



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:49 PM UTC

PDB ID : 4PJU / pdb_00004pju
Title : crystal structure of human Stromal Antigen 2 (SA2) in complex with Sister Chromatid Cohesion protein 1 (Scc1)
Authors : Hara, K.; Chen, Z.; Tomchick, D.R.; Yu, H.
Deposited on : 2014-05-12
Resolution : 3.05 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

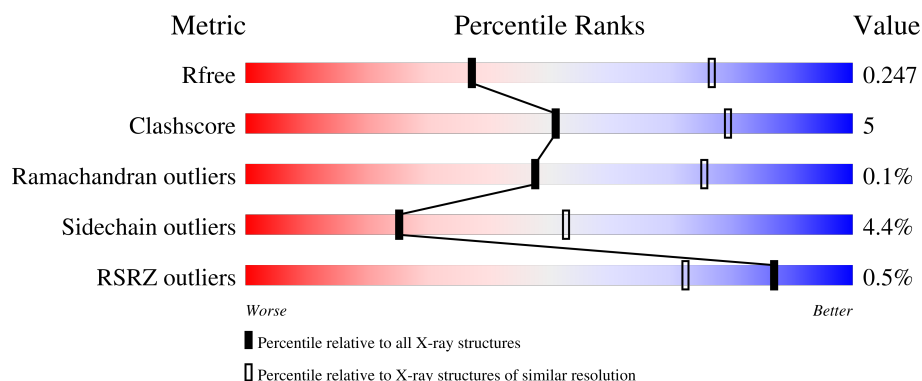
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

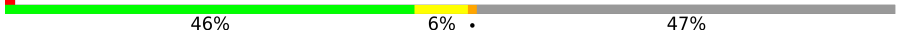
The reported resolution of this entry is 3.05 Å.

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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	981	
2	B	140	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15923 atoms, of which 7992 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-2.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
1	A	896	Total	C	H	N	O	S	Se		0	0	0
			14666	4674	7353	1216	1369	20	34				

- Molecule 2 is a protein called Double-strand-break repair protein rad21 homolog.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
2	B	74	Total	C	H	N	O	S	Se		0	0	0
			1235	385	639	101	107	1	2				

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total	O		
			19	19	0	0
3	B	3	Total	O		
			3	3	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.61Å 108.75Å 181.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.45 – 3.05 45.45 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.45-3.05) 99.9 (45.45-3.05)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 3.06Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.195 , 0.238 0.204 , 0.247	Depositor DCC
R_{free} test set	1521 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	92.4	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 63.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15923	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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	0.44	0/7402	0.79	3/9914 (0.0%)
2	B	0.47	0/604	0.79	0/812
All	All	0.44	0/8006	0.79	3/10726 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	801	GLN	N-CA-C	-6.73	104.65	112.92
1	A	939	ASP	N-CA-C	6.53	124.21	114.09
1	A	595	PHE	N-CA-C	5.52	118.56	109.72

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	7313	7353	7331	81	0
2	B	596	639	639	5	0
3	A	19	0	0	1	0
3	B	3	0	0	0	0
All	All	7931	7992	7970	83	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 5.

