



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:36 PM GMT

PDB ID : 1L3A
Title : Structure of the plant transcriptional regulator PBF-2
Authors : Desveaux, D.; Allard, J.; Brisson, N.; Sygusch, J.
Deposited on : 2002-02-26
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

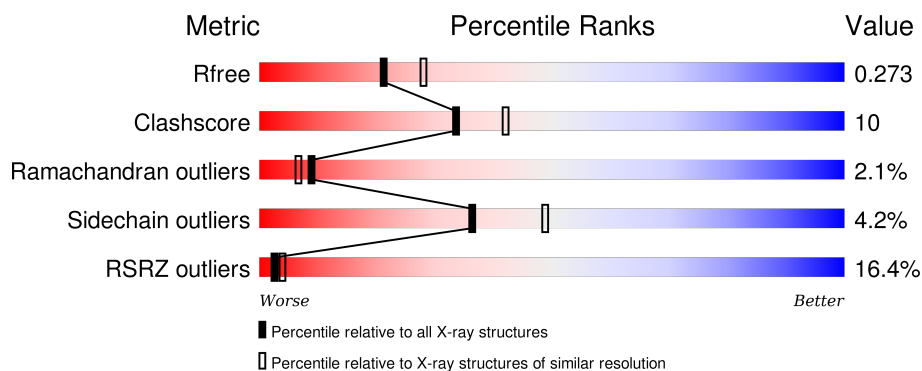
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 $\leq 5\%$. 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	227	<div> <div>14%</div> <div>55%</div> <div>17%</div> <div>27%</div> </div>
1	B	227	<div> <div>11%</div> <div>58%</div> <div>15%</div> <div>25%</div> </div>
1	C	227	<div> <div>16%</div> <div>59%</div> <div>19%</div> <div>20%</div> </div>
1	D	227	<div> <div>8%</div> <div>59%</div> <div>15%</div> <div>25%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5912 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 p24: plant transcriptional regulator PBF-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	0	0
			1307	847	218	238	4			
1	B	170	Total	C	N	O	S	0	0	0
			1338	866	222	246	4			
1	C	182	Total	C	N	O	S	0	0	0
			1448	933	248	263	4			
1	D	171	Total	C	N	O	S	0	0	0
			1342	868	223	247	4			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	MET	-	CLONING ARTIFACT	UNP Q9LL85
A	56	ALA	-	CLONING ARTIFACT	UNP Q9LL85
A	57	SER	-	CLONING ARTIFACT	UNP Q9LL85
A	58	MET	-	CLONING ARTIFACT	UNP Q9LL85
A	59	THR	-	CLONING ARTIFACT	UNP Q9LL85
A	60	GLY	-	CLONING ARTIFACT	UNP Q9LL85
A	61	GLY	-	CLONING ARTIFACT	UNP Q9LL85
A	62	GLN	-	CLONING ARTIFACT	UNP Q9LL85
A	63	GLN	-	CLONING ARTIFACT	UNP Q9LL85
A	64	MET	-	CLONING ARTIFACT	UNP Q9LL85
A	65	GLY	-	CLONING ARTIFACT	UNP Q9LL85
A	66	ARG	-	CLONING ARTIFACT	UNP Q9LL85
A	67	GLY	-	CLONING ARTIFACT	UNP Q9LL85
A	166	THR	-	ENGINEERED	UNP Q9LL85
A	274	LEU	-	CLONING ARTIFACT	UNP Q9LL85
A	275	GLU	-	CLONING ARTIFACT	UNP Q9LL85
A	276	HIS	-	EXPRESSION TAG	UNP Q9LL85
A	277	HIS	-	EXPRESSION TAG	UNP Q9LL85
A	278	HIS	-	EXPRESSION TAG	UNP Q9LL85
A	279	HIS	-	EXPRESSION TAG	UNP Q9LL85
A	280	HIS	-	EXPRESSION TAG	UNP Q9LL85

