



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:29 PM EDT

PDB ID : 4PJW / pdb_00004pjw
Title : crystal structure of human Stromal Antigen 2 (SA2) in complex with Sister Chromatid Cohesion protein 1 (Scc1), with bound MES
Authors : Hara, K.; Chen, Z.; Tomchick, D.R.; Yu, H.
Deposited on : 2014-05-12
Resolution : 2.85 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

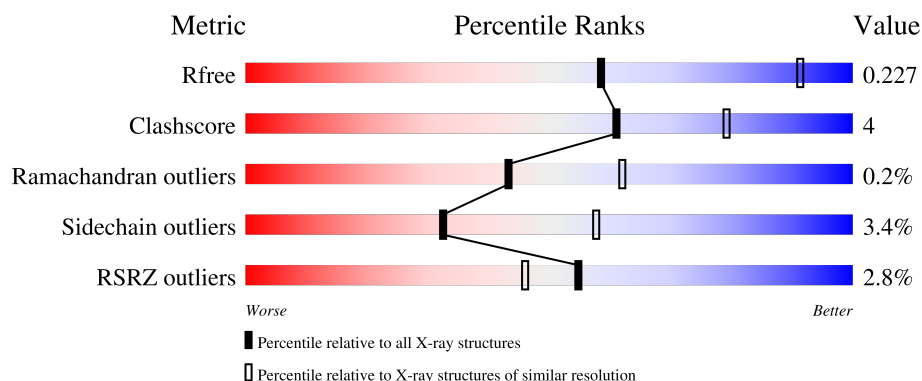
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

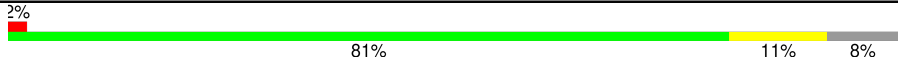
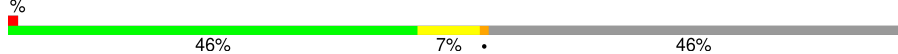
The reported resolution of this entry is 2.85 Å.

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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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 [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15768 atoms, of which 7768 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.

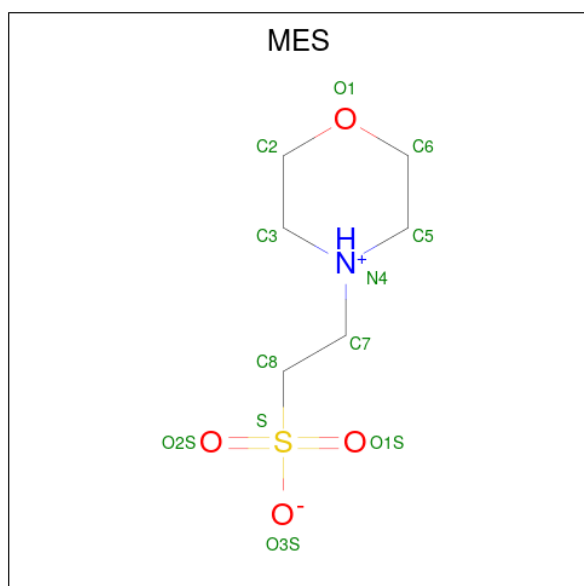
- Molecule 1 is a protein called Cohesin subunit SA-2.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
1	A	905	Total	C	H	N	O	S	Se		0	0	0
			14487	4705	7116	1228	1384	20	34				

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

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
2	B	75	Total	C	H	N	O	S	Se		0	0	0
			1242	390	639	102	108	1	2				

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms								ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S			0	0
			25	6	13	1	4	1				

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	11	Total 11	O 11	0	0
4	B	3	Total 3	O 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	78.73Å 108.05Å 180.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.70 – 2.85 41.70 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.70-2.85) 99.9 (41.70-2.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.210 , 0.225 0.213 , 0.227	Depositor DCC
R_{free} test set	1981 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	78.9	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.7	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	15768	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MES

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	0.35	0/7463	0.71	0/9997
2	B	0.39	0/612	0.71	0/824
All	All	0.35	0/8075	0.71	0/10821

