



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 02:47 AM UTC

PDB ID : 6R7O / pdb_00006r7o
Title : Crystal structure of the central region of human cohesin subunit STAG1
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Deposited on : 2019-03-29
Resolution : 2.31 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
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

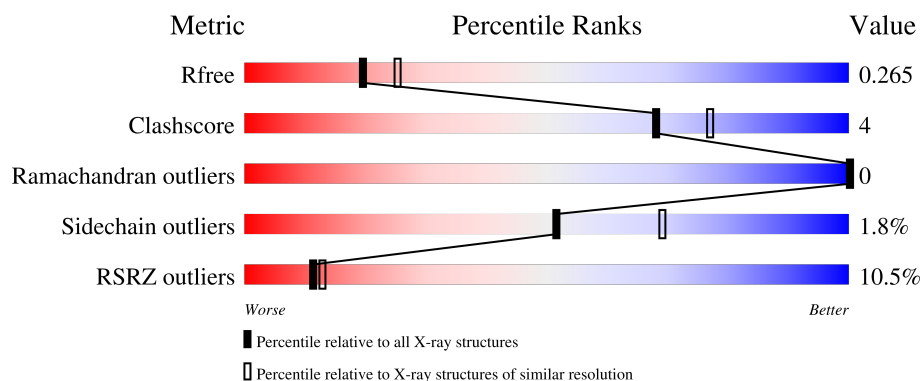
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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 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	459	6% 88% 6% • 6%
1	B	459	14% 81% 13% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7088 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 Cohesin subunit SA-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	0	0
			3458	2204	574	658	22			
1	B	430	Total	C	N	O	S	0	0	0
			3446	2195	577	652	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	457	SER	-	expression tag	UNP Q8WVM7
A	458	MET	-	expression tag	UNP Q8WVM7
B	457	SER	-	expression tag	UNP Q8WVM7
B	458	MET	-	expression tag	UNP Q8WVM7

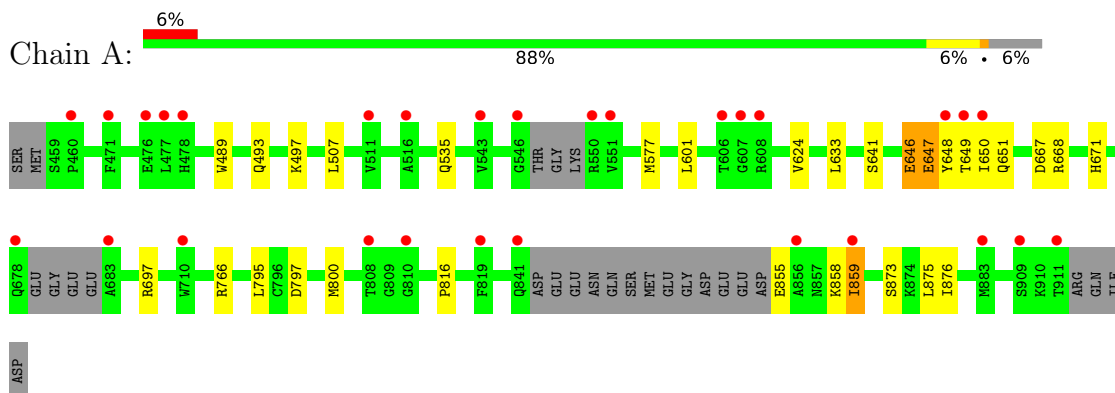
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	135	Total	O	0	0
			135	135		
2	B	49	Total	O	0	0
			49	49		

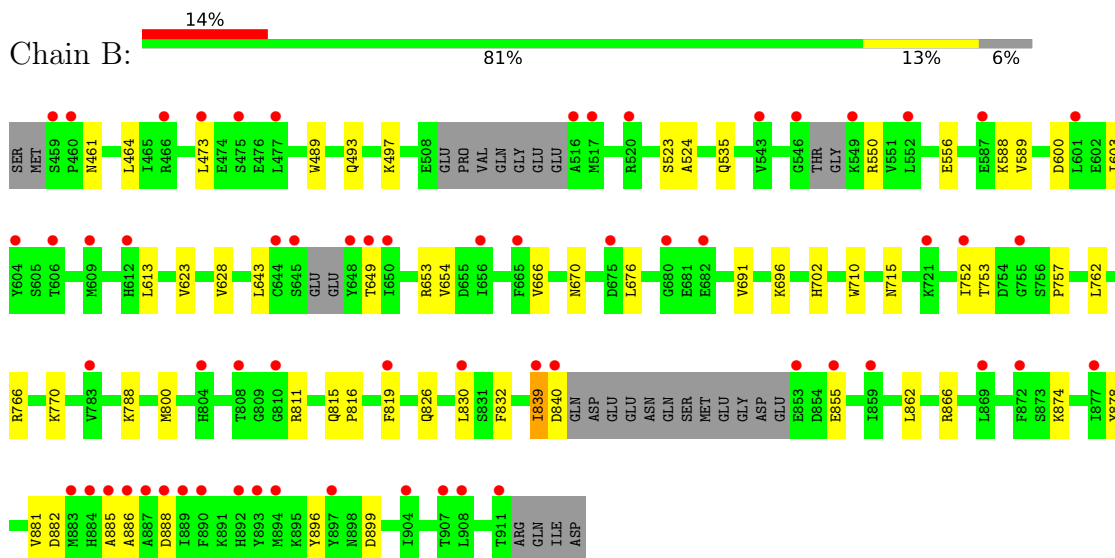
3 Residue-property plots [i](#)

