



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 24, 2024 – 04:38 PM EDT

PDB ID : 6QJ3
Title : Crystal structure of the *C. thermophilum* condensin Ycs4-Brn1 subcomplex
Authors : Hassler, M.; Haering, C.H.; Kschonsak, M.
Deposited on : 2019-01-22
Resolution : 3.30 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

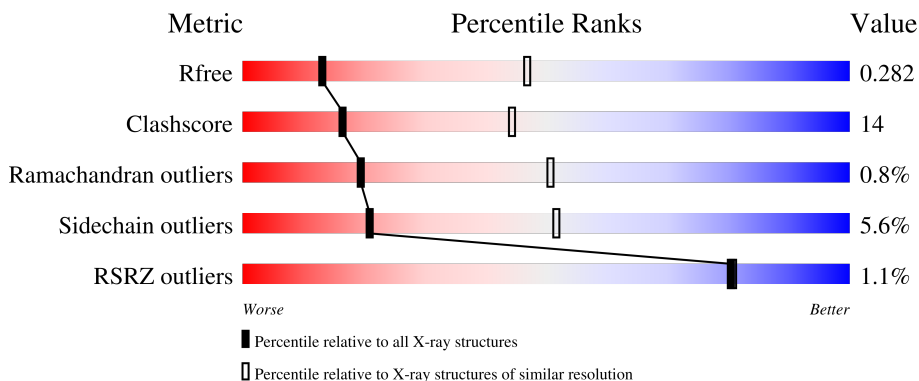
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



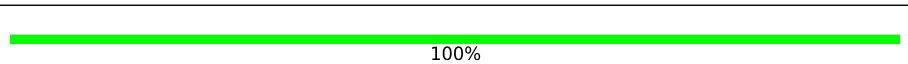
The reported resolution of this entry is 3.30 Å.

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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	1155	 65% 18% 15%
2	B	197	 16% 11% 72%
3	C	20	 100%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7700 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 Condensin complex subunit 1, Condensin complex subunit 1, Ycs4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	980	7187	4553	1251	1338	15	30	0	0	0

There are 121 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MSE	-	initiating methionine	UNP G0SB82
A	?	-	CYS	deletion	UNP G0SB82
A	?	-	ALA	deletion	UNP G0SB82
A	?	-	PRO	deletion	UNP G0SB82
A	?	-	ILE	deletion	UNP G0SB82
A	?	-	PHE	deletion	UNP G0SB82
A	?	-	PRO	deletion	UNP G0SB82
A	?	-	HIS	deletion	UNP G0SB82
A	?	-	PRO	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	LEU	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	PHE	deletion	UNP G0SB82
A	?	-	PRO	deletion	UNP G0SB82
A	?	-	TYR	deletion	UNP G0SB82
A	?	-	GLY	deletion	UNP G0SB82
A	?	-	ALA	deletion	UNP G0SB82
A	?	-	GLU	deletion	UNP G0SB82
A	?	-	ASP	deletion	UNP G0SB82
A	?	-	GLY	deletion	UNP G0SB82
A	?	-	PRO	deletion	UNP G0SB82
A	?	-	LEU	deletion	UNP G0SB82
A	?	-	LEU	deletion	UNP G0SB82
A	?	-	ALA	deletion	UNP G0SB82
A	?	-	ALA	deletion	UNP G0SB82
A	?	-	ASP	deletion	UNP G0SB82

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	CYS	deletion	UNP G0SB82
A	?	-	PRO	deletion	UNP G0SB82
A	?	-	THR	deletion	UNP G0SB82
A	?	-	HIS	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	ALA	deletion	UNP G0SB82
A	?	-	THR	deletion	UNP G0SB82
A	?	-	LYS	deletion	UNP G0SB82
A	?	-	ASP	deletion	UNP G0SB82
A	?	-	LYS	deletion	UNP G0SB82
A	?	-	ASP	deletion	UNP G0SB82
A	?	-	ILE	deletion	UNP G0SB82
A	?	-	HIS	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	ARG	deletion	UNP G0SB82
A	?	-	LEU	deletion	UNP G0SB82
A	?	-	ARG	deletion	UNP G0SB82
A	?	-	ASP	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	ASP	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	GLU	deletion	UNP G0SB82
A	?	-	LEU	deletion	UNP G0SB82
A	?	-	VAL	deletion	UNP G0SB82
A	?	-	LYS	deletion	UNP G0SB82
A	?	-	LYS	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	ARG	deletion	UNP G0SB82
A	?	-	GLN	deletion	UNP G0SB82
A	?	-	GLN	deletion	UNP G0SB82
A	?	-	GLU	deletion	UNP G0SB82
A	?	-	PRO	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	ARG	deletion	UNP G0SB82
A	?	-	PRO	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	ARG	deletion	UNP G0SB82
A	?	-	ASP	deletion	UNP G0SB82
A	?	-	GLU	deletion	UNP G0SB82
A	?	-	MET	deletion	UNP G0SB82

