



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 19, 2022 – 05:31 AM JST

PDB ID : 7FDM
Title : Crystal structure of transcription factor MYB29 in complex with MYC3
Authors : Luo, Q.; Wang, B.
Deposited on : 2021-07-17
Resolution : 2.50 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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.29
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)	:	2.29

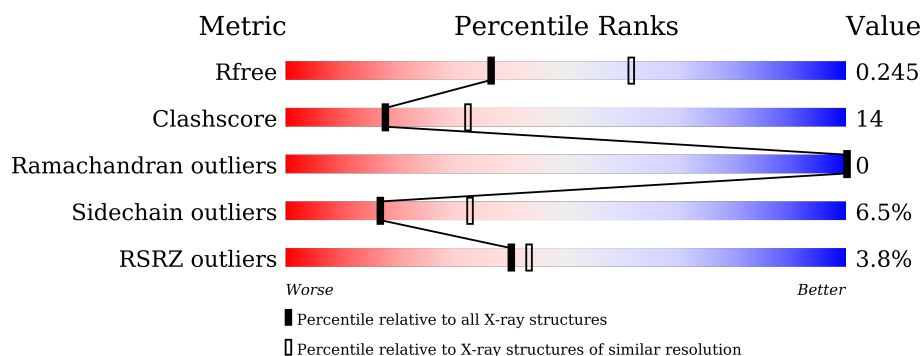
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	195	<div> <div>3%</div> <div>60%</div> <div>26%</div> <div>•</div> <div>13%</div> </div>
1	B	195	<div> <div>4%</div> <div>58%</div> <div>25%</div> <div>•</div> <div>14%</div> </div>
2	C	49	<div> <div>33%</div> <div>8%</div> <div>59%</div> </div>
2	D	49	<div> <div>18%</div> <div>12%</div> <div>69%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2870 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 Transcription factor MYC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	170	Total	C	N	O	S	0	0	0
			1321	829	224	263	5			
1	B	167	Total	C	N	O	S	0	0	0
			1290	811	220	254	5			

- Molecule 2 is a protein called Transcription factor MYB29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	20	Total	C	N	O	S	0	0	0
			139	84	26	28	1			
2	D	15	Total	C	N	O		0	0	0
			106	64	21	21				

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		
3	B	8	Total	O	0	0
			8	8		

- Molecule 1: Transcription factor MYC3



Chain D: 18% 12% 69%

SER	SER	LYS	ARG	CYS	PHE	LYS	ARG	SER	S184	S185	T186	S187	K188	L189	L190	A195	S198	SER	MET	GLY	THR	ILE	LEU	GLY	ALA	SER	ILE	GLU	GLY	THR	LEU	ILE	SER	SER	THR	PRO	LEU	SER	SER	CYS	LEU
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4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	85.25Å 85.25Å 57.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.90 – 2.50 27.90 – 2.49	Depositor EDS
% Data completeness (in resolution range)	78.9 (27.90-2.50) 78.0 (27.90-2.49)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.232 , 0.268 0.235 , 0.245	Depositor DCC
R_{free} test set	573 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 21.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.044 for -h,-k,l 0.489 for h,-h-k,-l 0.045 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2870	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.95% 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	0.28	0/1344	0.50	0/1814
1	B	0.27	0/1312	0.52	1/1771 (0.1%)
2	C	0.22	0/138	0.44	0/183
2	D	0.25	0/105	0.54	0/139
All	All	0.27	0/2899	0.51	1/3907 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	141	ASP	N-CA-C	-5.02	97.44	111.00

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	1321	0	1241	38	0
1	B	1290	0	1217	36	0
2	C	139	0	152	3	0
2	D	106	0	117	6	0
3	A	6	0	0	0	0
3	B	8	0	0	0	0
All	All	2870	0	2727	76	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 14.

