wwPDB X-ray Structure Validation Summary Report (i)

Oct 11, 2021 – 06:00 AM EDT

PDB ID	:	3CET
Title	:	Crystal structure of the pantheonate kinase-like protein Q6M145 at the resolution 1.8 A. Northeast Structural Genomics Consortium target MrR63
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Deposited on	:	2008-02-29
Resolution	:	1.80 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 (i)) were used in the production of this report:

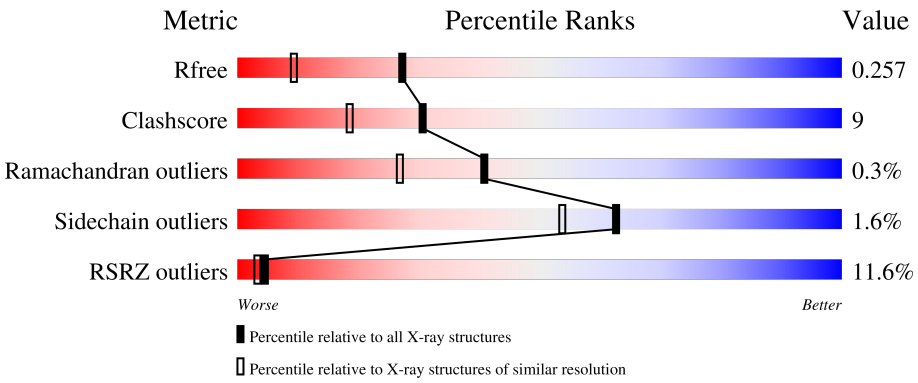
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 <=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	334	17%; 70%; 19%; • ; 10%
1	B	334	4%; 82%; 16%; •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5178 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 Conserved archaeal protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	300	2308	1452	377	471	4	4	0	0	0
1	B	330	2556	1611	416	520	4	5	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	ASN	LYS	engineered mutation	UNP Q6M145
A	50	VAL	ILE	engineered mutation	UNP Q6M145
A	93	ASN	ASP	engineered mutation	UNP Q6M145
A	101	SER	GLY	engineered mutation	UNP Q6M145
A	106	ASN	TYR	engineered mutation	UNP Q6M145
A	146	GLU	ASP	engineered mutation	UNP Q6M145
A	182	SER	LEU	engineered mutation	UNP Q6M145
A	187	ASP	ASN	engineered mutation	UNP Q6M145
A	254	ASN	THR	engineered mutation	UNP Q6M145
A	268	GLU	LYS	engineered mutation	UNP Q6M145
A	269	ASN	LYS	engineered mutation	UNP Q6M145
A	284	LEU	ILE	engineered mutation	UNP Q6M145
A	294	ALA	GLY	engineered mutation	UNP Q6M145
A	327	LEU	-	expression tag	UNP Q6M145
A	328	GLU	-	expression tag	UNP Q6M145
A	329	HIS	-	expression tag	UNP Q6M145
A	330	HIS	-	expression tag	UNP Q6M145
A	331	HIS	-	expression tag	UNP Q6M145
A	332	HIS	-	expression tag	UNP Q6M145
A	333	HIS	-	expression tag	UNP Q6M145
A	334	HIS	-	expression tag	UNP Q6M145
B	48	ASN	LYS	engineered mutation	UNP Q6M145
B	50	VAL	ILE	engineered mutation	UNP Q6M145
B	93	ASN	ASP	engineered mutation	UNP Q6M145
B	101	SER	GLY	engineered mutation	UNP Q6M145

