Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:00 PM GMT

PDB ID	:	4NHJ
Title	:	Crystal structure of Klebsiella pneumoniae RstA DNA-binding domain in complex with RstA box
Authors	:	Li, Y.C.; Hsiao, C.D.
Deposited on	:	2013-11-05
Resolution	:	2.70 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

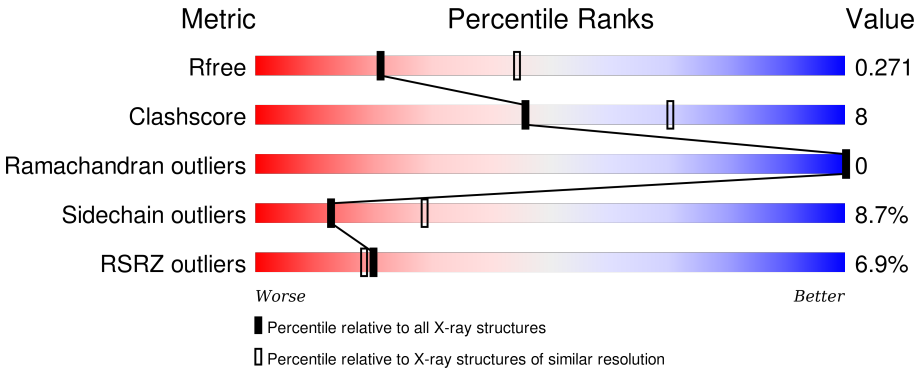
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	119	4% 63% 21% • 14%
1	B	119	9% 61% 24% 15%
2	C	23	61% 30% • •
3	D	23	4% 70% 30%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2582 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 DNA-binding transcriptional regulator RstA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	102	Total	C	N	O	S	0	0	0
			804	506	146	148	4			
1	B	101	Total	C	N	O	S	0	0	0
			797	501	145	147	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	121	MET	-	EXPRESSION TAG	UNP G0GNT0
A	122	HIS	-	EXPRESSION TAG	UNP G0GNT0
A	123	HIS	-	EXPRESSION TAG	UNP G0GNT0
A	124	HIS	-	EXPRESSION TAG	UNP G0GNT0
A	125	HIS	-	EXPRESSION TAG	UNP G0GNT0
A	126	HIS	-	EXPRESSION TAG	UNP G0GNT0
A	127	HIS	-	EXPRESSION TAG	UNP G0GNT0
A	128	ALA	-	EXPRESSION TAG	UNP G0GNT0
A	129	MET	-	EXPRESSION TAG	UNP G0GNT0
A	130	GLY	-	EXPRESSION TAG	UNP G0GNT0
A	153	MET	LEU	ENGINEERED MUTATION	UNP G0GNT0
A	168	MET	LEU	ENGINEERED MUTATION	UNP G0GNT0
B	121	MET	-	EXPRESSION TAG	UNP G0GNT0
B	122	HIS	-	EXPRESSION TAG	UNP G0GNT0
B	123	HIS	-	EXPRESSION TAG	UNP G0GNT0
B	124	HIS	-	EXPRESSION TAG	UNP G0GNT0
B	125	HIS	-	EXPRESSION TAG	UNP G0GNT0
B	126	HIS	-	EXPRESSION TAG	UNP G0GNT0
B	127	HIS	-	EXPRESSION TAG	UNP G0GNT0
B	128	ALA	-	EXPRESSION TAG	UNP G0GNT0
B	129	MET	-	EXPRESSION TAG	UNP G0GNT0
B	130	GLY	-	EXPRESSION TAG	UNP G0GNT0
B	153	MET	LEU	ENGINEERED MUTATION	UNP G0GNT0
B	168	MET	LEU	ENGINEERED MUTATION	UNP G0GNT0

- Molecule 2 is a DNA chain called 5'-D(*GP*GP*TP*TP*GP*TP*AP*CP*AP*TP*TP*C P*CP*GP*TP*TP*AP*CP*TP*CP*CP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	22	Total	C	N	O	P	0	0	0
			442	213	69	138	22			

- Molecule 3 is a DNA chain called 5'-D(*CP*AP*GP*GP*GP*AP*GP*TP*AP*AP*CP*G P*GP*AP*AP*TP*GP*TP*AP*CP*AP*AP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	23	Total	C	N	O	P	0	0	0
			476	226	98	130	22			

- Molecule 4 is water.

