



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 8J09 / pdb_00008j09
Title : Crystal structure of the Sld3 Cdc45-binding-domain, in complex with Cdc45
Authors : Li, H.; Ishizaka, I.; Kato, K.; Sun, X.; Muramatsu, S.; Itou, H.; Ose, T.; Araki, H.; Yao, M.
Deposited on : 2023-04-10
Resolution : 2.61 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
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

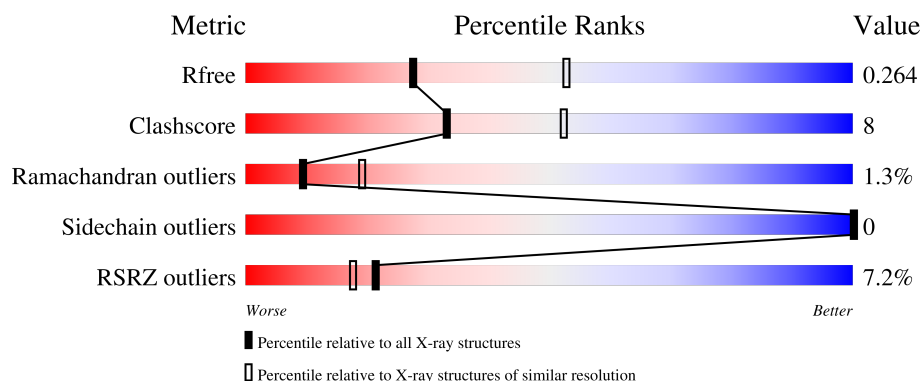
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	267	6% 73% 16% • 10%
2	B	650	6% 69% 16% • 15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6516 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 DNA replication regulator SLD3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	0
			1983	1286	332	359	6			

- Molecule 2 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	555	Total	C	N	O	S	0	0	0
			4493	2876	754	849	14			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		
3	B	24	Total	O	0	0
			24	24		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.77Å 107.57Å 128.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.47 – 2.61 43.47 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.47-2.61) 99.9 (43.47-2.61)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.219 , 0.262 0.220 , 0.264	Depositor DCC
R_{free} test set	1570 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.1	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	6516	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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	0.13	0/2018	0.34	0/2713
2	B	0.13	0/4578	0.38	1/6199 (0.0%)
All	All	0.13	0/6596	0.37	1/8912 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	53	LEU	N-CA-C	5.42	122.35	110.80

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	1983	0	2061	26	0
2	B	4493	0	4489	76	0
3	A	16	0	0	0	0
3	B	24	0	0	0	0
All	All	6516	0	6550	102	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 8.