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP G0SB82
A	?	-	ILE	deletion	UNP G0SB82
A	?	-	GLU	deletion	UNP G0SB82
A	?	-	PRO	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	GLN	deletion	UNP G0SB82
A	?	-	ALA	deletion	UNP G0SB82
A	?	-	PRO	deletion	UNP G0SB82
A	?	-	THR	deletion	UNP G0SB82
A	?	-	LEU	deletion	UNP G0SB82
A	?	-	ASP	deletion	UNP G0SB82
A	?	-	GLY	deletion	UNP G0SB82
A	?	-	ALA	deletion	UNP G0SB82
A	?	-	ASP	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	THR	deletion	UNP G0SB82
A	?	-	VAL	deletion	UNP G0SB82
A	?	-	PRO	deletion	UNP G0SB82
A	?	-	ALA	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	GLN	deletion	UNP G0SB82
A	?	-	ALA	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	PRO	deletion	UNP G0SB82
A	?	-	THR	deletion	UNP G0SB82
A	?	-	LYS	deletion	UNP G0SB82
A	?	-	ARG	deletion	UNP G0SB82
A	?	-	GLN	deletion	UNP G0SB82
A	?	-	ASN	deletion	UNP G0SB82
A	?	-	LYS	deletion	UNP G0SB82
A	?	-	ASP	deletion	UNP G0SB82
A	?	-	ARG	deletion	UNP G0SB82
A	?	-	HIS	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	LEU	deletion	UNP G0SB82
A	?	-	GLY	deletion	UNP G0SB82
A	?	-	ALA	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	THR	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	ARG	deletion	UNP G0SB82

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	deletion	UNP G0SB82
A	?	-	GLY	deletion	UNP G0SB82
A	?	-	GLY	deletion	UNP G0SB82
A	?	-	GLY	deletion	UNP G0SB82
A	?	-	GLN	deletion	UNP G0SB82
A	?	-	ASN	deletion	UNP G0SB82
A	?	-	LYS	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	LYS	deletion	UNP G0SB82
A	?	-	GLN	deletion	UNP G0SB82
A	?	-	GLN	deletion	UNP G0SB82

- Molecule 2 is a protein called Condensin complex subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
2	B	56	413	266	67	79	1	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	222	GLY	-	expression tag	UNP G0SBJ6
B	223	HIS	-	expression tag	UNP G0SBJ6
B	224	MSE	-	expression tag	UNP G0SBJ6

- Molecule 3 is a protein called Brn1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	20	100	60	20	20	0	0	0

UNK
UNK
UNK
UNK
UNK

• Molecule 2: Condensin complex subunit 2



GLY

• Molecule 3: Brn1



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.61Å 81.76Å 132.88Å 90.00° 93.15° 90.00°	Depositor
Resolution (Å)	45.11 – 3.30 45.11 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (45.11-3.30) 99.4 (45.11-3.30)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 3.32Å)	Xtrriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.231 , 0.284 0.230 , 0.282	Depositor DCC
R_{free} test set	1984 reflections (7.11%)	wwPDB-VP
Wilson B-factor (Å ²)	96.9	Xtrriage
Anisotropy	0.389	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 114.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7700	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% 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

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	0.32	0/7122	0.52	2/9609 (0.0%)
2	B	0.44	0/418	0.87	4/561 (0.7%)
All	All	0.32	0/7540	0.55	6/10170 (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
2	B	0	3
All	All	0	6

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	285	ASN	O-C-N	7.35	134.47	122.70
2	B	254	LEU	CA-CB-CG	6.42	130.07	115.30
2	B	285	ASN	C-N-CA	5.64	135.81	121.70
1	A	18	ASP	C-N-CD	5.27	139.47	128.40
2	B	285	ASN	CA-C-N	-5.27	105.61	117.20

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1061	ASN	Peptide
1	A	450	GLY	Peptide
1	A	783	PRO	Peptide
2	B	253	GLN	Peptide

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Mol	Chain	Res	Type	Group
2	B	259	LEU	Peptide

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	7187	0	6776	192	0
2	B	413	0	395	35	0
3	C	100	0	27	0	0
All	All	7700	0	7198	213	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 213 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)
2:B:270:ALA:HA	2:B:286:HIS:CE1	1.67	1.30
1:A:335:ASP:OD2	2:B:241:SER:N	1.71	1.23
1:A:28:ASP:O	1:A:31:LEU:CD1	1.91	1.18
1:A:28:ASP:O	1:A:31:LEU:HD11	1.43	1.17
1:A:27:ALA:HB1	1:A:73:SER:OG	1.46	1.15

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	930/1155 (80%)	865 (93%)	57 (6%)	8 (1%)	17	48
2	B	52/197 (26%)	42 (81%)	10 (19%)	0	100	100
All	All	982/1352 (73%)	907 (92%)	67 (7%)	8 (1%)	19	51

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	HIS
1	A	784	THR
1	A	1062	THR
1	A	1148	ILE
1	A	875	ILE

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	686/923 (74%)	650 (95%)	36 (5%)	23	54
2	B	41/163 (25%)	36 (88%)	5 (12%)	5	20
All	All	727/1086 (67%)	686 (94%)	41 (6%)	21	52

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1027	LEU
1	A	1119	MSE
1	A	1032	GLU
1	A	1071	ASP
2	B	288	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	HIS

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Mol	Chain	Res	Type
1	A	443	HIS
1	A	1003	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 monosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1180:UNK	C	1188:UNK	N	13.39
1	C	6:UNK	C	8:UNK	N	4.62

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	922/1155 (79%)	-0.15	10 (1%) 80 81	43, 114, 203, 272	0
2	B	55/197 (27%)	0.23	1 (1%) 68 67	54, 139, 170, 192	0
3	C	0/20	-	-	-	-
All	All	977/1372 (71%)	-0.13	11 (1%) 80 81	43, 115, 202, 272	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1139	PHE	3.8
2	B	286	HIS	3.3
1	A	764	SER	3.0
1	A	803	LEU	2.8
1	A	1016	SER	2.6

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 monosaccharides 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.