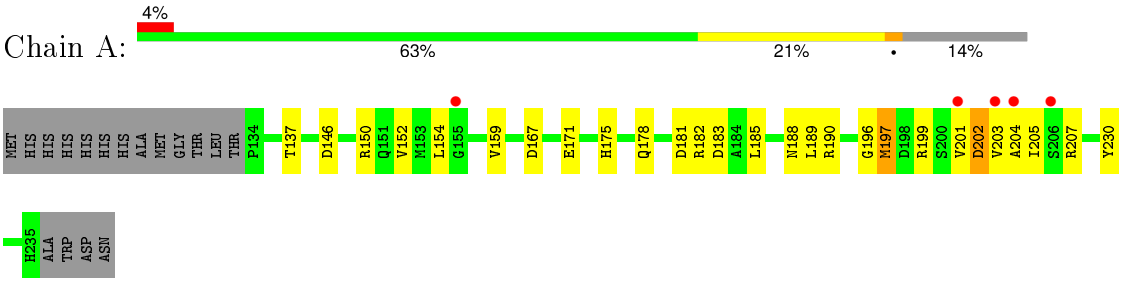
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total	O	0	0
			18	18		
4	B	19	Total	O	0	0
			19	19		
4	C	13	Total	O	0	0
			13	13		
4	D	13	Total	O	0	0
			13	13		

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.

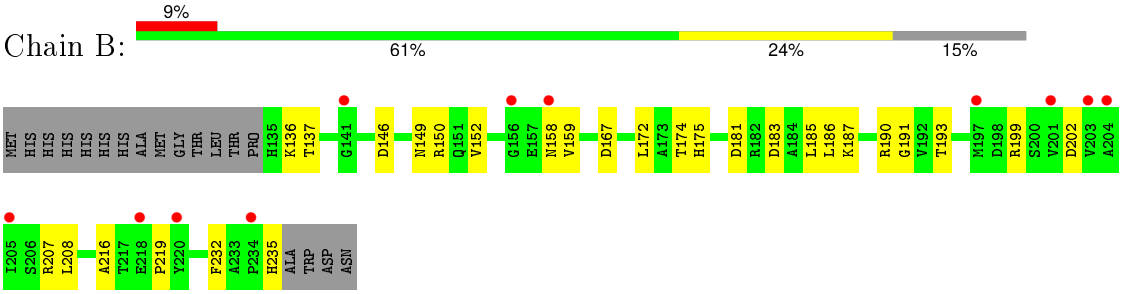
• Molecule 1: DNA-binding transcriptional regulator RstA

Chain A:



• Molecule 1: DNA-binding transcriptional regulator RstA

Chain B:

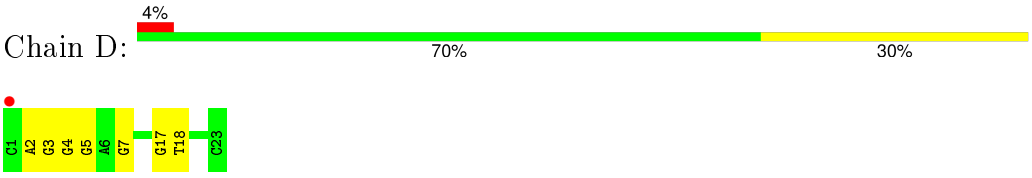


• Molecule 2: 5'-D(*GP*GP*TP*TP*GP*TP*AP*CP*AP*TP*TP*CP*CP*GP*TP*TP*AP*CP*TP*CP*CP*CP*T)-3'

Chain C:

• Molecule 3: 5'-D(*CP*AP*GP*GP*GP*AP*GP*TP*AP*AP*CP*GP*GP*AP*AP*TP*GP*TP*AP*CP*AP*AP*C)-3'

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	159.94Å 33.31Å 72.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.03 – 2.70 25.03 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.7 (25.03-2.70) 90.8 (25.03-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	8.01 (at 2.72Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.216 , 0.271 0.209 , 0.271	Depositor DCC
R_{free} test set	1025 reflections (10.04%)	DCC
Wilson B-factor (Å^2)	58.7	Xtriage
Anisotropy	0.766	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 44.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	1 of 10418 reflections (0.010%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2582	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

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	0.28	0/818	0.46	0/1104
1	B	0.24	0/810	0.46	0/1093
2	C	0.50	0/491	1.28	3/754 (0.4%)
3	D	0.52	0/537	1.13	1/828 (0.1%)
All	All	0.38	0/2656	0.85	4/3779 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	DG	O4'-C4'-C3'	-5.97	102.11	104.50
2	C	2	DG	C4'-C3'-C2'	-5.20	98.42	103.10
3	D	18	DT	O4'-C4'-C3'	-5.14	102.44	104.50
2	C	10	DT	N3-C4-O4	5.06	122.94	119.90

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	804	0	816	15	0
1	B	797	0	808	15	0
2	C	442	0	252	6	0
3	D	476	0	258	4	0
4	A	18	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	19	0	0	1	0
4	C	13	0	0	0	0
4	D	13	0	0	0	0
All	All	2582	0	2134	35	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 8.

