



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:43 AM UTC

PDB ID : 6QJ1 / pdb_00006qj1
Title : Crystal structure of the C. thermophilum condensin Smc2 ATPase head (crystal from I)
Authors : Hassler, M.; Haering, C.H.
Deposited on : 2019-01-22
Resolution : 2.56 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

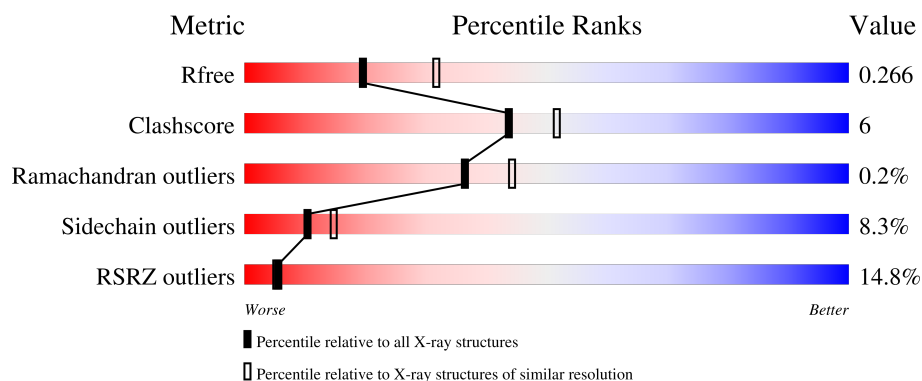
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	430	13% 76% 15% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3246 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 Structural maintenance of chromosomes protein, Structural maintenance of chromosomes protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	Se	0	0	0
			3205	2038	555	597	1	14			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP G0S5H7
A	200	ALA	ARG	conflict	UNP G0S5H7
A	974	SER	-	linker	UNP G0S5H7
A	975	GLY	-	linker	UNP G0S5H7
A	976	GLY	-	linker	UNP G0S5H7
A	977	SER	-	linker	UNP G0S5H7
A	978	GLY	-	linker	UNP G0S5H7
A	979	GLY	-	linker	UNP G0S5H7
A	980	SER	-	linker	UNP G0S5H7

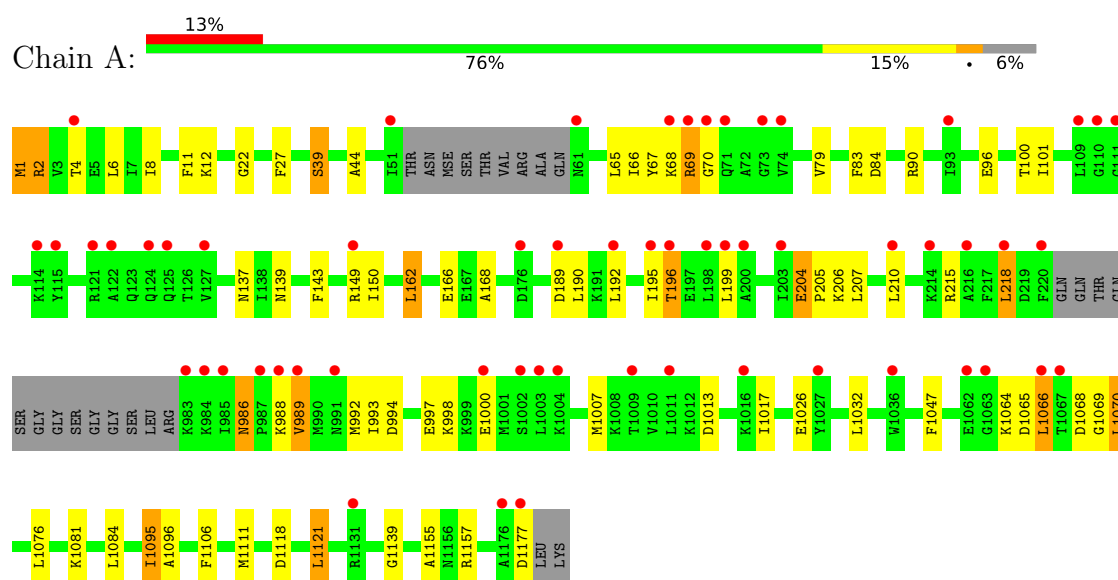
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	41	Total	O	0	0
			41	41		

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: Structural maintenance of chromosomes protein, Structural maintenance of chromosomes protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.32Å 107.98Å 174.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.89 – 2.56 45.89 – 2.56	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.89-2.56) 100.0 (45.89-2.56)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.51Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.233 , 0.262 0.238 , 0.266	Depositor DCC
R_{free} test set	1585 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	72.6	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3246	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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	0.14	0/3234	0.36	1/4323 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	ARG	N-CA-C	6.15	122.44	113.40

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	3205	0	3324	40	0
2	A	41	0	0	2	0
All	All	3246	0	3324	40	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 6.

