



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 07:23 pm GMT

PDB ID : 4WZS
Title : Crystal structure of the Mot1 N-terminal domain in complex with TBP and NC2 bound to a promoter DNA fragment
Authors : Butryn, A.; Hopfner, K.-P.
Deposited on : 2014-11-20
Resolution : 3.78 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

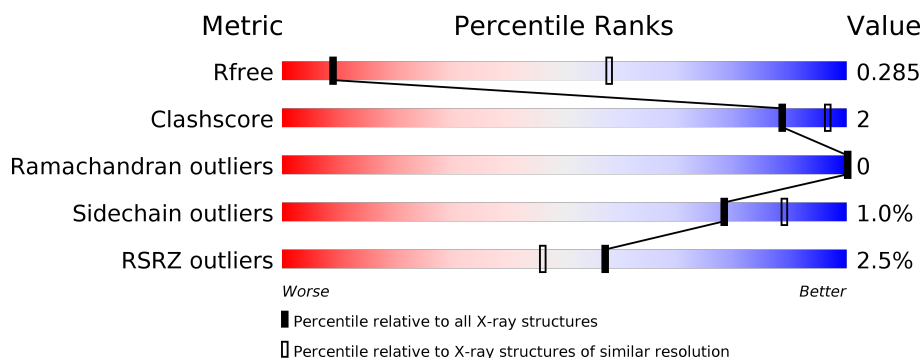
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.78 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}	111664	1061 (4.00-3.56)
Clashscore	122126	1132 (4.00-3.56)
Ramachandran outliers	120053	1094 (4.00-3.56)
Sidechain outliers	120020	1088 (4.00-3.56)
RSRZ outliers	108989	1015 (4.02-3.54)

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	95	<div> <div>5%</div> <div> <div></div> <div>68%</div> <div>31%</div> </div> </div>
2	B	149	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>24%</div> </div> </div>
3	C	780	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>6%</div> <div>7%</div> </div> </div>
4	D	200	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>12%</div> <div>11%</div> </div> </div>
5	E	24	<div> <div></div> <div> <div></div> <div>63%</div> <div>21%</div> <div>17%</div> </div> </div>
6	F	24	<div> <div></div> <div> <div></div> <div>79%</div> <div>21%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9037 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 ECU11_1470 protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	66	Total	C	N	O	0	0	0
			327	195	66	66			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP Q8SQT6

- Molecule 2 is a protein called TATA-binding protein-associated phosphoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	113	Total	C	N	O	Se	0	0	0
			657	401	125	130	1			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP M1K2J7
B	0	HIS	-	expression tag	UNP M1K2J7
B	1	MSE	-	expression tag	UNP M1K2J7

- Molecule 3 is a protein called Similarity to HELICASE MOT1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	722	Total	C	N	O	S	Se	0	0	0
			5845	3774	940	1108	9	14			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP Q8SVZ5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP Q8SVZ5
C	1	MSE	-	expression tag	UNP Q8SVZ5

- Molecule 4 is a protein called ECU04_1440 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
4	D	178	Total	C	N	O	S	Se	0	0	0
			1409	911	247	244	3	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP Q8ST28
D	0	HIS	-	expression tag	UNP Q8ST28
D	1	MSE	-	expression tag	UNP Q8ST28

- Molecule 5 is a DNA chain called DNA (5'-D(P*CP*CP*AP*CP*CP*CP*CP*TP*TP*TP*TP*AP*TP*AP*GP*CP*CP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	20	Total	C	N	O	P	0	0	0
			395	190	62	123	20			

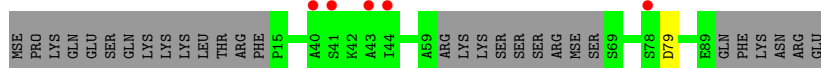
- Molecule 6 is a DNA chain called DNA (5'-D(P*GP*GP*GP*CP*TP*AP*TP*AP*AP*AP*AP*GP*GP*GP*GP*GP*GP*TP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	19	Total	C	N	O	P	0	0	0
			404	189	84	112	19			

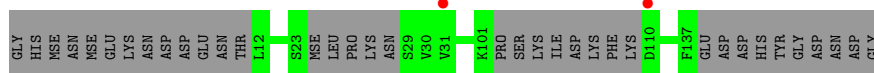
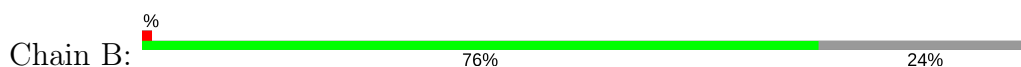
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

