



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:31 PM UTC

PDB ID : 4F3L / pdb_00004f3l
Title : Crystal Structure of the Heterodimeric CLOCK:BMAL1 Transcriptional Activator Complex
Authors : Huang, N.; Chelliah, Y.; Shan, Y.; Taylor, C.; Yoo, S.; Partch, C.; Green, C.B.; Zhang, H.; Takahashi, J.
Deposited on : 2012-05-09
Resolution : 2.27 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

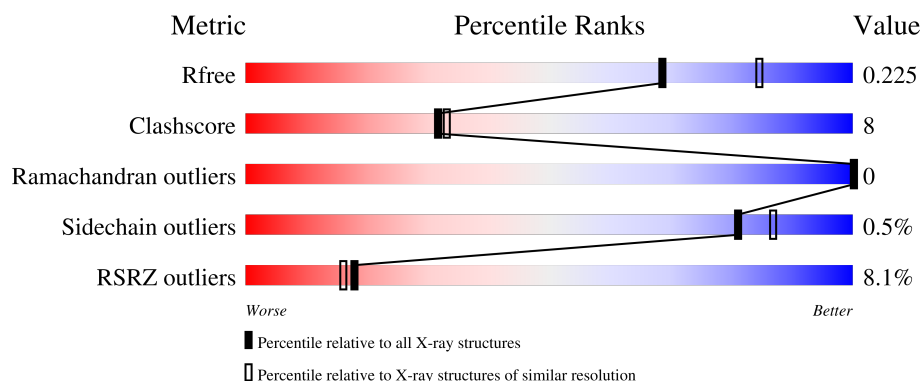
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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 $\leq 5\%$. 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	B	387	7% 64% 13% 22%
2	A	361	6% 71% 18% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5278 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 BMAL1b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	302	Total	C	N	O	S	0	3	0
			2459	1558	446	437	18			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	61	MET	-	expression tag	UNP Q6F6D6

- Molecule 2 is a protein called Circadian locomoter output cycles protein kaput.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	319	Total	C	N	O	S	0	1	0
			2642	1698	435	495	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	GLY	-	expression tag	UNP O08785
A	25	ALA	-	expression tag	UNP O08785

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	89	Total	O	0	0
			89	89		
3	A	88	Total	O	0	0
			88	88		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.24Å 71.95Å 173.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.12 – 2.27 37.12 – 2.27	Depositor EDS
% Data completeness (in resolution range)	92.3 (37.12-2.27) 98.1 (37.12-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.27Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.184 , 0.217 0.192 , 0.225	Depositor DCC
R_{free} test set	1978 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 74.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5278	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	B	0.39	0/2505	0.71	1/3362 (0.0%)
2	A	0.39	1/2712 (0.0%)	0.73	2/3670 (0.1%)
All	All	0.39	1/5217 (0.0%)	0.72	3/7032 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	280	HIS	ND1-CE1	5.30	1.37	1.32

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	280	HIS	CB-CG-CD2	-6.54	122.70	131.20
1	B	136	ASN	N-CA-C	6.35	118.77	111.02
2	A	280	HIS	CB-CG-ND1	5.55	131.02	122.70

