



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 : unknown
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

<http://wwpdb.org/validation/2016/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)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

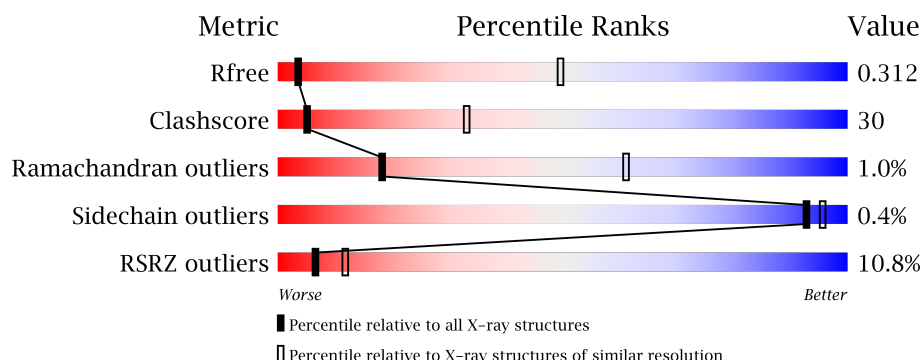
1 Overall quality at a glance

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}	100719	1077 (7.88-3.70)
Clashscore	112137	1007 (7.80-3.80)
Ramachandran outliers	110173	1106 (7.88-3.70)
Sidechain outliers	110143	1078 (7.88-3.70)
RSRZ outliers	101464	1086 (7.88-3.70)

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. 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	703	<div> <div>7%</div> <div>47%</div> <div>49%</div> <div>• •</div> </div>
1	B	703	<div> <div>13%</div> <div>46%</div> <div>47%</div> <div>• 6%</div> </div>

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			

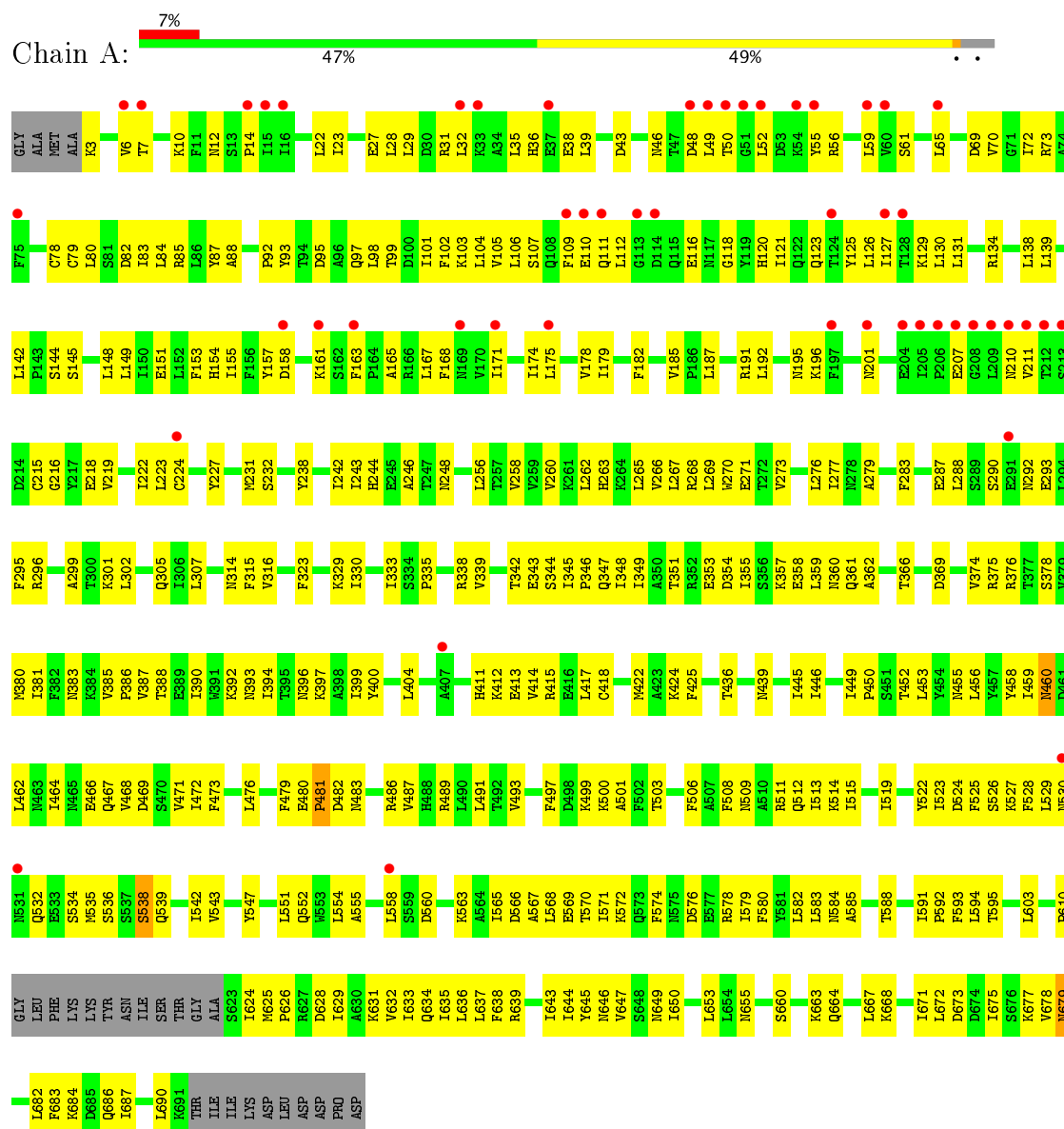
There are 4 discrepancies between the modelled and reference sequences:

