Full wwPDB X-ray Structure Validation Report (i)

Feb 11, 2024 – 03:54 PM EST

PDB ID	:	3CFS
Title	:	Structural basis of the interaction of RbAp46/RbAp48 with histone H4
Authors	:	Murzina, N.V.; Pei, X.-Y.; Pratap, J.V.; Sparkes, M.; Vicente-Garcia, J.; Ben-Shahar, T.R.; Verreault, A.; Luisi, B.F.; Laue, E.D.
Deposited on	:	2008-03-04
Resolution	:	2.40 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

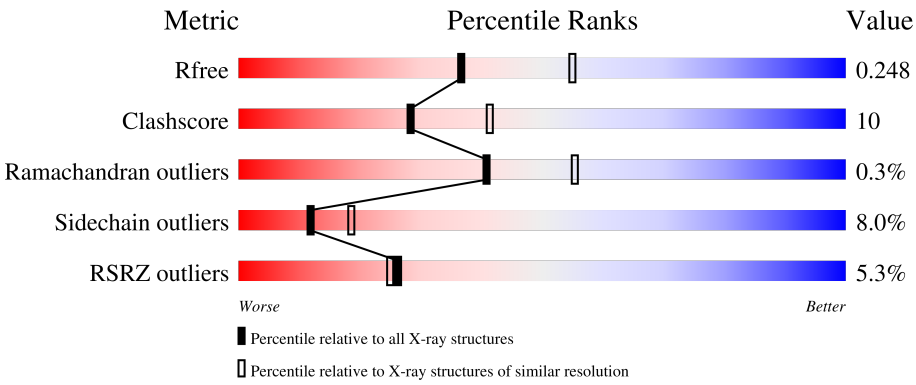
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	B	414	5%; 71%; 19%; • ; 7%
2	E	15	40%; 47%; 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ARS	B	412	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3397 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 Histone-binding protein RBBP7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	383	3068	1940	525	593	10	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	cloning artifact	UNP Q16576
B	-1	MSE	-	cloning artifact	UNP Q16576
B	0	ALA	-	cloning artifact	UNP Q16576

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	15	118	72	29	17	0	0	0

- Molecule 3 is ARSENIC (three-letter code: ARS) (formula: As).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	As		
3	B	1	1	1	0	0

- Molecule 4 is water.

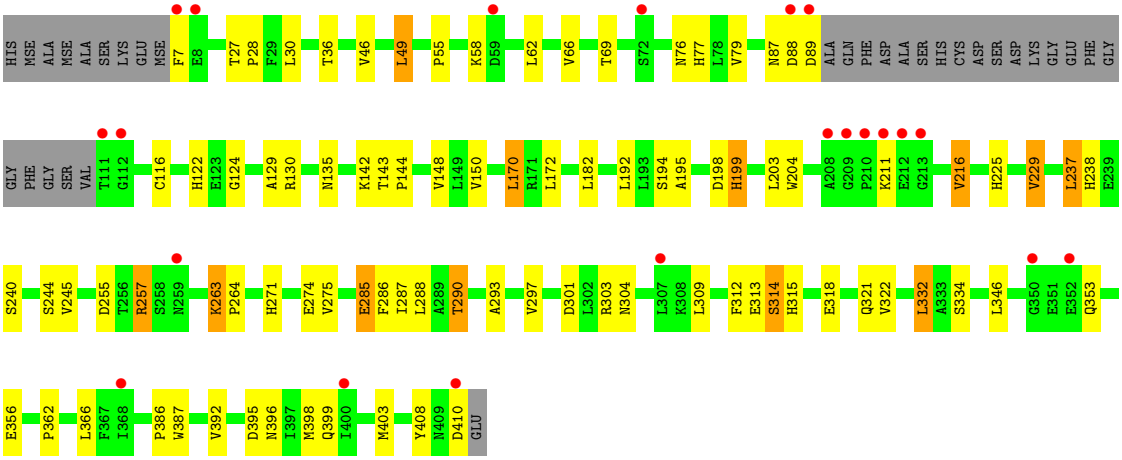
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	B	206	206	206	0	0
4	E	4	4	4	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

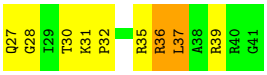
- Molecule 1: Histone-binding protein RBBP7

Chain B:



- Molecule 2: Histone H4

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	44.66Å 85.72Å 117.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.53 – 2.40 19.53 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.53-2.40) 99.9 (19.53-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	4.38 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.184 , 0.249 0.185 , 0.248	Depositor DCC
R_{free} test set	935 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	28.7	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 51.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3397	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: ARS

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	B	0.22	0/3155	0.43	0/4303
2	E	0.96	0/118	0.67	0/155
All	All	0.28	0/3273	0.44	0/4458

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
2	E	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	36	ARG	Sidechain

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	B	3068	0	2916	59	0
2	E	118	0	135	7	0
3	B	1	0	0	1	0
4	B	206	0	0	0	0
4	E	4	0	0	0	0
All	All	3397	0	3051	61	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 10.

