



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 04:40 am GMT

PDB ID : 5A3F  
Title : Crystal structure of the dynamin tetramer  
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Deposited on : 2015-05-29  
Resolution : 3.70 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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

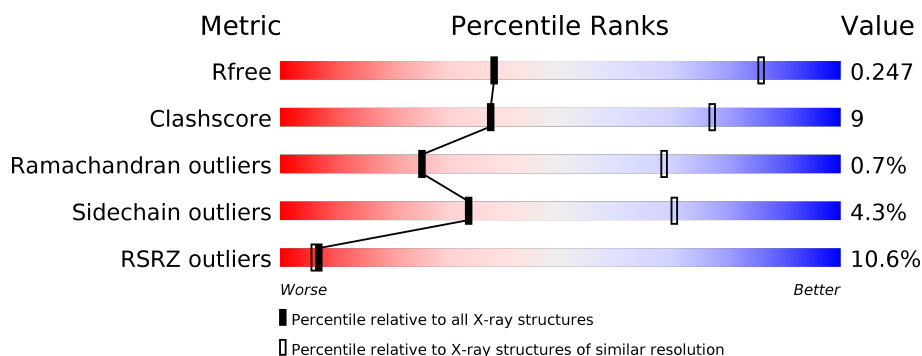
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 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))
$R_{free}$	100719	1234 (3.90-3.50)
Clashscore	112137	1377 (3.90-3.50)
Ramachandran outliers	110173	1323 (3.90-3.50)
Sidechain outliers	110143	1320 (3.90-3.50)
RSRZ outliers	101464	1262 (3.90-3.50)

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 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	754	<div> <div>15%</div> <div>66% 23% 8%</div> </div>
1	B	754	<div> <div>15%</div> <div>65% 9% 26%</div> </div>
1	C	754	<div> <div>2%</div> <div>67% 23% 7%</div> </div>
1	D	754	<div> <div>17%</div> <div>64% 8% 27%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18654 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 DYNAMIN 3.

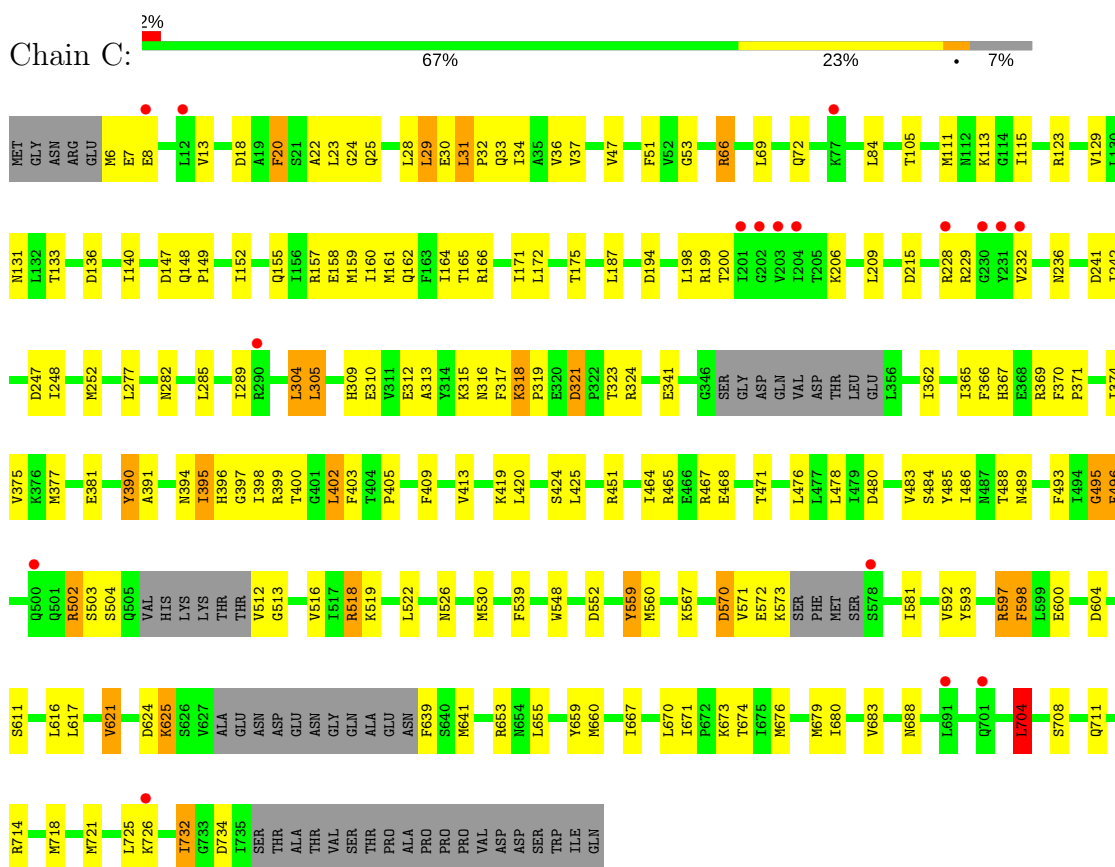
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	691	Total	C	N	O	S	0	0	0
			5548	3520	967	1035	26			
1	B	555	Total	C	N	O	S	0	0	0
			3751	2325	688	724	14			
1	C	700	Total	C	N	O	S	0	0	0
			5616	3557	983	1050	26			
1	D	554	Total	C	N	O	S	0	0	0
			3739	2316	687	722	14			

