



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 28, 2016 – 05:53 PM EST

PDB ID : 5LSK  
Title : CRYSTAL STRUCTURE OF THE HUMAN KINETOCHORE MIS12-CENP-C COMPLEX  
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Deposited on : 2016-09-02  
Resolution : 3.50 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  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028320  
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) : rb-20028320

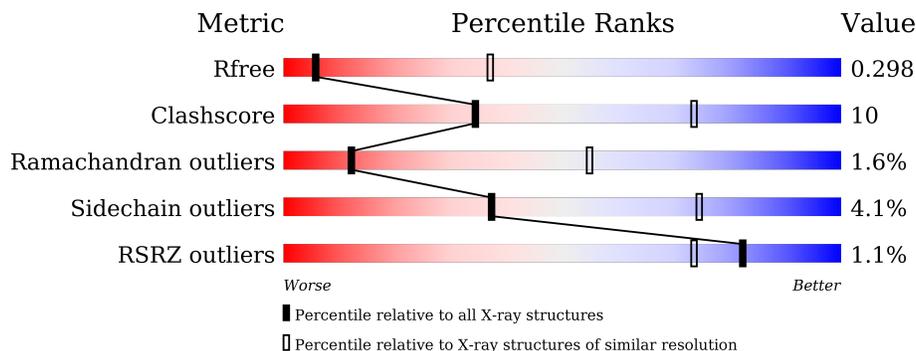
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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  $\geq 3$ , 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	205	
2	B	176	
3	D	296	
4	N	206	
5	P	76	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6192 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 Protein MIS12 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	199	1642	1049	270	312	11	0	0	0

- Molecule 2 is a protein called Polyamine-modulated factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	173	1412	886	256	265	5	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	30	MET	-	initiating methionine	UNP Q6P1K2

- Molecule 3 is a protein called Kinetochores-associated protein DSN1 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	178	1424	896	233	287	8	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	67	MET	-	initiating methionine	UNP Q9H410
D	357	HIS	-	expression tag	UNP Q9H410
D	358	HIS	-	expression tag	UNP Q9H410
D	359	HIS	-	expression tag	UNP Q9H410
D	360	HIS	-	expression tag	UNP Q9H410
D	361	HIS	-	expression tag	UNP Q9H410
D	362	HIS	-	expression tag	UNP Q9H410

- Molecule 4 is a protein called Kinetochores-associated protein NSL1 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	173	Total	C	N	O	S	0	0	0
			1390	874	241	266	9			

- Molecule 5 is a protein called Centromere protein C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	P	38	Total	C	N	O	S	0	0	0
			318	195	62	59	2			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	-4	GLY	-	expression tag	UNP Q03188
P	-3	PRO	-	expression tag	UNP Q03188
P	-2	LEU	-	expression tag	UNP Q03188
P	-1	GLY	-	expression tag	UNP Q03188
P	0	SER	-	expression tag	UNP Q03188

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total	O	0	0
			4	4		
6	B	1	Total	O	0	0
			1	1		
6	P	1	Total	O	0	0
			1	1		

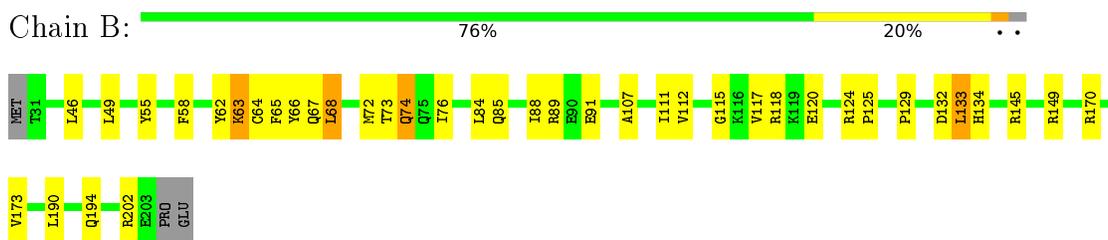
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

