



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 02:19 PM UTC

PDB ID : 5TD8 / pdb_00005td8
Title : Crystal structure of an Extended Dwarf Ndc80 Complex
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Deposited on : 2016-09-17
Resolution : 7.53 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 : 4-5-2 with Phenix2.0
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

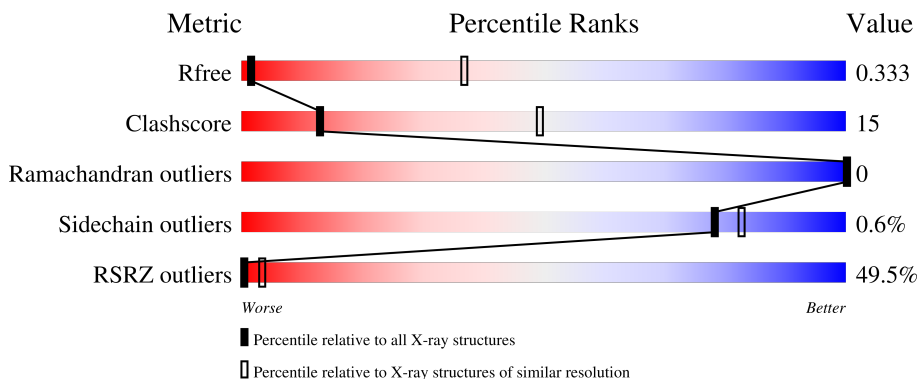
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.53 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	1167 (10.00-4.00)
Clashscore	190562	1000 (10.00-4.06)
Ramachandran outliers	187476	1054 (10.00-4.00)
Sidechain outliers	187428	1017 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

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 $\leq 5\%$. 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	279	
2	B	198	
3	C	114	
4	D	129	
5	E	145	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12626 atoms, of which 6191 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 Kinetochores protein NDC80.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	256	4302	1385	2144	363	404	6	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	111	SER	-	expression tag	UNP P40460
A	112	ASN	-	expression tag	UNP P40460
A	113	ALA	-	expression tag	UNP P40460

- Molecule 2 is a protein called Kinetochores protein NUF2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	186	2902	964	1376	247	303	12	0	0	0

- Molecule 3 is a protein called Kinetochores protein SPC24.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	C	111	1839	578	917	162	181	1	0	0	0

- Molecule 4 is a protein called Kinetochores protein SPC25.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	D	128	2011	632	998	190	186	5	0	0	0

- Molecule 5 is a protein called nanobody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
5	E	105	1566	512	756	143	152	3	0	0	0

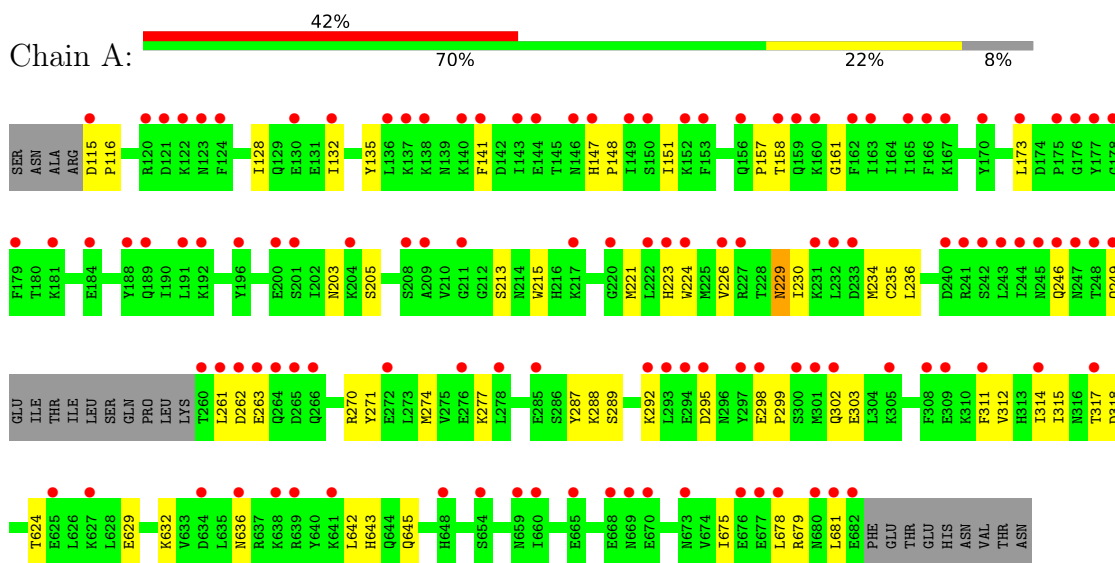
- Molecule 6 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total 2	Hg 2	0	0
6	B	2	Total 2	Hg 2	0	0
6	D	2	Total 2	Hg 2	0	0

