



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 10:14 AM UTC

PDB ID : 4XM4 / pdb_00004xm4
Title : Structure of Chaetomium Mex67:Mtr2 subunits
Authors : Aibara, S.; Valkov, M.; Stewart, M.
Deposited on : 2015-01-14
Resolution : 2.95 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
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

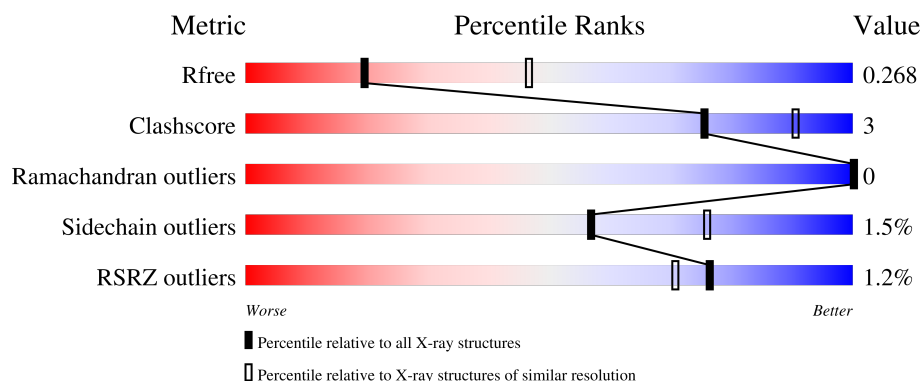
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	386	
1	B	386	
1	C	386	
1	D	386	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10475 atoms, of which 5201 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 Mex67.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	176	Total	C	H	N	O	S	0	0	0
			2745	891	1349	240	258	7			
1	B	183	Total	C	H	N	O	S	0	0	0
			2834	920	1389	249	269	7			
1	C	147	Total	C	H	N	O	S	0	0	0
			2369	746	1190	206	225	2			
1	D	157	Total	C	H	N	O	S	0	0	0
			2527	789	1273	219	244	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	179	SER	-	expression tag	UNP G0SET4
B	179	SER	-	expression tag	UNP G0SET4
C	179	SER	-	expression tag	UNP G0SET4
D	179	SER	-	expression tag	UNP G0SET4

- Molecule 1: Mex67

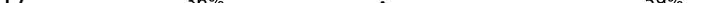


SER	SER	SER	CYS	LYS	PHE	SER	ARG	ASN	ASN	ILE	LEU	SER	SER	PRO	ARG	HIS	PRO	SER	THR	LEU	LEU	GLN	ARG	LEU	PHE	VAL	GLY	GLY	ASN	ASN	LEU	ILE	ALA	ASP	LEU	TRP	LYS	VAL	LEU	PRO	ALA	THR	ARG	HIS	PRO	SER	SER	LEU	ASP	GLN	THR	THR	GLN	TRP	LEU	ILE	CYS	HIS	THR	THR
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PRO	HIS	LEU	ALA	ASP	PRO	THR	GLY	MET	ALA	ALA	PRO	TYR	ALA	ASN	ILE	MET	GLY	LEU	GLN	CYS	GLU	GLU	ALA	ALA	ASP	ASP	ILE	SER	GLN	ASN	LEU	TYR	GLY	THR	ARG	THR	PHE	SER	SER	ARG	CYS	PHE	ILE	LEU	GLY	PRO	SER	LYS	PRO	GLY	ALA	PRO	HIS	PRO	TYR	ARG	VAL	LEU	SER
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ASP GLN LEU THR LEU HIS THR TRP LYS PRO GLN PRO ALA PRO GLN VAL GLY THR VAL

- Molecule 1: Mex67

Chain D:  36% . 59%

SER	MEI	PRO	ALA	LEU	SER	SER	GLN	LYS	LEU	SER	GLN	ALA	ALA	GLN	GLU	T196	D223	E224	T225	LEU	SER	SER	LEU	GLY	PHE	ASN	ASN	GLN	S236	L237	A238	E239	K259	D272	Q278	T285	R290	N297	Q310	R313	E316	P340	Q349	T351
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Q354	S362	PHE	PRO	THR	PRO	PRO	LEU	GLN	GLN	LEU	PRO	SER	ASN	VAL	ARG	ASP	GLY	GLU	ASN	ASN	ASN	VAL	ALA	SER	THR	PHE	LEU	GLN	ALA	PHE	PHE	GLN	LEU	THR	ASP	HTS	ASP	ARG	LEU	THR	LEU	ILE	PRO	GLN	PHE	THR	THR	PHE	SER	VAL	VAL	PHE	PHE	ALA	THR
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ASP SER PRO GLN ASP PRO ALA SER SER SER CYS LYS PHE SER SER ARG ASN LEU ASN ILE LEU SER PRO ARG HIS PRO SER THR LEU GLN ARG LEU PHE VAL GLY SER ASN LEU ILE ALA ASP LEU LYS VAL LEU PRO THR ALA ARG HIS PRO SER LEU ASP GLN THR SER GLN THR

LEU ILE ASP CYS HIS THR PHE PRO LEU ALA ASP PRO THR GLY MET MET PRO TYR ALA MET GLY LEU MET ILE ASN ASN ASN GLN CYS GLU GLU ALA ASP SER GLN ASN ASN LEU TYR GLY THR ARG ARG CYS PHE ILE LEU LEU GLY PRO SER LYS PRO GLY ALA PRO

