



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:52 PM UTC

PDB ID : 5OID / pdb_00005oid
Title : Complex Trichoplax STIL-NTD:human CEP85 coiled coil domain 4
Authors : van Breugel, M.
Deposited on : 2017-07-18
Resolution : 4.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

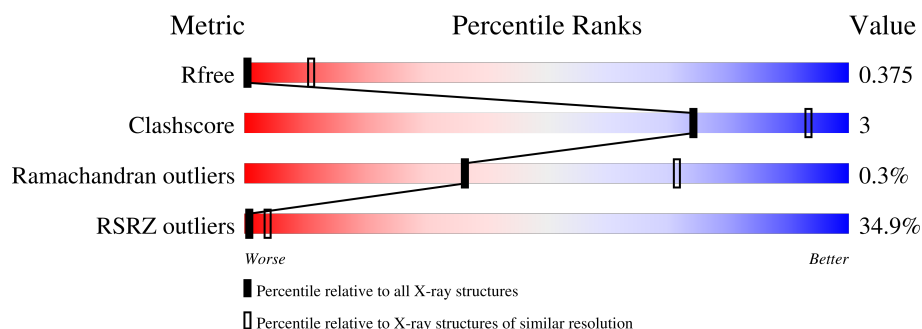
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.60 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}	180053	1007 (5.28-3.92)
Clashscore	190562	1022 (5.26-3.94)
Ramachandran outliers	187476	1069 (5.30-3.90)
RSRZ outliers	180081	1002 (5.28-3.92)

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 $\leq 5\%$. 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	360	
2	B	88	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1829 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 Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	0	0	0
			1634	974	330	330			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP B3S3X5
A	-1	GLY	-	expression tag	UNP B3S3X5
A	0	SER	-	expression tag	UNP B3S3X5
A	349	GLU	-	expression tag	UNP B3S3X5
A	350	PHE	-	expression tag	UNP B3S3X5
A	351	GLY	-	expression tag	UNP B3S3X5
A	352	GLU	-	expression tag	UNP B3S3X5
A	353	ASN	-	expression tag	UNP B3S3X5
A	354	LEU	-	expression tag	UNP B3S3X5
A	355	TYR	-	expression tag	UNP B3S3X5
A	356	PHE	-	expression tag	UNP B3S3X5
A	357	GLN	-	expression tag	UNP B3S3X5

- Molecule 2 is a protein called Centrosomal protein of 85 kDa.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	39	Total	C	N	O	0	0	0
			195	117	39	39			

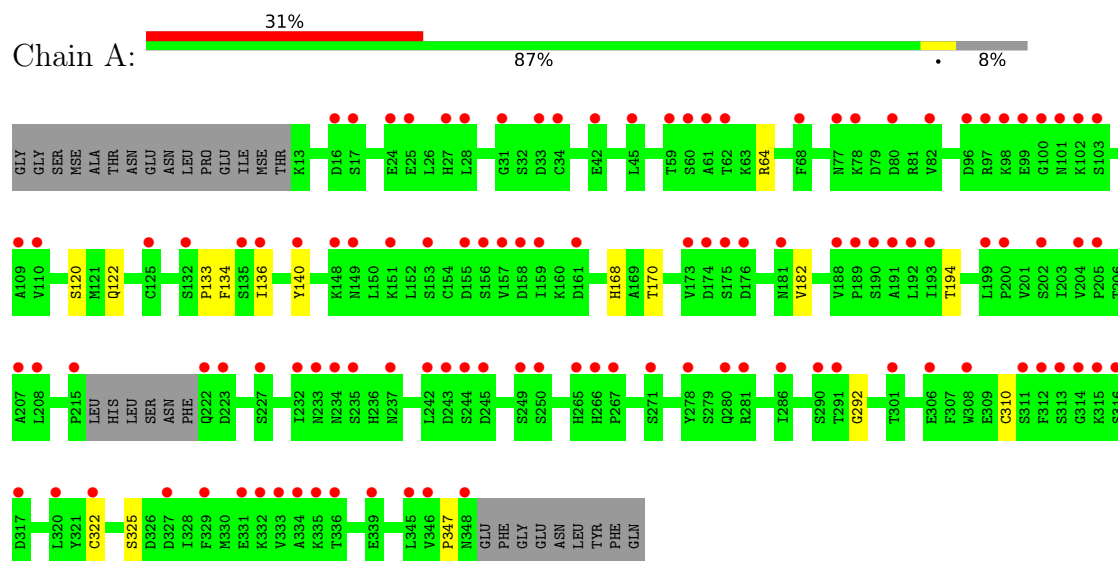
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	569	GLY	-	expression tag	UNP Q6P2H3

