

wwPDB X-ray Structure Validation Summary Report (i)

Sep 5, 2024 – 04:13 pm BST

PDB ID	:	8ROD
Title	:	Human cohesin SMC1A-HD(shortCC-EQ)/RAD21-C complex - Open/closed
		P-loop conformation
Authors	:	Vitoria Gomes, M.; Romier, C.
Deposited on	:	2024-01-11
Resolution	:	1.50 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.50 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	164625	3717 (1.50-1.50)
Clashscore	180529	4048 (1.50-1.50)
Ramachandran outliers	177936	3970(1.50-1.50)
Sidechain outliers	177891	3967 (1.50-1.50)
RSRZ outliers	164620	3718 (1.50-1.50)

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 <=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	А	366	19%	12% ••				
2	В	81	5% 67% ·	30%				



 $\mathbf{2}$

Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3678 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 1A.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	357	Total 2865	C 1831	N 482	0 542	S 10	0	17	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	176	GLY	-	linker	UNP Q14683
А	177	SER	-	linker	UNP Q14683
А	178	GLY	-	linker	UNP Q14683
А	179	SER	-	linker	UNP Q14683
А	180	LEU	-	linker	UNP Q14683
А	181	VAL	-	linker	UNP Q14683
А	182	PRO	-	linker	UNP Q14683
А	183	ARG	-	linker	UNP Q14683
А	184	GLY	-	linker	UNP Q14683
А	185	SER	-	linker	UNP Q14683
А	1053	GLY	-	linker	UNP Q14683
А	1054	SER	-	linker	UNP Q14683
А	1055	ALA	-	linker	UNP Q14683
A	1056	LYS	-	linker	UNP Q14683
А	1157	GLN	GLU	engineered mutation	UNP Q14683

There are 15 discrepancies between the modelled and reference sequences:

• Molecule 2 is a protein called 64-kDa C-terminal product.

Mol	Chain	Residues		Ato	\mathbf{ms}			ZeroOcc	AltConf	Trace
2	В	57	Total 448	C 284	N 78	O 85	S 1	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	557	MET	-	initiating methionine	UNP O60216

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Chain	Residue	Modelled	Actual	Comment	Reference
В	630	GLY	-	expression tag	UNP O60216
В	631	SER	-	expression tag	UNP O60216
В	632	LEU	-	expression tag	UNP O60216
В	633	GLU	-	expression tag	UNP O60216
В	634	VAL	-	expression tag	UNP O60216
В	635	LEU	-	expression tag	UNP O60216
В	636	PHE	-	expression tag	UNP O60216
В	637	GLN	-	expression tag	UNP O60216

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	А	1	Total 5	0 4	S 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	287	Total O 287 287	0	0
4	В	73	TotalO7373	0	0



MET LYS THR GLN GGLN MET LEU GLN GLN GLN GLN CGLN CGLN CLYS

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.



CEU VAL VAL CEU

• Molecule 1: Structural maintenance of chromosomes protein 1A



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants	66.11Å 113.84Å 134.47Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution (Å)	43.55 - 1.50	Depositor
Resolution (A)	43.55 - 1.50	EDS
% Data completeness	99.9(43.55-1.50)	Depositor
(in resolution range)	99.8 (43.55 - 1.50)	EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.36 (at 1.50 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.17_3644	Depositor
P. P.	0.198 , 0.232	Depositor
n, n_{free}	0.199 , 0.233	DCC
R_{free} test set	3994 reflections $(4.92%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	21.4	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.34 , 45.4	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3678	wwPDB-VP
Average B, all atoms $(Å^2)$	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.56% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: $\mathrm{SO4}$

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).

Mal	Chain	Bond	lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.34	0/2968	0.56	0/3993	
2	В	0.36	0/456	0.54	0/614	
All	All	0.35	0/3424	0.55	0/4607	

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	А	2865	0	2916	29	0
2	В	448	0	450	2	0
3	А	5	0	0	0	0
4	А	287	0	0	9	0
4	В	73	0	0	0	0
All	All	3678	0	3366	29	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.

The worst 5 of 29 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:143:ILE:HD13	1:A:1141[B]:LEU:HD21	1.65	0.79
1:A:1216:LEU:HD11	2:B:611:LEU:HD13	1.74	0.70
1:A:1177:GLN:O	1:A:1181:ASN:N	2.25	0.69
1:A:49:LEU:HD21	1:A:82[A]:MET:HE1	1.75	0.68
1:A:62:ARG:NH1	4:A:2104:HOH:O	2.26	0.62

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	Percer	ntiles
1	А	370/366~(101%)	364~(98%)	4 (1%)	2(0%)	25	8
2	В	55/81~(68%)	55 (100%)	0	0	100	100
All	All	425/447~(95%)	419 (99%)	4 (1%)	2 (0%)	25	8

All (2) Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	1125	MET
1	А	1124	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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.

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Mol	Chain	Analysed	d Rotameric Outliers		Percentiles	
Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	А	315/307~(103%)	311 (99%)	4 (1%)	65 41	
2	В	48/69~(70%)	47 (98%)	1 (2%)	48 20	
All	All	363/376~(96%)	358~(99%)	5 (1%)	67 38	

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All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	82[A]	MET
1	А	82[B]	MET
1	А	109	ASN
1	А	149	LYS
2	В	615	GLU

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

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)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Tuno	Chain	Dog	Link	В	ond leng	gths	E	Bond ang	gles
	Type	Ullalli	an Res Link		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
3	SO4	А	2000	-	$4,\!4,\!4$	0.68	0	$6,\!6,\!6$	0.54	0

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, 95^{th} 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	А	357/366~(97%)	0.98	71 (19%) 3 3	12, 28, 61, 113	17 (4%)
2	В	57/81~(70%)	0.34	4 (7%) 24 24	15, 23, 48, 92	0
All	All	414/447 (92%)	0.89	75 (18%) 4 3	12, 27, 59, 113	17 (4%)

The worst 5 of 75 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	1097	PHE	6.9
1	А	1090	ARG	6.3
1	А	1123	ARG	5.4
1	А	1210	CYS	5.2
1	А	1122	PHE	5.1

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)

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, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
3	SO4	А	2000	5/5	0.99	0.05	21,21,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.

