



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 9HX9 / pdb_00009hx9
Title : Structure of the SA2/SCC1/MCM3 complex
Authors : Patel, A.; Panne, D.
Deposited on : 2025-01-07
Resolution : 3.07 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 ⓘ 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

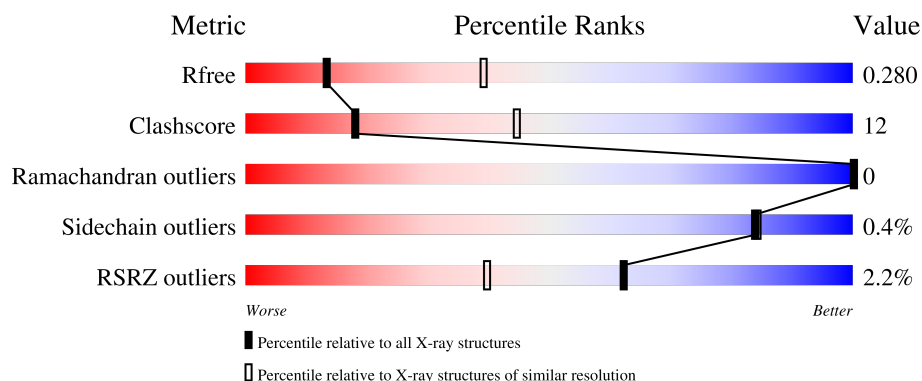
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.07 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	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)

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% 68% 27% 5%
2	B	140	44% 9% 47%
3	C	12	58% 33% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16614 atoms, of which 8304 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	935	Total	C	H	N	O	S	0	1	0
			15209	4848	7596	1268	1441	56			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	74	Total	C	H	N	O	S	0	0	0
			1235	385	639	101	107	3			

- Molecule 3 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	11	Total	C	H	N	O	0	0	0
			166	61	69	11	25			

- Molecule 4 is water.

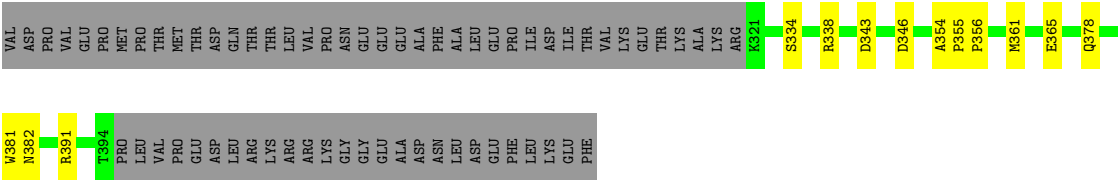
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	B	1	Total	O	0	0
			1	1		

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.

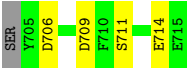
Chain A:

E80	E81	E82	E83	E84	E88	E91	E92	S93	V99	M240	M241	Y248	M255	I103	N119	F120	S125	V131	T132	A133	E134	F136	R137	H138	M139	E143	I144	Q167	W168	K169	E177	F178	V181	S189	I190	I191	L201	S207	L208	S219	T220	L221	L222																																				
M223	M224	K225	L226	M227	T228	M240	M241	Y248	M255	I103	M240	M241	Y248	M255	I103	N119	F120	S125	V131	T132	A133	E134	F136	R137	H138	M139	E143	I144	Q167	W168	K169	E177	F178	V181	S189	I190	I191	L201	S207	L208	S219	T220	L221	L222																																			
D338	K339	ASP	PRQ	GLU	GLU	ASP	GLY	MET	L351	L354	Y355	Y355	Y356	K358	GLY	L360	N361	S362	K363	L364	E365	L366	F371	K372	D373	M378	Y384	E282	M283	M284	L288	L393	L394	T395	L398	S401	E402	E403	E411	Y414	Y418	H421	R422	P423	G429	L432	K435	G436																															
ARG	ARG	ASP	PRQ	GLU	GLU	ASP	GLY	MET	L351	L354	Y355	Y355	Y356	K358	GLY	L360	N361	S362	K363	L364	E365	L366	F371	K372	D373	M378	Y384	E282	M283	M284	L288	L393	L394	T395	L398	S401	E402	E403	E411	Y414	Y418	H421	R422	P423	G429	L432	K435	G436																															
Q527	Q531	Q531	E534	V539	K545	T549	K551	E552	L557	D558	D559	R560	T561	L566	F567	A570	L571	P572	K584	V585	T586	L591	P592	D596	L597	E598	I599	Y600	T601	L605	E606	L609	Q615	I616	R617	K622	E630	Y636	H637	T645	I646	R649	L657	F665	L669	D682	L688	K692	H698	R699	A700	H701	L702	L703	F709	L715	D724	E727	Q728	I731	H732	W743	I748	T749	E750	S753	F756	D757	L758	L759	R760	L761	K762	K763	Q764	R765	R766	Y775	V779
ARG	ARG	ASP	PRQ	GLU	GLU	ASP	GLY	MET	L351	L354	Y355	Y355	Y356	K358	GLY	L360	N361	S362	K363	L364	E365	L366	F371	K372	D373	M378	Y384	E282	M283	M284	L288	L393	L394	T395	L398	S401	E402	E403	E411	Y414	Y418	H421	R422	P423	G429	L432	K435	G436																															
Q527	Q531	Q531	E534	V539	K545	T549	K551	E552	L557	D558	D559	R560	T561	L566	F567	A570	L571	P572	K584	V585	T586	L591	P592	D596	L597	E598	I599	Y600	T601	L605	E606	L609	Q615	I616	R617	K622	E630	Y636	H637	T645	I646	R649	L657	F665	L669	D682	L688	K692	H698	R699	A700	H701	L702	L703	F709	L715	D724	E727	Q728	I731	H732	W743	I748	T749	E750	S753	F756	D757	L758	L759	R760	L761	K762	K763	Q764	R765	R766	Y775	V779
ARG	ARG	ASP	PRQ	GLU	GLU	ASP	GLY	MET	L351	L354	Y355	Y355	Y356	K358	GLY	L360	N361	S362	K363	L364	E365	L366	F371	K372	D373	M378	Y384	E282	M283	M284	L288	L393	L394	T395	L398	S401	E402	E403	E411	Y414	Y418	H421	R422	P423	G429	L432	K435	G436																															
Q527	Q531	Q531	E534	V539	K545	T549	K551	E552	L557	D558	D559	R560	T561	L566	F567	A570	L571	P572	K584	V585	T586	L591	P592	D596	L597	E598	I599	Y600	T601	L605	E606	L609	Q615	I616	R617	K622	E630	Y636	H637	T645	I646	R649	L657	F665	L669	D682	L688	K692	H698	R699	A700	H701	L702	L703	F709	L7																							

