



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:56 AM GMT

PDB ID : 3GLW  
Title : Quaternary Structure of Drosophila melanogaster IC/Tctex-1/LC8; Allosteric Interactions of Dynein Light Chains with Dynein Intermediate Chain  
Authors : Hall, J.D.; Karplus, P.A.; Barbar, E.J.  
Deposited on : 2009-03-12  
Resolution : 3.15 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

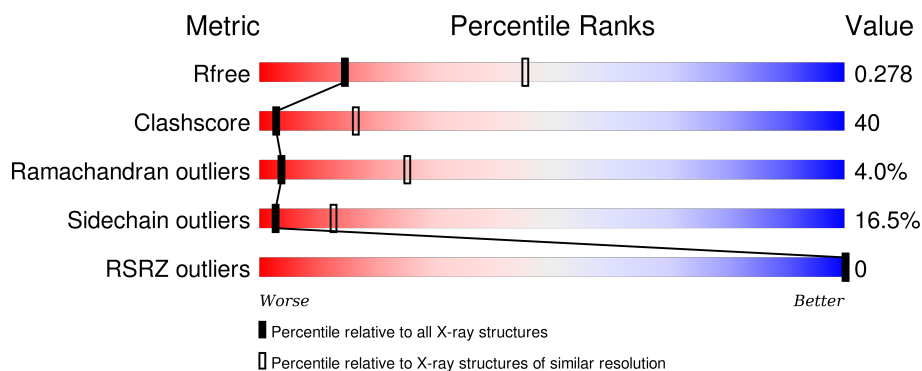
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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))
$R_{free}$	91344	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	89	 30% 58% 7% . .
2	Z	28	 18% 32% 11% 39%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 870 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 Dynein light chain 1, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	86	Total	C	N	O	S	0	5	0
			731	469	125	132	5			

- Molecule 2 is a protein called Dynein intermediate Chain.

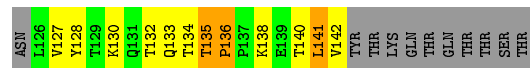
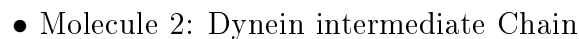
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	Z	17	Total	C	N	O	0	0	0
			136	88	21	27			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		



- Molecule 1: Dynein light chain 1, cytoplasmic



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.65Å 44.65Å 219.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.66 – 3.15 36.46 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.66-3.15) 100.0 (36.46-3.15)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	33.04 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.5.0046	Depositor
R, $R_{free}$	0.203 , 0.271 0.210 , 0.278	Depositor DCC
$R_{free}$ test set	118 reflections (4.68%)	DCC
Wilson B-factor (Å <sup>2</sup> )	68.0	Xtriage
Anisotropy	0.921	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 94.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 2638 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	870	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.21	0/763	0.30	0/1023
2	Z	0.25	0/138	0.44	0/189
All	All	0.22	0/901	0.33	0/1212

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	ALA	Peptide
1	A	78[A]	LEU	Peptide
1	A	88	SER	Peptide

### 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	731	0	721	57	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Z	136	0	145	21	3
3	A	3	0	0	0	0
All	All	870	0	866	68	3

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 40.

The worst 5 of 68 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:Z:134:THR:O	2:Z:136:PRO:HD3	1.24	1.26
1:A:35:GLU:OE2	1:A:60[B]:ARG:NH2	1.83	1.12
1:A:18:GLN:O	1:A:22:VAL:HG23	1.56	1.03
1:A:68:HIS:O	2:Z:127:VAL:HG13	1.63	0.96
2:Z:134:THR:O	2:Z:136:PRO:CD	2.14	0.94

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:128:TYR:N	2:Z:142:VAL:C[1_655]	1.17	1.03
2:Z:128:TYR:N	2:Z:142:VAL:O[1_655]	1.96	0.24
2:Z:128:TYR:N	2:Z:142:VAL:CA[1_655]	2.19	0.01

## 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	89/89 (100%)	73 (82%)	15 (17%)	1 (1%)	17 61
2	Z	15/28 (54%)	11 (73%)	1 (7%)	3 (20%)	0 0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	104/117 (89%)	84 (81%)	16 (15%)	4 (4%)	4	26

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Z	141	LEU
2	Z	135	THR
1	A	79	GLY
2	Z	136	PRO

### 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	78/77 (101%)	63 (81%)	15 (19%)	2	9
2	Z	17/28 (61%)	15 (88%)	2 (12%)	6	28
All	All	95/105 (90%)	78 (82%)	17 (18%)	3	11

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	HIS
1	A	60[A]	ARG
1	A	78[A]	LEU
1	A	50	TYR
1	A	78[B]	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	72	HIS
1	A	55	HIS
1	A	27	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	68	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	86/89 (96%)	-0.38	0 100 100	27, 47, 81, 112	0
2	Z	17/28 (60%)	-0.05	0 100 100	27, 42, 70, 77	9 (52%)
All	All	103/117 (88%)	-0.32	0 100 100	27, 47, 80, 112	9 (8%)

There are no RSRZ outliers to report.

### 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.