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: Cohesin subunit SA-1



• Molecule 1: Cohesin subunit SA-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	154.65Å 166.72Å 46.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	113.36 – 2.31 113.36 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.6 (113.36-2.31) 99.9 (113.36-2.31)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.32Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.226 , 0.264 0.229 , 0.265	Depositor DCC
R_{free} test set	2728 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7088	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.88% 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	0.08	0/3520	0.23	0/4762
1	B	0.08	0/3506	0.25	0/4737
All	All	0.08	0/7026	0.24	0/9499

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	3458	0	3425	17	0
1	B	3446	0	3427	32	0
2	A	135	0	0	2	0
2	B	49	0	0	0	0
All	All	7088	0	6852	49	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 4.

All (49) 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:B:523:SER:OG	1:B:588:LYS:NZ	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:800:MET:HE3	1:B:874:LYS:HG2	1.74	0.70
1:B:613:LEU:HD23	1:B:653:ARG:HD2	1.74	0.70
1:B:589:VAL:HG11	1:B:623:VAL:HG11	1.76	0.68
1:A:601:LEU:HB2	1:A:646:GLU:HG3	1.76	0.67
1:B:550:ARG:NH1	1:B:556:GLU:OE2	2.33	0.61
1:B:752:ILE:HG23	1:B:757:PRO:HG3	1.82	0.61
1:B:676:LEU:HD22	1:B:691:VAL:HG21	1.82	0.61
1:A:855:GLU:HG2	1:A:858:LYS:HE3	1.82	0.60
1:A:493:GLN:HG2	1:A:497:LYS:HE2	1.84	0.58
1:A:648:TYR:HA	1:A:651:GLN:HB3	1.86	0.58
1:B:770:LYS:HG2	1:B:819:PHE:HE1	1.70	0.57
1:A:667:ASP:O	1:A:671:HIS:ND1	2.35	0.56
1:A:766:ARG:NH1	1:A:816:PRO:O	2.41	0.52
1:B:839:ILE:HG22	1:B:840:ASP:H	1.74	0.52
1:B:862:LEU:HD11	1:B:899:ASP:HB3	1.92	0.52
1:B:493:GLN:HG2	1:B:497:LYS:HE2	1.90	0.51
1:A:507:LEU:HD13	1:A:577:MET:HE2	1.92	0.51
1:B:830:LEU:HD11	1:B:886:ALA:HA	1.92	0.50
1:B:473:LEU:HD13	1:B:524:ALA:HB2	1.95	0.49
1:A:668:ARG:NH2	2:A:1007:HOH:O	2.46	0.48
1:A:489:TRP:CD2	1:A:535:GLN:HG2	2.49	0.48
1:B:600:ASP:HB3	1:B:603:ILE:HD13	1.97	0.47
1:B:752:ILE:HD13	1:B:762:LEU:HD23	1.95	0.47
1:B:753:THR:O	1:B:811:ARG:NH2	2.47	0.47
1:B:826:GLN:HG2	1:B:881:VAL:HG12	1.97	0.47
1:A:800:MET:HE2	1:A:875:LEU:HD23	1.97	0.46
1:B:866:ARG:NH1	1:B:899:ASP:O	2.47	0.46
1:B:489:TRP:CD2	1:B:535:GLN:HG2	2.51	0.45
1:B:770:LYS:HG2	1:B:819:PHE:CE1	2.51	0.45
1:A:859:ILE:H	1:A:859:ILE:HG13	1.57	0.45
1:A:647:GLU:CD	1:A:649:THR:HB	2.42	0.45
1:B:628:VAL:O	1:B:696:LYS:HE3	2.17	0.45
1:B:788:LYS:HB3	1:B:832:PHE:HE1	1.81	0.44
1:B:800:MET:HG2	1:B:874:LYS:HE2	1.98	0.44
1:B:670:ASN:OD1	1:B:715:ASN:ND2	2.51	0.44
1:A:489:TRP:CE2	1:A:535:GLN:HG2	2.53	0.43
1:B:766:ARG:O	1:B:770:LYS:HG3	2.19	0.42
1:A:873:SER:HA	1:A:876:ILE:HD12	2.01	0.42
1:B:489:TRP:O	1:B:493:GLN:HB2	2.20	0.42
1:B:882:ASP:OD2	1:B:885:ALA:N	2.47	0.42
1:A:493:GLN:NE2	2:A:1012:HOH:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:839:ILE:O	1:B:896:TYR:OH	2.31	0.41
1:B:815:GLN:N	1:B:816:PRO:HD2	2.36	0.41
1:B:666:VAL:HG21	1:B:710:TRP:CD1	2.56	0.41
1:B:461:ASN:HA	1:B:464:LEU:HB2	2.02	0.41
1:A:633:LEU:HD13	1:A:697:ARG:HA	2.03	0.40
1:A:624:VAL:O	1:A:697:ARG:NE	2.54	0.40
1:B:800:MET:HE1	1:B:878:TYR:HB2	2.04	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	425/459 (93%)	415 (98%)	10 (2%)	0	100	100
1	B	420/459 (92%)	408 (97%)	12 (3%)	0	100	100
All	All	845/918 (92%)	823 (97%)	22 (3%)	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	385/415 (93%)	378 (98%)	7 (2%)	51	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	384/415 (92%)	377 (98%)	7 (2%)	51	69
All	All	769/830 (93%)	755 (98%)	14 (2%)	51	69