There are 4 discrepancies between the modelled and reference sequences:

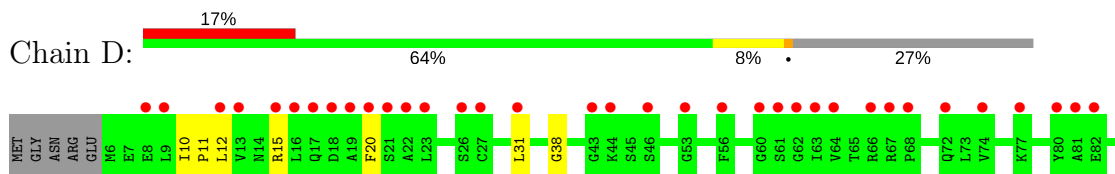
Chain	Residue	Modelled	Actual	Comment	Reference
A	361	SER	LYS	ENGINEERED MUTATION	UNP Q9UQ16
B	361	SER	LYS	ENGINEERED MUTATION	UNP Q9UQ16
C	361	SER	LYS	ENGINEERED MUTATION	UNP Q9UQ16
D	361	SER	LYS	ENGINEERED MUTATION	UNP Q9UQ16

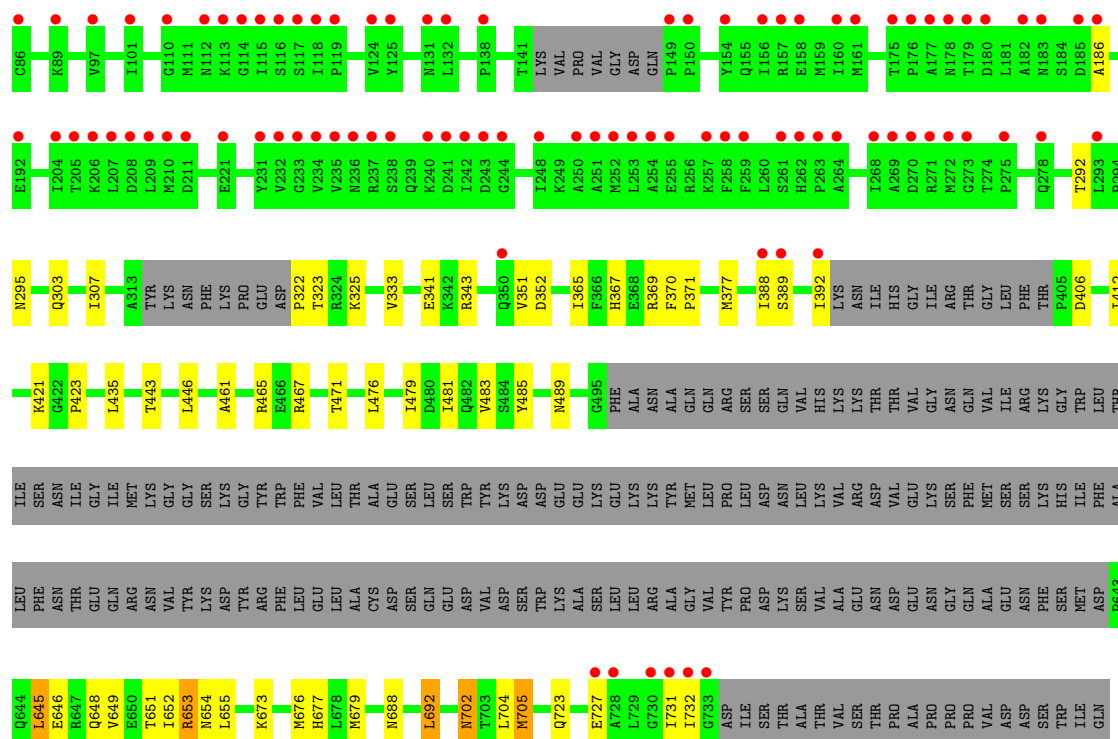


- Molecule 1: DYNAMIN 3



- Molecule 1: DYNAMIN 3





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.70Å 98.00Å 401.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.47 – 3.70 49.46 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.47-3.70) 98.8 (49.46-3.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 3.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.9_1692)	Depositor
R, $R_{free}$	0.232 , 0.278 0.233 , 0.247	Depositor DCC
$R_{free}$ test set	2103 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	142.0	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 134.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.368 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18654	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	211.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0/5635	0.47	2/7588 (0.0%)
1	B	0.25	0/3782	0.46	0/5134
1	C	0.25	0/5703	0.46	2/7679 (0.0%)
1	D	0.25	0/3769	0.46	0/5116
All	All	0.25	0/18889	0.46	4/25517 (0.0%)

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	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	704	LEU	CA-CB-CG	6.24	129.65	115.30
1	C	495	GLY	N-CA-C	-6.00	98.10	113.10
1	A	495	GLY	N-CA-C	-5.39	99.62	113.10
1	C	704	LEU	CA-CB-CG	5.15	127.14	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	625	LYS	Peptide
1	C	625	LYS	Peptide



## 5.2 Too-close contacts

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	5548	0	5670	120	0
1	B	3751	0	3183	43	0
1	C	5616	0	5733	132	0
