



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2017 – 09:22 PM EDT

PDB ID : 5MSM
Title : Structure of the Dcc1-Ctf8-Ctf18C Trimer
Authors : Wade, B.O.; Singleton, M.R.
Deposited on : unknown
Resolution : 2.29 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

<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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
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)	:	rb-20029824

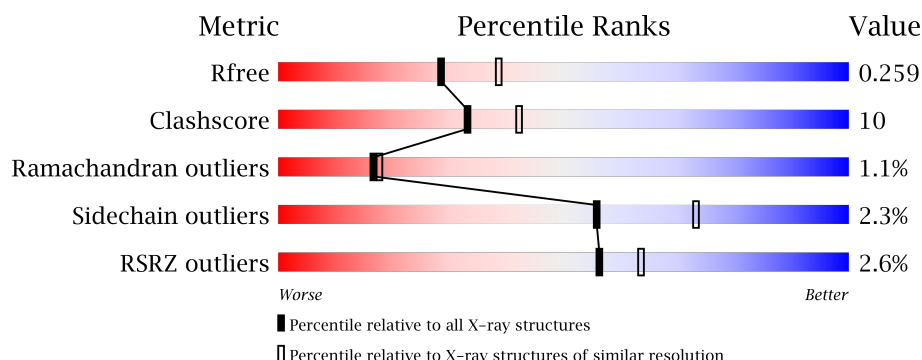
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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 ≥ 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	380	
1	D	380	
2	B	133	
2	E	133	
3	C	78	

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Mol	Chain	Length	Quality of chain
3	F	78	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a green segment on the left labeled '29%', a yellow segment in the middle, and a grey segment on the right labeled '67%'. A small black dot is located at the boundary between the yellow and grey segments.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8784 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 Sister chromatid cohesion protein DCC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	0	0
			3021	1947	502	558	14			
1	D	370	Total	C	N	O	S	0	0	0
			3016	1942	503	557	14			

- Molecule 2 is a protein called Chromosome transmission fidelity protein 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	132	Total	C	N	O	S	0	0	0
			1040	659	178	196	7			
2	E	124	Total	C	N	O	S	0	0	0
			980	624	167	183	6			

- Molecule 3 is a protein called Chromosome transmission fidelity protein 18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	27	Total	C	N	O	0	0	0
			234	153	42	39			
3	F	26	Total	C	N	O	0	0	0
			227	149	40	38			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	664	SER	-	expression tag	UNP P49956
C	665	GLY	-	expression tag	UNP P49956
F	664	SER	-	expression tag	UNP P49956
F	665	GLY	-	expression tag	UNP P49956

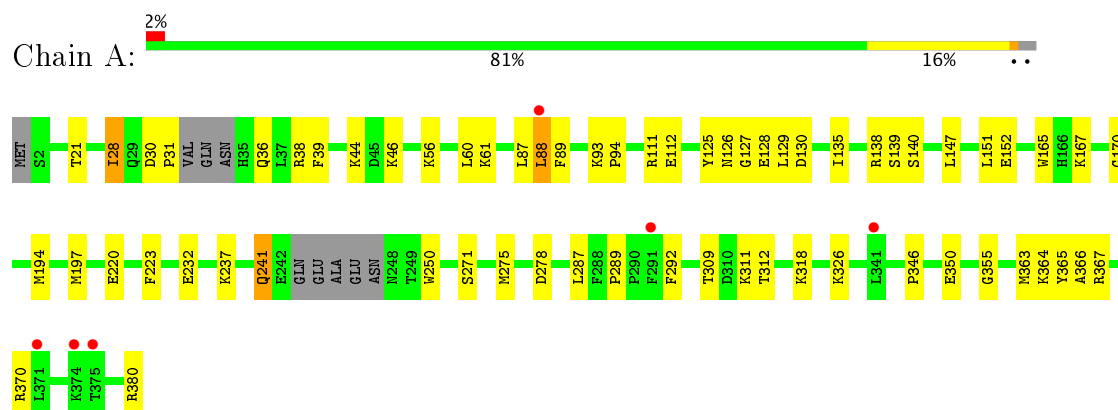
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	86	Total 86	O 86	0	0
4	B	39	Total 39	O 39	0	0
4	C	6	Total 6	O 6	0	0
4	D	90	Total 90	O 90	0	0
4	E	37	Total 37	O 37	0	0
4	F	8	Total 8	O 8	0	0