All (35) 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:199:ARG:NH1	3:D:7:DG:N7	2.41	0.68
1:B:172:LEU:HB3	1:B:232:PHE:HB2	1.81	0.63
1:A:182:ARG:NE	4:A:308:HOH:O	2.34	0.60
1:A:196:GLY:HA3	1:A:197:MET:HG2	1.90	0.54
1:B:187:LYS:NZ	1:B:193:THR:HA	2.23	0.54
1:B:183:ASP:O	1:B:187:LYS:HG2	2.09	0.53
1:A:190:ARG:NH2	2:C:5:DG:OP1	2.42	0.52
1:A:189:LEU:HG	1:A:190:ARG:HG3	1.92	0.52
1:B:207:ARG:NH2	2:C:14:DG:O6	2.37	0.51
2:C:2:DG:H1'	2:C:3:DT:H5"	1.92	0.51
3:D:2:DA:H2'	3:D:3:DG:C8	2.45	0.51
1:B:187:LYS:HZ2	1:B:193:THR:HA	1.76	0.51
1:A:199:ARG:NH1	3:D:17:DG:O6	2.44	0.50
1:B:152:VAL:HG13	1:B:159:VAL:HG13	1.94	0.50
1:A:204:ALA:HA	1:A:207:ARG:NH1	2.28	0.49
1:B:174:THR:HG22	1:B:175:HIS:CD2	2.48	0.49
1:B:207:ARG:NE	4:B:304:HOH:O	2.27	0.48
2:C:5:DG:H2"	2:C:6:DT:H71	1.95	0.48
1:A:201:VAL:O	1:A:205:ILE:HG12	2.14	0.48
1:A:207:ARG:HE	2:C:4:DT:H72	1.79	0.47
1:A:152:VAL:HG13	1:A:159:VAL:HB	1.97	0.46
1:B:186:LEU:O	1:B:191:GLY:HA2	2.16	0.45
1:B:183:ASP:OD2	1:B:187:LYS:NZ	2.50	0.44
1:A:171:GLU:OE1	1:A:188:ASN:ND2	2.50	0.44
3:D:4:DG:H2"	3:D:5:DG:C8	2.53	0.44
1:A:137:THR:HG22	1:A:146:ASP:HA	1.99	0.44
2:C:6:DT:H2"	2:C:7:DA:C8	2.53	0.44
1:B:150:ARG:NH1	1:B:167:ASP:OD1	2.49	0.43
1:A:175:HIS:O	1:A:178:GLN:HB3	2.19	0.42
1:B:216:ALA:HA	1:B:219:PRO:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:TYR:HE1	4:A:308:HOH:O	2.03	0.42
1:B:136:LYS:HA	1:B:136:LYS:HD2	1.84	0.41
1:A:202:ASP:OD1	1:A:202:ASP:N	2.52	0.41
1:A:150:ARG:NH1	1:A:167:ASP:OD1	2.54	0.41
1:B:146:ASP:OD2	1:B:149:ASN:ND2	2.32	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	100/119 (84%)	94 (94%)	6 (6%)	0	100	100
1	B	99/119 (83%)	92 (93%)	7 (7%)	0	100	100
All	All	199/238 (84%)	186 (94%)	13 (6%)	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	87/101 (86%)	80 (92%)	7 (8%)	15	33
1	B	86/101 (85%)	78 (91%)	8 (9%)	11	25
All	All	173/202 (86%)	158 (91%)	15 (9%)	13	29

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	LEU
1	A	181	ASP
1	A	183	ASP
1	A	185	LEU
1	A	197	MET
1	A	202	ASP
1	A	203	VAL
1	B	137	THR
1	B	158	ASN
1	B	181	ASP
1	B	185	LEU
1	B	190	ARG
1	B	202	ASP
1	B	208	LEU
1	B	235	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	158	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)

There are no ligands in this entry.

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^{th} 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	102/119 (85%)	0.37	5 (4%) 33 32	45, 62, 76, 86	0
1	B	101/119 (84%)	0.69	11 (10%) 7 5	41, 68, 91, 103	0
2	C	22/23 (95%)	-0.23	0 100 100	45, 57, 74, 77	0
3	D	23/23 (100%)	0.26	1 (4%) 39 38	44, 59, 72, 82	0
All	All	248/284 (87%)	0.43	17 (6%) 20 18	41, 64, 87, 103	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	141	GLY	6.8
3	D	1	DC	5.0
1	B	220	TYR	4.6
1	B	158	ASN	4.3
1	B	204	ALA	3.5
1	B	234	PRO	3.3
1	B	156	GLY	3.2
1	B	201	VAL	3.1
1	A	204	ALA	2.9
1	B	203	VAL	2.6
1	A	203	VAL	2.6
1	B	197	MET	2.3
1	B	205	ILE	2.3
1	A	206	SER	2.1
1	B	218	GLU	2.1
1	A	155	GLY	2.0
1	A	201	VAL	2.0

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.