1	D	3739	0	3174	43	0
All	All	18654	0	17760	322	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 322 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:22:ALA:HB2	1:A:84:LEU:HD21	1.59	0.85
1:C:451:ARG:HD2	1:C:704:LEU:HA	1.64	0.80
1:A:23:LEU:O	1:A:25:GLN:N	2.16	0.77
1:C:6:MET:HG3	1:C:7:GLU:H	1.50	0.76
1:A:451:ARG:HD2	1:A:704:LEU:HA	1.68	0.74

There are no symmetry-related clashes.

## 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	681/754 (90%)	654 (96%)	21 (3%)	6 (1%)	20 64
1	B	545/754 (72%)	528 (97%)	15 (3%)	2 (0%)	38 77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	690/754 (92%)	660 (96%)	22 (3%)	8 (1%)	15 59
1	D	544/754 (72%)	530 (97%)	13 (2%)	1 (0%)	51 85
All	All	2460/3016 (82%)	2372 (96%)	71 (3%)	17 (1%)	25 68

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	GLY
1	A	397	GLY
1	A	398	ILE
1	C	24	GLY
1	C	398	ILE

### 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	617/671 (92%)	588 (95%)	29 (5%)	30 68
1	B	293/671 (44%)	282 (96%)	11 (4%)	38 73
1	C	624/671 (93%)	595 (95%)	29 (5%)	31 68
1	D	292/671 (44%)	283 (97%)	9 (3%)	45 77
All	All	1826/2684 (68%)	1748 (96%)	78 (4%)	33 70

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	435	LEU
1	C	66	ARG
1	D	483	VAL
1	B	439	VAL
1	B	653	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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	691/754 (91%)	-0.28	9 (1%) 77 65	86, 200, 339, 531	0
1	B	555/754 (73%)	1.07	113 (20%) 1 1	92, 227, 356, 545	253 (45%)
1	C	700/754 (92%)	-0.25	17 (2%) 59 47	87, 201, 333, 458	0
1	D	554/754 (73%)	1.13	127 (22%) 1 1	93, 225, 352, 464	253 (45%)
All	All	2500/3016 (82%)	0.34	266 (10%) 7 6	86, 211, 346, 545	506 (20%)

The worst 5 of 266 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	241	ASP	22.7
1	D	116	SER	22.3
1	B	60	GLY	21.7
1	B	61	SER	16.3
1	D	233	GLY	15.9

### 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.