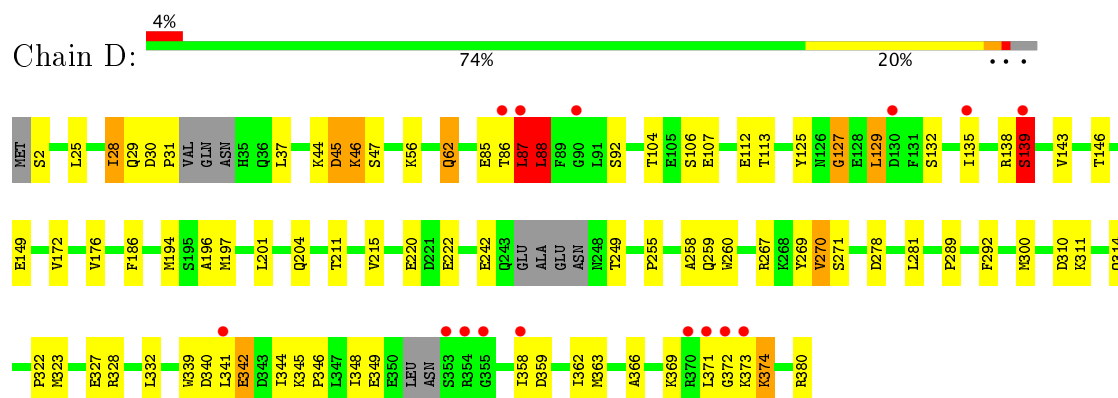
3 Residue-property plots [i](#)

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

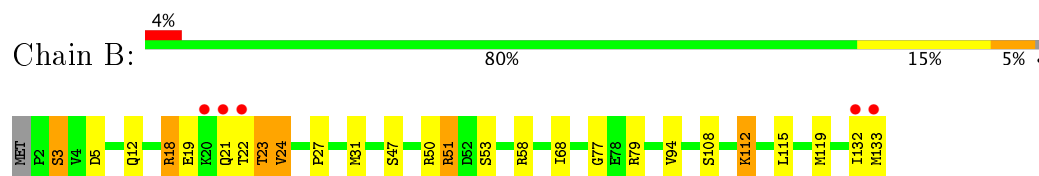
- Molecule 1: Sister chromatid cohesion protein DCC1



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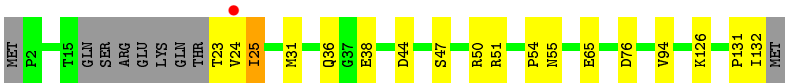


- Molecule 2: Chromosome transmission fidelity protein 8

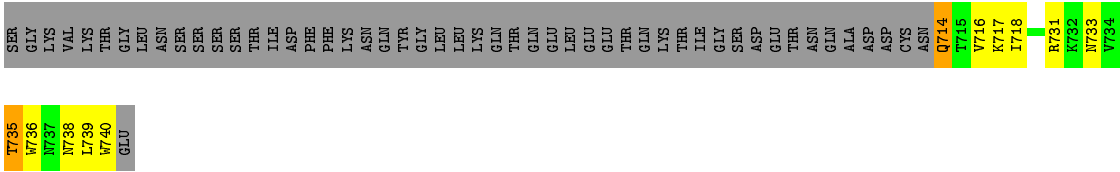


- Molecule 2: Chromosome transmission fidelity protein 8

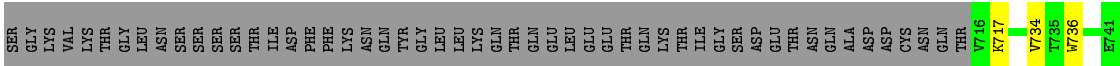




● Molecule 3: Chromosome transmission fidelity protein 18



● Molecule 3: Chromosome transmission fidelity protein 18



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.61Å 164.22Å 60.64Å 90.00° 90.55° 90.00°	Depositor
Resolution (Å)	60.64 – 2.29 82.11 – 2.29	Depositor EDS
% Data completeness (in resolution range)	89.9 (60.64-2.29) 88.4 (82.11-2.29)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.200 , 0.260 0.200 , 0.259	Depositor DCC
R_{free} test set	2250 reflections (4.87%)	DCC
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 29.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for l,k,-h 0.178 for h,-k,-l 0.032 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8784	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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	0.48	0/3090	0.68	0/4174
1	D	0.50	0/3084	0.75	4/4164 (0.1%)
2	B	0.54	0/1056	0.77	0/1418
2	E	0.51	0/995	0.78	4/1336 (0.3%)
3	C	0.54	0/241	0.83	0/328
3	F	0.73	0/234	0.61	0/318
All	All	0.51	0/8700	0.73	8/11738 (0.1%)

