

wwPDB X-ray Structure Validation Summary Report (i)

May 26, 2020 – 09:28 pm BST

PDB ID	:	6BZ1
Title	:	MEF2 Chimera D83V mutant/DNA complex
Authors	:	Lei, X.; Chen, L.
Deposited on	:	2017-12-21
Resolution	:	2.97 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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

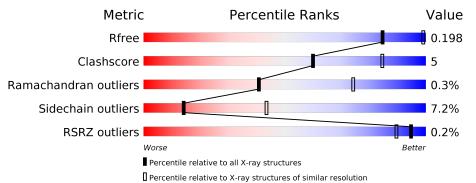
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\operatorname{CCP4}$:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.97 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
R _{free}	130704	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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 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 <=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	А	95	74%	19% • 6%
1	В	95	73%	19% • 6%
1	С	95	% 8 0%	15% 5%
1	D	95	80%	11% • 8%
2	Е	14	50% 36%	7% 7%
2	G	14	79%	21%

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Mol	Chain	Length	Quality of chain				
3	F	15	40%	47%		13%	
3	Н	15	60%	13%	13%	13%	



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4026 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	C	C 90	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	U		748	473	133	137	5	0	0	0
1	л	87	Total	С	Ν	Ο	S	0	0	0
	D	01	717	455	123	134	5	0		0
1	Δ	89	Total	С	Ν	Ο	S	0	0	0
	А	09	737	467	129	136	5	0	0	0
1	р	80	Total	С	Ν	Ο	S	0	0	0
		89	737	467	129	136	5	0	U	U

• Molecule 1 is a protein called MEF2 CHIMERA.

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	83	VAL	ASP	engineered mutation	UNP Q02080
D	83	VAL	ASP	engineered mutation	UNP Q02080
A	83	VAL	ASP	engineered mutation	UNP Q02080
В	83	VAL	ASP	engineered mutation	UNP Q02080

• Molecule 2 is a DNA chain called DNA (5'-D(P*AP*AP*CP*TP*AP*TP*TP*TP*AP*TP *AP*AP*GP*A)-3').

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
0	C	1.4	Total	С	Ν	Ο	Р	0	0	0
	G	14	288	139	53	82	14	0		
0	Е	13	Total	С	Ν	Ο	Р	0	0	0
	Ľ	15	267	129	48	77	13	0	0	0

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	Н	13	Total 266	C 129	N 45	O 79	Р 13	0	0	0

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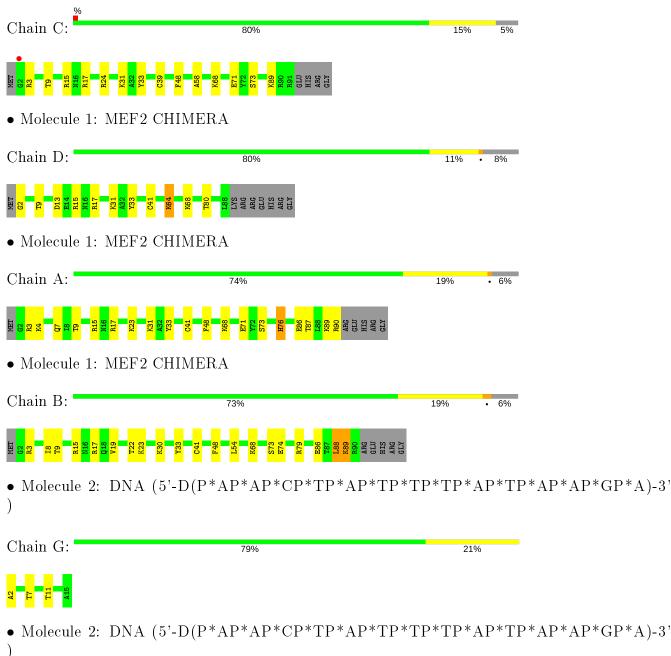
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Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
3	F	13	Total 266	C 129	N 45	O 79	Р 13	0	0	0



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: MEF2 CHIMERA



DT DT

Chain E:	50%	36%	7%	7%
DA 74 74 75 75 71 110 710 711 711 711 711 711 711 711				
• Molecule 3: DNA ((5'-D(P*TP*TP*CP*TP*TF	P*AP*TP*AP*A	AP*A	P*TP*AP*GP*TP*T)-3'
Chain H:	60%	13% 13%	13%	_
년 12 23 14 11 11 11 11				
• Molecule 3: DNA ((5'-D(P*TP*TP*CP*TP*TF	P*AP*TP*AP*A	AP*A	P*TP*AP*GP*TP*T)-3'
Chain F:	40%	47%	13%	b



