



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 5FRR
Title : Structure of the Pds5-Scc1 complex and implications for cohesin function
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Deposited on : 2015-12-22
Resolution : 5.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

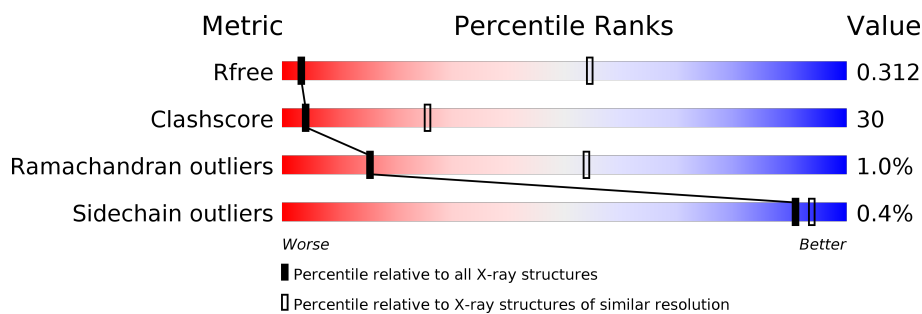
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.80 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}	130704	1008 (7.70-3.86)
Clashscore	141614	1035 (7.70-3.90)
Ramachandran outliers	138981	1003 (7.70-3.86)
Sidechain outliers	138945	1006 (7.78-3.82)

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 on 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	703	
1	B	703	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10858 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 SISTER CHROMATID COHESION PROTEIN PDS5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	677	Total	C	N	O	S	0	0	0
			5494	3526	914	1041	13			
1	B	660	Total	C	N	O	S	0	0	0
			5364	3455	889	1009	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q04264
A	0	ALA	-	expression tag	UNP Q04264
B	-1	GLY	-	expression tag	UNP Q04264
B	0	ALA	-	expression tag	UNP Q04264

- Molecule 1: SISTER CHROMATID COHESION PROTEIN PDS5



I633	E569	F502	L406	I330	I243	Y157	I83	GLY
I634	T570	T503	H411	I333	D249	D158	L84	ALA
I635	I571	F506	K412	V339	D250	P159	Y87	MET
I636	K572		E413	E340	N251	K161	A88	ALA
I637			V414	W341		S162		K3
I638	I575					D95		V6
I639	ASP	N509	R415	T342	R254	F163		
	GLU	A510	E416	E343	L255	P164	A96	
P642	R578	R511	L417	S344	L256	A165	Q97	S17
I643	I579	Q512	C418	S344	R166	A165	L98	T18
I644	F580	I514		I345	V258	L167	T99	
I645	I514	K514	M422	P346	V259	F168	D100	Q21
I646	L582	I515	Q347	Q347	V260		I101	L22
I647	I583	S516	F425	I348	K261	I171	F102	I23
S648	N584				L262		K103	T25
I649	A585	I519	L430	T351	H263	I174	L104	T26
I650	C586	S520	M431	R352	K264	L175	V105	N26
S651	S587	K521	I442	E553	L265	V178	L106	E27
I652	T588	Y522	D354	I355	L267		S107	L28
I653	N589	I523	L355	S356	L267	F182	Q108	L29
I654	D590	F524	I446	S356	R268		E109	D30
I655	I591	D525	T447	K357	L269		E110	R31
	P592	S526	T448	D447	W270	V185	Q111	D31
I656	F593	K527	I449	E358	E271	P186		L32
S657		F528	P450	L359	T272	L187	E116	K33
ASN	F594	F528	S451	N360	V273	E188	A34	A34
ASN	T595	ASN	T452	A362		V189	H120	L35
S660	K597	GLN	L453	L363	L276	I121	I121	E37
		GLN			I277	R191	Q122	E38
K663	C599	GLU	L456	T366		L192	Q123	L39
L667		SER			T283		T124	
	L603	SER	D461	P372	I284	N195	Y125	L42
K668	V604	SER	L462	R373			L126	
I671		SER	N463	V374	E287	N201	I127	N46
L672		SER	I464	R375	L288	P202	T47	T47
	L607	SER		R376		N203	K129	D48
Q608	GLN	GLN				E204	L130	L49
I675	T609	GLY	Q467	T377	N292	E204	L130	
S676	PRO	PRO	V468	S378	E293	L131	E132	T50
K677	GLY	I542	D469	V379	L294	P206	E132	G51
V678	LEU	V543	S470	N380	F295	E207	Y133	L52
	PHE	M544	V471	I381	R296	C208		
T681	LYS		I472			L209	I136	R56
L682	LYS	Y547	F473	V385	A299		V137	
F683	TYR		T300	P386	T300	C215	L137	L59
K684	ASN	L551	L476	V387	K301		L139	V60
	ILE	Q552			L302	E218	S61	
Q685	ILE	SER	F479	I390		V219	L142	R62
SER	THR	L554	E480		Q305		P143	
I686	GLY	A555	P481	I394	T308	T222	S144	L65
I687	ALA	S556	D482	N396	L223	C224	S145	K66
L690	SER		N483	K397	L233			
I693	ILE	S559	D484	I398	N314	E230	L148	V70
I694	MET	D560	K485	I399	F315		L149	G71
	PRO		R486	V400	V316	T236	I150	I72
	ARG	K563	V487	T401	S320	R237	L152	R73
ASP	D628	A564		S402		Y238	E151	
ASP	I639	I565	L490	L903	K324	Y239	F153	C78
PRO	A630	D566	L491	L403			H154	C79
ASP	K631	A567	L404	L404			I155	L80
	V679	L568	V400	H405			F156	

