



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:39 AM GMT

PDB ID : 3MMN
Title : Crystal structure of the receiver domain of the histidine kinase CKI1 from *Arabidopsis thaliana* complexed with Mg²⁺
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Deposited on : 2010-04-20
Resolution : 2.20 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

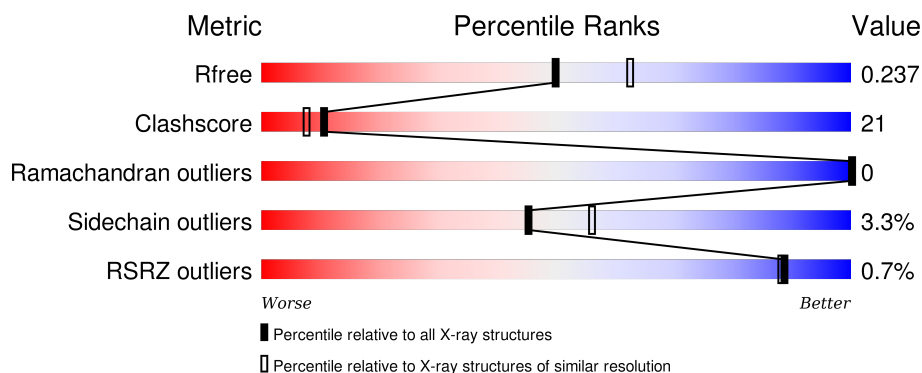
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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 $\leq 5\%$. 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	206	 49% 18% • 30%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1249 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 Histidine kinase homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	145	Total	C	N	O	S	0	1	0
			1129	701	197	224	7			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	925	GLY	-	EXPRESSION TAG	UNP O22267
A	926	SER	-	EXPRESSION TAG	UNP O22267
A	927	SER	-	EXPRESSION TAG	UNP O22267
A	928	HIS	-	EXPRESSION TAG	UNP O22267
A	929	HIS	-	EXPRESSION TAG	UNP O22267
A	930	HIS	-	EXPRESSION TAG	UNP O22267
A	931	HIS	-	EXPRESSION TAG	UNP O22267
A	932	HIS	-	EXPRESSION TAG	UNP O22267
A	933	HIS	-	EXPRESSION TAG	UNP O22267
A	934	SER	-	EXPRESSION TAG	UNP O22267
A	935	SER	-	EXPRESSION TAG	UNP O22267
A	936	GLY	-	EXPRESSION TAG	UNP O22267
A	937	LEU	-	EXPRESSION TAG	UNP O22267
A	938	VAL	-	EXPRESSION TAG	UNP O22267
A	939	PRO	-	EXPRESSION TAG	UNP O22267
A	940	ARG	-	EXPRESSION TAG	UNP O22267
A	941	GLY	-	EXPRESSION TAG	UNP O22267
A	942	SER	-	EXPRESSION TAG	UNP O22267
A	943	HIS	-	EXPRESSION TAG	UNP O22267
A	1123	LEU	-	EXPRESSION TAG	UNP O22267
A	1124	GLU	-	EXPRESSION TAG	UNP O22267
A	1125	HIS	-	EXPRESSION TAG	UNP O22267
A	1126	HIS	-	EXPRESSION TAG	UNP O22267
A	1127	HIS	-	EXPRESSION TAG	UNP O22267
A	1128	HIS	-	EXPRESSION TAG	UNP O22267
A	1129	HIS	-	EXPRESSION TAG	UNP O22267
A	1130	HIS	-	EXPRESSION TAG	UNP O22267

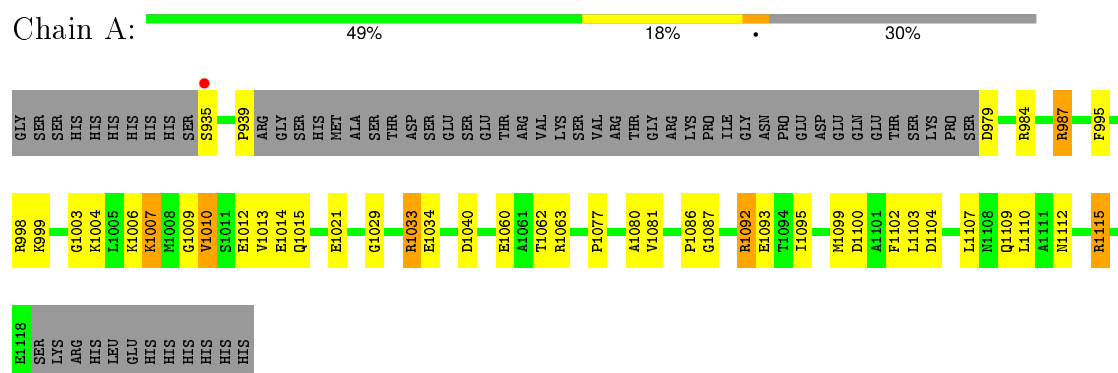
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mg 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	119	Total 119	O 119	0	0

- Molecule 1: Histidine kinase homolog



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	54.14Å 100.92Å 80.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.20 5.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (5.00-2.20) 99.0 (5.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.174 , 0.237 0.175 , 0.237	Depositor DCC
R_{free} test set	489 reflections (4.97%)	DCC
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.53 , 82.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 10328 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1249	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows:

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	1.20	5/1146 (0.4%)	1.01	4/1533 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1021	GLU	CG-CD	8.16	1.64	1.51
1	A	1034	GLU	CB-CG	5.57	1.62	1.52
1	A	1021	GLU	CB-CG	5.50	1.62	1.52
1	A	1115	ARG	CG-CD	5.23	1.65	1.51
1	A	1021	GLU	CD-OE2	5.20	1.31	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1033	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	A	1103	LEU	CA-CB-CG	6.34	129.88	115.30
1	A	1092	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	1081	VAL	CG1-CB-CG2	-5.02	102.88	110.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	1129	0	1125	48	0
2	A	1	0	0	0	0
3	A	119	0	0	20	0
All	All	1249	0	1125	48	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 21.