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

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	7371	7116	7374	65	0
2	B	603	639	646	6	0
3	A	12	13	13	0	0
4	A	11	0	0	1	0
4	B	3	0	0	0	0
All	All	8000	7768	8033	67	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 (67) 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:986:ASN:HD22	1:A:994:PRO:HB3	1.49	0.78
1:A:678:GLU:HB3	1:A:679:PRO:C	2.16	0.70
1:A:1015:LYS:HD3	1:A:1048:LEU:HA	1.76	0.67
1:A:989:GLY:N	1:A:990:GLU:HA	2.09	0.65
1:A:1011:LEU:O	1:A:1015:LYS:N	2.29	0.65
1:A:802:ILE:HG12	1:A:810:LEU:HB3	1.78	0.64
1:A:803:MSE:HA	1:A:807:ARG:HB2	1.79	0.64
1:A:316:MSE:HE1	1:A:329:LEU:HG	1.80	0.62
1:A:756:GLU:N	1:A:756:GLU:OE2	2.33	0.62
1:A:225:LYS:NZ	1:A:311:GLU:OE2	2.33	0.61
1:A:950:GLU:OE2	1:A:953:ARG:NH2	2.34	0.60
1:A:917:LYS:NZ	1:A:976:ASP:OD2	2.37	0.57
1:A:224:MSE:HB3	1:A:311:GLU:HG3	1.88	0.56
1:A:937:ASN:O	1:A:939:ASP:N	2.39	0.56
1:A:807:ARG:HG3	1:A:810:LEU:HD12	1.87	0.55
1:A:227:MSE:HG2	1:A:315:TRP:CZ2	2.42	0.54
1:A:990:GLU:OE2	1:A:1033:ARG:NH2	2.40	0.54
1:A:316:MSE:HE1	1:A:329:LEU:CG	2.40	0.51
1:A:811:GLU:N	1:A:812:PRO:CD	2.74	0.51
1:A:90:MSE:O	1:A:91:GLY:C	2.54	0.51
1:A:676:GLY:O	1:A:677:GLU:HG3	2.12	0.50
1:A:183:VAL:HG21	1:A:226:LEU:HD12	1.94	0.49
1:A:197:MSE:HE2	1:A:284:MSE:HE3	1.93	0.49
1:A:374:ARG:HG3	1:A:378:MSE:HE2	1.95	0.49
1:A:122:ILE:HG21	1:A:148:MSE:CE	2.43	0.48
1:A:693:ARG:NH2	4:A:1201:HOH:O	2.45	0.48
1:A:213:ARG:NH2	2:B:327:ASP:OD1	2.43	0.48
1:A:591:LEU:HB2	1:A:592:PRO:HD3	1.95	0.47
1:A:609:LEU:HD21	1:A:646:ILE:HG23	1.96	0.47
1:A:862:ARG:NH2	1:A:898:ASP:OD1	2.47	0.47
1:A:989:GLY:H	1:A:990:GLU:HA	1.80	0.47
1:A:243:ASN:OD1	1:A:246:ARG:NH2	2.45	0.46
1:A:678:GLU:N	1:A:679:PRO:HA	2.30	0.46
1:A:129:GLY:C	1:A:148:MSE:HE1	2.41	0.45
2:B:349:THR:OG1	2:B:350:THR:N	2.49	0.45
1:A:994:PRO:HA	1:A:995:LEU:HA	1.72	0.45
1:A:898:ASP:OD1	1:A:898:ASP:N	2.49	0.45
1:A:919:LEU:HD21	1:A:955:PHE:HB3	1.98	0.45
1:A:329:LEU:HD13	1:A:367:PHE:CG	2.52	0.44
1:A:382:LYS:NZ	2:B:346:ASP:O	2.50	0.44
1:A:958:THR:HG22	1:A:958:THR:O	2.18	0.44
1:A:987:PRO:O	1:A:991:SER:OG	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:SER:N	1:A:809:MSE:HE1	2.32	0.43
1:A:890:MSE:HE2	1:A:950:GLU:HG3	1.99	0.43
1:A:807:ARG:CG	1:A:810:LEU:HD12	2.47	0.43
1:A:335:THR:HG22	1:A:343:VAL:HG12	2.00	0.43
1:A:647:PHE:CD1	1:A:647:PHE:C	2.97	0.43
1:A:231:VAL:HG22	1:A:285:MSE:HE1	2.00	0.42
1:A:309:ILE:HG13	1:A:335:THR:HG21	2.00	0.42
1:A:359:GLU:HB3	1:A:360:LEU:CA	2.49	0.42
1:A:316:MSE:HE1	1:A:329:LEU:CD2	2.49	0.42
2:B:394:THR:HG22	2:B:395:PRO:HD2	2.01	0.42
1:A:312:ILE:HA	1:A:315:TRP:CE3	2.54	0.42
1:A:1039:LEU:N	1:A:1040:PRO:CD	2.83	0.42
1:A:298:ARG:NH2	2:B:331:GLU:OE1	2.50	0.42
1:A:678:GLU:HB3	1:A:680:ASP:N	2.35	0.41
1:A:1010:LEU:HB3	1:A:1011:LEU:HB2	2.03	0.41
1:A:1010:LEU:HD22	1:A:1011:LEU:HB2	2.03	0.41
1:A:803:MSE:CA	1:A:807:ARG:HB2	2.50	0.41
1:A:807:ARG:HD2	1:A:810:LEU:CD1	2.51	0.41
1:A:1026:MSE:HE2	1:A:1031:SER:HB2	2.02	0.41
1:A:298:ARG:HG3	2:B:337:ILE:HD11	2.03	0.40
1:A:359:GLU:HB3	1:A:360:LEU:HA	2.03	0.40
1:A:643:GLU:HG2	1:A:643:GLU:O	2.22	0.40
1:A:677:GLU:OE1	1:A:677:GLU:N	2.54	0.40
1:A:658:ILE:HD13	1:A:703:LEU:CD2	2.52	0.40
1:A:244:THR:HG21	1:A:274:LEU:HD12	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	883/981 (90%)	856 (97%)	25 (3%)	2 (0%)	43 62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	73/140 (52%)	72 (99%)	1 (1%)	0	100	100
All	All	956/1121 (85%)	928 (97%)	26 (3%)	2 (0%)	43	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	938	PHE
1	A	727	GLU

