W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Oct 18, 2023 – 08:58 AM EDT

PDB ID	:	2DUT
Title	:	Crystal structure of a M-loop deletion variant of MENT in the native conformation
Authors	:	Whisstock, J.C.; Buckle, A.M.; McGowan, S.; Irving, J.A.
Deposited on	:	2006-07-26
Resolution	:	3.00 Å(reported)

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

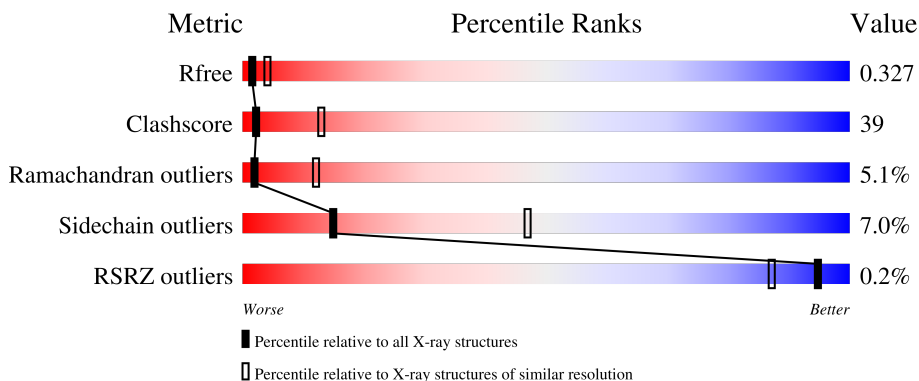|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.00 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	Percentile Ranks	Value
Rfree		0.327
Clashscore		39
Ramachandran outliers		5.1%
Sidechain outliers		7.0%
RSRZ outliers		0.2%

Worse 　　　　　 *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=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	423	39% / 41% / 6% / 13%
1	B	423	39% / 42% / 6% / 13%
1	C	423	39% / 42% / 6% / 13%
1	D	423	38% / 42% / 6% / 13%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 11020 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 Heterochromatin-associated protein MENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total 2721	C 1753	N 441	O 512	S 15	0	0	0
1	B	366	Total 2721	C 1753	N 441	O 512	S 15	0	0	0
1	C	366	Total 2721	C 1753	N 441	O 512	S 15	0	0	0
1	D	366	Total 2721	C 1753	N 441	O 512	S 15	0	0	0

There are 276 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-40	MET	-	cloning artifact	UNP O73790
A	-39	GLY	-	cloning artifact	UNP O73790
A	-38	GLY	-	cloning artifact	UNP O73790
A	-37	SER	-	cloning artifact	UNP O73790
A	-36	HIS	-	cloning artifact	UNP O73790
A	-35	HIS	-	cloning artifact	UNP O73790
A	-34	HIS	-	cloning artifact	UNP O73790
A	-33	HIS	-	cloning artifact	UNP O73790
A	-32	HIS	-	cloning artifact	UNP O73790
A	-31	HIS	-	cloning artifact	UNP O73790
A	-30	GLY	-	cloning artifact	UNP O73790
A	-29	MET	-	cloning artifact	UNP O73790
A	-28	ALA	-	cloning artifact	UNP O73790
A	-27	SER	-	cloning artifact	UNP O73790
A	-26	MET	-	cloning artifact	UNP O73790
A	-25	THR	-	cloning artifact	UNP O73790
A	-24	GLY	-	cloning artifact	UNP O73790
A	-23	GLY	-	cloning artifact	UNP O73790
A	-22	GLN	-	cloning artifact	UNP O73790
A	-21	GLN	-	cloning artifact	UNP O73790
A	-20	MET	-	cloning artifact	UNP O73790