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

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

• Molecule 1: SISTER CHROMATID COHESION PROTEIN PDS5



• Molecule 1: SISTER CHROMATID COHESION PROTEIN PDS5



L653	L654	N655	L656	S657	ASN	ASN	S660	K663	L667	K668	I671	L672	I675	S676	K677	V678	T681	L682	F683	K684	D685	Q686	I687	L690	I693	I694	L697	ASP	ASP	PRO	ASP																											
N589	D590	I591	P592	F593	L594	T595	F596	K597	N598	C599	L603	V604	L607	Q608	T609	PRO	GLY	LEU	PHE	LYS	LYS	TYR	ASN	ILE	THR	GLY	ALA	SER	ILE	PRO	ARG	D628	I629	A630	K631	V632	I633	Q634	I635	L636	L637	F638	R639	P642	I643	I644	Y645	N646	V647	S648	N649	I650	S651	V652				
I523	D524	F525	S526	K527	F528	LEU	ASN	ASN	GLN	GLU	SER	MET	SER	SER	SER	GLN	GLY	PRO	I542	Y543	M544	Y547	L551	Q552	M553	L554	A555	S556	S559	D560	K563	A564	I565	D566	A567	L568	E569	T570	Q571	I572	K573	N574	ASP	GLU	R575	L576	F577	P578	Q579	I580	V581	L582	L583	N584	I585	S586	V587	T588
I446	D447	T448	I449	Q450	A451	A452	L453	L456	D461	L462	M463	I464	Q467	V468	D469	S470	V471	I472	F473	L476	F479	E480	F481	D482	M483	D484	K485	R486	V487	L490	T491	S492	L493	L494	H495	L496	H411	K412	E413	V414	R415	E416	L417	C418	M422	F425	L430	M431	I442									
S356	K357	E358	L359	Q360	A361	A362	L363	T366	P372	R373	T374	R375	R376	T377	S378	V379	M380	I381	F382	V385	P386	V387	T390	I394	F395	M396	K397	I398	T399	Y400	T401	S402	L403	L404	H405	L406	H411	K412	E413	V414	R415	E416	L417	C418	M422	F425	L430	M431	I442									
L276	L277	V280	F283	L284	E287	L288	N292	E293	L294	R295	R296	K297	E298	A299	T300	K301	L302	Q305	T308	N314	F315	V316	S320	K324	K329	L330	A331	D332	L333	V337	R338	E340	K341	T342	E343	S344	L345	P346	L348	M422	F425	L430	M431	I442														
N195	N201	P202	N203	E204	I205	P206	E207	G208	L209	N210	V211	L212	C215	E218	V219	I222	L223	C224	R230	H234	L235	T236	K237	Y238	Y239	I242	I243	D249	D250	N251	R254	L255	T256	V258	V259	V260	R261	H263	K264	L265	V266	L267	R268	V269	M270	T271	T272	V273										
T128	K129	L130	L131	E132	Y133	I136	V137	L138	L139	R140	D141	L142	P143	S144	S145	L148	L149	I150	E151	L152	F153	H154	I155	F156	Y157	D158	P159	M160	K161	S162	F163	P164	A165	R166	L167	F168	M169	V170	I171	I174	L175	V178	I179	F182	V185	P186	L187	E188	V189	L190	R191	L192						
R62	A63	L64	L65	K66	H67	V68	D69	V70	I72	R73	A74	F75	A77	C78	C79	L80	T83	L84	H87	A88	F89	D90	D95	A96	Q97	L98	T99	D100	I101	F102	K103	L104	V105	L106	S107	Q108	F109	E110	Q111	L112	G113	D114	Q115	E116	M117	H120	I121	Q122	Q123	T124	Y125	L126	I127					
GLY	ALA	MET	ALA	K3	V6	T7	K8	L9	K10	F11	N12	I15	I16	S17	T18	S19	D20	Q21	L22	L23	S24	T25	H26	E27	L28	L29	D30	R31	L32	K33	A34	R35	E36	E37	E38	L39	A40	S41	L42	D45	M46	T47	D48	L49	T50	G51	L52	D53	K54	Y55	R56	D57	A58	V60	S61			

4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	283.69 Å 283.69 Å 172.79 Å 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 5.73 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.249 , 0.311 0.251 , 0.312	Depositor DCC
R_{free} test set	No test flags present.	DCC
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 , 402.2	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%)	15	58
1	B	650/703 (92%)	582 (90%)	63 (10%)	5 (1%)	22	66
All	All	1323/1406 (94%)	1183 (89%)	127 (10%)	13 (1%)	18	61

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%)	94	96
1	B	611/650 (94%)	608 (100%)	3 (0%)	91	95
All	All	1240/1300 (95%)	1235 (100%)	5 (0%)	93	95

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 [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	677/703 (96%)	0.54	51 (7%) 15 19	217, 391, 564, 683	0
1	B	660/703 (93%)	0.81	94 (14%) 3 9	260, 428, 646, 847	0
All	All	1337/1406 (95%)	0.67	145 (10%) 6 12	217, 407, 606, 847	0

The worst 5 of 145 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	61	SER	9.3
1	B	208	GLY	8.3
1	B	65	LEU	8.2
1	B	114	ASP	7.6
1	B	209	LEU	7.5

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 carbohydrates 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.