All (61) 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:271:HIS:HE1	1:B:290:THR:HG22	1.11	1.13
1:B:257:ARG:HH11	1:B:257:ARG:HG3	1.18	1.06
1:B:271:HIS:CE1	1:B:290:THR:HG22	1.94	1.03
1:B:257:ARG:HG3	1:B:257:ARG:NH1	1.82	0.90
1:B:271:HIS:HE1	1:B:290:THR:CG2	1.84	0.89
1:B:143:THR:HG22	1:B:144:PRO:HD2	1.56	0.87
1:B:271:HIS:CE1	1:B:290:THR:CG2	2.64	0.79
1:B:143:THR:CG2	1:B:144:PRO:HD2	2.14	0.76
1:B:257:ARG:HH11	1:B:257:ARG:CG	1.97	0.74
2:E:30:THR:OG1	2:E:32:PRO:HD2	1.87	0.74
1:B:69:THR:HG22	1:B:76:ASN:OD1	1.94	0.67
1:B:410:ASP:HB3	2:E:35:ARG:NH1	2.10	0.67
1:B:195:ALA:HB1	1:B:229:VAL:HG22	1.77	0.66
1:B:198:ASP:O	1:B:199:HIS:HB2	1.94	0.66
1:B:238:HIS:HD2	1:B:240:SER:H	1.43	0.64
1:B:237:LEU:HD13	1:B:285:GLU:HG2	1.80	0.63
1:B:122:HIS:HD2	1:B:124:GLY:O	1.82	0.62
1:B:143:THR:HG22	1:B:144:PRO:CD	2.26	0.62
1:B:263:LYS:HE3	1:B:264:PRO:HD2	1.82	0.62
1:B:312:PHE:HZ	1:B:346:LEU:HD22	1.67	0.60
1:B:321:GLN:HE21	1:B:322:VAL:H	1.50	0.59
1:B:315:HIS:HE1	1:B:334:SER:OG	1.87	0.56
1:B:225:HIS:HE1	1:B:244:SER:OG	1.88	0.56
1:B:142:LYS:HZ3	1:B:194:SER:HG	1.49	0.55
1:B:116:CYS:HB2	3:B:412:ARS:AS	2.67	0.54
1:B:410:ASP:HB3	2:E:35:ARG:HH12	1.71	0.54
1:B:313:GLU:O	1:B:314:SER:HB2	2.11	0.51
1:B:286:PHE:CG	1:B:303:ARG:HD2	2.47	0.50
1:B:356:GLU:OE1	2:E:36:ARG:CZ	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ASP:OD2	1:B:303:ARG:HD3	2.13	0.48
1:B:395:ASP:O	1:B:396:ASN:HB2	2.14	0.48
1:B:30:LEU:HD21	2:E:37:LEU:HB3	1.96	0.47
1:B:182:LEU:HD22	1:B:192:LEU:HD11	1.96	0.47
1:B:403:MET:HE2	1:B:408:TYR:HB3	1.97	0.47
1:B:36:THR:HG22	1:B:399:GLN:HG2	1.97	0.46
1:B:286:PHE:HB3	1:B:303:ARG:HD2	1.97	0.46
1:B:255:ASP:OD1	1:B:257:ARG:HG3	2.16	0.46
1:B:255:ASP:OD1	1:B:257:ARG:CG	2.64	0.46
1:B:297:VAL:HB	1:B:312:PHE:HB2	1.98	0.46
1:B:293:ALA:HA	1:B:318:GLU:HG2	1.98	0.45
1:B:49:LEU:HD12	1:B:49:LEU:HA	1.88	0.45
1:B:245:VAL:HG13	1:B:275:VAL:O	2.17	0.45
1:B:312:PHE:CZ	1:B:346:LEU:HD22	2.48	0.45
1:B:55:PRO:HB2	1:B:58:LYS:HG3	2.00	0.44
1:B:275:VAL:CG1	1:B:290:THR:HG23	2.48	0.44
1:B:150:VAL:HB	1:B:170:LEU:HB2	2.00	0.43
1:B:172:LEU:HD23	1:B:216:VAL:HG13	2.00	0.43
1:B:172:LEU:HB3	1:B:204:TRP:CE2	2.53	0.43
1:B:392:VAL:HG12	1:B:398:MET:HB3	1.99	0.43
1:B:27:THR:N	1:B:28:PRO:CD	2.82	0.42
1:B:198:ASP:O	1:B:199:HIS:CB	2.63	0.42
1:B:386:PRO:O	1:B:387:TRP:HB2	2.18	0.42
1:B:87:ASN:C	1:B:89:ASP:H	2.22	0.42
1:B:322:VAL:HG22	1:B:332:LEU:HD21	2.02	0.42
1:B:362:PRO:O	2:E:39:ARG:NH2	2.54	0.41
1:B:49:LEU:HD13	1:B:66:VAL:HG23	2.02	0.41
1:B:69:THR:HB	1:B:77:HIS:H	1.85	0.41
1:B:129:ALA:O	1:B:130:ARG:HD3	2.21	0.41
1:B:274:GLU:HG2	1:B:293:ALA:CB	2.51	0.41
1:B:49:LEU:HD13	1:B:66:VAL:CG2	2.51	0.40
2:E:27:GLN:HB3	2:E:28:GLY:H	1.72	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	B	379/414 (92%)	365 (96%)	13 (3%)	1 (0%)	41	55
2	E	13/15 (87%)	13 (100%)	0	0	100	100
All	All	392/429 (91%)	378 (96%)	13 (3%)	1 (0%)	41	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	314	SER