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	B	2459	0	2484	42	0
2	A	2642	0	2566	50	0
3	A	88	0	0	1	0
3	B	89	0	0	4	0
All	All	5278	0	5050	82	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 (82) 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)
2:A:83:LYS:HE3	2:A:180:LEU:HD13	1.55	0.87
2:A:66:ARG:HG3	2:A:68:MET:HE3	1.69	0.74
1:B:142:LEU:HD11	2:A:252:VAL:HG21	1.71	0.73
2:A:175:LEU:HD22	2:A:189:ASN:HD21	1.55	0.72
1:B:135:ALA:HB3	2:A:133:TYR:HE1	1.58	0.68
2:A:324:CYS:HB3	2:A:355[B]:TYR:OH	1.94	0.67
1:B:115:LEU:HB3	2:A:53:LEU:HD13	1.77	0.66
1:B:321:HIS:HE1	3:B:523:HOH:O	1.81	0.63
1:B:327:GLN:O	1:B:327:GLN:HG3	2.02	0.58
1:B:135:ALA:HB1	1:B:138:LYS:O	2.03	0.58
2:A:177:SER:HB3	2:A:183:GLU:HG2	1.86	0.57
1:B:289:LYS:HG2	2:A:104:PHE:HE1	1.72	0.55
1:B:442:LEU:HD12	1:B:442:LEU:N	2.22	0.55
1:B:442:LEU:HD12	1:B:442:LEU:H	1.71	0.55
2:A:126:MET:HE2	2:A:132:ILE:HG21	1.88	0.55
1:B:120:GLN:O	1:B:123:LYS:HB2	2.07	0.55
2:A:102:PRO:HG2	2:A:105:LEU:HB2	1.89	0.54
1:B:247:PHE:HA	1:B:355:GLN:OE1	2.07	0.54
1:B:135:ALA:HB3	2:A:133:TYR:CE1	2.40	0.53
2:A:177:SER:CB	2:A:183:GLU:HG2	2.38	0.53
1:B:327:GLN:N	1:B:328:PRO:HD3	2.24	0.53
1:B:248:PHE:CE1	1:B:283:HIS:HB2	2.43	0.53
2:A:125:ILE:HG22	2:A:131:ILE:HA	1.91	0.52
2:A:178:ASP:OD1	2:A:181:THR:HB	2.09	0.52
2:A:126:MET:HE1	2:A:222:LEU:HD22	1.93	0.51
1:B:112:LEU:O	1:B:116:ARG:HG3	2.11	0.51
1:B:323:HIS:CD2	1:B:324:MET:HG2	2.46	0.51
2:A:269:VAL:HG12	2:A:271:GLU:O	2.10	0.50
1:B:323:HIS:NE2	1:B:324:MET:HG2	2.26	0.50
1:B:353:VAL:HG22	1:B:357:ALA:CB	2.41	0.50
1:B:239:LEU:HD12	2:A:112:GLN:CD	2.38	0.49
2:A:51:ASN:OD1	2:A:70:LYS:HE2	2.12	0.49
2:A:342:LEU:HB2	2:A:348:TRP:CZ3	2.47	0.49
2:A:68:MET:HA	2:A:68:MET:HE2	1.95	0.49
2:A:165:GLU:O	2:A:168:LYS:HB3	2.13	0.48
1:B:389:HIS:O	1:B:392:VAL:HG12	2.13	0.48
1:B:88:MET:O	1:B:92:ILE:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:87:THR:HG21	2:A:185:LEU:HB3	1.95	0.48
2:A:94:SER:O	2:A:98:GLN:HG3	2.13	0.48
1:B:122:MET:HE1	2:A:80:PHE:CD2	2.49	0.48
2:A:83:LYS:CD	2:A:180:LEU:HB3	2.44	0.48
2:A:175:LEU:HD13	2:A:189:ASN:OD1	2.14	0.47
1:B:346:ILE:HG12	3:B:518:HOH:O	2.13	0.47
2:A:125:ILE:O	2:A:125:ILE:HG13	2.15	0.47
1:B:119:VAL:O	1:B:123:LYS:HG3	2.15	0.47
1:B:398:LYS:N	1:B:398:LYS:HD2	2.30	0.47
2:A:173:HIS:HB3	2:A:219:PHE:CZ	2.50	0.47
2:A:48:ASP:O	2:A:52:VAL:HG23	2.15	0.46
2:A:383:ALA:O	2:A:384:GLU:HB2	2.14	0.46
1:B:139:PRO:HD3	2:A:133:TYR:CE2	2.50	0.46
1:B:119:VAL:HG12	1:B:123:LYS:HE3	1.98	0.45
2:A:50:PHE:O	2:A:54:ILE:HG12	2.17	0.45
2:A:319:GLU:HB3	3:A:405:HOH:O	2.17	0.45
1:B:354:ASP:C	1:B:354:ASP:OD1	2.60	0.45
2:A:54:ILE:HG21	2:A:70:LYS:HA	1.98	0.45
2:A:145:LEU:HD12	2:A:382:ARG:NH2	2.32	0.45
2:A:270:GLU:HG3	2:A:271:GLU:N	2.31	0.45
2:A:325:HIS:O	2:A:329:MET:HG3	2.17	0.45