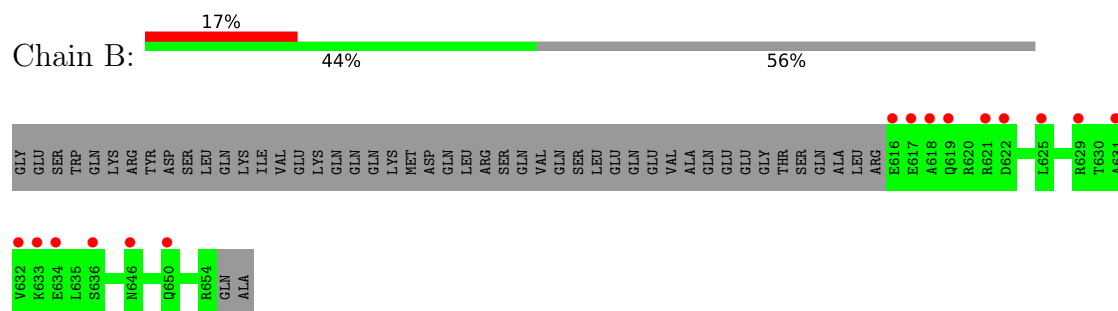
3 Residue-property plots [i](#)

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 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: Putative uncharacterized protein



• Molecule 2: Centrosomal protein of 85 kDa



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	268.70Å 268.70Å 268.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.00 – 4.60 95.00 – 4.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (95.00-4.60) 99.9 (95.00-4.60)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 4.66Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.353 , 0.365 0.361 , 0.375	Depositor DCC
R_{free} test set	492 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å ²)	228.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	1829	wwPDB-VP
Average B, all atoms (Å ²)	271.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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	0.23	0/1627	0.66	0/2257
2	B	0.14	0/194	0.43	0/270
All	All	0.22	0/1821	0.64	0/2527

There are no bond length outliers.

There are no bond angle outliers.

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	1634	0	706	8	0
2	B	195	0	86	0	0
All	All	1829	0	792	8	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 3.

All (8) 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:182:VAL:O	1:A:325:SER:HA	1.90	0.71
1:A:136:ILE:O	1:A:140:TYR:CB	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:THR:O	1:A:310:CYS:HA	2.07	0.54
1:A:122:GLN:O	1:A:170:THR:HA	2.12	0.50
1:A:120:SER:O	1:A:168:HIS:HA	2.13	0.49
1:A:322:CYS:CB	1:A:347:PRO:HA	2.43	0.49
1:A:292:GLY:HA2	1:A:310:CYS:O	2.14	0.48
1:A:133:PRO:O	1:A:134:PHE:C	2.63	0.41

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	326/360 (91%)	311 (95%)	14 (4%)	1 (0%)	36	71
2	B	37/88 (42%)	37 (100%)	0	0	100	100
All	All	363/448 (81%)	348 (96%)	14 (4%)	1 (0%)	36	71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	ARG

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 oligosaccharides 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

