



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 6QT8 / pdb_00006qt8
Title : Crystal structure of Rea1-MIDAS domain from Chaetomium thermophilum
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Deposited on : 2019-02-22
Resolution : 2.33 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
Mogul : 2022.3.0, CSD as543be (2022)
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

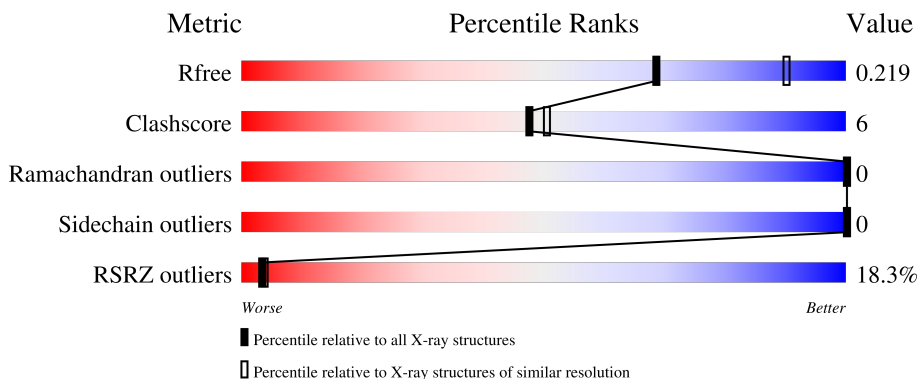
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	336	16% 77% 9% 14%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2360 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 Midasin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	289	2291	1453	404	424	10	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4670	MET	-	initiating methionine	UNP G0SHE6
A	4998	GLY	-	expression tag	UNP G0SHE6
A	4999	SER	-	expression tag	UNP G0SHE6
A	5000	HIS	-	expression tag	UNP G0SHE6
A	5001	HIS	-	expression tag	UNP G0SHE6
A	5002	HIS	-	expression tag	UNP G0SHE6
A	5003	HIS	-	expression tag	UNP G0SHE6
A	5004	HIS	-	expression tag	UNP G0SHE6
A	5005	HIS	-	expression tag	UNP G0SHE6

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0

- Molecule 4 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total I 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	23	Total 23	O 23	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	85.85Å 85.85Å 156.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.54 – 2.33 44.54 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.54-2.33) 99.9 (44.54-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.34Å)	Xtriage
Refinement program	REFMAC, PHENIX 1.12_2829	Depositor
R, R_{free}	0.181 , 0.212 0.193 , 0.219	Depositor DCC
R_{free} test set	1295 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.5	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	0.95	EDS
Total number of atoms	2360	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL, IOD

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	0.39	0/2333	0.59	0/3156

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	2291	0	2308	26	0
2	A	25	0	0	2	0
3	A	18	0	24	2	0
4	A	3	0	0	0	0
5	A	23	0	0	1	0
All	All	2360	0	2332	26	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 6.

All (26) 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:4906:GLN:O	1:A:4906:GLN:NE2	2.02	0.91
1:A:4999:SER:O	1:A:5000:HIS:ND1	2.23	0.67
1:A:4798:SER:O	1:A:4799:THR:HG22	1.95	0.66
1:A:4792:MET:HE1	1:A:4932:MET:HE1	1.82	0.62
1:A:4761:SER:HA	3:A:5108:GOL:H2	1.86	0.58
1:A:4765:ARG:HH21	3:A:5108:GOL:H12	1.69	0.57
1:A:4943:VAL:HA	1:A:4946:LEU:HD12	1.87	0.56
1:A:4906:GLN:O	1:A:4907:SER:HB3	2.05	0.55
1:A:4701:ARG:NH2	1:A:4856:PHE:O	2.38	0.55
1:A:4803:LEU:HD21	1:A:4946:LEU:HD22	1.90	0.54
1:A:4883:GLN:NE2	5:A:5202:HOH:O	2.42	0.52
1:A:4878:GLU:HA	1:A:4881:LEU:HD12	1.91	0.52
1:A:4914:ARG:NH1	2:A:5101:SO4:O2	2.43	0.52
1:A:4907:SER:HA	1:A:4910:HIS:ND1	2.28	0.49
1:A:4777:LYS:HE2	1:A:4891:GLU:N	2.30	0.47
1:A:4907:SER:HA	1:A:4910:HIS:CG	2.50	0.46
1:A:4906:GLN:HG3	1:A:4908:ARG:HB3	2.00	0.44
1:A:4900:LEU:HB3	1:A:4932:MET:HE2	1.99	0.43
1:A:4905:VAL:HG12	1:A:4910:HIS:CD2	2.52	0.43
1:A:4754:LYS:HE3	1:A:4754:LYS:HB3	1.70	0.43
1:A:4914:ARG:NH2	2:A:5105:SO4:O4	2.43	0.42
1:A:4739:LYS:HA	1:A:4739:LYS:HD2	1.60	0.42
1:A:4905:VAL:HG13	1:A:4909:ASP:HB2	2.01	0.42
1:A:4794:ASP:HB3	1:A:4798:SER:HB3	2.01	0.41
1:A:4796:ASN:OD1	1:A:4796:ASN:N	2.53	0.41
1:A:4794:ASP:O	1:A:4797:ARG:HB3	2.21	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	281/336 (84%)	275 (98%)	6 (2%)	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	250/291 (86%)	250 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	4875	HIS
1	A	4960	HIS
1	A	4975	HIS