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	GLY	-	cloning artifact	UNP O73790
A	-18	ARG	-	cloning artifact	UNP O73790
A	-17	ASP	-	cloning artifact	UNP O73790
A	-16	LEU	-	cloning artifact	UNP O73790
A	-15	TYR	-	cloning artifact	UNP O73790
A	-14	ASP	-	cloning artifact	UNP O73790
A	-13	ASP	-	cloning artifact	UNP O73790
A	-12	ASP	-	cloning artifact	UNP O73790
A	-11	ASP	-	cloning artifact	UNP O73790
A	-10	LYS	-	cloning artifact	UNP O73790
A	-9	ASP	-	cloning artifact	UNP O73790
A	-8	ARG	-	cloning artifact	UNP O73790
A	-7	TRP	-	cloning artifact	UNP O73790
A	-6	GLY	-	cloning artifact	UNP O73790
A	-5	SER	-	cloning artifact	UNP O73790
A	-4	GLU	-	cloning artifact	UNP O73790
A	-3	LEU	-	cloning artifact	UNP O73790
A	-2	GLU	-	cloning artifact	UNP O73790
A	-1	ILE	-	cloning artifact	UNP O73790
A	0	SER	-	cloning artifact	UNP O73790
A	?	-	THR	deletion	UNP O73790
A	?	-	GLU	deletion	UNP O73790
A	?	-	ALA	deletion	UNP O73790
A	?	-	VAL	deletion	UNP O73790
A	?	-	ARG	deletion	UNP O73790
A	?	-	ALA	deletion	UNP O73790
A	?	-	GLU	deletion	UNP O73790
A	?	-	SER	deletion	UNP O73790
A	?	-	SER	deletion	UNP O73790
A	?	-	SER	deletion	UNP O73790
A	?	-	VAL	deletion	UNP O73790
A	?	-	ALA	deletion	UNP O73790
A	?	-	ARG	deletion	UNP O73790
A	?	-	PRO	deletion	UNP O73790
A	?	-	SER	deletion	UNP O73790
A	?	-	ARG	deletion	UNP O73790
A	?	-	GLY	deletion	UNP O73790
A	?	-	ARG	deletion	UNP O73790
A	?	-	PRO	deletion	UNP O73790
A	?	-	LYS	deletion	UNP O73790
A	?	-	ARG	deletion	UNP O73790
A	?	-	ARG	deletion	UNP O73790

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	deletion	UNP O73790
A	?	-	MET	deletion	UNP O73790
A	?	-	ASP	deletion	UNP O73790
A	?	-	PRO	deletion	UNP O73790
A	?	-	GLU	deletion	UNP O73790
A	?	-	HIS	deletion	UNP O73790
B	-40	MET	-	cloning artifact	UNP O73790
B	-39	GLY	-	cloning artifact	UNP O73790
B	-38	GLY	-	cloning artifact	UNP O73790
B	-37	SER	-	cloning artifact	UNP O73790
B	-36	HIS	-	cloning artifact	UNP O73790
B	-35	HIS	-	cloning artifact	UNP O73790
B	-34	HIS	-	cloning artifact	UNP O73790
B	-33	HIS	-	cloning artifact	UNP O73790
B	-32	HIS	-	cloning artifact	UNP O73790
B	-31	HIS	-	cloning artifact	UNP O73790
B	-30	GLY	-	cloning artifact	UNP O73790
B	-29	MET	-	cloning artifact	UNP O73790
B	-28	ALA	-	cloning artifact	UNP O73790
B	-27	SER	-	cloning artifact	UNP O73790
B	-26	MET	-	cloning artifact	UNP O73790
B	-25	THR	-	cloning artifact	UNP O73790
B	-24	GLY	-	cloning artifact	UNP O73790
B	-23	GLY	-	cloning artifact	UNP O73790
B	-22	GLN	-	cloning artifact	UNP O73790
B	-21	GLN	-	cloning artifact	UNP O73790
B	-20	MET	-	cloning artifact	UNP O73790
B	-19	GLY	-	cloning artifact	UNP O73790
B	-18	ARG	-	cloning artifact	UNP O73790
B	-17	ASP	-	cloning artifact	UNP O73790
B	-16	LEU	-	cloning artifact	UNP O73790
B	-15	TYR	-	cloning artifact	UNP O73790
B	-14	ASP	-	cloning artifact	UNP O73790
B	-13	ASP	-	cloning artifact	UNP O73790
B	-12	ASP	-	cloning artifact	UNP O73790
B	-11	ASP	-	cloning artifact	UNP O73790
B	-10	LYS	-	cloning artifact	UNP O73790
B	-9	ASP	-	cloning artifact	UNP O73790
B	-8	ARG	-	cloning artifact	UNP O73790
B	-7	TRP	-	cloning artifact	UNP O73790
B	-6	GLY	-	cloning artifact	UNP O73790
B	-5	SER	-	cloning artifact	UNP O73790