1:B:174:GLU:HA	1:B:184:GLN:HG3	1.99	0.44
1:B:410:ASP:C	1:B:410:ASP:OD1	2.61	0.44
2:A:182:PRO:HD2	2:A:185:LEU:HD12	2.00	0.43
1:B:127:GLY:HA2	1:B:128:ALA:HA	1.75	0.43
2:A:88:THR:O	2:A:88:THR:HG22	2.18	0.43
2:A:165:GLU:O	2:A:169:ILE:HD13	2.18	0.43
2:A:313:TYR:CD2	2:A:321:LEU:HD13	2.54	0.43
1:B:176:VAL:HG13	1:B:182:TYR:O	2.19	0.43
2:A:378:TYR:CE2	2:A:382:ARG:HD3	2.53	0.42
1:B:407:LYS:HB2	1:B:413:PHE:CE1	2.54	0.42
1:B:311:LEU:HD12	3:B:528:HOH:O	2.19	0.42
1:B:333:ILE:HD13	2:A:159:PRO:HG2	2.02	0.42
2:A:150:VAL:O	2:A:151:ASP:HB2	2.19	0.42
1:B:126:ARG:HD3	2:A:60:MET:O	2.19	0.42
2:A:168:LYS:O	2:A:169:ILE:C	2.61	0.42
2:A:175:LEU:HD22	2:A:189:ASN:ND2	2.30	0.41
2:A:384:GLU:OE2	2:A:384:GLU:HA	2.20	0.41
1:B:289:LYS:HG3	1:B:290:SER:N	2.36	0.41
1:B:71:LYS:N	1:B:74:ARG:HH11	2.19	0.41
1:B:138:LYS:HD3	1:B:147:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:HIS:CE1	3:B:523:HOH:O	2.63	0.40
1:B:327:GLN:N	1:B:328:PRO:CD	2.84	0.40
2:A:120:GLY:HA2	2:A:255:VAL:O	2.21	0.40
1:B:79:GLN:HB3	1:B:83:ARG:NH1	2.36	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	295/387 (76%)	283 (96%)	12 (4%)	0	100	100
2	A	316/361 (88%)	311 (98%)	5 (2%)	0	100	100
All	All	611/748 (82%)	594 (97%)	17 (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	B	273/345 (79%)	270 (99%)	3 (1%)	65	75
2	A	296/332 (89%)	296 (100%)	0	100	100
All	All	569/677 (84%)	566 (100%)	3 (0%)	81	87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	337	SER
1	B	433	TYR
1	B	442	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	181	ASN
2	A	112	GLN
2	A	354	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	B	302/387 (78%)	0.38	27 (8%) 15 14	18, 62, 149, 204	3 (0%)
2	A	319/361 (88%)	0.34	23 (7%) 21 20	22, 64, 145, 217	1 (0%)
All	All	621/748 (83%)	0.36	50 (8%) 18 16	18, 63, 149, 217	4 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	325	VAL	7.0
2	A	204	PRO	5.2
1	B	329	ALA	4.8
2	A	172	THR	4.6
1	B	256	PRO	4.6
1	B	290	SER	3.6
2	A	42	SER	3.6
1	B	135	ALA	3.6
2	A	167	TYR	3.5
2	A	174	LEU	3.5
2	A	203	ASP	3.5
2	A	177	SER	3.4
1	B	128	ALA	3.4
2	A	180	LEU	3.3
1	B	73	ALA	3.3
2	A	272	PRO	3.2
1	B	112	LEU	3.0
1	B	442	LEU	3.0
1	B	326	PRO	3.0
1	B	324	MET	2.9
1	B	102	CYS	2.9
1	B	111	LYS	2.9
1	B	277	LYS	2.9
1	B	254	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	328	PRO	2.8
1	B	104	ALA	2.7
1	B	330	ASN	2.7
2	A	175	LEU	2.7
1	B	165	ASP	2.6
2	A	179	SER	2.6
1	B	310	ASN	2.5
2	A	91	SER	2.5
2	A	202	ILE	2.4
1	B	108	LYS	2.4
2	A	205	LYS	2.4
2	A	171	SER	2.4
2	A	270	GLU	2.4
1	B	211	SER	2.3
1	B	107	ARG	2.3
1	B	109	LEU	2.2
1	B	210	SER	2.2
2	A	182	PRO	2.2
1	B	323	HIS	2.1
2	A	223	THR	2.1
2	A	128	ASP	2.1
1	B	238	ARG	2.1
2	A	361	GLN	2.0
2	A	76	LYS	2.0
2	A	362	TRP	2.0
2	A	274	GLU	2.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.