5.3.2 Protein sidechains ⓘ

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	819/843 (97%)	793 (97%)	26 (3%)	34	59
2	B	70/125 (56%)	66 (94%)	4 (6%)	18	39
All	All	889/968 (92%)	859 (97%)	30 (3%)	32	58

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	294	VAL
1	A	298	ARG
1	A	325	ASN
1	A	327	SER
1	A	336	MSE
1	A	358	LYS
1	A	376	VAL
1	A	382	LYS
1	A	474	HIS
1	A	535	CYS
1	A	561	THR
1	A	585	VAL
1	A	626	THR
1	A	636	TYR

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Mol	Chain	Res	Type
1	A	669	LEU
1	A	708	LEU
1	A	724	ASP
1	A	737	THR
1	A	754	THR
1	A	809	MSE
1	A	816	THR
1	A	818	ASP
1	A	824	GLU
1	A	827	SER
1	A	894	ASN
1	A	1018	VAL
2	B	336	THR
2	B	337	ILE
2	B	348	VAL
2	B	362	MSE

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	247	GLN
1	A	295	HIS
1	A	573	GLN
1	A	608	HIS
1	A	618	ASN
1	A	735	GLN
1	A	764	GLN
1	A	925	GLN
1	A	934	ASN
2	B	378	GLN

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 [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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	MES	A	1101	-	12,12,12	2.25	1 (8%)	15,16,16	1.72	3 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MES	A	1101	-	-	2/6/14/14	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	MES	C8-S	-7.52	1.67	1.77

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	MES	C6-C5-N4	-3.38	104.99	110.12
3	A	1101	MES	C5-N4-C3	3.05	115.40	108.84
3	A	1101	MES	O1S-S-C8	2.37	110.30	106.73

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	MES	C8-C7-N4-C5
3	A	1101	MES	C8-C7-N4-C3

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 ⓘ

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	871/981 (88%)	-0.27	24 (2%) 55 46	14, 60, 121, 172	0
2	B	73/140 (52%)	-0.41	2 (2%) 56 47	22, 46, 85, 122	0
All	All	944/1121 (84%)	-0.28	26 (2%) 55 46	14, 59, 120, 172	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	938	PHE	5.1
1	A	260	ALA	4.5
1	A	994	PRO	4.2
1	A	91	GLY	4.1
1	A	254	LYS	3.7
2	B	395	PRO	3.3
1	A	835	ILE	3.2
1	A	853	SER	2.9
1	A	966	THR	2.9
1	A	1010	LEU	2.8
1	A	965	LYS	2.8
1	A	455	GLY	2.8
1	A	990	GLU	2.7
1	A	989	GLY	2.6
1	A	967	ARG	2.6
1	A	808	ASP	2.5
1	A	548	LEU	2.5
1	A	991	SER	2.4
1	A	677	GLU	2.3
1	A	1032	LEU	2.3
1	A	1033	ARG	2.3
1	A	1035	GLU	2.2
2	B	394	THR	2.2
1	A	167	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	836	GLU	2.1
1	A	1048	LEU	2.1

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 oligosaccharides 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, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
3	MES	A	1101	12/12	0.70	0.14	40,52,83,97	0

6.5 Other polymers [i](#)

There are no such residues in this entry.