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLU	-	cloning artifact	UNP O73790
B	-3	LEU	-	cloning artifact	UNP O73790
B	-2	GLU	-	cloning artifact	UNP O73790
B	-1	ILE	-	cloning artifact	UNP O73790
B	0	SER	-	cloning artifact	UNP O73790
B	?	-	THR	deletion	UNP O73790
B	?	-	GLU	deletion	UNP O73790
B	?	-	ALA	deletion	UNP O73790
B	?	-	VAL	deletion	UNP O73790
B	?	-	ARG	deletion	UNP O73790
B	?	-	ALA	deletion	UNP O73790
B	?	-	GLU	deletion	UNP O73790
B	?	-	SER	deletion	UNP O73790
B	?	-	SER	deletion	UNP O73790
B	?	-	SER	deletion	UNP O73790
B	?	-	VAL	deletion	UNP O73790
B	?	-	ALA	deletion	UNP O73790
B	?	-	ARG	deletion	UNP O73790
B	?	-	PRO	deletion	UNP O73790
B	?	-	SER	deletion	UNP O73790
B	?	-	ARG	deletion	UNP O73790
B	?	-	GLY	deletion	UNP O73790
B	?	-	ARG	deletion	UNP O73790
B	?	-	PRO	deletion	UNP O73790
B	?	-	LYS	deletion	UNP O73790
B	?	-	ARG	deletion	UNP O73790
B	?	-	ARG	deletion	UNP O73790
B	?	-	ARG	deletion	UNP O73790
B	?	-	MET	deletion	UNP O73790
B	?	-	ASP	deletion	UNP O73790
B	?	-	PRO	deletion	UNP O73790
B	?	-	GLU	deletion	UNP O73790
B	?	-	HIS	deletion	UNP O73790
C	-40	MET	-	cloning artifact	UNP O73790
C	-39	GLY	-	cloning artifact	UNP O73790
C	-38	GLY	-	cloning artifact	UNP O73790
C	-37	SER	-	cloning artifact	UNP O73790
C	-36	HIS	-	cloning artifact	UNP O73790
C	-35	HIS	-	cloning artifact	UNP O73790
C	-34	HIS	-	cloning artifact	UNP O73790
C	-33	HIS	-	cloning artifact	UNP O73790
C	-32	HIS	-	cloning artifact	UNP O73790

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-31	HIS	-	cloning artifact	UNP O73790
C	-30	GLY	-	cloning artifact	UNP O73790
C	-29	MET	-	cloning artifact	UNP O73790
C	-28	ALA	-	cloning artifact	UNP O73790
C	-27	SER	-	cloning artifact	UNP O73790
C	-26	MET	-	cloning artifact	UNP O73790
C	-25	THR	-	cloning artifact	UNP O73790
C	-24	GLY	-	cloning artifact	UNP O73790
C	-23	GLY	-	cloning artifact	UNP O73790
C	-22	GLN	-	cloning artifact	UNP O73790
C	-21	GLN	-	cloning artifact	UNP O73790
C	-20	MET	-	cloning artifact	UNP O73790
C	-19	GLY	-	cloning artifact	UNP O73790
C	-18	ARG	-	cloning artifact	UNP O73790
C	-17	ASP	-	cloning artifact	UNP O73790
C	-16	LEU	-	cloning artifact	UNP O73790
C	-15	TYR	-	cloning artifact	UNP O73790
C	-14	ASP	-	cloning artifact	UNP O73790
C	-13	ASP	-	cloning artifact	UNP O73790
C	-12	ASP	-	cloning artifact	UNP O73790
C	-11	ASP	-	cloning artifact	UNP O73790
C	-10	LYS	-	cloning artifact	UNP O73790
C	-9	ASP	-	cloning artifact	UNP O73790
C	-8	ARG	-	cloning artifact	UNP O73790
C	-7	TRP	-	cloning artifact	UNP O73790
C	-6	GLY	-	cloning artifact	UNP O73790
C	-5	SER	-	cloning artifact	UNP O73790
C	-4	GLU	-	cloning artifact	UNP O73790
C	-3	LEU	-	cloning artifact	UNP O73790
C	-2	GLU	-	cloning artifact	UNP O73790
C	-1	ILE	-	cloning artifact	UNP O73790
C	0	SER	-	cloning artifact	UNP O73790
C	?	-	THR	deletion	UNP O73790
C	?	-	GLU	deletion	UNP O73790
C	?	-	ALA	deletion	UNP O73790
C	?	-	VAL	deletion	UNP O73790
C	?	-	ARG	deletion	UNP O73790
C	?	-	ALA	deletion	UNP O73790
C	?	-	GLU	deletion	UNP O73790
C	?	-	SER	deletion	UNP O73790
C	?	-	SER	deletion	UNP O73790
C	?	-	SER	deletion	UNP O73790