All (40) 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:69:ARG:N	1:A:70:GLY:HA2	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MSE:HE1	1:A:101:ILE:HD12	1.80	0.63
1:A:2:ARG:HD3	1:A:84:ASP:HB3	1.81	0.63
1:A:96:GLU:OE1	1:A:96:GLU:N	2.34	0.57
1:A:150:ILE:HG23	1:A:1096:ALA:HB3	1.88	0.56
1:A:192:LEU:O	1:A:196:THR:OG1	2.19	0.56
1:A:1:MSE:N	2:A:1205:HOH:O	2.39	0.55
1:A:1065:ASP:OD2	1:A:1066:LEU:N	2.41	0.52
1:A:215:ARG:HA	1:A:218:LEU:HD12	1.91	0.52
1:A:986:ASN:HB3	1:A:989:VAL:HG23	1.91	0.52
1:A:44:ALA:HB1	1:A:79:VAL:HG11	1.93	0.51
1:A:162:LEU:HD21	1:A:1032:LEU:HD21	1.93	0.50
1:A:1118:ASP:HA	1:A:1121:LEU:HD22	1.94	0.50
1:A:162:LEU:HD22	1:A:166:GLU:HG3	1.92	0.49
1:A:1013:ASP:O	1:A:1017:ILE:HG12	2.12	0.49
1:A:195:ILE:HG21	1:A:1007:MSE:HG2	1.95	0.48
1:A:68:LYS:C	1:A:70:GLY:HA2	2.39	0.47
1:A:196:THR:HG23	1:A:1007:MSE:HE1	1.97	0.47
1:A:90:ARG:NH1	1:A:1139:GLY:O	2.42	0.47
1:A:27:PHE:CD1	1:A:1155:ALA:HA	2.51	0.46
1:A:215:ARG:HA	1:A:218:LEU:CD1	2.45	0.46
1:A:204:GLU:N	1:A:205:PRO:HD2	2.31	0.45
1:A:83:PHE:HE1	1:A:1111:MSE:HE1	1.81	0.45
1:A:168:ALA:HB1	1:A:1106:PHE:CG	2.52	0.45
1:A:66:ILE:HG22	1:A:67:TYR:H	1.82	0.44
1:A:67:TYR:CZ	1:A:68:LYS:HE2	2.52	0.44
1:A:1081:LYS:HA	1:A:1081:LYS:HD3	1.80	0.43
1:A:988:LYS:HB2	1:A:992:MSE:HE3	2.01	0.42
1:A:1068:ASP:OD2	1:A:1068:ASP:N	2.51	0.42
1:A:12:LYS:HE3	1:A:65:LEU:HD22	2.01	0.42
1:A:39:SER:HB3	2:A:1204:HOH:O	2.19	0.42
1:A:1064:LYS:HD3	1:A:1064:LYS:HA	1.76	0.42
1:A:1047:PHE:CE1	1:A:1095:ILE:HG12	2.55	0.42
1:A:1070:LEU:HD12	1:A:1070:LEU:HA	1.86	0.42
1:A:8:ILE:HG22	1:A:11:PHE:HB3	2.01	0.42
1:A:993:ILE:O	1:A:997:GLU:HB2	2.19	0.41
1:A:22:GLY:O	1:A:1157:ARG:NE	2.44	0.41
1:A:162:LEU:HB2	1:A:1069:GLY:HA2	2.02	0.41
1:A:994:ASP:O	1:A:998:LYS:HG2	2.21	0.41
1:A:143:PHE:HB2	1:A:1111:MSE:O	2.21	0.40

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	400/430 (93%)	384 (96%)	15 (4%)	1 (0%)	36	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	ASN

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	351/358 (98%)	322 (92%)	29 (8%)	10	15

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	2	ARG
1	A	4	THR
1	A	6	LEU
1	A	39	SER
1	A	100	THR
1	A	139	ASN
1	A	149	ARG
1	A	162	LEU
1	A	189	ASP

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Mol	Chain	Res	Type
1	A	190	LEU
1	A	196	THR
1	A	199	LEU
1	A	204	GLU
1	A	206	LYS
1	A	207	LEU
1	A	210	LEU
1	A	218	LEU
1	A	986	ASN
1	A	989	VAL
1	A	1000	GLU
1	A	1026	GLU
1	A	1066	LEU
1	A	1070	LEU
1	A	1076	LEU
1	A	1084	LEU
1	A	1095	ILE
1	A	1121	LEU
1	A	1177	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides 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

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	392/430 (91%)	1.00	58 (14%) 5 5	52, 85, 133, 149	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	51	ILE	8.9
1	A	220	PHE	7.3
1	A	73	GLY	4.9
1	A	69	ARG	4.5
1	A	1176	ALA	3.8
1	A	198	LEU	3.5
1	A	195	ILE	3.5
1	A	988	LYS	3.4
1	A	203	ILE	3.4
1	A	1011	LEU	3.4
1	A	218	LEU	3.3
1	A	71	GLN	3.3
1	A	111	GLY	3.2
1	A	989	VAL	3.2
1	A	70	GLY	3.1
1	A	109	LEU	3.1
1	A	1002	SER	3.1
1	A	983	LYS	3.0
1	A	985	ILE	3.0
1	A	74	VAL	3.0
1	A	984	LYS	2.9
1	A	1003	LEU	2.9
1	A	1027	TYR	2.8
1	A	216	ALA	2.8
1	A	124	GLN	2.8
1	A	1004	LYS	2.8
1	A	1062	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	115	TYR	2.7
1	A	1000	GLU	2.7
1	A	61	ASN	2.7
1	A	210	LEU	2.7
1	A	1066	LEU	2.7
1	A	125	GLN	2.6
1	A	1067	THR	2.6
1	A	4	THR	2.6
1	A	200	ALA	2.6
1	A	987	PRO	2.5
1	A	199	LEU	2.5
1	A	1063	GLY	2.5
1	A	114	LYS	2.4
1	A	1177	ASP	2.4
1	A	1036	TRP	2.3
1	A	176	ASP	2.2
1	A	121	ARG	2.2
1	A	991	ASN	2.2
1	A	196	THR	2.2
1	A	110	GLY	2.2
1	A	189	ASP	2.2
1	A	68	LYS	2.2
1	A	192	LEU	2.1
1	A	214	LYS	2.1
1	A	122	ALA	2.1
1	A	93	ILE	2.1
1	A	1016	LYS	2.1
1	A	127	VAL	2.1
1	A	149	ARG	2.0
1	A	1131	ARG	2.0
1	A	1009	THR	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.