



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:43 AM UTC

PDB ID : 7JFM / pdb_00007jfm
Title : Crystal structure of mouse phosphorylated IRF-3 bound to CBP
Authors : Li, P.; Jing, T.; Zhao, B.
Deposited on : 2020-07-17
Resolution : 2.23 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
Mogul : 2022.3.0, CSD as543be (2022)
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

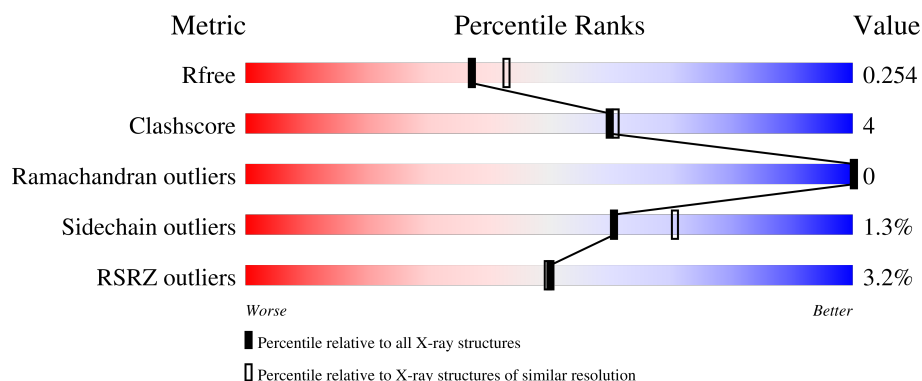
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	A	210	84% 10% 6%
1	B	210	4% 80% 12% 8%
2	C	47	70% 13% 17%
2	D	47	11% 64% 13% • 21%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3715 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 Interferon regulatory factor 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	P	S	0	0	0
			1565	1007	264	283	1	10			
1	B	194	Total	C	N	O	P	S	0	0	0
			1528	979	260	278	1	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	SER	-	expression tag	UNP P70671
A	182	GLU	-	expression tag	UNP P70671
A	183	PHE	-	expression tag	UNP P70671
B	181	SER	-	expression tag	UNP P70671
B	182	GLU	-	expression tag	UNP P70671
B	183	PHE	-	expression tag	UNP P70671

- Molecule 2 is a protein called CREB-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	39	Total	C	N	O	S	0	0	0
			310	195	58	56	1			
2	D	37	Total	C	N	O	S	0	0	0
			298	188	56	53	1			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	4	Total	O	0	0
			4	4		

i

- Molecule 1: Interferon regulatory factor 3



-
- The diagram illustrates a protein structure with various residues highlighted in yellow and red. The residues are labeled with their three-letter codes and positions. The structure is a long, thin, and somewhat irregular shape, possibly representing a protein backbone or a specific domain. The residues are distributed along the length of the structure, with some clusters and some gaps. The labels are in a small, black, sans-serif font. The background is white.
- Residues shown (from left to right):
- M341
 - G376
 - S379
 - T382
 - I387
 - S388
 - N389
 - S390
 - SER
 - GLU
 - PHE
 - GLU
 - ASN
 - PRO
 - LEU
 - LYS
 - GLN
 - LEU
 - LEU
 - ALA
 - GLU
 - Q195
 - L214
 - R217
 - R221
 - L222
 - V223
 - G224
 - S225
 - T226
 - A227
 - T230
 - L231
 - PRO
 - TRP
 - Q234
 - P235
 - K248
 - Y253
 - L265
 - L274
 - A275
 - A276
 - E291
 - H305
 - K308
 - D309
 - G310
 - F313
 - D321
 - P333
 - R334
 - Y335

- | | | | | | | | | | | | | | | | |
|-----|-------|-------|-------|-------|-------|-------|-------|-------|-----|-----|-----|-----|-----|-----|-----|
| SER | A2066 | L2067 | Q2068 | D2069 | L2070 | L2096 | F2100 | R2104 | THR | ALA | LYS | TYR | VAL | ALA | ASN |
|-----|-------|-------|-------|-------|-------|-------|-------|-------|-----|-----|-----|-----|-----|-----|-----|

-

4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	118.80Å 118.80Å 72.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	51.44 – 2.23 51.44 – 2.23	Depositor EDS
% Data completeness (in resolution range)	99.9 (51.44-2.23) 99.9 (51.44-2.23)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.17_3644	Depositor
R, R_{free}	0.231 , 0.252 0.235 , 0.254	Depositor DCC
R_{free} test set	1408 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	67.0	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.165 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3715	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.69% 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

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

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	0.09	0/1599	0.26	0/2170
1	B	0.08	0/1558	0.24	0/2109
2	C	0.08	0/313	0.23	0/421
2	D	0.08	0/299	0.25	0/400
All	All	0.08	0/3769	0.25	0/5100

There are no bond length outliers.

There are no bond angle outliers.

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	1565	0	1526	13	0
1	B	1528	0	1491	15	0
2	C	310	0	333	4	0
2	D	298	0	322	6	0
3	A	10	0	0	0	0
3	B	4	0	0	0	0
All	All	3715	0	3672	32	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 4.