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	VAL	deletion	UNP O73790
C	?	-	ALA	deletion	UNP O73790
C	?	-	ARG	deletion	UNP O73790
C	?	-	PRO	deletion	UNP O73790
C	?	-	SER	deletion	UNP O73790
C	?	-	ARG	deletion	UNP O73790
C	?	-	GLY	deletion	UNP O73790
C	?	-	ARG	deletion	UNP O73790
C	?	-	PRO	deletion	UNP O73790
C	?	-	LYS	deletion	UNP O73790
C	?	-	ARG	deletion	UNP O73790
C	?	-	ARG	deletion	UNP O73790
C	?	-	ARG	deletion	UNP O73790
C	?	-	MET	deletion	UNP O73790
C	?	-	ASP	deletion	UNP O73790
C	?	-	PRO	deletion	UNP O73790
C	?	-	GLU	deletion	UNP O73790
C	?	-	HIS	deletion	UNP O73790
D	-40	MET	-	cloning artifact	UNP O73790
D	-39	GLY	-	cloning artifact	UNP O73790
D	-38	GLY	-	cloning artifact	UNP O73790
D	-37	SER	-	cloning artifact	UNP O73790
D	-36	HIS	-	cloning artifact	UNP O73790
D	-35	HIS	-	cloning artifact	UNP O73790
D	-34	HIS	-	cloning artifact	UNP O73790
D	-33	HIS	-	cloning artifact	UNP O73790
D	-32	HIS	-	cloning artifact	UNP O73790
D	-31	HIS	-	cloning artifact	UNP O73790
D	-30	GLY	-	cloning artifact	UNP O73790
D	-29	MET	-	cloning artifact	UNP O73790
D	-28	ALA	-	cloning artifact	UNP O73790
D	-27	SER	-	cloning artifact	UNP O73790
D	-26	MET	-	cloning artifact	UNP O73790
D	-25	THR	-	cloning artifact	UNP O73790
D	-24	GLY	-	cloning artifact	UNP O73790
D	-23	GLY	-	cloning artifact	UNP O73790
D	-22	GLN	-	cloning artifact	UNP O73790
D	-21	GLN	-	cloning artifact	UNP O73790
D	-20	MET	-	cloning artifact	UNP O73790
D	-19	GLY	-	cloning artifact	UNP O73790
D	-18	ARG	-	cloning artifact	UNP O73790
D	-17	ASP	-	cloning artifact	UNP O73790

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	LEU	-	cloning artifact	UNP O73790
D	-15	TYR	-	cloning artifact	UNP O73790
D	-14	ASP	-	cloning artifact	UNP O73790
D	-13	ASP	-	cloning artifact	UNP O73790
D	-12	ASP	-	cloning artifact	UNP O73790
D	-11	ASP	-	cloning artifact	UNP O73790
D	-10	LYS	-	cloning artifact	UNP O73790
D	-9	ASP	-	cloning artifact	UNP O73790
D	-8	ARG	-	cloning artifact	UNP O73790
D	-7	TRP	-	cloning artifact	UNP O73790
D	-6	GLY	-	cloning artifact	UNP O73790
D	-5	SER	-	cloning artifact	UNP O73790
D	-4	GLU	-	cloning artifact	UNP O73790
D	-3	LEU	-	cloning artifact	UNP O73790
D	-2	GLU	-	cloning artifact	UNP O73790
D	-1	ILE	-	cloning artifact	UNP O73790
D	0	SER	-	cloning artifact	UNP O73790
D	?	-	THR	deletion	UNP O73790
D	?	-	GLU	deletion	UNP O73790
D	?	-	ALA	deletion	UNP O73790
D	?	-	VAL	deletion	UNP O73790
D	?	-	ARG	deletion	UNP O73790
D	?	-	ALA	deletion	UNP O73790
D	?	-	GLU	deletion	UNP O73790
D	?	-	SER	deletion	UNP O73790
D	?	-	SER	deletion	UNP O73790
D	?	-	SER	deletion	UNP O73790
D	?	-	VAL	deletion	UNP O73790
D	?	-	ALA	deletion	UNP O73790
D	?	-	ARG	deletion	UNP O73790
D	?	-	PRO	deletion	UNP O73790
D	?	-	SER	deletion	UNP O73790
D	?	-	ARG	deletion	UNP O73790
D	?	-	GLY	deletion	UNP O73790
D	?	-	ARG	deletion	UNP O73790
D	?	-	PRO	deletion	UNP O73790
D	?	-	LYS	deletion	UNP O73790
D	?	-	ARG	deletion	UNP O73790
D	?	-	ARG	deletion	UNP O73790
D	?	-	ARG	deletion	UNP O73790
D	?	-	MET	deletion	UNP O73790
D	?	-	ASP	deletion	UNP O73790

