



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 17, 2024 – 07:44 AM EDT

PDB ID : 5LSJ
Title : CRYSTAL STRUCTURE OF THE HUMAN KINETOCHORE MIS12-CENP-C delta-HEAD2 COMPLEX
Authors : Vetter, I.R.; Petrovic, A.; Keller, J.; Liu, Y.
Deposited on : 2016-09-02
Resolution : 3.25 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)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

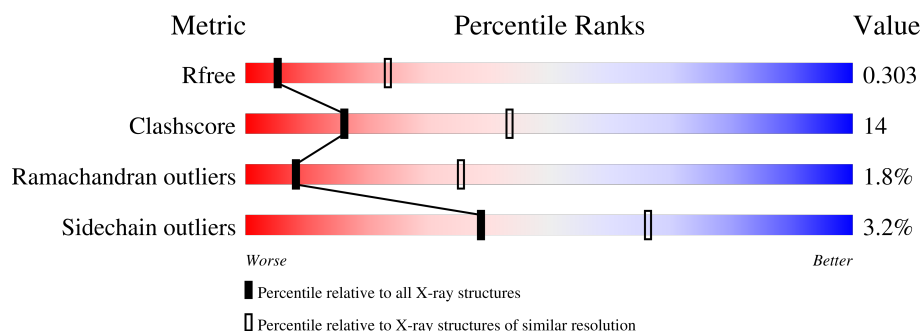
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	205	66% 29% . .
1	C	205	60% 34% . .
2	B	176	61% 35% . .
2	E	176	66% 30% . . .
3	D	178	39% 17% . 43%
3	F	178	42% 15% 43%
4	G	116	54% 33% . 12%

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Mol	Chain	Length	Quality of chain
4	N	116	<div> <div></div> <div>51%</div> <div>33%</div> <div>2%</div> <div>13%</div> </div>
5	P	76	<div> <div></div> <div>11%</div> <div>7%</div> <div>83%</div> </div>
5	Q	76	<div> <div></div> <div>8%</div> <div>11%</div> <div>80%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9621 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
1	A	199	Total	C	N	O	S	0	0	0
			1642	1049	270	312	11			
1	C	199	Total	C	N	O	S	0	0	0
			1642	1049	270	312	11			

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	101	Total	C	N	O	S	0	0	0
			815	509	134	166	6			
3	F	101	Total	C	N	O	S	0	0	0
			815	509	134	166	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	185	MET	-	initiating methionine	UNP Q9H410
D	357	HIS	-	expression tag	UNP Q9H410

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Chain	Residue	Modelled	Actual	Comment	Reference
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
F	185	MET	-	initiating methionine	UNP Q9H410
F	357	HIS	-	expression tag	UNP Q9H410
F	358	HIS	-	expression tag	UNP Q9H410
F	359	HIS	-	expression tag	UNP Q9H410
F	360	HIS	-	expression tag	UNP Q9H410
F	361	HIS	-	expression tag	UNP Q9H410
F	362	HIS	-	expression tag	UNP Q9H410

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	101	Total	C	N	O	S	0	0	0
			810	516	135	154	5			
4	G	102	Total	C	N	O	S	0	0	0
			821	525	136	155	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	91	MET	-	initiating methionine	UNP Q96IY1
G	91	MET	-	initiating methionine	UNP Q96IY1

- Molecule 5 is a protein called Centromere protein C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	P	13	Total	C	N	O	S	0	0	0
			117	73	26	17	1			
5	Q	15	Total	C	N	O	S	0	0	0
			135	84	31	19	1			

