



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 03:13 am BST

PDB ID : 4DRA
Title : Crystal structure of MHF complex
Authors : Tao, Y.; Niu, L.; Teng, M.
Deposited on : 2012-02-17
Resolution : 2.41 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 ⓘ symbol.

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	:	2.11
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)	:	2.11

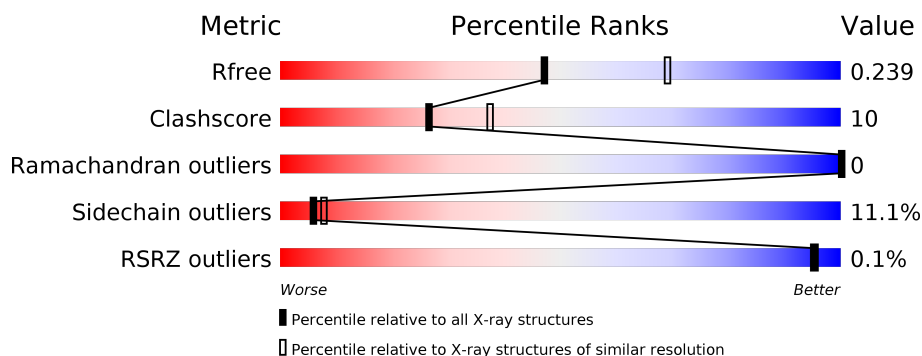
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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 $\leq 5\%$. 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	113	
1	B	113	
1	C	113	
1	D	113	
2	E	84	
2	F	84	

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Mol	Chain	Length	Quality of chain
2	G	84	<div><div></div><div>73%12%•12%</div></div>
2	H	84	<div><div></div><div>65%21%•10%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5387 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 Centromere protein S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	93	Total	C	N	O	S	1	4	0
			773	483	135	150	5			
1	B	95	Total	C	N	O	S	0	1	0
			764	481	134	144	5			
1	C	98	Total	C	N	O	S	0	0	0
			735	464	127	139	5			
1	D	93	Total	C	N	O	S	0	0	0
			686	431	114	136	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
A	-4	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
A	-3	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
A	-2	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
A	-1	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
A	0	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
B	-5	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
B	-4	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
B	-3	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
B	-2	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
B	-1	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
B	0	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
C	-5	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
C	-4	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
C	-3	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
C	-2	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
C	-1	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
C	0	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
D	-5	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
D	-4	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
D	-3	HIS	-	EXPRESSION TAG	UNP Q8N2Z9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
D	-1	HIS	-	EXPRESSION TAG	UNP Q8N2Z9
D	0	HIS	-	EXPRESSION TAG	UNP Q8N2Z9

- Molecule 2 is a protein called Centromere protein X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	74	Total	C	N	O	S	0	0	0
			573	369	98	105	1			
2	F	74	Total	C	N	O	S	0	0	0
			584	374	102	107	1			
2	G	74	Total	C	N	O	S	0	0	0
			576	368	102	105	1			
2	H	76	Total	C	N	O	S	0	0	0
			580	369	102	108	1			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	EXPRESSION TAG	UNP A8MT69
E	-1	SER	-	EXPRESSION TAG	UNP A8MT69
E	0	HIS	-	EXPRESSION TAG	UNP A8MT69
F	-2	GLY	-	EXPRESSION TAG	UNP A8MT69
F	-1	SER	-	EXPRESSION TAG	UNP A8MT69
F	0	HIS	-	EXPRESSION TAG	UNP A8MT69
G	-2	GLY	-	EXPRESSION TAG	UNP A8MT69
G	-1	SER	-	EXPRESSION TAG	UNP A8MT69
G	0	HIS	-	EXPRESSION TAG	UNP A8MT69
H	-2	GLY	-	EXPRESSION TAG	UNP A8MT69
H	-1	SER	-	EXPRESSION TAG	UNP A8MT69
H	0	HIS	-	EXPRESSION TAG	UNP A8MT69

- Molecule 3 is water.

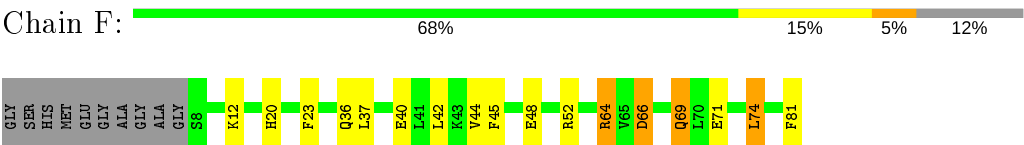
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	17	Total	O	0	0
			17	17		
3	B	25	Total	O	0	0
			25	25		
3	C	16	Total	O	0	0
			16	16		

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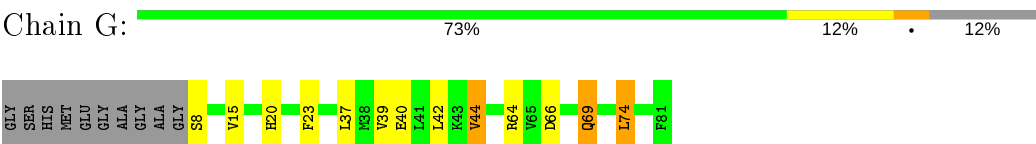
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	8	Total 8	O 8	0	0
3	E	19	Total 19	O 19	0	0
3	F	12	Total 12	O 12	0	0
3	G	11	Total 11	O 11	0	0
3	H	8	Total 8	O 8	0	0