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(Å ²)	Q<0.9
1	A	325/360 (90%)	1.70	112 (34%)  	98, 269, 380, 525	0
2	B	39/88 (44%)	1.75	15 (38%)  	225, 278, 433, 450	0
All	All	364/448 (81%)	1.71	127 (34%)  	98, 274, 395, 525	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	348	ASN	9.4
1	A	99	GLU	9.0
1	A	244	SER	7.9
1	A	333	VAL	7.2
1	A	60	SER	7.1
1	A	176	ASP	6.1
2	B	616	GLU	6.1
1	A	215	PRO	6.0
2	B	617	GLU	5.8
1	A	132	SER	5.6
1	A	175	SER	5.4
1	A	135	SER	5.2
1	A	334	ALA	5.1
1	A	235	SER	5.1
1	A	286	ILE	5.0
1	A	109	ALA	4.9
1	A	327	ASP	4.8
1	A	290	SER	4.6
1	A	322	CYS	4.6
1	A	100	GLY	4.5
1	A	101	ASN	4.5
1	A	313	SER	4.5
1	A	149	ASN	4.4
1	A	332	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	291	THR	4.3
1	A	200	PRO	4.2
1	A	306	GLU	4.2
1	A	315	LYS	4.1
1	A	148	LYS	4.0
1	A	191	ALA	4.0
1	A	96	ASP	3.9
2	B	631	ALA	3.9
1	A	234	ASN	3.9
1	A	188	VAL	3.9
1	A	189	PRO	3.9
1	A	158	ASP	3.7
1	A	346	VAL	3.7
1	A	103	SER	3.7
1	A	266	HIS	3.7
1	A	173	VAL	3.6
1	A	136	ILE	3.6
1	A	314	GLY	3.6
1	A	80	ASP	3.5
1	A	78	LYS	3.5
1	A	25	GLU	3.5
1	A	242	LEU	3.5
1	A	320	LEU	3.5
1	A	278	TYR	3.4
1	A	34	CYS	3.4
1	A	202	SER	3.4
1	A	336	THR	3.4
1	A	222	GLN	3.4
2	B	633	LYS	3.4
2	B	622	ASP	3.3
1	A	161	ASP	3.2
1	A	125	CYS	3.2
1	A	243	ASP	3.1
1	A	265	HIS	3.1
1	A	155	ASP	3.1
1	A	335	LYS	3.0
1	A	61	ALA	3.0
2	B	618	ALA	3.0
1	A	98	LYS	3.0
1	A	17	SER	3.0
1	A	249	SER	3.0
1	A	316	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	159	ILE	3.0
1	A	102	LYS	2.9
1	A	27	HIS	2.9
1	A	271	SER	2.9
1	A	42	GLU	2.9
1	A	190	SER	2.8
1	A	329	PHE	2.8
1	A	68	PHE	2.8
2	B	629	ARG	2.7
1	A	157	VAL	2.7
1	A	193	ILE	2.7
1	A	233	ASN	2.7
1	A	250	SER	2.7
1	A	181	ASN	2.6
2	B	646	ASN	2.6
1	A	192	LEU	2.6
1	A	59	THR	2.6
1	A	223	ASP	2.6
1	A	24	GLU	2.6
1	A	345	LEU	2.6
2	B	632	VAL	2.5
1	A	267	PRO	2.5
1	A	28	LEU	2.5
1	A	140	TYR	2.5
1	A	232	ILE	2.5
2	B	650	GLN	2.5
1	A	16	ASP	2.5
1	A	301	THR	2.4
1	A	227	SER	2.4
1	A	110	VAL	2.4
1	A	281	ARG	2.4
1	A	207	ALA	2.4
1	A	97	ARG	2.3
1	A	156	SER	2.3
1	A	205	PRO	2.3
1	A	280	GLN	2.3
1	A	31	GLY	2.3
1	A	317	ASP	2.3
1	A	62	THR	2.2
2	B	634	GLU	2.2
1	A	208	LEU	2.2
1	A	204	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	45	LEU	2.2
1	A	245	ASP	2.2
1	A	82	VAL	2.2
1	A	331	GLU	2.2
2	B	636	SER	2.2
1	A	151	LYS	2.1
1	A	312	PHE	2.1
1	A	153	SER	2.1
1	A	311	SER	2.1
1	A	77	ASN	2.1
1	A	308	TRP	2.1
1	A	199	LEU	2.1
1	A	339	GLU	2.0
1	A	174	ASP	2.0
1	A	237	ASN	2.0
2	B	619	GLN	2.0
2	B	621	ARG	2.0
1	A	33	ASP	2.0
2	B	625	LEU	2.0

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 oligosaccharides 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.