4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 32	Depositor	
Cell constants	78.44Å 78.44Å 111.04Å	Deperitor	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor	
Resolution (Å)	42.99 - 2.97	Depositor	
Resolution (A)	42.99 - 2.97	EDS	
% Data completeness	99.7 (42.99-2.97)	Depositor	
(in resolution range)	99.7 (42.99 - 2.97)	EDS	
R _{merge}	(Not available)	Depositor	
$\frac{\mathrm{R}_{sym}}{< I/\sigma(I) > 1}$	(Not available)	Depositor	
$< I/\sigma(I) > 1$	$1.82 (at 2.95 \text{\AA})$	Xtriage	
Refinement program	REFMAC 5.8.0189	Depositor	
D D	0.139 , 0.190	Depositor	
R, R_{free}	0.146 , 0.198	DCC	
R _{free} test set	756 reflections (4.81%)	wwPDB-VP	
Wilson B-factor $(Å^2)$	65.0	Xtriage	
Anisotropy	0.042	Xtriage	
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33 , 30.7	EDS	
L-test for twinning ²	$< L > = 0.42, < L^2 > = 0.25$	Xtriage	
	0.447 for -h,-k,l		
Estimated twinning fraction	0.469 for h,-h-k,-l	Xtriage	
	0.447 for -k,-h,-l		
	0.281 for H, K, L		
Depented twinning freetien	0.206 for -K, -H, -L	Deperitor	
Reported twinning fraction	0.312 for -h,-k,l	Depositor	
	0.201 for K, H, -L		
Outliers	0 of 15721 reflections	Xtriage	
F_o, F_c correlation	0.96	EDS	
Total number of atoms	4026	wwPDB-VP	
Average B, all atoms $(Å^2)$	67.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.42% of the height of the origin peak. No significant pseudotranslation is detected.

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.



 $^{^1 {\}rm Intensities}$ estimated from amplitudes.

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	Boi	nd lengths	Bo	ond angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.61	0/746	0.83	1/997~(0.1%)
1	В	0.60	0/746	0.83	2/997~(0.2%)
1	С	0.58	0/757	0.82	2/1011~(0.2%)
1	D	0.58	0/726	0.80	0/972
2	Е	0.60	1/299~(0.3%)	0.95	1/459~(0.2%)
2	G	0.58	1/323~(0.3%)	0.94	1/496~(0.2%)
3	F	0.58	0/297	1.02	1/456~(0.2%)
3	Н	0.75	0/297	1.06	2/456~(0.4%)
All	All	0.60	2/4191~(0.0%)	0.88	10/5844~(0.2%)

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	А	0	1

All (2) bond length outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
2	Е	11	DA	O3'-P	-6.06	1.53	1.61
2	G	11	DT	O3'-P	-5.96	1.54	1.61

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	F	3	DT	C1'-O4'-C4'	-8.36	101.74	110.10
1	В	79	ARG	NE-CZ-NH1	5.88	123.24	120.30
3	Н	3	DC	P-O3'-C3'	5.79	126.64	119.70
2	Е	11	DA	C1'-O4'-C4'	-5.53	104.57	110.10
1	С	24	ARG	NE-CZ-NH1	5.52	123.06	120.30



There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Group
1	А	87	THR	Peptide

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	А	737	0	768	8	0
1	В	737	0	768	14	0
1	С	748	0	781	6	0
1	D	717	0	742	9	0
2	Ε	267	0	149	6	0
2	G	288	0	160	2	0
3	F	266	0	150	6	0
3	Н	266	0	150	5	0
All	All	4026	0	3668	33	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 5.

The worst 5 of 33 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:8:ILE:N	1:B:8:ILE:HD12	2.15	0.62
1:D:15:ARG:HD3	1:B:19:VAL:HG21	1.83	0.61
1:A:48:PHE:O	1:B:41:CYS:HB2	2.02	0.60
1:D:13:ASP:OD2	1:B:15:ARG:HD3	2.01	0.59
3:H:3:DC:H2"	3:H:4:DT:O5'	2.02	0.59

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	Perce	ntiles
1	А	87/95~(92%)	82 (94%)	5~(6%)	0	100	100
1	В	87/95~(92%)	82 (94%)	4 (5%)	1 (1%)	14	47
1	С	88/95~(93%)	83 (94%)	5~(6%)	0	100	100
1	D	85/95~(90%)	81 (95%)	4 (5%)	0	100	100
All	All	347/380~(91%)	328~(94%)	18 (5%)	1 (0%)	41	74

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	89	LYS

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	А	84/89~(94%)	76~(90%)	8 (10%)	8 30		
1	В	84/89~(94%)	76~(90%)	8 (10%)	8 30		
1	С	85/89~(96%)	80 (94%)	5(6%)	19 52		
1	D	82/89~(92%)	79~(96%)	3 (4%)	34 68		
All	All	335/356~(94%)	311~(93%)	24 (7%)	14 43		

5 of 24 residues with a non-rotameric side chain are listed below:



Mol	Chain	Res	Type
1	А	23	LYS
1	А	76	HIS
1	В	86	GLU
1	А	33	TYR
1	А	73	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 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, 95^{th} 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 $>$	$\# RSRZ {>}2$	$\mathbf{OWAB}(\mathrm{\AA}^2)$	$\mathbf{Q}{<}0.9$
1	А	89/95~(93%)	0.25	0 100 100	51,65,83,92	0
1	В	89/95~(93%)	0.21	0 100 100	52,67,88,94	0
1	С	90/95~(94%)	0.22	1 (1%) 80 63	50,63,85,89	0
1	D	87/95~(91%)	0.21	0 100 100	50,61,76,88	0
2	Ε	13/14~(92%)	-0.39	0 100 100	67, 75, 92, 96	0
2	G	14/14~(100%)	-0.31	0 100 100	41, 57, 86, 102	0
3	F	13/15~(86%)	-0.36	0 100 100	70, 75, 87, 93	0
3	Н	13/15~(86%)	-0.28	0 100 100	36, 57, 71, 72	0
All	All	408/438~(93%)	0.15	1 (0%) 95 89	36,66,87,102	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	2	GLY	2.2

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.

