W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 27, 2014 – 06:30 PM GMT

PDB ID   :   3MVD
Title   :   Crystal structure of the chromatin factor RCC1 in complex with the nucleo-
              some core particle
Authors   :   Makde, R.D.; England, J.R.; Yennawar, H.P.; Tan, S.
Deposited on :   2010-05-04
Resolution   :   2.90 Å(reported)

<div style="border:1px solid red; background:#ffcccc; padding:10px;">

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
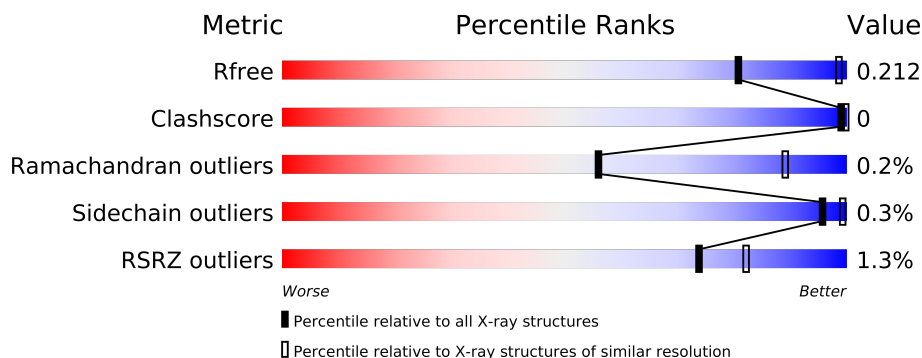
A user guide is available at http://wwpdb.org/ValidationPDFNotes.html

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1   Overall quality at a glance ⓘ

The reported resolution of this entry is 2.90 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	Percentile Ranks	Value
Rfree		0.212
Clashscore		0
Ramachandran outliers		0.2%
Sidechain outliers		0.3%
RSRZ outliers		1.3%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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	135	
1	E	135	
2	B	102	
2	F	102	
3	C	129	
3	G	129	
4	D	122	
4	H	122	
5	I	147	
6	J	147	
7	K	423	
7	L	423	

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 17743 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 Histone H3.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	98	Total	C	N	O	S	0	0	0
			801	506	153	139	3			
1	E	95	Total	C	N	O	S	0	0	0
			779	492	148	136	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	GLY	SEE REMARK 999	UNP P84233
E	102	ALA	GLY	SEE REMARK 999	UNP P84233

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	82	Total	C	N	O	S	0	0	0
			653	413	127	112	1			
2	F	86	Total	C	N	O	S	0	0	0
			672	424	130	117	1			

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	107	Total	C	N	O	0	0	0
			811	510	158	143			
3	G	107	Total	C	N	O	0	0	0
			815	513	159	143			

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	93	Total	C	N	O	S	0	0	0
			718	451	128	137	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	93	726	457	130	137	2	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	SEE REMARK 999	UNP P02281
H	29	THR	SER	SEE REMARK 999	UNP P02281

- Molecule 5 is a DNA chain called DNA (146-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
5	I	146	2975	1413	540	876	146	0	0	0

- Molecule 6 is a DNA chain called DNA (146-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
6	J	146	3011	1425	564	876	146	0	0	0

- Molecule 7 is a protein called Regulator of chromosome condensation.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	K	391	2893	1802	516	559	16	0	0	0
7	L	394	2889	1798	515	560	16	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

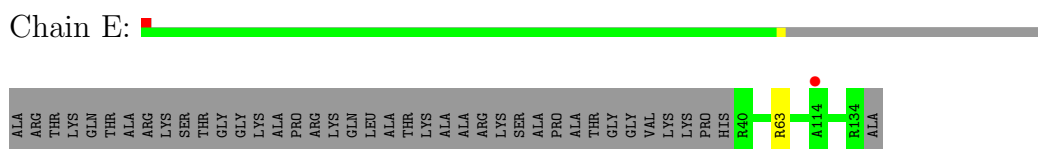| Chain	Residue	Modelled	Actual	Comment	Reference
K	0	GLY	-	EXPRESSION TAG	UNP P25171
K	1	SER	-	EXPRESSION TAG	UNP P25171
L	0	GLY	-	EXPRESSION TAG	UNP P25171
L	1	SER	-	EXPRESSION TAG	UNP P25171