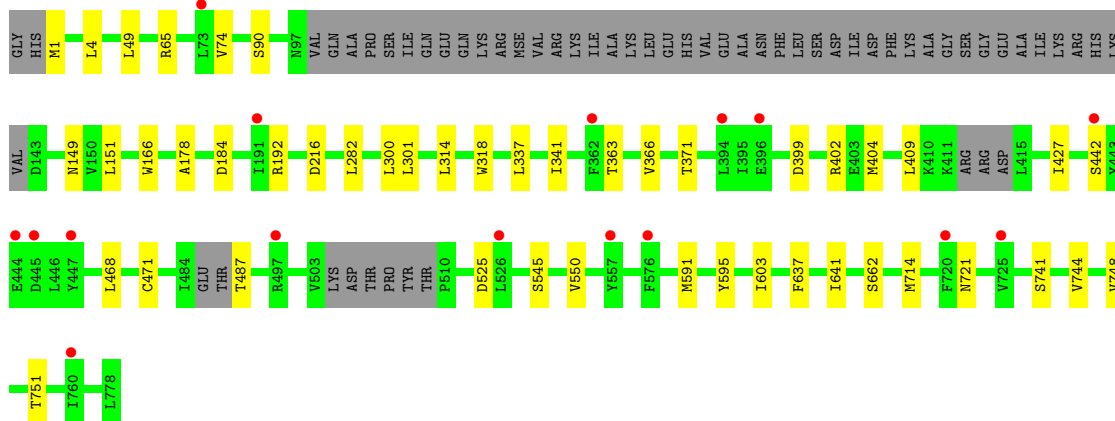
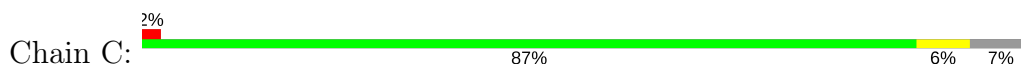
- Molecule 1: ECU11_1470 protein



- Molecule 2: TATA-binding protein-associated phosphoprotein

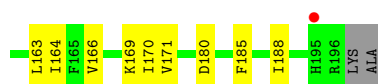


- Molecule 3: Similarity to HELICASE MOT1



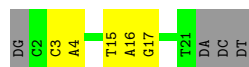
- Molecule 4: ECU04_1440 protein





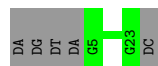
- Molecule 5: DNA (5'-D(P*CP*CP*AP*CP*CP*CP*CP*TP*TP*TP*TP*AP*TP*AP*GP*CP*CP*CP*T)-3')

Chain E: 63% 21% 17%



- Molecule 6: DNA (5'-D(P*GP*GP*GP*CP*TP*AP*TP*AP*AP*AP*AP*GP*GP*GP*GP*GP*TP*GP*G)-3')

Chain F: 79% 21%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	150.63Å 140.27Å 90.78Å 90.00° 113.70° 90.00°	Depositor
Resolution (Å)	49.17 – 3.78 49.17 – 3.78	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.17-3.78) 98.7 (49.17-3.78)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.77Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.235 , 0.258 0.251 , 0.285	Depositor DCC
R_{free} test set	861 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	152.2	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 72.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9037	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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 [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	0.40	0/322	0.41	0/441
2	B	0.40	0/654	0.39	0/888
3	C	0.43	0/5943	0.46	0/7989
4	D	0.41	0/1431	0.46	0/1923
5	E	1.14	0/438	0.92	0/670
6	F	0.96	0/456	0.80	0/705
All	All	0.52	0/9244	0.52	0/12616

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
1	A	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
1	A	79	ASP	Mainchain

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	327	0	149	0	0
2	B	657	0	408	0	0
3	C	5845	0	5902	20	2
4	D	1409	0	1482	14	0
5	E	395	0	227	3	1
6	F	404	0	213	0	0
All	All	9037	0	8381	36	2

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 2.