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	B	341/361 (94%)	315 (92%)	26 (8%)	13	20
2	E	11/11 (100%)	9 (82%)	2 (18%)	1	2
All	All	352/372 (95%)	324 (92%)	28 (8%)	12	18

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	7	PHE
1	B	46	VAL
1	B	49	LEU
1	B	62	LEU
1	B	79	VAL
1	B	88	ASP
1	B	135	ASN
1	B	148	VAL
1	B	170	LEU
1	B	199	HIS
1	B	203	LEU

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Mol	Chain	Res	Type
1	B	211	LYS
1	B	216	VAL
1	B	229	VAL
1	B	237	LEU
1	B	257	ARG
1	B	263	LYS
1	B	285	GLU
1	B	287	ILE
1	B	288	LEU
1	B	290	THR
1	B	304	ASN
1	B	309	LEU
1	B	332	LEU
1	B	353	GLN
1	B	366	LEU
2	E	31	LYS
2	E	37	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	26	ASN
1	B	75	GLN
1	B	87	ASN
1	B	122	HIS
1	B	135	ASN
1	B	137	HIS
1	B	175	HIS
1	B	191	HIS
1	B	225	HIS
1	B	238	HIS
1	B	249	GLN
1	B	271	HIS
1	B	304	ASN
1	B	315	HIS
1	B	321	GLN
1	B	342	ASN
1	B	384	ASN
1	B	399	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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 (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 (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	B	383/414 (92%)	-0.08	21 (5%) 25 24	5, 27, 57, 119	7 (1%)
2	E	15/15 (100%)	0.08	0 100 100	18, 38, 57, 73	0
All	All	398/429 (92%)	-0.08	21 (5%) 26 25	5, 27, 58, 119	7 (1%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	213	GLY	8.3
1	B	212	GLU	7.7
1	B	210	PRO	7.0
1	B	211	LYS	6.6
1	B	111	THR	5.4
1	B	209	GLY	4.6
1	B	368	ILE	4.4
1	B	7	PHE	4.4
1	B	88	ASP	4.3
1	B	400	ILE	4.1
1	B	259	ASN	3.9
1	B	72	SER	3.9
1	B	89	ASP	3.8
1	B	352	GLU	2.8
1	B	112	GLY	2.6
1	B	8	GLU	2.4
1	B	307	LEU	2.4
1	B	208	ALA	2.4
1	B	350	GLY	2.3
1	B	59	ASP	2.1
1	B	410	ASP	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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
3	ARS	B	412	1/1	0.66	0.57	120,120,120,120	0

6.5 Other polymers (i)

There are no such residues in this entry.