All (102) 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)
2:B:16:LEU:HD21	2:B:52:GLN:HE22	1.47	0.80
2:B:506:ILE:HG13	2:B:547:ARG:HD3	1.67	0.73
2:B:526:ARG:NH1	2:B:558:GLU:OE2	2.22	0.71
2:B:312:THR:HG22	2:B:314:ASP:H	1.56	0.70
2:B:537:ASP:O	2:B:539:TYR:N	2.26	0.68
2:B:31:VAL:HG22	2:B:42:THR:HG21	1.78	0.66
2:B:537:ASP:C	2:B:539:TYR:H	2.02	0.66
2:B:231:HIS:O	2:B:231:HIS:ND1	2.25	0.65
2:B:19:SER:HA	2:B:26:GLN:HG3	1.77	0.65
2:B:556:CYS:SG	2:B:563:GLN:NE2	2.73	0.62
2:B:464:GLN:O	2:B:467:THR:OG1	2.19	0.60
2:B:282:ILE:HD12	2:B:283:ALA:N	2.18	0.58
2:B:546:LEU:HD11	2:B:629:ILE:HD11	1.84	0.58
2:B:249:ASN:ND2	2:B:250:SER:H	2.01	0.58
1:A:228:LEU:HD22	1:A:244:LEU:HD21	1.86	0.57
2:B:249:ASN:HD22	2:B:250:SER:H	1.52	0.57
2:B:531:GLN:HA	2:B:572:ILE:HG22	1.87	0.56
2:B:633:ARG:NH1	2:B:635:GLU:OE2	2.39	0.56
2:B:344:VAL:HG12	2:B:401:LEU:HD22	1.87	0.55
1:A:357:LEU:HD11	1:A:378:LYS:HE2	1.89	0.55
2:B:1:MET:N	2:B:137:SER:O	2.32	0.55
1:A:206:ALA:O	1:A:210:LYS:HG2	2.07	0.54
2:B:463:ALA:O	2:B:464:GLN:HG3	2.08	0.54
2:B:267:LEU:HB3	2:B:316:LEU:HD22	1.88	0.54
2:B:399:TYR:HB2	2:B:401:LEU:HD12	1.90	0.53
2:B:101:GLN:HA	2:B:104:VAL:HG23	1.90	0.53
1:A:271:ILE:HG21	1:A:350:ALA:HB2	1.89	0.52
2:B:354:ASN:O	2:B:358:ARG:HG3	2.09	0.52
2:B:382:HIS:HA	2:B:385:LYS:HD3	1.92	0.51
2:B:386:ARG:HG2	2:B:386:ARG:NH1	2.25	0.51
1:A:360:GLU:O	1:A:361:THR:HG22	2.10	0.51
2:B:531:GLN:O	2:B:533:GLY:N	2.44	0.51
2:B:311:LYS:O	2:B:312:THR:OG1	2.25	0.50
1:A:258:THR:HG23	1:A:374:ILE:HG21	1.94	0.49
2:B:538:LEU:HD21	2:B:573:ASP:HA	1.94	0.49
1:A:204:TYR:CZ	1:A:208:LEU:HD11	2.47	0.49
2:B:158:ALA:HB1	2:B:233:TYR:HB3	1.95	0.49
2:B:561:ASP:OD2	2:B:561:ASP:N	2.46	0.49
2:B:410:VAL:HG13	2:B:418:SER:HB2	1.95	0.49
2:B:610:GLN:HB2	2:B:627:SER:HB3	1.94	0.48
2:B:325:TYR:HB3	2:B:404:ILE:HA	1.95	0.48
2:B:353:GLU:O	2:B:357:LYS:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:357:LYS:O	2:B:361:LYS:HG3	2.14	0.48
1:A:379:LYS:N	1:A:379:LYS:HD3	2.28	0.48
2:B:90:ILE:O	2:B:133:ASN:ND2	2.46	0.48
2:B:595:ILE:C	2:B:597:THR:H	2.22	0.48
2:B:16:LEU:HD21	2:B:52:GLN:NE2	2.24	0.47
1:A:157:PRO:HA	1:A:160:TYR:HB3	1.94	0.47
1:A:361:THR:O	1:A:362:PRO:C	2.57	0.47
2:B:633:ARG:HB3	2:B:635:GLU:OE2	2.15	0.47
2:B:635:GLU:H	2:B:635:GLU:CD	2.24	0.46
1:A:390:LEU:HB3	1:A:417:LEU:HD13	1.95	0.46
2:B:564:LEU:HD22	2:B:600:PRO:HD3	1.98	0.46
2:B:587:ARG:HD3	2:B:587:ARG:HA	1.62	0.45
2:B:356:LYS:HE2	2:B:360:HIS:CE1	2.51	0.45
2:B:610:GLN:HB2	2:B:627:SER:CB	2.46	0.45
1:A:205:GLN:HB2	1:A:284:LEU:HD13	1.99	0.45
2:B:52:GLN:O	2:B:54:VAL:N	2.50	0.45
2:B:553:ILE:HG23	2:B:563:GLN:OE1	2.17	0.45
2:B:325:TYR:CZ	2:B:590:ARG:HB3	2.52	0.45
1:A:337:LEU:HG	1:A:338:ASP:N	2.31	0.44
1:A:179:PHE:HD1	1:A:183:ASN:HD22	1.66	0.44
1:A:248:VAL:HG21	1:A:259:ILE:HD11	1.99	0.44
2:B:351:TRP:CD1	2:B:351:TRP:H	2.35	0.44
2:B:490:GLU:H	2:B:490:GLU:CD	2.25	0.44
2:B:604:ASN:HB2	2:B:607:MET:HE3	2.00	0.44
2:B:538:LEU:O	2:B:538:LEU:HD23	2.16	0.44
2:B:598:LYS:HE3	2:B:598:LYS:HB3	1.84	0.44
2:B:386:ARG:HG2	2:B:386:ARG:HH11	1.80	0.44
1:A:254:LYS:HE3	1:A:254:LYS:HB2	1.78	0.44
2:B:161:LYS:HG3	2:B:233:TYR:CE2	2.52	0.43
2:B:479:LEU:HD22	2:B:491:LEU:HD21	2.00	0.43
1:A:375:GLN:O	1:A:378:LYS:N	2.50	0.43
2:B:163:LEU:HD23	2:B:163:LEU:H	1.84	0.43
2:B:351:TRP:HB3	2:B:511:VAL:HG22	2.01	0.43
2:B:521:HIS:CE1	2:B:562:LYS:HD3	2.53	0.43
1:A:298:TYR:OH	1:A:341:GLU:OE2	2.31	0.43
1:A:406:VAL:HG13	1:A:406:VAL:O	2.17	0.43
2:B:15:ILE:HD13	2:B:82:LEU:HD11	1.99	0.43
1:A:163:SER:O	1:A:167:ASP:HB2	2.19	0.43
2:B:45:LEU:HD21	2:B:255:ILE:HD12	2.00	0.43
2:B:526:ARG:NH2	2:B:563:GLN:OE1	2.41	0.43
2:B:572:ILE:HB	2:B:579:TYR:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ASP:OD1	1:A:240:ARG:NE	2.41	0.42
2:B:381:ASP:HB3	2:B:384:ILE:HD12	2.01	0.42
2:B:334:LEU:HB2	2:B:380:MET:HE1	2.01	0.42
2:B:435:GLY:O	2:B:494:ARG:NH1	2.52	0.42
1:A:248:VAL:HG13	1:A:249:ILE:HG13	2.01	0.42
2:B:360:HIS:CE1	2:B:370:LEU:HD21	2.55	0.42
2:B:535:ASP:OD1	2:B:536:LEU:N	2.51	0.42
2:B:128:PRO:HB2	2:B:240:TYR:CZ	2.55	0.42
1:A:386:LYS:O	1:A:392:GLY:HA3	2.20	0.41
2:B:573:ASP:O	2:B:577:ASP:N	2.52	0.41
1:A:222:HIS:CE1	1:A:267:LYS:HA	2.56	0.41
1:A:375:GLN:C	1:A:379:LYS:HE2	2.46	0.41
2:B:537:ASP:C	2:B:539:TYR:N	2.72	0.41
1:A:302:LEU:HD12	1:A:302:LEU:HA	1.92	0.41
2:B:228:LYS:HB3	2:B:229:GLN:H	1.77	0.41
2:B:282:ILE:HD12	2:B:283:ALA:H	1.86	0.41
2:B:388:LEU:HD23	2:B:388:LEU:HA	1.87	0.41
2:B:436:ASN:ND2	2:B:475:SER:OG	2.51	0.41
2:B:517:LYS:HA	2:B:517:LYS:HD3	1.91	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	235/267 (88%)	225 (96%)	6 (3%)	4 (2%)	7	14
2	B	545/650 (84%)	509 (93%)	30 (6%)	6 (1%)	11	23
All	All	780/917 (85%)	734 (94%)	36 (5%)	10 (1%)	9	19