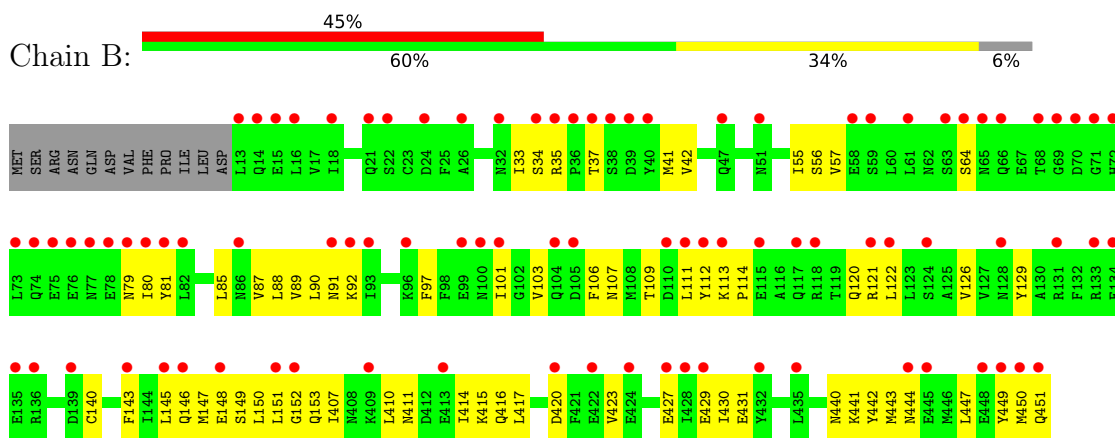
3 Residue-property plots [i](#)

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: Kinetochores protein NDC80

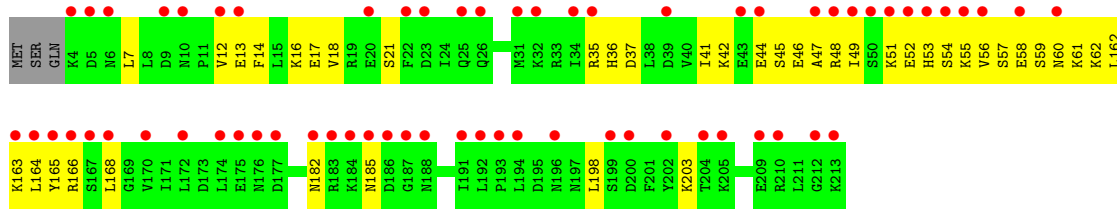


- Molecule 2: Kinetochores protein NUF2

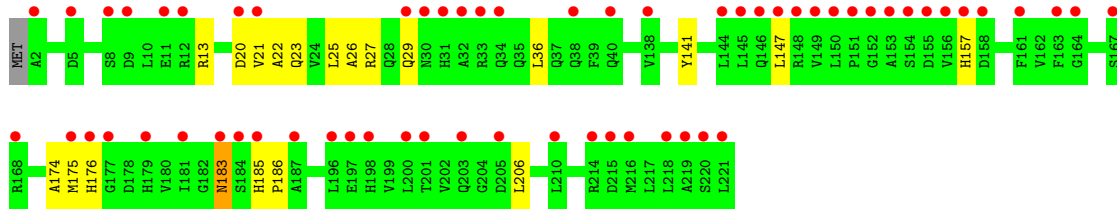
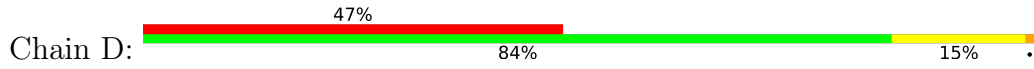


- Molecule 3: Kinetochores protein SPC24

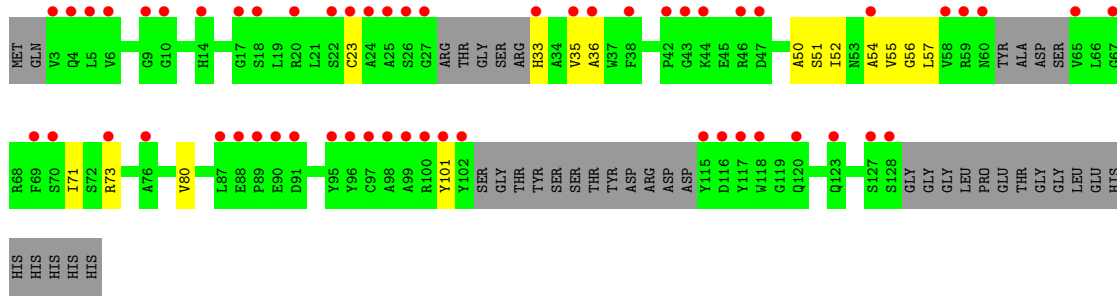
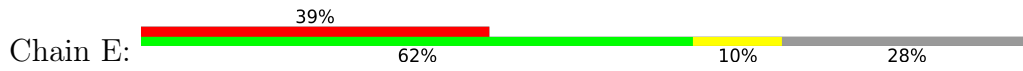