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
1	D	0	1
2	B	0	1
2	E	0	1
All	All	0	6

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	88	LEU	CA-CB-CG	10.00	138.30	115.30
1	D	88	LEU	CB-CG-CD2	-9.13	95.47	111.00
2	E	54	PRO	N-CA-C	6.68	129.47	112.10
2	E	54	PRO	CA-C-N	6.58	131.68	117.20
2	E	54	PRO	C-N-CA	6.17	137.13	121.70

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	ASN	Peptide
1	A	241	GLN	Peptide
1	A	88	LEU	Peptide
2	B	18	ARG	Peptide
1	D	374	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	3021	0	3037	50	0
1	D	3016	0	3027	73	0
2	B	1040	0	1060	31	0
2	E	980	0	1006	12	0
3	C	234	0	228	19	0
3	F	227	0	219	3	0
4	A	86	0	0	10	0
4	B	39	0	0	2	0
4	C	6	0	0	1	0
4	D	90	0	0	14	0
4	E	37	0	0	3	0
4	F	8	0	0	0	0
All	All	8784	0	8577	167	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 167 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:D:85:GLU:HB3	1:D:88:LEU:HD21	1.43	1.00
1:D:380:ARG:NH2	4:D:402:HOH:O	1.96	0.98
1:A:197:MET:HE1	1:A:292:PHE:HD1	1.31	0.94
2:B:21:GLN:HG3	2:B:27:PRO:HD3	1.53	0.90
1:D:62:GLN:HG2	3:F:734:VAL:HG22	1.52	0.88

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	365/380 (96%)	352 (96%)	11 (3%)	2 (0%)	32	39
1	D	362/380 (95%)	344 (95%)	11 (3%)	7 (2%)	9	8
2	B	130/133 (98%)	124 (95%)	5 (4%)	1 (1%)	22	26
2	E	120/133 (90%)	117 (98%)	2 (2%)	1 (1%)	22	26
3	C	25/78 (32%)	25 (100%)	0	0	100	100
3	F	24/78 (31%)	24 (100%)	0	0	100	100
All	All	1026/1182 (87%)	986 (96%)	29 (3%)	11 (1%)	17	18

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	88	LEU
1	D	270	VAL
1	D	372	GLY
1	D	127	GLY
1	A	139	SER

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	342/352 (97%)	338 (99%)	4 (1%)	75	87
1	D	341/352 (97%)	331 (97%)	10 (3%)	48	64
2	B	116/120 (97%)	110 (95%)	6 (5%)	27	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	110/120 (92%)	110 (100%)	0	100	100
3	C	25/71 (35%)	23 (92%)	2 (8%)	14	17
3	F	24/71 (34%)	24 (100%)	0	100	100
All	All	958/1086 (88%)	936 (98%)	22 (2%)	56	73

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	112	LYS
1	D	28	ILE
1	D	342	GLU
3	C	714	GLN
3	C	735	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	67	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 carbohydrates 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 [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, 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(Å ²)	Q<0.9
1	A	371/380 (97%)	-0.26	6 (1%) 72 77	34, 48, 77, 105	0
1	D	370/380 (97%)	-0.05	15 (4%) 38 45	34, 51, 92, 132	0
2	B	132/133 (99%)	-0.26	5 (3%) 41 48	33, 47, 81, 96	0
2	E	124/133 (93%)	-0.34	1 (0%) 86 89	30, 45, 67, 76	0
3	C	27/78 (34%)	-0.33	0 100 100	39, 44, 61, 96	0
3	F	26/78 (33%)	-0.31	0 100 100	36, 43, 54, 60	0
All	All	1050/1182 (88%)	-0.20	27 (2%) 56 63	30, 49, 84, 132	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	370	ARG	5.6
1	D	372	GLY	5.3
1	D	86	THR	5.2
2	B	22	THR	4.8
1	D	353	SER	4.4

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 [i](#)

There are no such residues in this entry.