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Chain	Residue	Modelled	Actual	Comment	Reference
A	281	HIS	-	EXPRESSION TAG	UNP Q9LL85
B	55	MET	-	CLONING ARTIFACT	UNP Q9LL85
B	56	ALA	-	CLONING ARTIFACT	UNP Q9LL85
B	57	SER	-	CLONING ARTIFACT	UNP Q9LL85
B	58	MET	-	CLONING ARTIFACT	UNP Q9LL85
B	59	THR	-	CLONING ARTIFACT	UNP Q9LL85
B	60	GLY	-	CLONING ARTIFACT	UNP Q9LL85
B	61	GLY	-	CLONING ARTIFACT	UNP Q9LL85
B	62	GLN	-	CLONING ARTIFACT	UNP Q9LL85
B	63	GLN	-	CLONING ARTIFACT	UNP Q9LL85
B	64	MET	-	CLONING ARTIFACT	UNP Q9LL85
B	65	GLY	-	CLONING ARTIFACT	UNP Q9LL85
B	66	ARG	-	CLONING ARTIFACT	UNP Q9LL85
B	67	GLY	-	CLONING ARTIFACT	UNP Q9LL85
B	166	THR	-	ENGINEERED	UNP Q9LL85
B	274	LEU	-	CLONING ARTIFACT	UNP Q9LL85
B	275	GLU	-	CLONING ARTIFACT	UNP Q9LL85
B	276	HIS	-	EXPRESSION TAG	UNP Q9LL85
B	277	HIS	-	EXPRESSION TAG	UNP Q9LL85
B	278	HIS	-	EXPRESSION TAG	UNP Q9LL85
B	279	HIS	-	EXPRESSION TAG	UNP Q9LL85
B	280	HIS	-	EXPRESSION TAG	UNP Q9LL85
B	281	HIS	-	EXPRESSION TAG	UNP Q9LL85
C	55	MET	-	CLONING ARTIFACT	UNP Q9LL85
C	56	ALA	-	CLONING ARTIFACT	UNP Q9LL85
C	57	SER	-	CLONING ARTIFACT	UNP Q9LL85
C	58	MET	-	CLONING ARTIFACT	UNP Q9LL85
C	59	THR	-	CLONING ARTIFACT	UNP Q9LL85
C	60	GLY	-	CLONING ARTIFACT	UNP Q9LL85
C	61	GLY	-	CLONING ARTIFACT	UNP Q9LL85
C	62	GLN	-	CLONING ARTIFACT	UNP Q9LL85
C	63	GLN	-	CLONING ARTIFACT	UNP Q9LL85
C	64	MET	-	CLONING ARTIFACT	UNP Q9LL85
C	65	GLY	-	CLONING ARTIFACT	UNP Q9LL85
C	66	ARG	-	CLONING ARTIFACT	UNP Q9LL85
C	67	GLY	-	CLONING ARTIFACT	UNP Q9LL85
C	166	THR	-	ENGINEERED	UNP Q9LL85
C	274	LEU	-	CLONING ARTIFACT	UNP Q9LL85
C	275	GLU	-	CLONING ARTIFACT	UNP Q9LL85
C	276	HIS	-	EXPRESSION TAG	UNP Q9LL85
C	277	HIS	-	EXPRESSION TAG	UNP Q9LL85
C	278	HIS	-	EXPRESSION TAG	UNP Q9LL85

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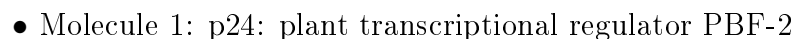
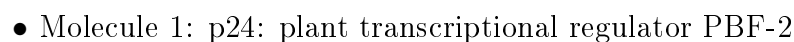
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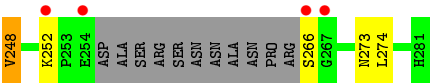
Chain	Residue	Modelled	Actual	Comment	Reference
C	279	HIS	-	EXPRESSION TAG	UNP Q9LL85
C	280	HIS	-	EXPRESSION TAG	UNP Q9LL85
C	281	HIS	-	EXPRESSION TAG	UNP Q9LL85
D	55	MET	-	CLONING ARTIFACT	UNP Q9LL85
D	56	ALA	-	CLONING ARTIFACT	UNP Q9LL85
D	57	SER	-	CLONING ARTIFACT	UNP Q9LL85
D	58	MET	-	CLONING ARTIFACT	UNP Q9LL85
D	59	THR	-	CLONING ARTIFACT	UNP Q9LL85
D	60	GLY	-	CLONING ARTIFACT	UNP Q9LL85
D	61	GLY	-	CLONING ARTIFACT	UNP Q9LL85
D	62	GLN	-	CLONING ARTIFACT	UNP Q9LL85
D	63	GLN	-	CLONING ARTIFACT	UNP Q9LL85
D	64	MET	-	CLONING ARTIFACT	UNP Q9LL85
D	65	GLY	-	CLONING ARTIFACT	UNP Q9LL85
D	66	ARG	-	CLONING ARTIFACT	UNP Q9LL85
D	67	GLY	-	CLONING ARTIFACT	UNP Q9LL85
D	166	THR	-	ENGINEERED	UNP Q9LL85
D	274	LEU	-	CLONING ARTIFACT	UNP Q9LL85
D	275	GLU	-	CLONING ARTIFACT	UNP Q9LL85
D	276	HIS	-	EXPRESSION TAG	UNP Q9LL85
D	277	HIS	-	EXPRESSION TAG	UNP Q9LL85
D	278	HIS	-	EXPRESSION TAG	UNP Q9LL85
D	279	HIS	-	EXPRESSION TAG	UNP Q9LL85
D	280	HIS	-	EXPRESSION TAG	UNP Q9LL85
D	281	HIS	-	EXPRESSION TAG	UNP Q9LL85

- Molecule 2 is water.