All (76) 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:142:GLU:HG3	1:B:143:GLU:H	1.43	0.84
1:A:119:LYS:HG3	1:B:160:VAL:HG11	1.72	0.72
1:B:59:LEU:HD21	1:B:231:VAL:HG22	1.73	0.70
1:B:148:GLU:HB3	2:D:190:LEU:HD11	1.74	0.69
1:A:210:ASN:HB2	1:A:236:ASN:HB2	1.74	0.69
1:B:162:GLY:HA3	1:B:171:LEU:HD12	1.74	0.68
1:A:162:GLY:HA3	1:A:171:LEU:HD12	1.77	0.66
1:A:51:THR:HG23	1:A:55:ARG:NE	2.11	0.64
1:A:55:ARG:NH1	1:A:234:LEU:O	2.29	0.64
1:B:46:GLN:HB3	1:B:236:ASN:OD1	1.98	0.63
1:B:51:THR:O	1:B:55:ARG:HG3	2.00	0.62
1:B:142:GLU:CG	1:B:143:GLU:H	2.11	0.62
2:D:185:SER:HA	2:D:188:LYS:HG3	1.82	0.60
1:A:52:LEU:HA	1:A:55:ARG:HH21	1.66	0.60
1:A:78:ASP:OD1	1:A:79:PHE:N	2.35	0.60
1:B:208:THR:HG22	1:B:210:ASN:N	2.17	0.59
2:D:187:SER:HA	2:D:190:LEU:HD12	1.85	0.59
1:B:208:THR:HG23	1:B:236:ASN:O	2.04	0.58
1:A:52:LEU:HD22	1:A:94:ASP:HB2	1.86	0.57
1:B:55:ARG:HD2	1:B:234:LEU:O	2.05	0.57
1:A:163:VAL:HG13	1:B:116:GLU:HG3	1.86	0.56
1:A:115:GLN:H	1:A:115:GLN:CD	2.09	0.56
1:A:60:ILE:HD11	1:A:70:ALA:HB2	1.88	0.56
1:A:154:SER:HA	1:A:157:GLN:HG3	1.88	0.56
1:B:208:THR:HG22	1:B:210:ASN:H	1.70	0.55
1:A:55:ARG:HB3	1:A:234:LEU:HB3	1.88	0.55
1:A:48:ASN:O	1:A:51:THR:HG22	2.07	0.55
1:B:62:SER:HB2	1:B:230:LYS:HE2	1.89	0.54
1:B:50:ASP:OD1	1:B:50:ASP:N	2.27	0.54
1:B:68:THR:HG23	1:B:217:SER:HA	1.91	0.53
1:B:128:LEU:HD13	2:D:189:LEU:HD13	1.91	0.52
2:C:184:SER:N	2:C:187:SER:HG	2.07	0.52
1:A:150:PHE:O	1:A:154:SER:OG	2.26	0.51
1:A:165:LEU:HB3	1:A:166:PRO:HD3	1.93	0.50
1:A:75:ILE:HD11	1:A:211:GLY:HA2	1.93	0.50
1:B:165:LEU:HB3	1:B:166:PRO:HD3	1.94	0.50
1:A:50:ASP:OD1	1:A:50:ASP:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:THR:N	1:A:148:GLU:OE2	2.32	0.49
1:A:51:THR:HG23	1:A:55:ARG:HE	1.75	0.49
1:A:48:ASN:H	1:A:51:THR:HG22	1.76	0.49
1:A:55:ARG:HD2	1:A:234:LEU:O	2.13	0.49
2:C:196:ARG:O	2:C:196:ARG:HG3	2.12	0.49
1:B:53:GLN:HE21	2:D:195:ALA:HB2	1.76	0.48
1:A:117:HIS:O	1:A:121:VAL:HG22	2.13	0.48
1:A:56:LEU:HD22	1:A:70:ALA:HB1	1.95	0.48
1:A:52:LEU:HA	1:A:55:ARG:NH2	2.28	0.47
1:A:190:GLU:OE1	1:B:194:GLN:NE2	2.45	0.47
1:B:75:ILE:HD11	1:B:211:GLY:HA2	1.96	0.47
1:B:57:GLN:O	1:B:61:GLU:HG2	2.15	0.47
1:A:120:ARG:HB3	1:A:144:VAL:HG11	1.95	0.47
1:B:142:GLU:CG	1:B:143:GLU:N	2.79	0.46
1:B:159:PHE:CE1	1:B:166:PRO:HG2	2.50	0.46
1:A:177:TRP:CZ3	1:A:223:GLN:HG3	2.52	0.45
1:B:88:VAL:O	1:B:89:ILE:HD13	2.16	0.45
1:A:149:TRP:HD1	1:A:198:TYR:CE2	2.35	0.45
1:B:57:GLN:HG2	1:B:96:TYR:CD1	2.51	0.45
1:A:93:GLY:O	2:C:198:SER:OG	2.34	0.45
1:A:55:ARG:NH1	1:A:235:PHE:HA	2.32	0.44
1:A:159:PHE:CE2	1:A:166:PRO:HG2	2.52	0.44
1:B:46:GLN:HG2	1:B:47:PHE:CD2	2.53	0.44
2:D:189:LEU:H	2:D:189:LEU:HD23	1.82	0.44
1:A:69:TYR:HE1	1:A:200:LEU:HD21	1.83	0.44
1:B:92:TRP:HH2	1:B:151:PHE:CE1	2.37	0.42
1:A:65:GLU:HB3	1:A:221:ILE:HD12	2.02	0.42
1:B:67:TRP:HA	1:B:217:SER:HB2	2.02	0.42
1:B:210:ASN:HB2	1:B:236:ASN:HB2	2.02	0.42
1:B:115:GLN:H	1:B:115:GLN:CD	2.24	0.42
1:B:206:ILE:HB	1:B:213:VAL:HG13	2.01	0.42
1:B:69:TYR:CD2	1:B:71:ILE:HG13	2.55	0.41
1:B:177:TRP:CZ3	1:B:223:GLN:HG3	2.55	0.41
1:B:71:ILE:HD13	1:B:92:TRP:HZ3	1.85	0.41
1:A:73:TRP:HB2	1:A:90:LEU:HD12	2.02	0.41
1:A:65:GLU:HG2	1:A:221:ILE:HG23	2.03	0.41
1:B:227:LEU:O	1:B:231:VAL:HG23	2.21	0.40
1:A:115:GLN:H	1:A:115:GLN:NE2	2.19	0.40
1:A:120:ARG:HB3	1:A:144:VAL:CG1	2.52	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	A	162/195 (83%)	160 (99%)	2 (1%)	0	100	100
1	B	159/195 (82%)	156 (98%)	3 (2%)	0	100	100
2	C	18/49 (37%)	18 (100%)	0	0	100	100
2	D	13/49 (26%)	13 (100%)	0	0	100	100
All	All	352/488 (72%)	347 (99%)	5 (1%)	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	142/167 (85%)	132 (93%)	10 (7%)	15	29
1	B	137/167 (82%)	127 (93%)	10 (7%)	14	27
2	C	16/42 (38%)	16 (100%)	0	100	100
2	D	12/42 (29%)	12 (100%)	0	100	100
All	All	307/418 (73%)	287 (94%)	20 (6%)	17	33