All (48) 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:1107:LEU:HD12	3:A:83:HOH:O	1.58	1.03
1:A:1093:GLU:HG2	3:A:20:HOH:O	1.74	0.88
1:A:1109:GLN:HE22	1:A:1112:ASN:HD22	1.21	0.86
1:A:987[B]:ARG:HG3	1:A:1012:GLU:HB3	1.58	0.83
1:A:1109:GLN:NE2	1:A:1112:ASN:HD22	1.81	0.78
1:A:1040:ASP:HB3	3:A:21:HOH:O	1.85	0.75
1:A:1115:ARG:HD2	3:A:106:HOH:O	1.86	0.75
1:A:1014:GLU:HB2	3:A:112:HOH:O	1.93	0.66
1:A:999:LYS:NZ	1:A:1015:GLN:HE22	1.94	0.66
1:A:1107:LEU:HB2	3:A:1131:HOH:O	1.96	0.65
1:A:987[A]:ARG:HH11	1:A:987[A]:ARG:CG	2.09	0.63
1:A:1115:ARG:NE	3:A:106:HOH:O	2.30	0.63
1:A:1115:ARG:CD	3:A:106:HOH:O	2.43	0.63
1:A:1107:LEU:CD1	3:A:83:HOH:O	2.27	0.63
1:A:1086:PRO:HD3	1:A:1102:PHE:CE2	2.34	0.62
1:A:1003:GLY:O	1:A:1007:LYS:HD2	2.00	0.62
1:A:1086:PRO:HD3	1:A:1102:PHE:CZ	2.36	0.60
1:A:1092:ARG:CZ	3:A:103:HOH:O	2.49	0.60
1:A:998:ARG:HD2	1:A:1015:GLN:HE21	1.65	0.60
1:A:987[A]:ARG:HH11	1:A:987[A]:ARG:HG2	1.66	0.60
1:A:987[A]:ARG:CG	1:A:987[A]:ARG:NH1	2.66	0.59
1:A:1006:LYS:HD2	3:A:46:HOH:O	2.07	0.55
1:A:1087:GLY:HA3	3:A:22:HOH:O	2.06	0.54
1:A:935:SER:HB2	1:A:1109:GLN:HB3	1.89	0.54
1:A:1077:PRO:HA	1:A:1100:ASP:OD2	2.09	0.53
1:A:939:PRO:HG2	1:A:1095:ILE:HD11	1.90	0.53
1:A:987[B]:ARG:HE	1:A:1012:GLU:CD	2.13	0.52
1:A:935:SER:HB2	1:A:1109:GLN:CB	2.40	0.51
1:A:979:ASP:N	3:A:92:HOH:O	2.42	0.51
1:A:1010:VAL:HG11	1:A:1013:VAL:CG2	2.41	0.51
1:A:995:PHE:O	1:A:999:LYS:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1040:ASP:CB	3:A:21:HOH:O	2.53	0.48
1:A:1004:LYS:HE2	1:A:1107:LEU:O	2.15	0.47
1:A:1087:GLY:CA	3:A:22:HOH:O	2.62	0.46
1:A:1060:GLU:HG3	3:A:39:HOH:O	2.15	0.46
1:A:987[B]:ARG:HG3	1:A:1012:GLU:OE1	2.16	0.45
1:A:1104:ASP:CA	3:A:2:HOH:O	2.64	0.45
1:A:1063:ARG:NH1	3:A:20:HOH:O	2.35	0.43
1:A:984:ARG:HA	1:A:1009:GLY:O	2.19	0.43
1:A:998:ARG:HD2	1:A:1015:GLN:NE2	2.34	0.42
1:A:1062:THR:HG21	1:A:1099:MET:HG3	2.02	0.42
1:A:998:ARG:HG2	1:A:1015:GLN:NE2	2.34	0.42
1:A:987[A]:ARG:NH1	3:A:94:HOH:O	2.28	0.42
1:A:1080:ALA:HB2	1:A:1099:MET:SD	2.60	0.42
1:A:999:LYS:HD3	1:A:999:LYS:HA	1.78	0.41
1:A:1029:GLY:O	1:A:1033:ARG:HG2	2.21	0.40
1:A:1063:ARG:NE	3:A:109:HOH:O	2.51	0.40
1:A:1010:VAL:HG11	1:A:1013:VAL:HG22	2.03	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	142/206 (69%)	138 (97%)	4 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	124/181 (68%)	119 (96%)	5 (4%)	38 47

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

Mol	Chain	Res	Type
1	A	987[A]	ARG
1	A	987[B]	ARG
1	A	1007	LYS
1	A	1010	VAL
1	A	1110	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1015	GLN
1	A	1109	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 [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	145/206 (70%)	-0.84	1 (0%) 89 88	22, 36, 51, 61	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	935	SER	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(Å ²)	Q<0.9
2	MG	A	1	1/1	0.97	0.06	-1.20	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.