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	641	SER
1	A	646	GLU
1	A	647	GLU
1	A	650	ILE
1	A	795	LEU
1	A	797	ASP
1	A	859	ILE
1	B	643	LEU
1	B	649	THR
1	B	654	VAL
1	B	702	HIS
1	B	839	ILE
1	B	855	GLU
1	B	888	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	651	GLN
1	A	736	GLN
1	A	804	HIS
1	A	815	GLN
1	B	493	GLN
1	B	652	ASN
1	B	736	GLN
1	B	748	GLN
1	B	820	ASN
1	B	863	HIS

5.3.3 RNA ⓘ

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	433/459 (94%)	0.56	29 (6%) 24 26	32, 56, 89, 104	0
1	B	430/459 (93%)	1.06	62 (14%) 6 7	43, 69, 103, 124	0
All	All	863/918 (94%)	0.81	91 (10%) 11 13	32, 62, 98, 124	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	460	PRO	5.5
1	A	546	GLY	4.5
1	B	887	ALA	4.5
1	B	648	TYR	4.5
1	B	546	GLY	4.3
1	B	911	THR	4.2
1	B	869	LEU	4.2
1	B	853	GLU	4.1
1	B	459	SER	4.0
1	B	908	LEU	3.9
1	B	516	ALA	3.9
1	B	606	THR	3.9
1	B	892	HIS	3.9
1	A	511	VAL	3.8
1	A	683	ALA	3.8
1	B	872	PHE	3.7
1	B	907	THR	3.5
1	B	682	GLU	3.4
1	A	859	ILE	3.3
1	B	890	PHE	3.3
1	B	645	SER	3.3
1	A	606	THR	3.2
1	B	839	ILE	3.2
1	A	649	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	804	HIS	3.1
1	A	648	TYR	3.1
1	B	650	ILE	3.0
1	B	549	LYS	3.0
1	A	477	LEU	3.0
1	A	911	THR	3.0
1	B	877	ILE	3.0
1	B	680	GLY	3.0
1	B	477	LEU	2.9
1	A	841	GLN	2.8
1	B	819	PHE	2.8
1	B	894	MET	2.8
1	B	889	ILE	2.8
1	B	904	ILE	2.8
1	A	476	GLU	2.8
1	B	855	GLU	2.8
1	B	473	LEU	2.8
1	A	471	PHE	2.8
1	B	649	THR	2.7
1	A	650	ILE	2.7
1	B	612	HIS	2.7
1	A	819	PHE	2.7
1	A	856	ALA	2.6
1	B	886	ALA	2.6
1	B	552	LEU	2.6
1	B	830	LEU	2.6
1	A	608	ARG	2.6
1	B	609	MET	2.5
1	B	601	LEU	2.5
1	B	884	HIS	2.5
1	B	840	ASP	2.5
1	B	466	ARG	2.4
1	B	543	VAL	2.4
1	A	883	MET	2.4
1	A	678	GLN	2.4
1	B	897	TYR	2.4
1	A	607	GLY	2.4
1	A	810	GLY	2.4
1	A	551	VAL	2.4
1	B	885	ALA	2.3
1	B	783	VAL	2.3
1	A	516	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	644	CYS	2.3
1	B	808	THR	2.3
1	A	478	HIS	2.3
1	B	475	SER	2.3
1	B	520	ARG	2.2
1	B	893	TYR	2.2
1	B	665	PHE	2.2
1	B	883	MET	2.2
1	B	810	GLY	2.2
1	B	656	ILE	2.2
1	A	543	VAL	2.2
1	B	721	LYS	2.1
1	A	460	PRO	2.1
1	B	755	GLY	2.1
1	A	909	SER	2.1
1	B	752	ILE	2.1
1	A	710	TRP	2.1
1	B	587	GLU	2.1
1	B	859	ILE	2.1
1	B	604	TYR	2.1
1	A	808	THR	2.0
1	B	888	ASP	2.0
1	B	517	MET	2.0
1	B	675	ASP	2.0
1	A	550	ARG	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.