



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 8, 2024 – 01:28 AM EDT

PDB ID : 4LL8
Title : Complex of carboxy terminal domain of Myo4p and She3p middle fragment
Authors : Shi, H.; Singh, N.; Esselborn, F.; Blobel, G.
Deposited on : 2013-07-09
Resolution : 3.58 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 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	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

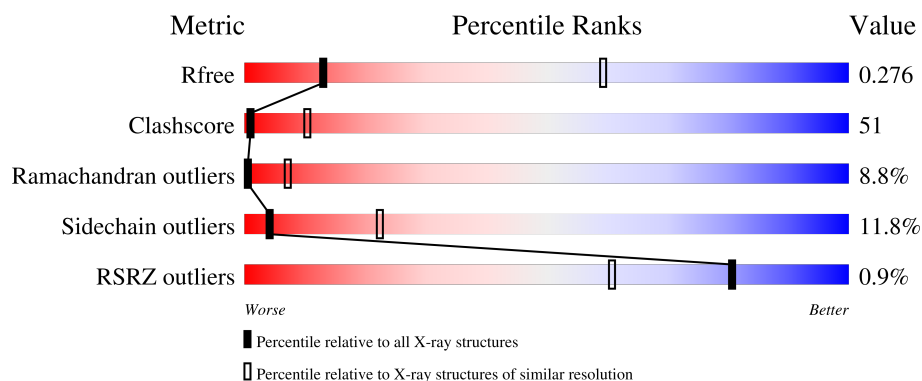
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.58 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}	164625	1360 (3.66-3.50)
Clashscore	180529	1456 (3.66-3.50)
Ramachandran outliers	177936	1438 (3.66-3.50)
Sidechain outliers	177891	1438 (3.66-3.50)
RSRZ outliers	164620	1360 (3.66-3.50)

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	539	<div> <div></div> <div>20% 45% 13% 21%</div> </div>
2	B	235	<div> <div></div> <div>20% 25% 52%</div> </div>
2	E	235	<div> <div></div> <div>25% 23% 49%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5337 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-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3421	2203	568	639	11			

There are 6 discrepancies between the modelled and reference sequences:

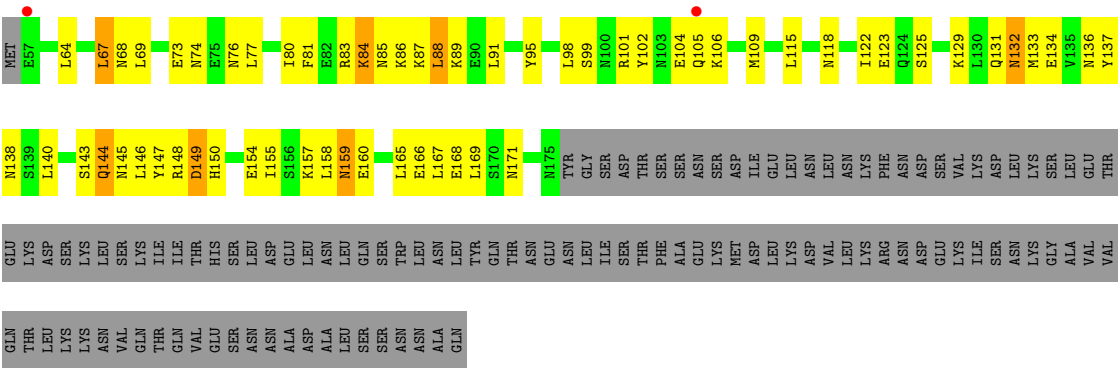
Chain	Residue	Modelled	Actual	Comment	Reference
A	1018	ALA	LYS	engineered mutation	UNP P32492
A	1019	ALA	LYS	engineered mutation	UNP P32492
A	1020	ALA	LYS	engineered mutation	UNP P32492
A	1113	SER	CYS	engineered mutation	UNP P32492
A	1288	SER	CYS	engineered mutation	UNP P32492
A	1320	SER	CYS	engineered mutation	UNP P32492

- Molecule 2 is a protein called SWI5-dependent HO expression protein 3.