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	THR
1	A	53	GLN

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Mol	Chain	Res	Type
1	A	115	GLN
1	A	117	HIS
1	A	141	ASP
1	A	175	VAL
1	A	215	LEU
1	A	218	SER
1	A	222	SER
1	A	227	LEU
1	B	50	ASP
1	B	51	THR
1	B	53	GLN
1	B	78	ASP
1	B	94	ASP
1	B	114	GLU
1	B	175	VAL
1	B	218	SER
1	B	225	SER
1	B	227	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	A	209	GLN
1	A	238	ASN
1	B	66	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	170/195 (87%)	0.08	6 (3%) 44 47	12, 52, 98, 112	0
1	B	167/195 (85%)	0.14	8 (4%) 30 32	12, 50, 100, 111	0
2	C	20/49 (40%)	-0.04	0 100 100	64, 87, 109, 114	0
2	D	15/49 (30%)	-0.10	0 100 100	66, 80, 92, 94	0
All	All	372/488 (76%)	0.09	14 (3%) 40 43	12, 58, 100, 114	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	78	ASP	5.4
1	B	131	GLY	4.7
1	A	52	LEU	3.7
1	B	46	GLN	3.0
1	B	100	GLU	2.9
1	B	210	ASN	2.8
1	B	236	ASN	2.8
1	A	118	ARG	2.7
1	A	236	ASN	2.7
1	A	143	GLU	2.6
1	A	210	ASN	2.5
1	B	129	ILE	2.3
1	A	231	VAL	2.2
1	B	47	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 monosaccharides 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.