All (83) 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:241:MSE:HE1	1:A:278:GLN:HB2	1.69	0.72
1:A:224:MSE:HB3	1:A:311:GLU:HG3	1.74	0.69
1:A:337:HIS:NE2	3:A:1117:HOH:O	2.26	0.68
1:A:296:ARG:NH1	1:A:299:ASP:OD1	2.34	0.60
1:A:228:THR:HG23	1:A:318:MSE:HE1	1.84	0.59
1:A:803:MSE:N	1:A:803:MSE:SE	2.85	0.58
2:B:349:THR:OG1	2:B:350:THR:N	2.33	0.56
1:A:862:ARG:NH2	1:A:898:ASP:OD1	2.38	0.56
2:B:387:LYS:O	2:B:391:ARG:HB2	2.06	0.56
1:A:122:ILE:HG21	1:A:148:MSE:CE	2.35	0.56
1:A:361:ASN:OD1	1:A:363:LYS:N	2.39	0.56
1:A:950:GLU:OE2	1:A:953:ARG:NH2	2.37	0.55
1:A:122:ILE:HG21	1:A:148:MSE:HE2	1.89	0.54
1:A:243:ASN:OD1	1:A:246:ARG:NH2	2.37	0.54
1:A:564:THR:OG1	1:A:595:PHE:HB2	2.07	0.54
1:A:129:GLY:C	1:A:148:MSE:HE1	2.33	0.53
1:A:139:MSE:HE2	1:A:143:GLU:HB2	1.89	0.53
1:A:374:ARG:HG3	1:A:378:MSE:HE2	1.90	0.53
1:A:917:LYS:NZ	1:A:976:ASP:OD2	2.42	0.52
1:A:900:ILE:HG22	1:A:904:MSE:HE3	1.92	0.52
1:A:932:GLN:N	1:A:932:GLN:OE1	2.43	0.52
1:A:744:GLN:NE2	1:A:764:GLN:OE1	2.44	0.51
1:A:799:SER:O	1:A:801:GLN:N	2.43	0.50
1:A:1035:GLU:HG3	1:A:1036:ASP:HA	1.92	0.50
1:A:966:THR:OG1	1:A:967:ARG:N	2.46	0.48
1:A:861:ARG:HA	1:A:864:LEU:HD12	1.95	0.48
1:A:940:ARG:HD3	1:A:941:SER:N	2.29	0.48
1:A:228:THR:CG2	1:A:318:MSE:HE1	2.43	0.48
1:A:375:ILE:HA	1:A:378:MSE:HE3	1.95	0.48
1:A:280:GLU:HG3	1:A:284:MSE:HE3	1.95	0.47
1:A:799:SER:C	1:A:801:GLN:H	2.21	0.47
1:A:241:MSE:SE	1:A:278:GLN:NE2	2.98	0.47
1:A:473:LEU:HD13	2:B:353:LEU:HD21	1.97	0.47
1:A:549:THR:O	1:A:553:LYS:HG2	2.15	0.46
1:A:913:ILE:HG13	1:A:914:GLN:N	2.30	0.46
1:A:988:GLN:NE2	1:A:990:GLU:OE2	2.46	0.46
1:A:724:ASP:OD1	1:A:724:ASP:N	2.48	0.46
1:A:600:TYR:CE2	1:A:609:LEU:HB2	2.51	0.46
1:A:982:PHE:CE1	1:A:1030:MSE:HE1	2.50	0.46
1:A:529:ILE:HG23	1:A:563:ILE:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:LEU:HB2	1:A:592:PRO:HD3	1.98	0.46
1:A:759:LEU:O	1:A:763:LYS:HG3	2.16	0.46
1:A:765:MSE:HE1	1:A:815:TYR:HB2	1.98	0.45
1:A:592:PRO:HA	1:A:595:PHE:CZ	2.51	0.45
1:A:332:VAL:HG11	1:A:351:LEU:CD1	2.47	0.45
1:A:744:GLN:HB2	1:A:761:LEU:HD13	1.97	0.45
1:A:811:GLU:N	1:A:812:PRO:HD2	2.31	0.45
1:A:127:CYS:SG	1:A:148:MSE:HE3	2.56	0.45
1:A:908:ARG:HG2	1:A:909:GLN:N	2.31	0.45
1:A:802:ILE:HB	1:A:803:MSE:SE	2.66	0.45
1:A:112:ILE:HG13	1:A:113:ALA:N	2.32	0.45
1:A:689:SER:O	1:A:693:ARG:HG3	2.17	0.45
1:A:810:LEU:HB3	1:A:813:LEU:HD12	1.99	0.44
1:A:462:LYS:O	1:A:466:PHE:HD1	2.01	0.44
1:A:312:ILE:HA	1:A:315:TRP:CE3	2.53	0.43
1:A:335:THR:HG22	1:A:343:VAL:HG12	2.00	0.43
1:A:784:LYS:HB3	1:A:828:PHE:HE1	1.83	0.43
1:A:309:ILE:HG13	1:A:335:THR:HG21	2.00	0.43
1:A:336:MSE:HE3	1:A:374:ARG:CG	2.48	0.43
1:A:1011:LEU:HD12	1:A:1012:ARG:H	1.84	0.43
1:A:558:ASP:O	1:A:561:THR:OG1	2.37	0.42
1:A:762:LYS:HG3	1:A:813:LEU:HD23	2.00	0.42
1:A:706:TRP:O	1:A:708:LEU:N	2.52	0.42
1:A:610:ASP:OD2	1:A:649:ARG:NH2	2.52	0.42
1:A:332:VAL:HG11	1:A:351:LEU:HD11	2.02	0.42
1:A:617:ARG:HD2	1:A:657:LEU:HB2	2.02	0.42
1:A:1034:ARG:HG2	1:A:1042:MSE:SE	2.69	0.42
1:A:335:THR:CG2	1:A:343:VAL:HG12	2.49	0.42
1:A:121:PHE:HE1	1:A:179:ILE:HD11	1.83	0.42
1:A:339:LYS:HE3	2:B:346:ASP:OD2	2.20	0.41
1:A:658:ILE:HD13	1:A:703:LEU:CD2	2.50	0.41
1:A:1039:LEU:N	1:A:1040:PRO:CD	2.83	0.41
1:A:1037:VAL:HG12	1:A:1037:VAL:O	2.20	0.41
1:A:817:PRO:HB3	1:A:821:LEU:HD23	2.02	0.41
1:A:809:MSE:HE3	1:A:811:GLU:HB2	2.03	0.41
1:A:336:MSE:SE	1:A:378:MSE:HE1	2.70	0.41
1:A:495:TRP:HA	1:A:498:MSE:HE3	2.02	0.41
1:A:211:GLN:HG2	2:B:330:LYS:HD3	2.01	0.40
1:A:535:CYS:HB3	1:A:548:LEU:HD11	2.02	0.40
1:A:135:MSE:HE3	1:A:139:MSE:SE	2.72	0.40
1:A:227:MSE:HE3	1:A:285:MSE:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1012:ARG:HA	1:A:1015:LYS:HB2	2.04	0.40
1:A:938:PHE:CE1	1:A:995:LEU:HG	2.56	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	870/981 (89%)	836 (96%)	33 (4%)	1 (0%)	48	75
2	B	72/140 (51%)	70 (97%)	2 (3%)	0	100	100
All	All	942/1121 (84%)	906 (96%)	35 (4%)	1 (0%)	48	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1037	VAL

