



wwPDB X-ray Structure Validation Summary Report ⓘ

May 27, 2020 – 01:12 am BST

PDB ID : 3AU4
Title : Structure of the human myosin-X MyTH4-FERM cassette bound to its specific cargo, DCC
Authors : Hirano, Y.; Hatano, T.; Hakoshima, T.
Deposited on : 2011-01-28
Resolution : 1.90 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

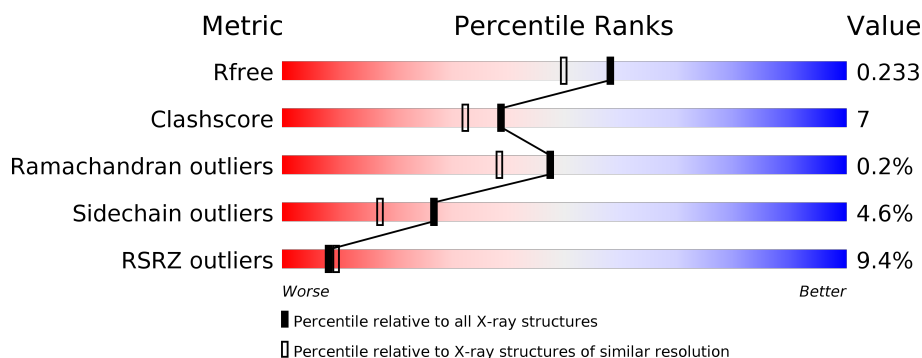
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	555	<div> <div>8%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>• 6%</div> </div> </div>
2	B	63	<div> <div>10%</div> <div> <div></div> <div>32%</div> <div>16%</div> <div>• 49%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4677 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 Myosin-X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	0	0
			4200	2696	703	779	22			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1484	GLY	-	EXPRESSION TAG	UNP Q9HD67
A	1485	PRO	-	EXPRESSION TAG	UNP Q9HD67
A	1663	THR	SER	SEE REMARK 999	UNP Q9HD67
A	?	-	THR	DELETION	UNP Q9HD67
A	?	-	PRO	DELETION	UNP Q9HD67
A	?	-	CYS	DELETION	UNP Q9HD67
A	?	-	GLU	DELETION	UNP Q9HD67
A	?	-	ARG	DELETION	UNP Q9HD67
A	?	-	LEU	DELETION	UNP Q9HD67
A	?	-	GLU	DELETION	UNP Q9HD67
A	?	-	LYS	DELETION	UNP Q9HD67
A	?	-	ARG	DELETION	UNP Q9HD67
A	?	-	ARG	DELETION	UNP Q9HD67
A	?	-	THR	DELETION	UNP Q9HD67
A	?	-	SER	DELETION	UNP Q9HD67
A	?	-	PHE	DELETION	UNP Q9HD67
A	?	-	LEU	DELETION	UNP Q9HD67
A	?	-	GLU	DELETION	UNP Q9HD67
A	?	-	GLY	DELETION	UNP Q9HD67
A	?	-	THR	DELETION	UNP Q9HD67
A	?	-	LEU	DELETION	UNP Q9HD67
A	?	-	ARG	DELETION	UNP Q9HD67
A	?	-	ARG	DELETION	UNP Q9HD67

- Molecule 2 is a protein called Netrin receptor DCC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	32	Total 234	C 141	N 38	O 53	S 2	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1385	GLY	-	EXPRESSION TAG	UNP P43146
B	1386	PRO	-	EXPRESSION TAG	UNP P43146
B	1387	GLY	-	EXPRESSION TAG	UNP P43146
B	1388	TYR	-	EXPRESSION TAG	UNP P43146
B	1389	GLN	-	EXPRESSION TAG	UNP P43146