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	deletion	UNP O73790
D	?	-	GLU	deletion	UNP O73790
D	?	-	HIS	deletion	UNP O73790

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	34	Total 34	O 34	0	0
2	B	34	Total 34	O 34	0	0
2	C	33	Total 33	O 33	0	0
2	D	35	Total 35	O 35	0	0

3 Residue-property plots ⓘ

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 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.
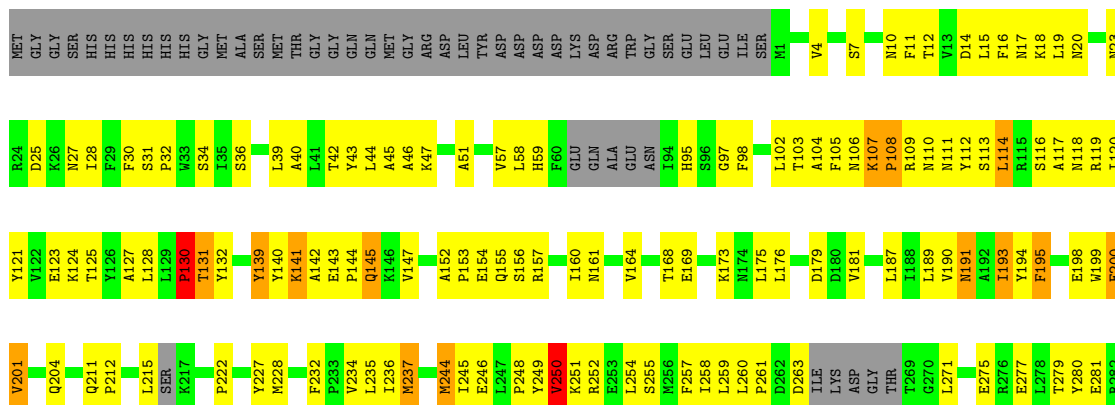
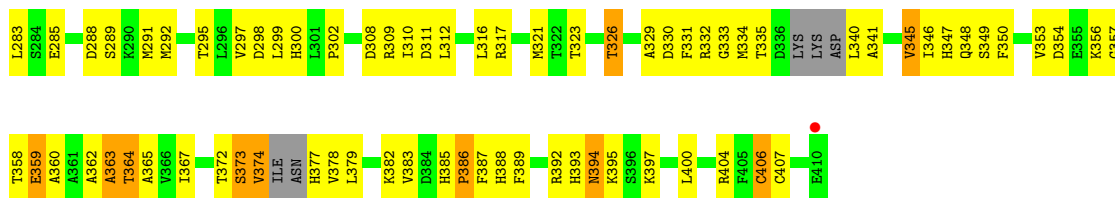• Molecule 1: Heterochromatin-associated protein MENT
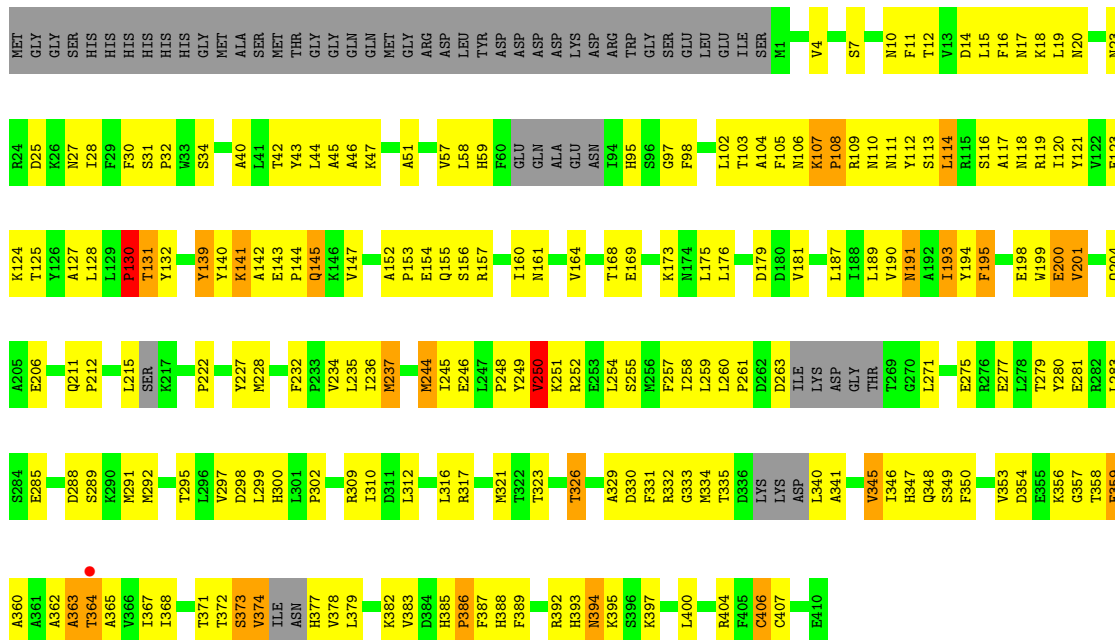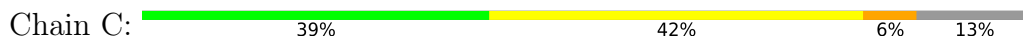
Chain A:

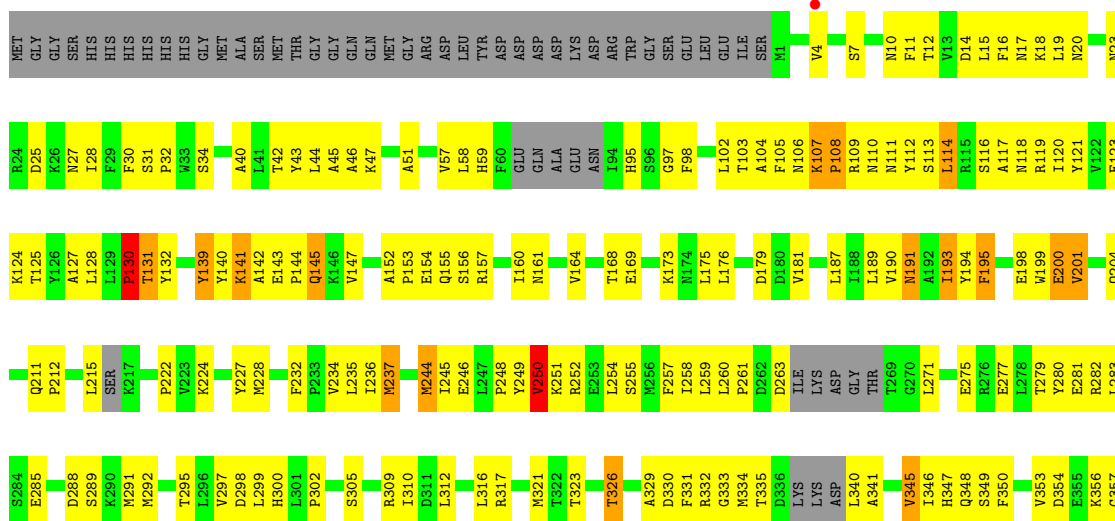• Molecule 1: Heterochromatin-associated protein MENT

Chain B:

L283 S284 E285 D288 S289 K290 M291 M292 T295 L296 V297 D298 L299 H300 L301 P302 D308 R309 I310 D311 L312 L316 R317 M321 T322 T323 T326 A329 D330 F331 R332 G333 M334 T335 D336 LYS LYS ASP L340 A341 V345 I346 H347 Q348 S349 F350 V353 D354 E355 K356 G357

T358 E359 A360 A361 A362 A363 T364 A365 V366 I367 T372 S373 V374 ILE H377 V378 L379 K382 V383 D384 H385 P386 F387 H388 F389 R392 H393 N394 K395 S396 K397 L400 R404 F405 C406 C407 E410