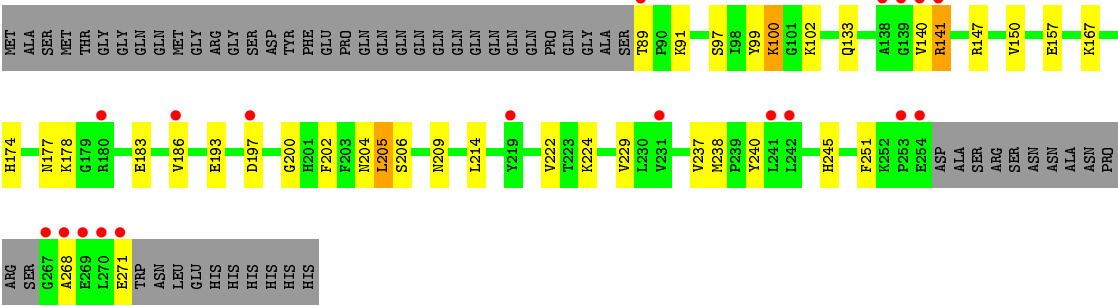
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	105	Total O 105 105	0	0
2	B	94	Total O 94 94	0	0
2	C	150	Total O 150 150	0	0
2	D	128	Total O 128 128	0	0

- Molecule 1: p24: plant transcriptional regulator PBF-2





● Molecule 1: p24: plant transcriptional regulator PBF-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.87Å 89.81Å 144.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.42 – 2.30 42.42 – 2.30	Depositor EDS
% Data completeness (in resolution range)	85.9 (42.42-2.30) 89.8 (42.42-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.72 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.216 , 0.267 0.222 , 0.273	Depositor DCC
R_{free} test set	3723 reflections (10.09%)	DCC
Wilson B-factor (Å ²)	47.7	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 40452 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5912	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.41	0/1342	0.56	0/1817
1	B	0.42	0/1372	0.57	0/1856
1	C	0.42	0/1490	0.57	0/2016
1	D	0.44	0/1376	0.60	0/1861
All	All	0.42	0/5580	0.58	0/7550

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 [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	A	1307	0	1303	28	0
1	B	1338	0	1330	33	0
1	C	1448	0	1413	36	0
1	D	1342	0	1333	24	0
2	A	105	0	0	5	0
2	B	94	0	0	4	0
2	C	150	0	0	3	0
2	D	128	0	0	5	0
All	All	5912	0	5379	110	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.

The worst 5 of 110 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:238:MET:HE1	1:D:229:VAL:HG22	1.48	0.94
1:A:185:ARG:HD3	1:A:210:LYS:HB3	1.53	0.87
1:A:133:GLN:HG2	1:A:150:VAL:HG12	1.60	0.83
1:B:180:ARG:HB3	1:B:180:ARG:HH11	1.42	0.81
1:C:180:ARG:HG2	1:C:181:SER:H	1.46	0.80

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	164/227 (72%)	148 (90%)	12 (7%)	4 (2%)	7	5
1	B	166/227 (73%)	151 (91%)	13 (8%)	2 (1%)	16	16
1	C	178/227 (78%)	163 (92%)	9 (5%)	6 (3%)	5	2
1	D	167/227 (74%)	155 (93%)	10 (6%)	2 (1%)	16	16
All	All	675/908 (74%)	617 (91%)	44 (6%)	14 (2%)	9	7

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	213	ASN
1	A	118	ASP
1	A	138	ALA
1	B	90	PRO
1	B	181	SER

5.3.2 Protein sidechains ⓘ

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	144/194 (74%)	138 (96%)	6 (4%)	36	49
1	B	147/194 (76%)	140 (95%)	7 (5%)	31	42
1	C	158/194 (81%)	155 (98%)	3 (2%)	65	81
1	D	147/194 (76%)	138 (94%)	9 (6%)	23	30
All	All	596/776 (77%)	571 (96%)	25 (4%)	36	49

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	209	ASN
1	C	209	ASN
1	D	222	VAL
1	B	271	GLU
1	C	248	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	245	HIS
1	D	133	GLN
1	D	208	GLN
1	C	174	HIS
1	D	217	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no carbohydrates 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 [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	A	166/227 (73%)	1.21	32 (19%) 2 2	32, 53, 101, 127	0
1	B	170/227 (74%)	0.91	26 (15%) 3 5	33, 52, 83, 95	4 (2%)
1	C	182/227 (80%)	1.18	36 (19%) 1 2	30, 48, 97, 124	0
1	D	171/227 (75%)	0.98	19 (11%) 7 11	29, 47, 85, 92	5 (2%)
All	All	689/908 (75%)	1.07	113 (16%) 2 4	29, 51, 93, 127	9 (1%)

The worst 5 of 113 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	181	SER	17.1
1	D	270	LEU	14.0
1	D	267	GLY	12.3
1	B	268	ALA	11.7
1	C	181	SER	11.3

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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.