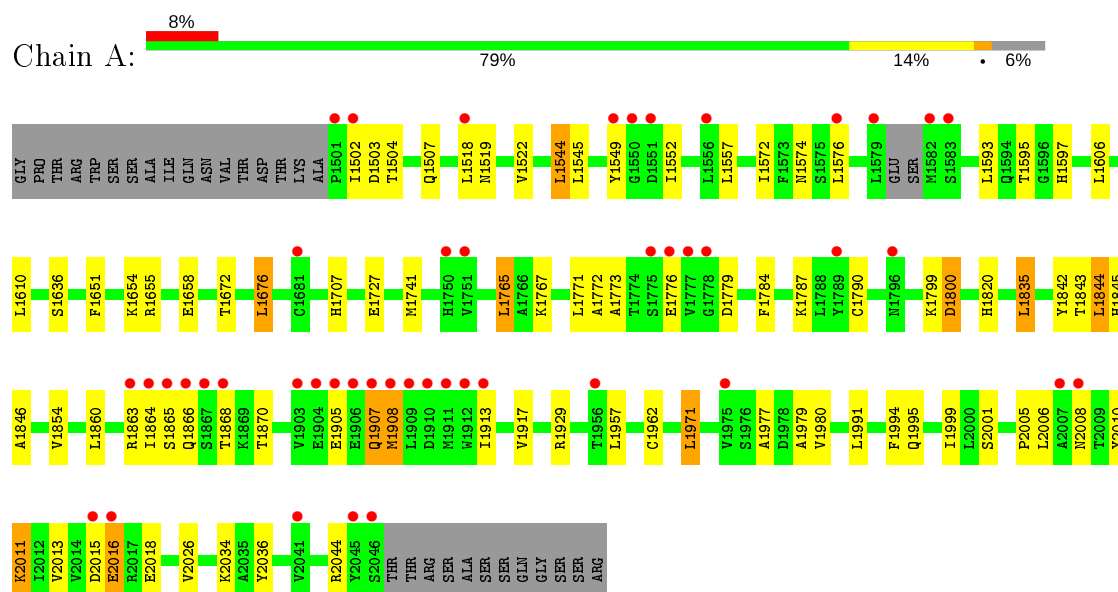
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	241	Total 241	O 241	0	0
3	B	2	Total 2	O 2	0	0

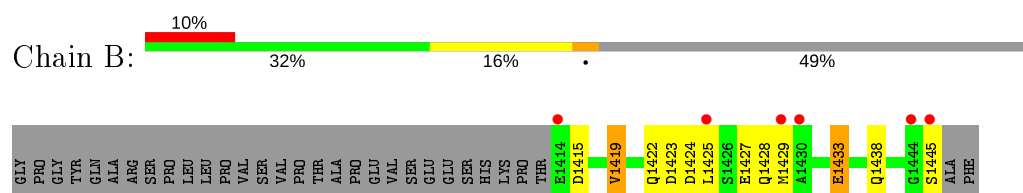
3 Residue-property plots [i](#)

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: Myosin-X



• Molecule 2: Netrin receptor DCC



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.22Å 49.56Å 93.98Å 90.00° 116.71° 90.00°	Depositor
Resolution (Å)	34.06 – 1.90 34.06 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.7 (34.06-1.90) 95.5 (34.06-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 1.89Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.215 , 0.233 0.215 , 0.233	Depositor DCC
R_{free} test set	2685 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4677	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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	0.45	5/4297 (0.1%)	0.57	0/5816
2	B	0.31	0/234	0.44	0/314
All	All	0.44	5/4531 (0.1%)	0.56	0/6130

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1507	GLN	C-O	-9.37	1.05	1.23
1	A	1507	GLN	CB-CG	-6.72	1.34	1.52
1	A	1507	GLN	CD-NE2	-6.50	1.16	1.32
1	A	1507	GLN	CD-OE1	-6.43	1.09	1.24
1	A	1597	HIS	C-O	-5.54	1.12	1.23

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	4200	0	4168	61	0
2	B	234	0	217	10	0
3	A	241	0	0	5	0
3	B	2	0	0	0	0
All	All	4677	0	4385	66	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 7.

The worst 5 of 66 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:1864:ILE:HD12	1:A:1913:ILE:HG22	1.52	0.91
1:A:1868:THR:HG23	1:A:1870:THR:H	1.41	0.85
2:B:1415:ASP:O	2:B:1419:VAL:HG12	1.88	0.72
1:A:1504:THR:HG21	1:A:1544:LEU:O	1.91	0.70
1:A:2013:VAL:HG22	1:A:2018:GLU:HG2	1.78	0.66

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	520/555 (94%)	505 (97%)	14 (3%)	1 (0%)	47	38
2	B	30/63 (48%)	30 (100%)	0	0	100	100
All	All	550/618 (89%)	535 (97%)	14 (2%)	1 (0%)	47	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1772	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	458/492 (93%)	439 (96%)	19 (4%)	30	21
2	B	25/53 (47%)	22 (88%)	3 (12%)	5	1
All	All	483/545 (89%)	461 (95%)	22 (5%)	27	17

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1844	LEU
1	A	1929	ARG
2	B	1423	ASP
1	A	1907	GLN
1	A	1908	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1817	HIS
1	A	1938	GLN
1	A	1845	HIS
1	A	1796	ASN
1	A	1820	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	524/555 (94%)	0.37	46 (8%)	10 11	21, 35, 67, 86	3 (0%)
2	B	32/63 (50%)	1.23	6 (18%)	1 1	41, 58, 70, 73	0
All	All	556/618 (89%)	0.42	52 (9%)	8 9	21, 36, 69, 86	3 (0%)

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1777	VAL	6.9
1	A	1778	GLY	5.7
1	A	1501	PRO	5.3
1	A	1864	ILE	5.2
1	A	1502	ILE	5.0

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 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.