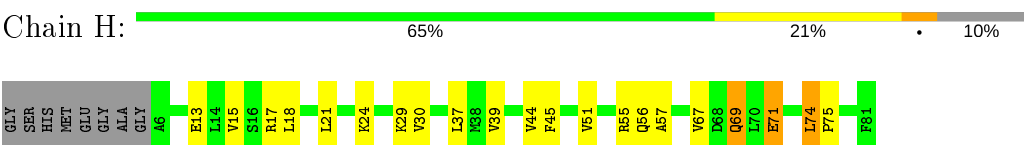
● Molecule 2: Centromere protein X



● Molecule 2: Centromere protein X



● Molecule 2: Centromere protein X



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	41.01Å 128.77Å 88.70Å 90.00° 100.74° 90.00°	Depositor
Resolution (Å)	34.15 – 2.41 41.27 – 2.41	Depositor EDS
% Data completeness (in resolution range)	90.3 (34.15-2.41) 93.9 (41.27-2.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.42Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6 _289)	Depositor
R, R_{free}	0.190 , 0.242 0.190 , 0.239	Depositor DCC
R_{free} test set	1643 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5387	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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	0.25	0/782	0.41	0/1050
1	B	0.24	0/773	0.39	0/1037
1	C	0.23	0/744	0.36	0/1005
1	D	0.22	0/694	0.37	0/942
2	E	0.23	0/579	0.33	0/782
2	F	0.23	0/590	0.37	0/795
2	G	0.22	0/582	0.35	0/785
2	H	0.22	0/586	0.34	0/792
All	All	0.23	0/5330	0.37	0/7188

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	773	0	755	29	0
1	B	764	0	765	25	0
1	C	735	0	695	14	0
1	D	686	0	630	15	0
2	E	573	0	582	14	0
2	F	584	0	602	16	0
2	G	576	0	587	9	0
2	H	580	0	580	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	17	0	0	0	0
3	B	25	0	0	0	0
3	C	16	0	0	0	0
3	D	8	0	0	0	0
3	E	19	0	0	0	0
3	F	12	0	0	0	0
3	G	11	0	0	0	0
3	H	8	0	0	0	0
All	All	5387	0	5196	108	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 10.

The worst 5 of 108 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)
2:F:48:GLU:HG3	2:F:52:ARG:HE	1.42	0.83
1:B:99:LYS:HG2	2:F:40:GLU:HG3	1.60	0.83
1:B:88:ARG:HH22	1:C:88:ARG:HH21	1.29	0.77
1:B:88:ARG:NH2	1:C:88:ARG:HH21	1.84	0.76
1:D:57:GLN:HG3	2:H:45:PHE:CZ	2.22	0.74

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	95/113 (84%)	93 (98%)	2 (2%)	0	100	100
1	B	94/113 (83%)	94 (100%)	0	0	100	100
1	C	96/113 (85%)	95 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	91/113 (80%)	91 (100%)	0	0	100	100
2	E	72/84 (86%)	71 (99%)	1 (1%)	0	100	100
2	F	72/84 (86%)	72 (100%)	0	0	100	100
2	G	72/84 (86%)	72 (100%)	0	0	100	100
2	H	74/84 (88%)	74 (100%)	0	0	100	100
All	All	666/788 (84%)	662 (99%)	4 (1%)	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	82/101 (81%)	73 (89%)	9 (11%)	6	8
1	B	81/101 (80%)	71 (88%)	10 (12%)	4	5
1	C	71/101 (70%)	62 (87%)	9 (13%)	4	5
1	D	67/101 (66%)	57 (85%)	10 (15%)	3	3
2	E	60/69 (87%)	53 (88%)	7 (12%)	5	6
2	F	63/69 (91%)	58 (92%)	5 (8%)	12	18
2	G	61/69 (88%)	57 (93%)	4 (7%)	16	25
2	H	60/69 (87%)	54 (90%)	6 (10%)	7	10
All	All	545/680 (80%)	485 (89%)	60 (11%)	6	8

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	92	LEU
1	D	75	THR
2	H	44	VAL
1	D	45	GLN
1	D	83	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	57	GLN
1	D	45	GLN
2	H	58	GLN
1	C	60	ASN
1	C	78	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 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, 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	93/113 (82%)	-0.06	0 100 100	20, 37, 65, 78	2 (2%)
1	B	95/113 (84%)	-0.07	0 100 100	23, 36, 60, 83	0
1	C	98/113 (86%)	-0.23	0 100 100	28, 42, 73, 83	0
1	D	93/113 (82%)	-0.09	1 (1%) 80 78	31, 52, 85, 115	0
2	E	74/84 (88%)	-0.18	0 100 100	19, 36, 57, 61	0
2	F	74/84 (88%)	-0.10	0 100 100	21, 38, 63, 69	0
2	G	74/84 (88%)	-0.21	0 100 100	28, 39, 60, 71	0
2	H	76/84 (90%)	0.03	0 100 100	29, 52, 73, 98	0
All	All	677/788 (85%)	-0.11	1 (0%) 95 95	19, 42, 70, 115	2 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	15	TYR	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.