There are 10 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

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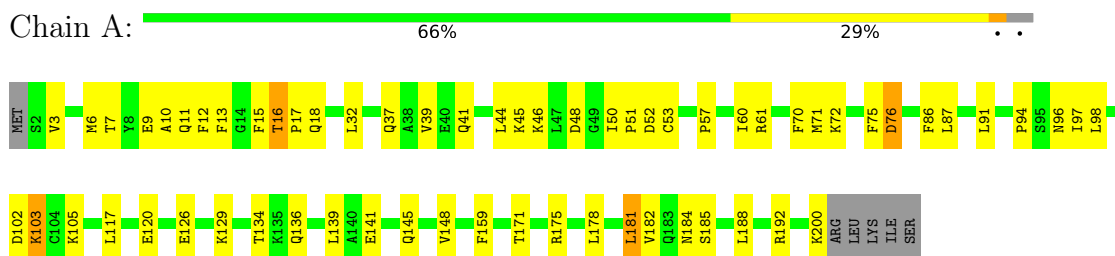
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Chain	Residue	Modelled	Actual	Comment	Reference
P	0	SER	-	expression tag	UNP Q03188
Q	-4	GLY	-	expression tag	UNP Q03188
Q	-3	PRO	-	expression tag	UNP Q03188
Q	-2	LEU	-	expression tag	UNP Q03188
Q	-1	GLY	-	expression tag	UNP Q03188
Q	0	SER	-	expression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

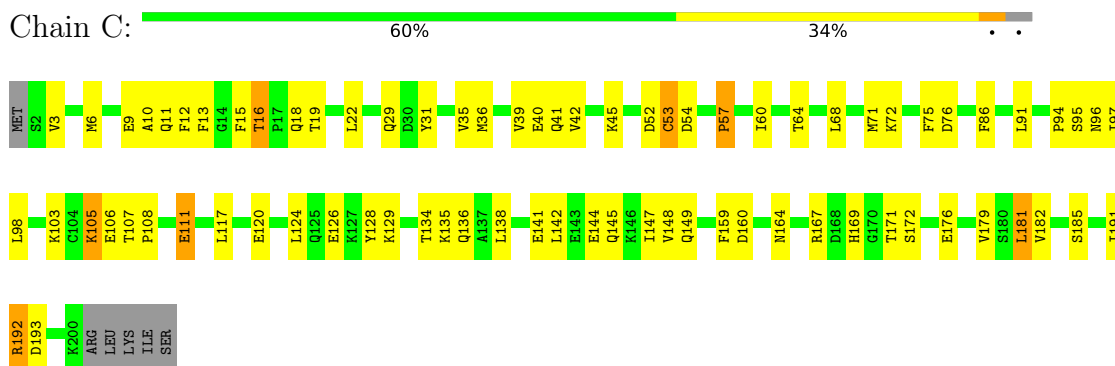
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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



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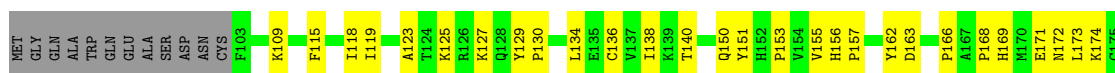


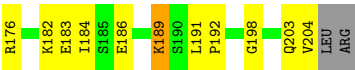
- Molecule 2: Polyamine-modulated factor 1



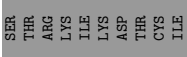
- Molecule 2: Polyamine-modulated factor 1







• Molecule 5: Centromere protein C



• Molecule 5: Centromere protein C



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.16Å 156.40Å 76.00Å 90.00° 102.82° 90.00°	Depositor
Resolution (Å)	19.99 – 3.25 45.55 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.99-3.25) 99.8 (45.55-2.80)	Depositor EDS
R_{merge}	0.35	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.246 , 0.297 0.251 , 0.303	Depositor DCC
R_{free} test set	1905 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.653	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 29.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	9621	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.08% 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