● Molecule 1: Heterochromatin-associated protein MENT

Chain C: 39% 42% 6% 13%

MET GLY GLY SER HIS HIS HIS HIS HIS HIS GLY MET ALA SER MET THR GLY GLN GLN GLN MET GLY ARG ASP LEU TYR ASP ASP ASP LYS ASP ARG TRP GLY SER GLU LEU GLU ILE SER M1 V4 S7 N10 F11 T12 V13 D14 L15 F16 N17 K18 L19 N20 N23

R24 D25 K26 N27 I28 F29 F30 S31 P32 W33 S34 A40 L41 T42 Y43 L44 A45 A46 K47 A51 V57 L58 H59 F60 GLU GLN ALA GLU ASN I94 H95 S96 G97 F98 L102 T103 A104 F105 N106 K107 P108 R109 N110 N111 Y112 S113 L114 R115 S116 A117 N118 R119 I120 Y121 V122 E123

K124 T125 Y126 A127 L128 L129 P130 T131 Y132 Y139 Y140 K141 A142 E143 P144 Q145 K146 V147 A152 P153 E154 Q155 S156 R157 I160 N161 V164 T168 E169 K173 N174 L175 L176 D179 D180 V181 L187 I188 L189 V190 N191 A192 I193 Y194 F195 E198 W199 E200 V201 Q204

A205 E206 Q211 P212 L215 SER K217 P222 Y227 M228 F232 P233 V234 L235 I236 M237 M244 I245 E246 L247 P248 Y249 V250 K251 R252 E253 L254 S255 M256 F257 I258 L259 L260 P261 D262 D263 ILE LYS ASP GLY THR T269 G270 L271 E275 R276 L277 L278 T279 Y280 E281 R282 L283

S284 E285 D288 S289 K290 M291 M292 T295 L296 V297 D298 L299 H300 L301 P302 R309 I310 D311 L312 L316 R317 M321 T322 T323 T326 A329 D330 F331 R332 G333 M334 T335 D336 LYS LYS ASP L340 A341 V345 I346 H347 Q348 S349 F350 V353 D354 E355 K356 G357 T358 E359

A360 A361 A362 A363 T364 A365 V366 I367 I368 T371 T372 S373 V374 ILE ASN H377 V378 L379 K382 V383 D384 H385 P386 F387 H388 F389 R392 H393 N394 K395 S396 K397 L400 R404 F405 C406 C407 E410
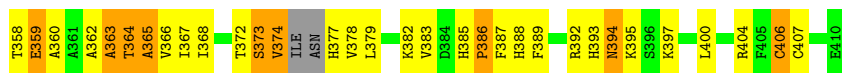
● Molecule 1: Heterochromatin-associated protein MENT

Chain D: 38% 42% 6% 13%

MET GLY GLY SER HIS HIS HIS HIS HIS HIS GLY MET ALA SER MET THR GLY GLN GLN GLN MET GLY ARG ASP LEU TYR ASP ASP ASP LYS ASP ARG TRP GLY SER GLU LEU GLU ILE SER M1 V4 S7 N10 F11 T12 V13 D14 L15 F16 N17 K18 L19 N20 N23

R24 D25 K26 N27 I28 F29 F30 S31 P32 W33 S34 A40 L41 T42 Y43 L44 A45 A46 K47 A51 V57 L58 H59 F60 GLU GLN ALA GLU ASN I94 H95 S96 G97 F98 L102 T103 A104 F105 N106 K107 P108 R109 N110 N111 Y112 S113 L114 R115 S116 A117 N118 R119 I120 Y121 V122 E123

K124 T125 Y126 A127 L128 L129 P130 T131 Y132 Y139 Y140 K141 A142 E143 P144 Q145 K146 V147 A152 P153 E154 Q155 S156 R157 I160 N161 V164 T168 E169 K173 N174 L175 L176 D179 D180 V181 L187 I188 L189 V190 N191 A192 I193 Y194 F195 E198 W199 E200 V201 Q204

Q211 P212 L215 SER K217 P222 V223 K224 Y227 M228 F232 P233 V234 L235 I236 M237 M244 I245 E246 L247 P248 Y249 V250 K251 R252 E253 L254 S255 M256 F257 I258 L259 L260 P261 D262 D263 ILE LYS ASP GLY THR T269 G270 L271 E275 R276 L277 L278 T279 Y280 E281 R282 L283