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](#)

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	A	5108	-	5,5,5	1.07	1 (20%)	5,5,5	1.07	0
3	GOL	A	5106	-	5,5,5	1.00	0	5,5,5	1.07	0
2	SO4	A	5104	-	4,4,4	0.22	0	6,6,6	0.04	0
2	SO4	A	5101	-	4,4,4	0.25	0	6,6,6	0.14	0
2	SO4	A	5102	-	4,4,4	0.23	0	6,6,6	0.13	0
2	SO4	A	5105	-	4,4,4	0.29	0	6,6,6	0.13	0
3	GOL	A	5107	-	5,5,5	0.96	0	5,5,5	1.11	0
2	SO4	A	5103	-	4,4,4	0.21	0	6,6,6	0.12	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	5106	-	-	0/4/4/4	-
3	GOL	A	5107	-	-	4/4/4/4	-
3	GOL	A	5108	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5108	GOL	C1-C2	2.04	1.59	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5107	GOL	C1-C2-C3-O3
3	A	5107	GOL	O1-C1-C2-C3
3	A	5107	GOL	O2-C2-C3-O3
3	A	5107	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5108	GOL	2	0
2	A	5101	SO4	1	0
2	A	5105	SO4	1	0

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	289/336 (86%)	0.88	53 (18%) 3 4	43, 68, 155, 192	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4904	LEU	7.2
1	A	4696	LEU	7.2
1	A	5000	HIS	6.8
1	A	4743	ALA	6.4
1	A	4943	VAL	6.2
1	A	4905	VAL	5.8
1	A	4903	GLY	5.6
1	A	4935	ALA	5.4
1	A	4798	SER	5.2
1	A	4886	SER	4.9
1	A	4944	LEU	4.8
1	A	4775	PRO	4.7
1	A	4946	LEU	4.6
1	A	4697	LYS	4.4
1	A	4774	ILE	4.0
1	A	4947	LYS	3.9
1	A	4739	LYS	3.7
1	A	4698	ARG	3.6
1	A	4741	SER	3.5
1	A	4742	GLY	3.5
1	A	4777	LYS	3.5
1	A	4841	PRO	3.2
1	A	4922	GLU	3.1
1	A	4942	SER	3.0
1	A	4799	THR	3.0
1	A	4778	ARG	3.0
1	A	4694	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	4999	SER	2.9
1	A	4910	HIS	2.9
1	A	4773	ALA	2.7
1	A	4695	GLN	2.7
1	A	4934	ASP	2.7
1	A	4821	GLY	2.6
1	A	4766	ASP	2.5
1	A	4945	GLU	2.5
1	A	4740	LEU	2.5
1	A	4771	ARG	2.4
1	A	4795	ASP	2.4
1	A	4820	ALA	2.4
1	A	4891	GLU	2.3
1	A	4892	ASP	2.2
1	A	4933	ASP	2.2
1	A	4764	LYS	2.2
1	A	4693	ASP	2.2
1	A	4950	ARG	2.1
1	A	4769	TRP	2.1
1	A	4908	ARG	2.1
1	A	4772	ARG	2.1
1	A	4776	SER	2.1
1	A	4770	MET	2.0
1	A	4870	ARG	2.0
1	A	4924	ARG	2.0
1	A	4978	GLU	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	5105	5/5	0.59	0.12	152,152,155,161	0
3	GOL	A	5107	6/6	0.63	0.22	124,131,143,154	0
3	GOL	A	5106	6/6	0.77	0.21	118,124,131,132	0
2	SO4	A	5104	5/5	0.80	0.14	119,131,139,145	0
3	GOL	A	5108	6/6	0.83	0.23	89,110,117,117	0
2	SO4	A	5103	5/5	0.86	0.16	78,88,111,120	0
2	SO4	A	5101	5/5	0.90	0.09	115,121,126,136	0
2	SO4	A	5102	5/5	0.91	0.13	105,107,117,126	0
4	IOD	A	5111	1/1	0.97	0.08	87,87,87,87	1
4	IOD	A	5110	1/1	0.99	0.04	65,65,65,65	1
4	IOD	A	5109	1/1	1.00	0.02	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.