● Molecule 4: Kinetochores protein SPC25



● Molecule 5: nanobody



4 Data and refinement statistics i

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	226.82Å 226.82Å 237.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	113.41 – 7.53 113.41 – 7.53	Depositor EDS
% Data completeness (in resolution range)	99.7 (113.41-7.53) 99.7 (113.41-7.53)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 7.45Å)	Xtrriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.312 , 0.328 0.314 , 0.333	Depositor DCC
R_{free} test set	204 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtrriage
Anisotropy	0.073	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	0.016 for -l,-k,-h 0.013 for -h,l,k	Xtrriage
F_o, F_c correlation	0.70	EDS
Total number of atoms	12626	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.47% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HG

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	0.24	0/2199	0.44	0/2958
2	B	0.20	0/1547	0.45	0/2083
3	C	0.29	0/933	0.62	0/1251
4	D	0.16	0/1030	0.40	0/1392
5	E	0.14	0/826	0.36	0/1116
All	All	0.22	0/6535	0.46	0/8800

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 [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	2158	2144	2171	54	2
2	B	1526	1376	1493	66	0
3	C	922	917	932	72	2
4	D	1013	998	999	16	0
5	E	810	756	771	17	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	D	2	0	0	0	0
All	All	6435	6191	6366	192	2

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 15.

The worst 5 of 192 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:249:GLN:OE1	1:A:270:ARG:NH1	2.07	0.88
3:C:21:SER:HB3	5:E:57:LEU:HG	1.57	0.86
2:B:148:GLU:O	2:B:152:GLY:N	2.13	0.81
3:C:61:LYS:O	3:C:164:LEU:HB2	1.81	0.80
3:C:61:LYS:O	3:C:164:LEU:CB	2.32	0.78

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:SER:N	3:C:37:ASP:OD1[3_745]	2.04	0.16
1:A:213:SER:H	3:C:37:ASP:OD1[3_745]	1.54	0.06

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	252/279 (90%)	232 (92%)	20 (8%)	0	100	100
2	B	184/198 (93%)	163 (89%)	21 (11%)	0	100	100
3	C	109/114 (96%)	104 (95%)	5 (5%)	0	100	100
4	D	126/129 (98%)	112 (89%)	14 (11%)	0	100	100
5	E	97/145 (67%)	94 (97%)	3 (3%)	0	100	100
All	All	768/865 (89%)	705 (92%)	63 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	246/268 (92%)	244 (99%)	2 (1%)	73	80
2	B	175/187 (94%)	174 (99%)	1 (1%)	78	83
3	C	106/109 (97%)	106 (100%)	0	100	100
4	D	107/108 (99%)	106 (99%)	1 (1%)	70	79
5	E	83/115 (72%)	83 (100%)	0	100	100
All	All	717/787 (91%)	713 (99%)	4 (1%)	78	83

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	229	ASN
1	A	681	LEU
2	B	103	VAL
4	D	183	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	176	HIS
4	D	203	GLN
2	B	438	HIS
3	C	188	ASN
4	D	28	GLN

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](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	256/279 (91%)	2.16	118 (46%) 0 4	16, 46, 102, 144	0
2	B	186/198 (93%)	2.30	90 (48%) 0 3	26, 59, 110, 129	0
3	C	111/114 (97%)	2.74	64 (57%) 0 3	20, 42, 54, 65	0
4	D	128/129 (99%)	2.21	61 (47%) 0 4	20, 40, 70, 82	1 (0%)
5	E	105/145 (72%)	2.21	56 (53%) 0 3	23, 38, 53, 69	0
All	All	786/865 (90%)	2.29	389 (49%) 0 3	16, 44, 89, 144	1 (0%)

The worst 5 of 389 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	70	ASP	11.9
1	A	208	SER	9.2
5	E	27	GLY	9.1
4	D	156	VAL	9.0
3	C	9	ASP	8.5

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	HG	B	501	1/1	0.71	0.21	208,208,208,208	0
6	HG	D	302	1/1	0.94	0.22	77,77,77,77	1
6	HG	D	301	1/1	0.97	0.08	68,68,68,68	1
6	HG	A	702	1/1	0.97	0.08	144,144,144,144	1
6	HG	A	701	1/1	0.98	0.24	81,81,81,81	1
6	HG	B	502	1/1	0.98	0.06	115,115,115,115	1

6.5 Other polymers [i](#)

There are no such residues in this entry.