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.
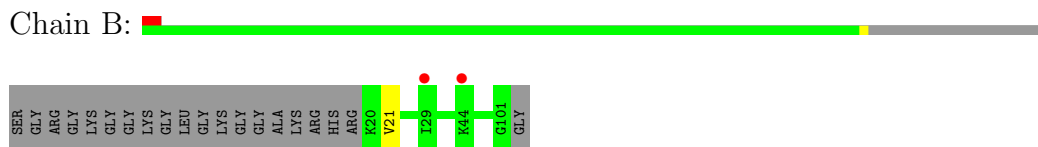
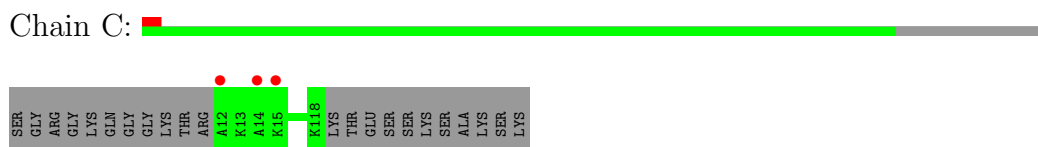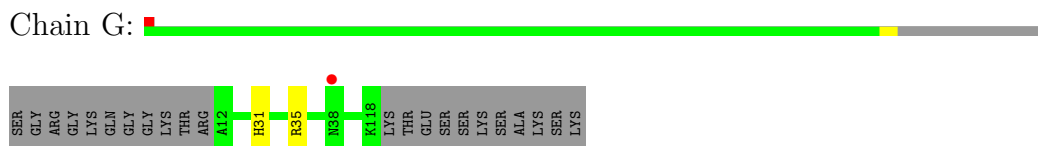• Molecule 1: Histone H3.2
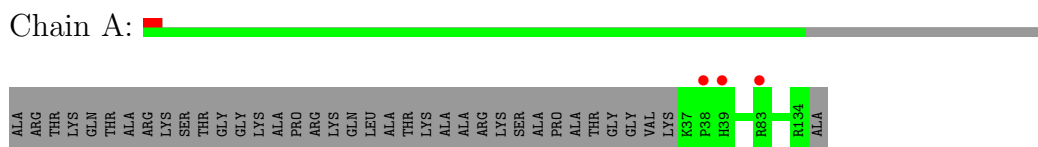
Chain A:

• Molecule 1: Histone H3.2

Chain E:

• Molecule 2: Histone H4

Chain B:

• Molecule 2: Histone H4

Chain F:

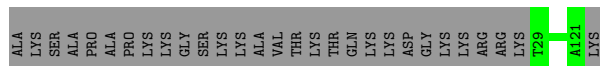• Molecule 3: Histone H2A

Chain C:
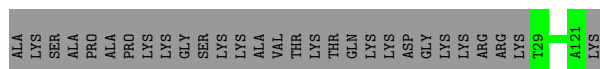
• Molecule 3: Histone H2A

Chain G:

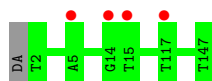- Molecule 4: Histone H2B 1.1

Chain D:

- Molecule 4: Histone H2B 1.1

Chain H:

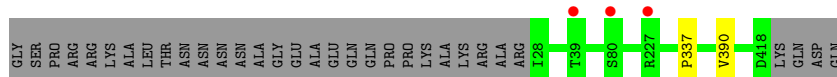- Molecule 5: DNA (146-MER)

Chain I:

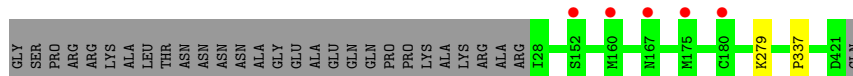- Molecule 6: DNA (146-MER)

Chain J:

- Molecule 7: Regulator of chromosome condensation

Chain K:

- Molecule 7: Regulator of chromosome condensation

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	102.68Å 183.04Å 107.03Å 90.00° 101.52° 90.00°	Depositor
Resolution (Å)	34.70 – 2.90 48.99 – 2.89	Depositor EDS
% Data completeness (in resolution range)	94.1 (34.70-2.90) 98.3 (48.99-2.89)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.34 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6_289)	Depositor
R, R_{free}	0.175 , 0.215 0.173 , 0.212	Depositor DCC
R_{free} test set	2105 reflections (2.48%)	DCC
Wilson B-factor (Å^2)	77.1	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 41.6	EDS
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
L-test for twinning	$<|L|> = 0.49, <L^2> = 0.33$	Xtriage
Outliers	0 of 85000 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17743	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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	0.21	0/813	0.35	0/1093
1	E	0.20	0/789	0.36	0/1059
2	B	0.20	0/660	0.37	0/885
2	F	0.20	0/680	0.37	0/912
3	C	0.19	0/821	0.34	0/1112
3	G	0.19	0/825	0.35	0/1116
4	D	0.21	0/729	0.37	0/985
4	H	0.21	0/737	0.37	0/993
5	I	0.41	0/3333	1.01	0/5137
6	J	0.41	0/3381	1.03	3/5221 (0.1%)
7	K	0.20	0/2938	0.38	0/3975
7	L	0.20	0/2934	0.38	0/3976
All	All	0.29	0/18640	0.70	3/26464 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	78	DG	O4'-C4'-C3'	-8.00	101.20	106.00
6	J	38	DG	O4'-C4'-C3'	-6.26	102.00	104.50
6	J	78	DG	C4'-C3'-C2'	-5.35	98.28	103.10

There are no chirality outliers.