S284 E285 D288 S289 K290 M291 M292 T295 L296 V297 D298 L299 H300 L301 P302 S305 R309 I310 D311 L312 L316 R317 M321 T322 T323 T326 A329 D330 F331 R332 G333 M334 T335 D336 LYS LYS ASP L340 A341 V345 I346 H347 Q348 S349 F350 V353 D354 E355 K356 G357

T358 E359 A360 A361 A362 A363 T364 A365 V366 I367 I368 T372 S373 V374 ILE ASN H377 V378 L379 K382 V383 D384 H385 P386 F387 H388 F389 R392 H393 N394 K395 S396 K397 L400 R404 F405 C406 C407 E410

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	182.56Å 182.56Å 96.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00 19.97 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.6 (20.00-3.00) 95.6 (19.97-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.02 (at 2.98Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.278 , 0.293 0.293 , 0.327	Depositor DCC
R_{free} test set	3090 reflections (4.49%)	wwPDB-VP
Wilson B-factor (Å^2)	55.4	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 65.0	EDS
L-test for twinning[2]	$< |L| > = 0.45, < L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.073 for -h,-k,l 0.073 for h,-h-k,-l 0.499 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	11020	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.50	0/2780	0.81	4/3785 (0.1%)
1	B	0.50	0/2780	0.81	4/3785 (0.1%)
1	C	0.50	0/2780	0.81	4/3785 (0.1%)
1	D	0.50	0/2780	0.81	4/3785 (0.1%)
All	All	0.50	0/11120	0.81	16/15140 (0.1%)

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	373	SER	N-CA-C	9.84	137.58	111.00
1	D	373	SER	N-CA-C	9.84	137.57	111.00
1	C	373	SER	N-CA-C	9.83	137.54	111.00
1	A	373	SER	N-CA-C	9.82	137.53	111.00
1	D	200	GLU	N-CA-C	-6.20	94.25	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2721	0	2497	206	0
1	B	2721	0	2497	210	0
1	C	2721	0	2497	202	0
1	D	2721	0	2497	227	0

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	34	0	0	2	0
2	B	34	0	0	2	0
2	C	33	0	0	2	0
2	D	35	0	0	3	0
All	All	11020	0	9988	821	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 39.

The worst 5 of 821 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:317:ARG:HA	1:A:321:MET:O	1.55	1.06
1:B:308:ASP:HB2	1:D:368:ILE:HG12	1.37	1.06
1:B:317:ARG:HA	1:B:321:MET:O	1.55	1.05
1:C:317:ARG:HA	1:C:321:MET:O	1.55	1.05
1:D:317:ARG:HA	1:D:321:MET:O	1.55	1.04

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	354/423 (84%)	275 (78%)	61 (17%)	18 (5%)	2	12
1	B	354/423 (84%)	275 (78%)	61 (17%)	18 (5%)	2	12
1	C	354/423 (84%)	276 (78%)	60 (17%)	18 (5%)	2	12
1	D	354/423 (84%)	275 (78%)	61 (17%)	18 (5%)	2	12
All	All	1416/1692 (84%)	1101 (78%)	243 (17%)	72 (5%)	2	12

5 of 72 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	LYS
1	A	108	PRO
1	A	130	PRO
1	A	173	LYS
1	A	251	LYS

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	270/379 (71%)	251 (93%)	19 (7%)	15	47
1	B	270/379 (71%)	251 (93%)	19 (7%)	15	47
1	C	270/379 (71%)	251 (93%)	19 (7%)	15	47
1	D	270/379 (71%)	251 (93%)	19 (7%)	15	47
All	All	1080/1516 (71%)	1004 (93%)	76 (7%)	15	47

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	114	LEU
1	D	283	LEU
1	D	130	PRO
1	D	190	VAL
1	D	378	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	204	GLN
1	D	118	ASN
1	C	211	GLN
1	D	20	ASN
1	D	191	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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(Å²)	Q<0.9
1	A	366/423 (86%)	-0.12	0	100	100	15, 40, 75, 99	0
1	B	366/423 (86%)	-0.17	1 (0%)	94	84	15, 40, 75, 99	0
1	C	366/423 (86%)	-0.18	1 (0%)	94	84	15, 40, 75, 99	0
1	D	366/423 (86%)	-0.19	1 (0%)	94	84	15, 40, 75, 99	0
All	All	1464/1692 (86%)	-0.16	3 (0%)	95	87	15, 40, 76, 99	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	410	GLU	2.4
1	C	364	THR	2.2
1	D	4	VAL	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.