All (32) 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:242:GLU:HA	1:A:251:LYS:HD2	1.69	0.73
2:D:2070:LEU:HD21	2:D:2100:PHE:HB3	1.77	0.66
1:B:221:ARG:NH1	1:B:230:THR:O	2.30	0.65
1:A:221:ARG:NH2	1:A:263:ASN:O	2.28	0.64
1:A:274:LEU:HB2	1:A:313:PHE:HB3	1.79	0.62
1:A:246:THR:HG21	2:D:2072:ARG:HH22	1.63	0.61
1:B:221:ARG:HH12	1:B:230:THR:H	1.49	0.61
1:B:274:LEU:HB2	1:B:313:PHE:HB3	1.84	0.59
1:A:282:SER:HA	1:B:387:ILE:HG22	1.88	0.56
1:B:195:GLN:O	2:D:2085:GLN:NE2	2.38	0.56
1:B:265:LEU:HD22	1:B:341:MET:HE1	1.88	0.55
1:A:330:GLY:HA3	1:A:381:LYS:HD3	1.90	0.53
1:B:305:HIS:ND1	1:B:309:ASP:O	2.42	0.52
2:D:2072:ARG:HD3	2:D:2074:LEU:HD13	1.91	0.52
2:C:2066:ALA:O	2:C:2068:GLN:N	2.42	0.51
1:A:229:MET:HE1	1:A:234:GLN:HG3	1.93	0.50
1:A:246:THR:HG21	2:D:2072:ARG:NH2	2.26	0.49
1:A:222:LEU:HD23	1:A:236:VAL:HB	1.95	0.48
1:A:319:VAL:HG13	2:C:2096:LEU:HB2	1.94	0.47
1:A:204:TYR:HB3	1:A:245:LEU:HD11	1.98	0.46
1:B:222:LEU:HD12	1:B:265:LEU:HD23	1.99	0.45
1:B:291:GLU:OE2	1:B:335:TYR:OH	2.29	0.45
1:B:321:ASP:HB2	1:B:333:PRO:HB3	2.01	0.42
1:B:234:GLN:HA	1:B:235:PRO:HD3	1.84	0.42
1:A:316:ARG:HB2	1:A:317:PRO:HD3	2.02	0.42
2:C:2070:LEU:HD21	2:C:2104:ARG:HD2	2.02	0.42
1:A:383:VAL:HG11	1:B:253:TYR:CZ	2.54	0.42
1:B:276:ALA:H	1:B:310:GLY:HA3	1.86	0.41
2:C:2070:LEU:HD22	2:C:2100:PHE:HB3	2.03	0.41
2:D:2081:GLN:CD	2:D:2081:GLN:H	2.29	0.41
1:B:214:LEU:HD13	1:B:214:LEU:HA	1.97	0.41
1:B:308:LYS:HG3	1:B:309:ASP:OD1	2.21	0.41

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	195/210 (93%)	188 (96%)	7 (4%)	0	100	100
1	B	189/210 (90%)	179 (95%)	10 (5%)	0	100	100
2	C	37/47 (79%)	36 (97%)	1 (3%)	0	100	100
2	D	33/47 (70%)	31 (94%)	2 (6%)	0	100	100
All	All	454/514 (88%)	434 (96%)	20 (4%)	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	163/175 (93%)	162 (99%)	1 (1%)	78	83
1	B	160/175 (91%)	158 (99%)	2 (1%)	61	71
2	C	36/42 (86%)	36 (100%)	0	100	100
2	D	34/42 (81%)	32 (94%)	2 (6%)	18	16
All	All	393/434 (91%)	388 (99%)	5 (1%)	61	71

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

Mol	Chain	Res	Type
1	A	274	LEU
1	B	248	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	382	THR
2	D	2067	LEU
2	D	2074	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	349	GLN
1	B	195	GLN
1	B	212	GLN
2	D	2103	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	SEP	B	379	1	8,9,10	1.61	1 (12%)	7,12,14	1.33	1 (14%)
1	SEP	A	379	1	8,9,10	1.62	1 (12%)	7,12,14	1.27	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	B	379	1	-	0/6/8/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	379	1	-	0/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	379	SEP	P-O1P	3.54	1.61	1.50
1	B	379	SEP	P-O1P	3.51	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	379	SEP	OG-CB-CA	2.90	110.97	108.14
1	A	379	SEP	OG-CB-CA	2.70	110.77	108.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	A	197/210 (93%)	-0.57	2 (1%) 79 81	50, 76, 109, 133	0
1	B	193/210 (91%)	-0.01	8 (4%) 41 41	59, 91, 139, 180	0
2	C	39/47 (82%)	-0.28	0 100 100	80, 97, 120, 142	0
2	D	37/47 (78%)	1.17	5 (13%) 7 6	115, 136, 170, 179	0
All	All	466/514 (90%)	-0.18	15 (3%) 50 50	50, 86, 142, 180	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	227	ALA	4.0
2	D	2098	ALA	3.8
1	B	226	THR	3.0
1	B	224	GLY	2.9
1	B	388	SER	2.7
1	B	376	GLY	2.7
1	A	191	LEU	2.4
1	B	217	PRO	2.4
2	D	2087	LEU	2.3
2	D	2099	ALA	2.2
1	B	390	SER	2.2
2	D	2071	LEU	2.1
1	A	192	ALA	2.1
1	B	231	LEU	2.1
2	D	2101	ILE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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($\text{\AA}^2$)	Q<0.9
1	SEP	B	379	10/11	0.98	0.06	65,77,82,84	0
1	SEP	A	379	10/11	0.99	0.04	69,72,79,80	0

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.