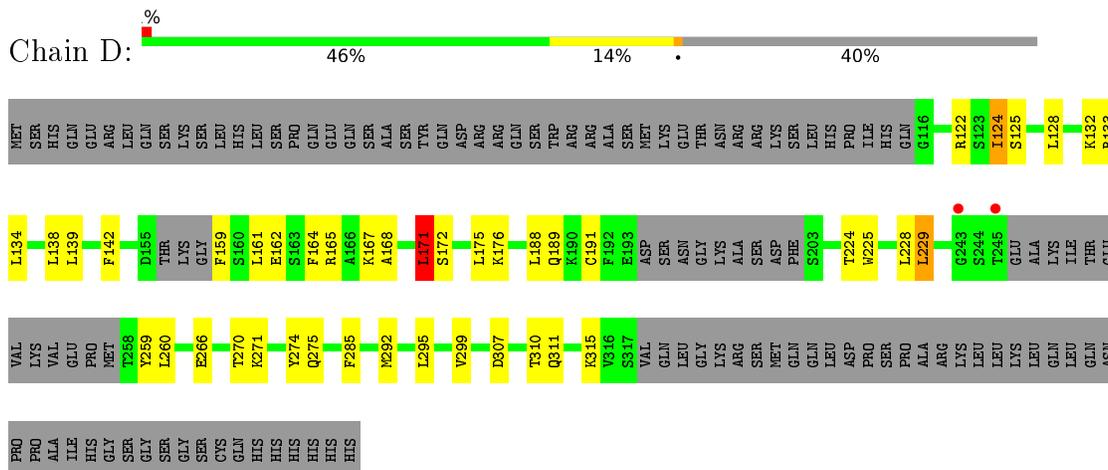
- Molecule 1: Protein MIS12 homolog



- Molecule 2: Polyamine-modulated factor 1

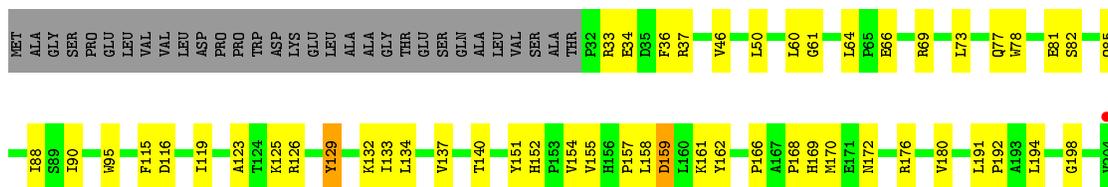


- Molecule 3: Kinetochores-associated protein DSN1 homolog



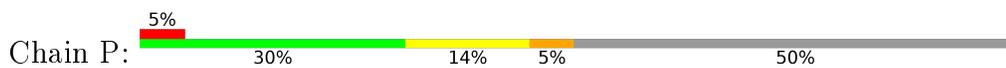
- Molecule 4: Kinetochores-associated protein NSL1 homolog





LEU  
ARG

• Molecule 5: Centromere protein C



ARG  
LYS  
ILE  
LYS  
THR  
CYS  
ILE

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.01Å 112.69Å 90.81Å 90.00° 114.18° 90.00°	Depositor
Resolution (Å)	19.74 – 3.50 19.74 – 3.50	Depositor EDS
% Data completeness (in resolution range)	83.7 (19.74-3.50) 83.8 (19.74-3.50)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 3.52Å)	Xtrriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, $R_{free}$	0.244 , 0.298 0.243 , 0.298	Depositor DCC
$R_{free}$ test set	711 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	74.6	Xtrriage
Anisotropy	0.059	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 26.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6192	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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 [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	0.26	0/1671	0.40	0/2246
2	B	0.24	0/1433	0.40	1/1933 (0.1%)
3	D	0.25	0/1441	0.46	1/1928 (0.1%)
4	N	0.24	0/1415	0.41	0/1908
5	P	0.24	0/321	0.55	0/426
All	All	0.25	0/6281	0.42	2/8441 (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
3	D	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	171	LEU	CA-CB-CG	5.66	128.32	115.30
2	B	68	LEU	CA-CB-CG	5.56	128.09	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	124	ILE	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	1642	0	1646	44	0
2	B	1412	0	1419	30	0
3	D	1424	0	1404	32	0
4	N	1390	0	1390	43	0
5	P	318	0	311	9	0
6	A	4	0	0	1	0
6	B	1	0	0	0	0
6	P	1	0	0	0	0
All	All	6192	0	6170	123	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 123 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)
3:D:128:LEU:HD13	3:D:132:LYS:HB3	1.57	0.86
4:N:158:LEU:HD23	4:N:159:ASP:H	1.38	0.85
1:A:72:LYS:O	1:A:76:ASP:HB2	1.85	0.76
2:B:63:LYS:O	2:B:66:TYR:N	2.20	0.74
1:A:130:THR:HG22	3:D:259:TYR:HD1	1.55	0.72

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	197/205 (96%)	184 (93%)	11 (6%)	2 (1%)	19	66
2	B	171/176 (97%)	162 (95%)	7 (4%)	2 (1%)	16	61
3	D	170/296 (57%)	159 (94%)	11 (6%)	0	100	100
4	N	171/206 (83%)	153 (90%)	13 (8%)	5 (3%)	6	42
5	P	34/76 (45%)	24 (71%)	7 (21%)	3 (9%)	1	12
All	All	743/959 (78%)	682 (92%)	49 (7%)	12 (2%)	12	55

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
2	B	64	CYS
4	N	155	VAL
5	P	13	TYR
5	P	34	VAL

### 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	188/194 (97%)	180 (96%)	8 (4%)	35	74
2	B	151/155 (97%)	146 (97%)	5 (3%)	45	79
3	D	163/269 (61%)	156 (96%)	7 (4%)	35	74
4	N	154/180 (86%)	149 (97%)	5 (3%)	46	80
5	P	35/67 (52%)	32 (91%)	3 (9%)	13	49
All	All	691/865 (80%)	663 (96%)	28 (4%)	37	74

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	202	ARG
3	D	164	PHE
5	P	9	LEU

*Continued on next page...*

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Mol	Chain	Res	Type
3	D	142	PHE
3	D	161	LEU

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	199/205 (97%)	-0.38	1 (0%) 91 88	27, 59, 112, 158	0
2	B	173/176 (98%)	-0.51	0 100 100	30, 56, 97, 108	0
3	D	178/296 (60%)	-0.24	2 (1%) 82 73	44, 80, 126, 142	0
4	N	173/206 (83%)	-0.20	1 (0%) 90 85	35, 83, 124, 141	0
5	P	38/76 (50%)	0.39	4 (10%) 8 8	54, 91, 129, 141	0
All	All	761/959 (79%)	-0.30	8 (1%) 82 73	27, 70, 121, 158	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	245	THR	4.4
5	P	46	SER	2.6
5	P	48	ALA	2.4
1	A	53	CYS	2.4
3	D	243	GLY	2.4

### 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

There are no such residues in this entry.