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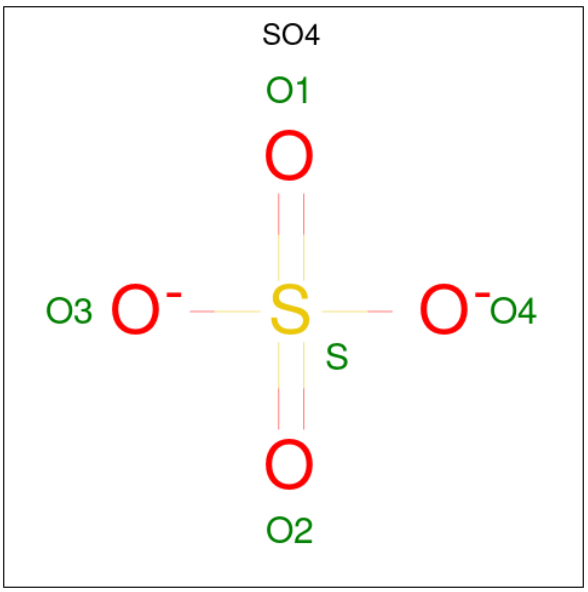
Chain	Residue	Modelled	Actual	Comment	Reference
B	106	ASN	TYR	engineered mutation	UNP Q6M145
B	146	GLU	ASP	engineered mutation	UNP Q6M145
B	182	SER	LEU	engineered mutation	UNP Q6M145
B	187	ASP	ASN	engineered mutation	UNP Q6M145
B	254	ASN	THR	engineered mutation	UNP Q6M145
B	268	GLU	LYS	engineered mutation	UNP Q6M145
B	269	ASN	LYS	engineered mutation	UNP Q6M145
B	284	LEU	ILE	engineered mutation	UNP Q6M145
B	294	ALA	GLY	engineered mutation	UNP Q6M145
B	327	LEU	-	expression tag	UNP Q6M145
B	328	GLU	-	expression tag	UNP Q6M145
B	329	HIS	-	expression tag	UNP Q6M145
B	330	HIS	-	expression tag	UNP Q6M145
B	331	HIS	-	expression tag	UNP Q6M145
B	332	HIS	-	expression tag	UNP Q6M145
B	333	HIS	-	expression tag	UNP Q6M145
B	334	HIS	-	expression tag	UNP Q6M145

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is water.

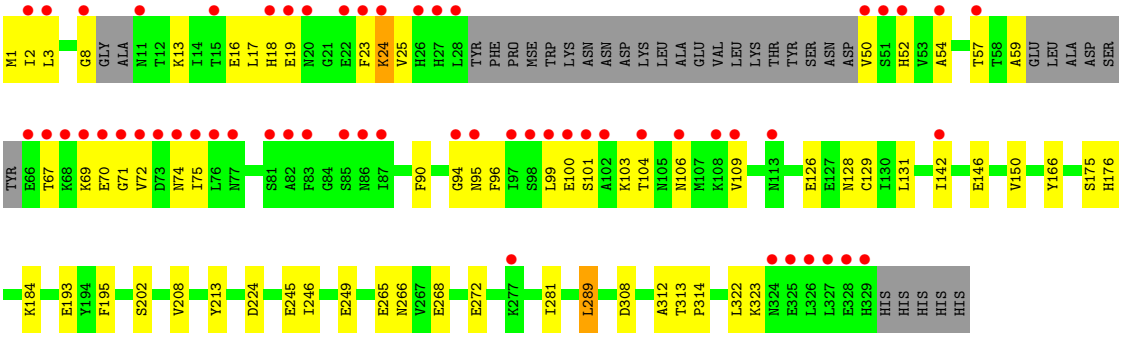
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	119	119	119	0	0
			Total	O		
3	B	185	185	185	0	0