HIS	PRO	TYR	ARG	VAL	LEU	SER	ASP	GLN	LEU	THR	LEU	HIS	THR	TRP	LYS	PRO	GLN	PRO	ALA	PRO	GLN	VAL	GLY	THR	VAL
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	43.75Å 96.09Å 194.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.04 – 2.95 48.04 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.04-2.95) 98.9 (48.04-2.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.227 , 0.265 0.232 , 0.268	Depositor DCC
R_{free} test set	924 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	69.0	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10475	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% 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	0.32	0/1440	0.64	0/1969
1	B	0.31	0/1491	0.63	0/2040
1	C	0.30	0/1199	0.65	0/1621
1	D	0.30	0/1272	0.67	0/1718
All	All	0.31	0/5402	0.64	0/7348

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	1396	1349	1347	8	0
1	B	1445	1389	1389	7	0
1	C	1179	1190	1190	2	0
1	D	1254	1273	1273	17	0
All	All	5274	5201	5199	31	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 3.

All (31) 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:D:236:SER:O	1:D:237:LEU:HG	1.57	1.04
1:B:382:VAL:O	1:B:385:THR:HG22	1.64	0.95
1:A:382:VAL:O	1:A:385:THR:HG22	1.67	0.95
1:D:237:LEU:HD12	1:D:237:LEU:O	1.70	0.90
1:D:237:LEU:HD13	1:D:278:GLN:OE1	1.78	0.83
1:A:475:THR:O	1:B:442:ARG:NH2	2.26	0.69
1:D:236:SER:C	1:D:237:LEU:HG	2.18	0.67
1:D:236:SER:O	1:D:237:LEU:CG	2.41	0.65
1:D:237:LEU:O	1:D:237:LEU:CD1	2.43	0.64
1:A:508:GLN:OE1	1:B:445:SER:OG	2.15	0.64
1:C:336:LYS:NZ	1:C:350:ILE:O	2.33	0.61
1:B:398:ARG:NH2	1:B:465:PRO:O	2.34	0.60
1:D:239:GLU:HG2	1:D:278:GLN:HA	1.84	0.60
1:A:382:VAL:C	1:A:385:THR:HG22	2.28	0.58
1:D:259:LYS:NZ	1:D:285:THR:O	2.38	0.54
1:A:478:TRP:O	1:B:442:ARG:NH2	2.42	0.52
1:D:237:LEU:HD12	1:D:237:LEU:C	2.35	0.49
1:D:340:PRO:O	1:D:351:ARG:NH1	2.46	0.48
1:D:223:ASP:HB3	1:D:225:THR:HG23	1.95	0.47
1:D:290:ARG:NH1	1:D:316:GLU:OE2	2.47	0.47
1:D:354:GLN:OE1	1:D:354:GLN:N	2.48	0.47
1:D:310:GLN:O	1:D:313:ARG:NH1	2.47	0.46
1:D:237:LEU:HD13	1:D:278:GLN:CD	2.40	0.45
1:D:272:ASP:N	1:D:297:ASN:OD1	2.49	0.45
1:B:428:SER:HB3	1:B:463:VAL:HG12	1.98	0.45
1:B:454:SER:HA	1:B:457:ILE:CD1	2.47	0.45
1:A:382:VAL:O	1:A:385:THR:CG2	2.52	0.44
1:D:237:LEU:HD22	1:D:272:ASP:O	2.18	0.44
1:C:364:PHE:N	1:C:365:PRO:HD2	2.35	0.42
1:A:428:SER:HB3	1:A:463:VAL:HG12	2.02	0.42
1:A:513:ASP:OD2	1:A:516:GLN:NE2	2.53	0.40

There are no symmetry-related clashes.

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	174/386 (45%)	171 (98%)	3 (2%)	0	100	100
1	B	181/386 (47%)	178 (98%)	3 (2%)	0	100	100
1	C	143/386 (37%)	140 (98%)	3 (2%)	0	100	100
1	D	153/386 (40%)	152 (99%)	1 (1%)	0	100	100
All	All	651/1544 (42%)	641 (98%)	10 (2%)	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	
1	A	158/344 (46%)	156 (99%)	2 (1%)	61	78
1	B	163/344 (47%)	160 (98%)	3 (2%)	51	72
1	C	131/344 (38%)	129 (98%)	2 (2%)	57	76
1	D	140/344 (41%)	138 (99%)	2 (1%)	59	77
All	All	592/1376 (43%)	583 (98%)	9 (2%)	57	76

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	388	GLN
1	A	494	MET
1	B	408	SER
1	B	497	TYR
1	B	543	VAL
1	C	220	LEU
1	C	313	ARG
1	D	349	GLN
1	D	354	GLN

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	422	GLN
1	A	551	HIS
1	D	198	GLN
1	D	298	ASN

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 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 [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	176/386 (45%)	0.01	2 (1%) 78 73	33, 63, 97, 126	0
1	B	183/386 (47%)	0.16	2 (1%) 78 73	39, 68, 106, 142	0
1	C	147/386 (38%)	0.35	3 (2%) 65 57	58, 104, 136, 146	0
1	D	157/386 (40%)	0.26	1 (0%) 85 82	78, 101, 124, 144	0
All	All	663/1544 (42%)	0.19	8 (1%) 76 71	33, 84, 124, 146	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	382	VAL	3.6
1	C	204	LEU	2.8
1	D	236	SER	2.3
1	C	268	LEU	2.2
1	B	558	ALA	2.1
1	A	497	TYR	2.1
1	C	245	LEU	2.0
1	A	382	VAL	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 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.