4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	283.69Å 283.69Å 172.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 5.80 49.19 – 5.79	Depositor EDS
% Data completeness (in resolution range)	95.0 (50.00-5.80) 99.6 (49.19-5.79)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 5.73Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.249 , 0.311 0.251 , 0.312	Depositor DCC
R_{free} test set	518 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	383.9	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 403.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	10858	wwPDB-VP
Average B, all atoms (Å ²)	424.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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

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	0.25	0/5600	0.42	0/7597
1	B	0.25	0/5464	0.41	0/7408
All	All	0.25	0/11064	0.41	0/15005

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	5494	0	5551	334	0
1	B	5364	0	5435	324	1
All	All	10858	0	10986	647	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 30.

The worst 5 of 647 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:333:ILE:HD12	1:B:333:ILE:H	1.29	0.97
1:A:98:LEU:HD23	1:A:142:LEU:HD21	1.51	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:ARG:HA	1:B:376:ARG:HH12	1.36	0.91
1:B:98:LEU:HD23	1:B:142:LEU:HD21	1.52	0.89
1:B:462:LEU:HD13	1:B:559:SER:HA	1.53	0.88

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:B:556:SER:CB	1:B:556:SER:CB[7_555]	2.12	0.08

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	673/703 (96%)	601 (89%)	64 (10%)	8 (1%)	13	49
1	B	650/703 (92%)	582 (90%)	63 (10%)	5 (1%)	19	60
All	All	1323/1406 (94%)	1183 (89%)	127 (10%)	13 (1%)	15	54

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	536	SER
1	A	538	SER
1	A	679	ASN
1	B	682	LEU
1	A	655	ASN

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	629/650 (97%)	627 (100%)	2 (0%)	92	94
1	B	611/650 (94%)	608 (100%)	3 (0%)	88	93
All	All	1240/1300 (95%)	1235 (100%)	5 (0%)	91	94

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

Mol	Chain	Res	Type
1	A	469	ASP
1	A	547	TYR
1	B	120	HIS
1	B	469	ASP
1	B	547	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	455	ASN
1	A	575	ASN
1	B	467	GLN
1	A	509	ASN
1	A	598	ASN

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 ⓘ

There are no carbohydrates 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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.