3 Residue-property plots (i)

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

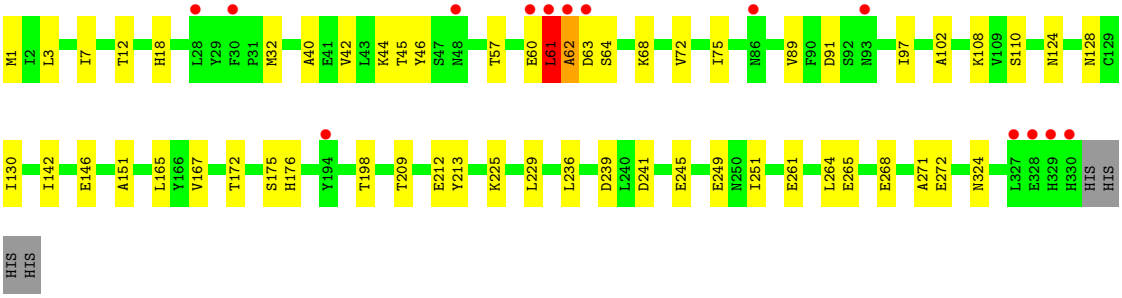
- Molecule 1: Conserved archaeal protein

Chain A:



- Molecule 1: Conserved archaeal protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.42Å 75.31Å 163.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 1.80 36.92 – 1.79	Depositor EDS
% Data completeness (in resolution range)	82.2 (19.98-1.80) 87.3 (36.92-1.79)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.26 (at 1.79Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.219 , 0.246 0.230 , 0.257	Depositor DCC
R_{free} test set	6616 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	19.5	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 50.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5178	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	1/2333 (0.0%)	0.59	1/3152 (0.0%)
1	B	0.29	0/2591	0.59	0/3506
All	All	0.31	1/4924 (0.0%)	0.59	1/6658 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	ASP	C-N	-5.93	1.20	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	184	LYS	CD-CE-NZ	6.49	126.62	111.70

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	2308	0	2307	51	0
1	B	2556	0	2537	40	0
2	B	10	0	0	0	0
3	A	119	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	185	0	0	0	0
All	All	5178	0	4844	89	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 9.

The worst 5 of 89 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:89:VAL:HG11	1:B:102:ALA:HB2	1.57	0.86
1:B:89:VAL:HG13	1:B:97:ILE:HG13	1.60	0.83
1:B:124:ASN:HD21	1:B:324:ASN:HD21	1.31	0.77
1:B:42:VAL:O	1:B:45:THR:HG22	1.85	0.77
1:A:128:ASN:ND2	1:A:146:GLU:H	1.95	0.65

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	292/334 (87%)	276 (94%)	16 (6%)	0	100 100
1	B	328/334 (98%)	317 (97%)	9 (3%)	2 (1%)	25 12
All	All	620/668 (93%)	593 (96%)	25 (4%)	2 (0%)	41 27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	61	LEU
1	B	62	ALA

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	262/287 (91%)	257 (98%)	5 (2%)	57	46
1	B	288/287 (100%)	284 (99%)	4 (1%)	67	59
All	All	550/574 (96%)	541 (98%)	9 (2%)	62	54

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	213	TYR
1	B	225	LYS
1	A	213	TYR
1	A	289	LEU
1	B	61	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	176	HIS
1	B	287	ASN
1	B	269	ASN
1	A	254	ASN
1	B	162	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	SO4	B	402	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	B	401	-	4,4,4	0.24	0	6,6,6	0.06	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	224:ASP	C	225:LYS	N	1.20

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	296/334 (88%)	0.82	58 (19%)	1	0	10, 26, 55, 74	0
1	B	325/334 (97%)	0.06	14 (4%)	35	29	11, 21, 40, 63	2 (0%)
All	All	621/668 (92%)	0.42	72 (11%)	4	3	10, 23, 52, 74	2 (0%)

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	329	HIS	8.2
1	A	329	HIS	7.7
1	A	327	LEU	7.7
1	A	328	GLU	6.9
1	B	62	ALA	6.7

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)

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(Å^2)	Q<0.9
2	SO4	B	402	5/5	0.96	0.10	45,47,47,47	0
2	SO4	B	401	5/5	0.99	0.08	24,25,26,28	0

6.5 Other polymers (i)

There are no such residues in this entry.