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	815/843 (97%)	779 (96%)	36 (4%)	25	53
2	B	69/125 (55%)	66 (96%)	3 (4%)	26	53
All	All	884/968 (91%)	845 (96%)	39 (4%)	25	53

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	LEU
1	A	92	LYS
1	A	130	VAL
1	A	142	SER
1	A	143	GLU
1	A	232	ASN
1	A	241	MSE
1	A	296	ARG
1	A	336	MSE
1	A	346	LYS
1	A	376	VAL
1	A	403	GLU
1	A	404	VAL
1	A	424	VAL
1	A	501	LEU
1	A	548	LEU
1	A	617	ARG
1	A	636	TYR
1	A	645	THR
1	A	650	VAL
1	A	677	GLU
1	A	703	LEU
1	A	711	CYS
1	A	748	ILE
1	A	754	THR
1	A	759	LEU
1	A	779	VAL
1	A	791	LEU
1	A	803	MSE
1	A	854	LYS
1	A	908	ARG
1	A	931	ILE
1	A	995	LEU
1	A	1012	ARG
1	A	1033	ARG
1	A	1036	ASP
2	B	334	SER
2	B	362	MSE
2	B	387	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	GLN
1	A	236	ASN
1	A	247	GLN
1	A	261	ASN
1	A	275	GLN
1	A	277	ASN
1	A	278	GLN
1	A	295	HIS
1	A	637	HIS
1	A	728	GLN
1	A	780	ASN
1	A	822	GLN
1	A	888	GLN
1	A	928	ASN
1	A	1046	ASN

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](#)

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 [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	862/981 (87%)	-0.48	4 (0%) 87 72	34, 85, 141, 192	0
2	B	72/140 (51%)	-0.61	1 (1%) 73 51	47, 74, 109, 141	0
All	All	934/1121 (83%)	-0.49	5 (0%) 87 72	34, 84, 140, 192	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	959	PHE	3.3
2	B	394	THR	3.0
1	A	966	THR	2.2
1	A	677	GLU	2.2
1	A	460	LEU	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.