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	THR
1	A	362	PRO
2	B	53	LEU
2	B	532	ASP
2	B	537	ASP
2	B	538	LEU
2	B	464	GLN
1	A	155	SER
2	B	627	SER
1	A	315	VAL

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	225/249 (90%)	225 (100%)	0	100	100
2	B	499/586 (85%)	499 (100%)	0	100	100
All	All	724/835 (87%)	724 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	ASN
1	A	395	ASN
2	B	26	GLN
2	B	52	GLN
2	B	57	GLN
2	B	114	GLN
2	B	249	ASN
2	B	321	GLN
2	B	464	GLN
2	B	493	ASN
2	B	624	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

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	241/267 (90%)	0.24	15 (6%) 26 22	26, 49, 101, 125	0
2	B	555/650 (85%)	0.39	42 (7%) 20 16	27, 52, 89, 121	0
All	All	796/917 (86%)	0.34	57 (7%) 21 18	26, 51, 93, 125	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	536	LEU	5.4
2	B	539	TYR	4.9
2	B	538	LEU	4.2
2	B	53	LEU	4.0
2	B	51	LYS	3.9
2	B	628	SER	3.8
1	A	370	SER	3.7
1	A	337	LEU	3.5
2	B	304	PRO	3.3
2	B	557	ALA	3.2
1	A	315	VAL	3.2
1	A	362	PRO	3.2
2	B	533	GLY	3.2
2	B	305	SER	3.1
2	B	230	ILE	3.0
2	B	312	THR	3.0
2	B	650	LEU	2.9
2	B	563	GLN	2.8
1	A	154	TYR	2.8
2	B	463	ALA	2.8
1	A	363	ASN	2.8
2	B	303	THR	2.7
2	B	561	ASP	2.7
2	B	111	SER	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	114	GLN	2.6
2	B	624	ASN	2.6
2	B	626	GLU	2.5
2	B	462	SER	2.5
2	B	50	LYS	2.5
2	B	165	LEU	2.5
2	B	587	ARG	2.5
2	B	473	TRP	2.4
2	B	54	VAL	2.4
1	A	207	MET	2.4
2	B	562	LYS	2.4
2	B	105	ILE	2.3
2	B	145	ASP	2.3
2	B	541	ASN	2.3
2	B	52	GLN	2.3
2	B	564	LEU	2.3
1	A	420	PRO	2.3
2	B	386	ARG	2.2
2	B	534	PRO	2.2
2	B	164	GLU	2.2
2	B	627	SER	2.2
2	B	313	PRO	2.2
1	A	199	SER	2.2
1	A	155	SER	2.2
1	A	359	SER	2.1
1	A	314	LEU	2.1
2	B	532	ASP	2.1
2	B	62	PHE	2.1
1	A	372	GLY	2.1
2	B	537	ASP	2.1
1	A	197	SER	2.1
1	A	157	PRO	2.1
2	B	112	GLY	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.