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	0.29	0/1671	0.48	0/2246
1	C	0.35	2/1671 (0.1%)	0.49	0/2246
2	B	0.26	0/1433	0.47	1/1933 (0.1%)
2	E	0.27	0/1433	0.49	1/1933 (0.1%)
3	D	0.26	0/824	0.49	0/1104
3	F	0.26	0/824	0.48	0/1104
4	G	0.27	0/836	0.46	0/1126
4	N	0.40	1/824 (0.1%)	0.58	2/1110 (0.2%)
5	P	0.24	0/119	0.59	0/156
5	Q	0.24	0/138	0.55	0/182
All	All	0.30	3/9773 (0.0%)	0.49	4/13140 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	152	HIS	C-N	8.33	1.50	1.34
1	C	111	GLU	CD-OE1	-5.93	1.19	1.25
1	C	111	GLU	CD-OE2	-5.37	1.19	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	173	LEU	CA-CB-CG	6.95	131.28	115.30
4	N	160	LEU	CA-CB-CG	6.46	130.16	115.30
2	E	68	LEU	CA-CB-CG	5.67	128.35	115.30
2	B	38	LEU	CA-CB-CG	5.21	127.29	115.30

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	1642	0	1646	65	0
1	C	1642	0	1646	77	0
2	B	1412	0	1419	54	0
2	E	1412	0	1419	48	0
3	D	815	0	801	29	0
3	F	815	0	801	24	0
4	G	821	0	842	33	0
4	N	810	0	833	29	0
5	P	117	0	116	6	0
5	Q	135	0	136	7	0
All	All	9621	0	9659	277	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 14.

The worst 5 of 277 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:181:LEU:HD21	3:D:302:LEU:HD22	1.63	0.79
1:A:6:MET:HG3	1:A:18:GLN:HE22	1.47	0.79
2:B:46:LEU:HD21	2:B:88:ILE:HG21	1.68	0.74
2:E:46:LEU:HD21	2:E:88:ILE:HG21	1.71	0.72
1:A:7:THR:OG1	4:N:126:ARG:NH1	2.23	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%)	187 (95%)	8 (4%)	2 (1%)	15	47
1	C	197/205 (96%)	181 (92%)	14 (7%)	2 (1%)	15	47
2	B	171/176 (97%)	161 (94%)	6 (4%)	4 (2%)	6	29
2	E	171/176 (97%)	164 (96%)	4 (2%)	3 (2%)	8	35
3	D	97/178 (54%)	96 (99%)	1 (1%)	0	100	100
3	F	97/178 (54%)	95 (98%)	2 (2%)	0	100	100
4	G	100/116 (86%)	90 (90%)	7 (7%)	3 (3%)	4	24
4	N	99/116 (85%)	86 (87%)	9 (9%)	4 (4%)	3	17
5	P	11/76 (14%)	8 (73%)	3 (27%)	0	100	100
5	Q	13/76 (17%)	8 (62%)	2 (15%)	3 (23%)	0	0
All	All	1153/1502 (77%)	1076 (93%)	56 (5%)	21 (2%)	8	35

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	117	VAL
2	E	117	VAL
5	Q	7	ASP
4	N	166	PRO
4	G	155	VAL

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	188/194 (97%)	182 (97%)	6 (3%)	39	66
1	C	188/194 (97%)	183 (97%)	5 (3%)	44	70
2	B	151/155 (97%)	146 (97%)	5 (3%)	38	65
2	E	151/155 (97%)	144 (95%)	7 (5%)	27	57
3	D	94/161 (58%)	92 (98%)	2 (2%)	53	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	94/161 (58%)	93 (99%)	1 (1%)	73	84
4	G	93/104 (89%)	91 (98%)	2 (2%)	52	74
4	N	92/104 (88%)	87 (95%)	5 (5%)	22	53
5	P	12/67 (18%)	12 (100%)	0	100	100
5	Q	14/67 (21%)	13 (93%)	1 (7%)	14	42
All	All	1077/1362 (79%)	1043 (97%)	34 (3%)	39	66

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	131	LYS
2	E	197	LEU
4	G	189	LYS
3	D	275	GLN
3	D	260	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	C	29	GLN

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 monosaccharides 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

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.