There are no planarity outliers.

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	801	0	0	0	0
1	E	779	0	0	0	0
2	B	653	0	0	0	0
2	F	672	0	0	0	0
3	C	811	0	0	0	0
3	G	815	0	0	1	0
4	D	718	0	0	0	0
4	H	726	0	0	0	0
5	I	2975	0	0	0	0
6	J	3011	0	0	0	0
7	K	2893	0	0	0	0
7	L	2889	0	0	0	0
All	All	17743	0	0	1	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 0.

All (1) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:G:31:HIS:CD2	3:G:35:ARG:NH1	2.82	0.48

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	96/135 (71%)	95 (99%)	1 (1%)	0	100	100
1	E	93/135 (69%)	90 (97%)	3 (3%)	0	100	100
2	B	80/102 (78%)	78 (98%)	2 (2%)	0	100	100
2	F	84/102 (82%)	81 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	105/129 (81%)	102 (97%)	3 (3%)	0	100	100
3	G	105/129 (81%)	104 (99%)	1 (1%)	0	100	100
4	D	91/122 (75%)	90 (99%)	1 (1%)	0	100	100
4	H	91/122 (75%)	89 (98%)	2 (2%)	0	100	100
7	K	389/423 (92%)	370 (95%)	18 (5%)	1 (0%)	50	85
7	L	392/423 (93%)	370 (94%)	20 (5%)	2 (0%)	38	79
All	All	1526/1822 (84%)	1469 (96%)	54 (4%)	3 (0%)	56	89

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	L	279	LYS
7	K	337	PRO
7	L	337	PRO

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	84/110 (76%)	84 (100%)	0	100	100
1	E	82/110 (74%)	81 (99%)	1 (1%)	82	96
2	B	67/78 (86%)	66 (98%)	1 (2%)	76	95
2	F	67/78 (86%)	66 (98%)	1 (2%)	76	95
3	C	81/101 (80%)	81 (100%)	0	100	100
3	G	82/101 (81%)	82 (100%)	0	100	100
4	D	77/102 (76%)	77 (100%)	0	100	100
4	H	79/102 (78%)	79 (100%)	0	100	100
7	K	308/342 (90%)	307 (100%)	1 (0%)	96	99
7	L	303/342 (89%)	303 (100%)	0	100	100
All	All	1230/1466 (84%)	1226 (100%)	4 (0%)	96	99

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	21	VAL
1	E	63	ARG
2	F	92	ARG
7	K	390	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

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, 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(Å²)	Q<0.9
1	A	98/135 (72%)	0.23	3 (3%) 47	55	42, 66, 97, 149	0
1	E	95/135 (70%)	0.14	1 (1%) 77	84	43, 61, 87, 110	0
2	B	82/102 (80%)	0.14	2 (2%) 56	65	41, 61, 97, 117	0
2	F	86/102 (84%)	-0.00	0 100	100	37, 56, 102, 149	0
3	C	107/129 (82%)	0.28	3 (2%) 50	59	42, 60, 94, 132	0
3	G	107/129 (82%)	0.09	1 (0%) 81	88	41, 63, 94, 138	0
4	D	93/122 (76%)	-0.03	0 100	100	41, 59, 95, 127	0
4	H	93/122 (76%)	-0.08	0 100	100	41, 61, 94, 118	0
5	I	146/147 (99%)	0.12	4 (2%) 52	61	70, 117, 150, 195	0
6	J	146/147 (99%)	0.14	2 (1%) 72	80	70, 112, 152, 183	0
7	K	391/423 (92%)	-0.07	3 (0%) 83	89	47, 73, 107, 134	0
7	L	394/423 (93%)	0.11	5 (1%) 74	82	50, 84, 118, 160	0
All	All	1838/2116 (86%)	0.07	24 (1%) 74	82	37, 74, 131, 195	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	L	167	ASN	4.2
7	L	180	CYS	4.1
7	L	152	SER	3.4
1	A	39	HIS	3.0
1	E	114	ALA	2.9

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.