All (36) 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)
3:C:545:SER:HB2	3:C:550:VAL:HG21	1.64	0.78
4:D:160:ILE:HD11	4:D:180:ASP:HB3	1.87	0.56
3:C:65:ARG:HB3	3:C:178:ALA:HB1	1.87	0.55
3:C:314:LEU:HD23	3:C:318:TRP:HE1	1.73	0.54
3:C:74:VAL:HG21	3:C:192:ARG:HG3	1.89	0.54
4:D:151:LEU:HD11	4:D:164:ILE:HD12	1.89	0.54
4:D:137:HIS:HB3	4:D:140:TYR:HB2	1.89	0.53
3:C:399:ASP:HA	3:C:402:ARG:HG2	1.91	0.53
4:D:143:TYR:HB2	4:D:151:LEU:HB3	1.89	0.53
4:D:164:ILE:HA	4:D:170:ILE:HG22	1.91	0.52
4:D:29:VAL:HG22	4:D:82:THR:HG23	1.91	0.52
3:C:721:ASN:HB3	3:C:748:VAL:HG13	1.92	0.51
4:D:185:PHE:HA	4:D:188:ILE:HG22	1.93	0.51
3:C:314:LEU:HD11	3:C:341:ILE:HG21	1.94	0.50
3:C:282:LEU:HD21	3:C:300:LEU:HD23	1.95	0.48
3:C:363:THR:HB	3:C:442:SER:HB2	1.96	0.48
4:D:99:LYS:HE3	4:D:103:LYS:HE3	1.95	0.47
4:D:163:LEU:HB2	4:D:171:VAL:HG23	1.97	0.47
5:E:16:DA:H2"	5:E:17:DG:C8	2.50	0.47
3:C:427:ILE:HD11	3:C:468:LEU:HD23	1.97	0.47
4:D:25:LEU:HA	4:D:120:SER:HA	1.96	0.46
3:C:301:LEU:HD23	3:C:337:LEU:HD21	1.98	0.46
4:D:130:LEU:HD13	4:D:166:VAL:HG22	1.98	0.46
3:C:371:THR:HG23	3:C:404:MSE:HE1	1.97	0.46
4:D:73:ILE:HG12	4:D:79:MSE:HE2	1.99	0.45
3:C:591:MSE:O	3:C:595:TYR:HD2	2.00	0.45
3:C:714:MSE:HE1	3:C:751:THR:HG21	2.00	0.43
3:C:409:LEU:HB3	3:C:471:CYS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:169:LYS:HD3	5:E:15:DT:H5''	2.02	0.42
3:C:1:MSE:HA	3:C:4:LEU:HD23	2.02	0.41
3:C:487:THR:HG21	3:C:525:ASP:HB2	2.02	0.41
3:C:90:SER:HA	3:C:166:TRP:HB3	2.01	0.41
4:D:23:PRO:HB3	4:D:122:CYS:HB2	2.01	0.41
5:E:3:DC:H2''	5:E:4:DA:H8	1.86	0.41
3:C:741:SER:HA	3:C:744:VAL:HG12	2.03	0.41
3:C:637:PHE:CE2	3:C:641:ILE:HD11	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:149:ASN:ND2	3:C:151:LEU:CD1[2_13510]	1.63	0.57
3:C:662:SER:CB	5:E:4:DA:OP1[4_13411]	2.04	0.16

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	62/95 (65%)	61 (98%)	1 (2%)	0	100	100
2	B	107/149 (72%)	105 (98%)	2 (2%)	0	100	100
3	C	712/780 (91%)	689 (97%)	23 (3%)	0	100	100
4	D	176/200 (88%)	168 (96%)	8 (4%)	0	100	100
All	All	1057/1224 (86%)	1023 (97%)	34 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	
2	B	26/131 (20%)	26 (100%)	0	100	100
3	C	663/698 (95%)	658 (99%)	5 (1%)	83	92
4	D	153/167 (92%)	150 (98%)	3 (2%)	58	81
All	All	842/996 (84%)	834 (99%)	8 (1%)	78	89

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	49	LEU
3	C	184	ASP
3	C	216	ASP
3	C	366	VAL
3	C	603	ILE
4	D	25	LEU
4	D	45	LEU
4	D	82	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	693	ASN
4	D	137	HIS

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

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	63/95 (66%)	0.35	5 (7%) 12 10	75, 108, 138, 199	0
2	B	109/149 (73%)	0.04	2 (1%) 68 59	64, 103, 132, 222	0
3	C	708/780 (90%)	0.13	16 (2%) 60 50	3, 63, 117, 203	0
4	D	174/200 (87%)	0.30	4 (2%) 60 50	21, 65, 105, 122	0
5	E	20/24 (83%)	-0.17	0 100 100	94, 124, 222, 255	0
6	F	19/24 (79%)	-0.40	0 100 100	98, 120, 210, 220	0
All	All	1093/1272 (85%)	0.15	27 (2%) 57 46	3, 70, 127, 255	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	447	TYR	5.4
2	B	110	ASP	4.7
3	C	362	PHE	4.0
3	C	396	GLU	3.5
3	C	576	PHE	3.1
1	A	78	SER	3.1
1	A	41	SER	2.9
1	A	40	ALA	2.7
3	C	725	VAL	2.7
4	D	153	TYR	2.7
3	C	760	ILE	2.6
4	D	90	SER	2.6
3	C	73	LEU	2.5
1	A	43	ALA	2.4
3	C	444	GLU	2.4
3	C	442	SER	2.3
3	C	191	ILE	2.2
3	C	394	LEU	2.2
1	A	44	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	31	VAL	2.2
3	C	557	TYR	2.1
4	D	195	HIS	2.1
4	D	81	ILE	2.1
3	C	497	ARG	2.1
3	C	526	LEU	2.1
3	C	445	ASP	2.0
3	C	720	PHE	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 carbohydrates 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.