	0.41
1:B:894:GLU:CD	1:B:969:ARG:HH22	2.24	0.41
1:B:793:ASN:C	1:B:793:ASN:ND2	2.74	0.41
1:B:621:ASP:OD1	1:B:621:ASP:C	2.59	0.41
1:A:896:LEU:CD1	1:A:936:ARG:HH22	2.34	0.40
1:A:811:GLU:CG	1:A:847:ARG:NH1	2.84	0.40
1:A:844:ASP:OD1	1:A:844:ASP:C	2.60	0.40
1:B:647:LEU:HD12	1:B:647:LEU:HA	1.89	0.40
1:B:613:VAL:CB	3:B:304:ATP:H5'1	2.45	0.40
1:B:856:LEU:HB2	4:B:53:HOH:O	2.21	0.40
1:B:942:PHE:CE1	1:B:955:LYS:HG3	2.57	0.40
1:A:834:ARG:HG2	1:A:906:ILE:HD11	2.03	0.40
1:B:965:ASP:HA	1:B:966:PRO:HD2	1.88	0.40

All (2) 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:B:949:ASN:OD1	1:B:949:ASN:OD1[2_555]	2.09	0.11
1:A:899:THR:OG1	4:A:1:HOH:O[1_554]	2.19	0.01

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	264/303 (87%)	239 (90%)	18 (7%)	7 (3%)	6	18
1	B	247/303 (82%)	222 (90%)	22 (9%)	3 (1%)	16	43
All	All	511/606 (84%)	461 (90%)	40 (8%)	10 (2%)	9	27

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	770	ASN
1	B	896	LEU
1	A	771	PHE
1	A	947	ASP
1	A	995	LYS
1	A	900	GLY
1	B	940	ILE
1	A	608	GLY
1	A	982	PRO
1	B	900	GLY

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	242/272 (89%)	232 (96%)	10 (4%)	37	69
1	B	226/272 (83%)	215 (95%)	11 (5%)	31	62
All	All	468/544 (86%)	447 (96%)	21 (4%)	34	66

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	593	LEU
1	A	605	LEU
1	A	769	ARG
1	A	793	ASN
1	A	794	ARG
1	A	805	LEU
1	A	806	ASN
1	A	839	MET
1	A	889	MET
1	A	904	GLU
1	B	593	LEU
1	B	647	LEU
1	B	793	ASN
1	B	794	ARG
1	B	805	LEU
1	B	809	ARG
1	B	812	TYR
1	B	926	MET
1	B	953	VAL
1	B	954	GLU
1	B	959	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	612	GLN
1	A	618	ASN
1	A	652	HIS
1	A	787	GLN
1	A	793	ASN
1	A	801	HIS
1	A	808	GLN
1	A	829	GLN
1	A	833	HIS
1	A	977	ASN
1	B	652	HIS
1	B	787	GLN
1	B	793	ASN
1	B	833	HIS
1	B	964	HIS
1	B	967	ASN

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Mol	Chain	Res	Type
1	B	977	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 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	303	2	24,33,33	0.83	0	31,52,52	1.27	4 (12%)
3	ATP	B	304	2	24,33,33	0.84	0	31,52,52	1.27	3 (9%)

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	303	2	-	0/18/38/38	0/3/3/3
3	ATP	B	304	2	-	0/18/38/38	0/3/3/3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	304	ATP	PB-O3B-PG	-2.93	122.86	132.67
3	A	303	ATP	PB-O3B-PG	-2.38	124.69	132.67
3	A	303	ATP	C1'-N9-C4	-2.22	123.59	126.94
3	B	304	ATP	C1'-N9-C4	-2.22	123.59	126.94
3	A	303	ATP	O5'-C5'-C4'	2.13	116.98	109.12
3	A	303	ATP	O2B-PB-O3B	2.97	118.55	105.09
3	B	304	ATP	O2B-PB-O3B	3.08	119.07	105.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	303	ATP	1	0
3	B	304	ATP	3	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 ⓘ

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	270/303 (89%)	0.29	15 (5%) 28 21	24, 48, 88, 104	0
1	B	253/303 (83%)	0.35	13 (5%) 32 24	27, 48, 84, 105	0
All	All	523/606 (86%)	0.32	28 (5%) 29 22	24, 48, 87, 105	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	900	GLY	5.5
1	B	899	THR	5.1
1	B	610	PHE	4.2
1	B	885	ILE	3.8
1	A	994	LEU	3.7
1	B	769	ARG	3.6
1	A	923	SER	3.4
1	A	944	PRO	3.3
1	A	899	THR	3.2
1	A	946	PHE	3.2
1	B	771	PHE	3.0
1	A	995	LYS	2.9
1	A	771	PHE	2.6
1	B	897	ASP	2.5
1	B	923	SER	2.4
1	A	901	HIS	2.4
1	B	896	LEU	2.4
1	B	902	TYR	2.4
1	A	900	GLY	2.3
1	B	607	GLN	2.3
1	A	887	THR	2.3
1	A	996	SER	2.3
1	A	922	PHE	2.2
1	A	950	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	845	GLU	2.2
1	A	858	LYS	2.2
1	A	772	VAL	2.1
1	B	901	HIS	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, 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(\AA^2)	Q<0.9
3	ATP	A	303	31/31	0.97	0.18	0.54	29,38,54,63	0
3	ATP	B	304	31/31	0.97	0.16	-0.48	37,45,59,62	0
2	MG	B	307	1/1	0.95	0.13	-	22,22,22,22	0
2	MG	B	308	1/1	0.96	0.29	-	42,42,42,42	0
2	MG	A	306	1/1	0.95	0.28	-	26,26,26,26	0
2	MG	A	305	1/1	0.93	0.23	-	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.