Chain B: 44% 9% 47%



● Molecule 3: DNA replication licensing factor MCM3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.30Å 108.23Å 177.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.41 – 3.07 92.41 – 3.08	Depositor EDS
% Data completeness (in resolution range)	76.6 (92.41-3.07) 76.6 (92.41-3.08)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.216 , 0.281 0.216 , 0.280	Depositor DCC
R_{free} test set	1142 reflections (3.92%)	wwPDB-VP
Wilson B-factor (Å ²)	70.0	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 67.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16614	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 3.46% 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	0.83	2/7750 (0.0%)	1.16	16/10448 (0.2%)
2	B	0.82	0/606	1.17	0/818
3	C	1.11	0/100	0.88	0/136
All	All	0.83	2/8456 (0.0%)	1.16	16/11402 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
2	B	0	2
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	225	LYS	C-N	8.34	1.44	1.33
1	A	83	MET	C-N	7.09	1.43	1.33

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	760	ARG	CG-CD-NE	7.53	128.57	112.00
1	A	227	MET	CG-SD-CE	-7.24	84.97	100.90
1	A	363	LYS	CA-C-N	7.20	131.25	120.31
1	A	363	LYS	C-N-CA	7.20	131.25	120.31
1	A	324	LEU	CD1-CG-CD2	-7.18	95.01	110.80

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1033	ARG	Sidechain
1	A	1034	ARG	Sidechain
1	A	240	ASN	Sidechain
1	A	263	ARG	Sidechain
2	B	338	ARG	Sidechain

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	7613	7596	7595	195	1
2	B	596	639	639	9	1
3	C	97	69	69	4	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
All	All	8310	8304	8303	203	1

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 12.

The worst 5 of 203 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:961:LEU:HD23	1:A:966:THR:HB	1.60	0.84
1:A:1015:LYS:HD3	1:A:1048:LEU:HD23	1.63	0.79
1:A:561:THR:HG22	1:A:599:ILE:HD11	1.66	0.78
1:A:432:LEU:HD23	1:A:484:MET:HE3	1.68	0.76
1:A:756:GLU:HA	1:A:759:LEU:HD12	1.66	0.76

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:SER:OG	2:B:343:ASP:OD2[4_445]	2.10	0.10

5.3 Torsion angles

5.3.1 Protein backbone

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	926/981 (94%)	878 (95%)	48 (5%)	0	100	100
2	B	72/140 (51%)	72 (100%)	0	0	100	100
3	C	9/12 (75%)	8 (89%)	1 (11%)	0	100	100
All	All	1007/1133 (89%)	958 (95%)	49 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	846/882 (96%)	843 (100%)	3 (0%)	84	84
2	B	69/129 (54%)	68 (99%)	1 (1%)	59	73
3	C	11/12 (92%)	11 (100%)	0	100	100
All	All	926/1023 (90%)	922 (100%)	4 (0%)	84	84

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	VAL
1	A	263	ARG
1	A	361	ASN
2	B	334	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	GLN
1	A	275	GLN
1	A	499	ASN
1	A	773	GLN

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	935/981 (95%)	0.04	22 (2%) 59 37	14, 93, 158, 216	1 (0%)
2	B	74/140 (52%)	-0.23	0 100 100	22, 60, 117, 129	0
3	C	11/12 (91%)	0.14	0 100 100	40, 70, 107, 111	0
All	All	1020/1133 (90%)	0.02	22 (2%) 62 40	14, 91, 156, 216	1 (0%)

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	357	ASN	4.6
1	A	360	LEU	3.6
1	A	715	LEU	3.4
1	A	875	THR	2.6
1	A	498	MET	2.5

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.