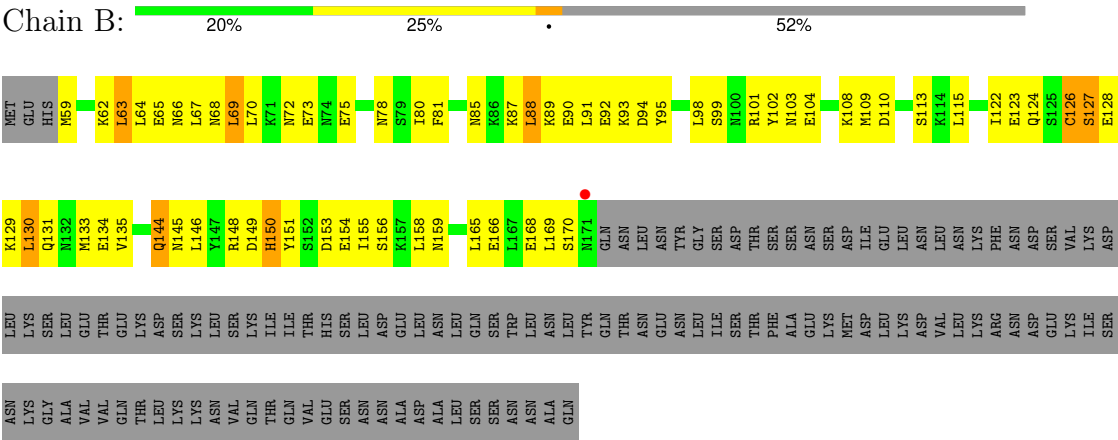
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	119	Total	C	N	O	S	0	0	0
			982	602	170	206	4			
2	B	113	Total	C	N	O	S	0	0	0
			934	574	159	197	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	56	MET	-	expression tag	UNP P38272
E	57	GLU	-	expression tag	UNP P38272
E	58	HIS	-	expression tag	UNP P38272
E	59	MET	-	expression tag	UNP P38272
B	56	MET	-	expression tag	UNP P38272
B	57	GLU	-	expression tag	UNP P38272
B	58	HIS	-	expression tag	UNP P38272
B	59	MET	-	expression tag	UNP P38272



● Molecule 2: SWI5-dependent HO expression protein 3



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	272.01Å 38.12Å 183.99Å 90.00° 125.24° 90.00°	Depositor
Resolution (Å)	50.00 – 3.58 50.00 – 3.58	Depositor EDS
% Data completeness (in resolution range)	75.5 (50.00-3.58) 89.8 (50.00-3.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.57Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.268 0.234 , 0.276	Depositor DCC
R_{free} test set	1794 reflections (9.59%)	wwPDB-VP
Wilson B-factor (Å ²)	87.7	Xtriage
Anisotropy	0.584	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 82.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5337	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.33% 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	0.48	0/3479	0.78	1/4702 (0.0%)
2	B	0.39	0/940	0.60	0/1253
2	E	0.41	0/989	0.62	0/1320
All	All	0.45	0/5408	0.73	1/7275 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1320	SER	N-CA-C	6.59	128.80	111.00

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	3421	0	3515	443	0
2	B	934	0	928	84	0
2	E	982	0	968	76	0
All	All	5337	0	5411	545	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 51.

The worst 5 of 545 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:E:91:LEU:HD23	2:B:91:LEU:HD22	1.37	1.05
2:E:123:GLU:HG3	2:B:122:ILE:HG21	1.42	1.02
1:A:1163:ILE:HD13	1:A:1226:LEU:HD11	1.40	1.01
1:A:1343:GLU:HB2	1:A:1344:PRO:HD3	1.40	1.00
2:E:166:GLU:HG2	2:B:165:LEU:HD13	1.46	0.97

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	422/539 (78%)	262 (62%)	110 (26%)	50 (12%)	0	4
2	B	111/235 (47%)	95 (86%)	13 (12%)	3 (3%)	4	28
2	E	117/235 (50%)	104 (89%)	9 (8%)	4 (3%)	3	25
All	All	650/1009 (64%)	461 (71%)	132 (20%)	57 (9%)	0	7

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1086	ASN
1	A	1096	ARG
1	A	1097	GLU
1	A	1098	SER
1	A	1109	MET

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	385/488 (79%)	336 (87%)	49 (13%)	3	19
2	B	110/225 (49%)	100 (91%)	10 (9%)	7	31
2	E	115/225 (51%)	102 (89%)	13 (11%)	4	24
All	All	610/938 (65%)	538 (88%)	72 (12%)	4	22

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	129	LYS
2	B	168	GLU
2	E	133	MET
2	B	94	ASP
1	A	1262	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1415	ASN
2	E	72	ASN
1	A	1435	GLN
2	E	132	ASN
1	A	1153	ASN

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 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	428/539 (79%)	-0.09	3 (0%) 84 66	24, 98, 162, 190	1 (0%)
2	B	113/235 (48%)	0.03	1 (0%) 81 61	59, 119, 161, 184	0
2	E	119/235 (50%)	0.04	2 (1%) 69 47	54, 125, 159, 186	0
All	All	660/1009 (65%)	-0.05	6 (0%) 81 61	24, 106, 161, 190	1 (0%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	171	ASN	3.1
1	A	1468	LEU	2.8
2	E	105	GLN	2.4
1	A	1098	SER	2.2
1	A	1132	ASN	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 monosaccharides 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.