



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:46 PM GMT

PDB ID : 4AEZ
Title : Crystal Structure of Mitotic Checkpoint Complex
Authors : Kulkarni, K.A.; Chao, W.C.H.; Zhang, Z.; Barford, D.
Deposited on : 2012-01-13
Resolution : 2.30 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

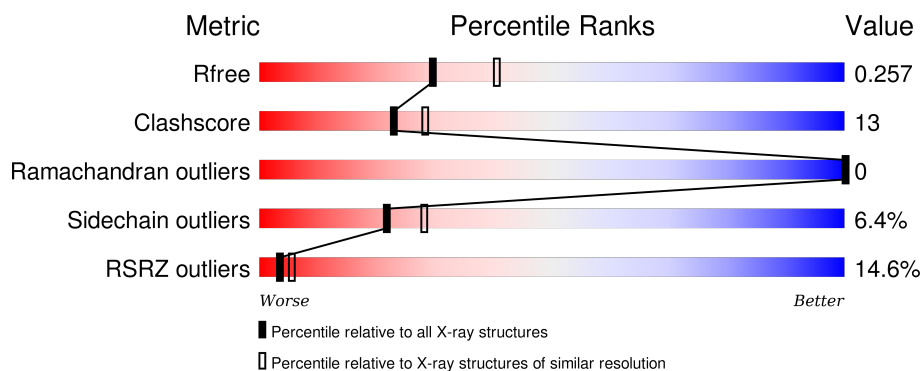
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	401	<div> <div>71%</div> <div>9% • 19%</div> </div>
1	D	401	<div> <div>3%</div> <div>61%</div> <div>16% • 22%</div> </div>
1	G	401	<div> <div>15%</div> <div>54%</div> <div>23% • 21%</div> </div>
2	B	203	<div> <div>71%</div> <div>16% • 11%</div> </div>
2	E	203	<div> <div>33%</div> <div>53%</div> <div>30% • 14%</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	203	<div><div></div><div>27%</div><div>60%</div><div>28%</div><div>9%</div></div>
3	C	223	<div><div></div><div>2%</div><div>77%</div><div>19%</div><div></div></div>
3	F	223	<div><div></div><div>8%</div><div>66%</div><div>19%</div><div>12%</div></div>
3	I	223	<div><div></div><div>38%</div><div>44%</div><div>34%</div><div>9%</div><div>13%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16896 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 WD REPEAT-CONTAINING PROTEIN SLP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2499	1565	445	483	6			
1	D	314	Total	C	N	O	S	0	0	0
			2406	1507	426	467	6			
1	G	317	Total	C	N	O	S	0	0	0
			2400	1502	425	467	6			

- Molecule 2 is a protein called MITOTIC SPINDLE CHECKPOINT COMPONENT MAD2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	180	Total	C	N	O	S	0	0	0
			1469	941	243	278	7			
2	E	175	Total	C	N	O	S	0	0	0
			1369	880	224	260	5			
2	H	185	Total	C	N	O	S	0	0	0
			1477	951	246	274	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	12	ALA	LEU	ENGINEERED MUTATION	UNP O14417
B	133	ALA	ARG	ENGINEERED MUTATION	UNP O14417
E	12	ALA	LEU	ENGINEERED MUTATION	UNP O14417
E	133	ALA	ARG	ENGINEERED MUTATION	UNP O14417
H	12	ALA	LEU	ENGINEERED MUTATION	UNP O14417
H	133	ALA	ARG	ENGINEERED MUTATION	UNP O14417

- Molecule 3 is a protein called MITOTIC SPINDLE CHECKPOINT COMPONENT MAD3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	215	Total	C	N	O	S	0	0	0
			1799	1142	313	339	5			

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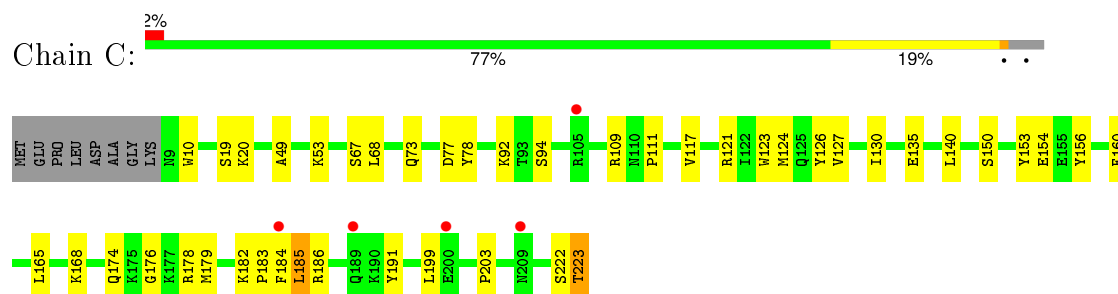
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	196	Total	C	N	O	S	0	0	0
			1585	1013	265	302	5			
3	I	193	Total	C	N	O	S	0	0	0
			1574	997	273	300	4			

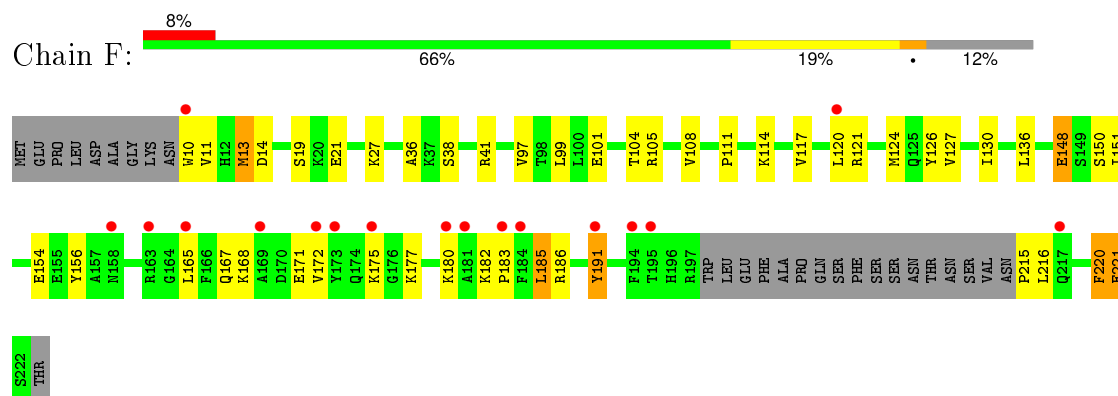
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	114	Total	O	0	0
			114	114		
4	B	33	Total	O	0	0
			33	33		
4	C	33	Total	O	0	0
			33	33		
4	D	61	Total	O	0	0
			61	61		
4	E	1	Total	O	0	0
			1	1		
4	F	48	Total	O	0	0
			48	48		
4	G	21	Total	O	0	0
			21	21		
4	H	6	Total	O	0	0
			6	6		
4	I	1	Total	O	0	0
			1	1		

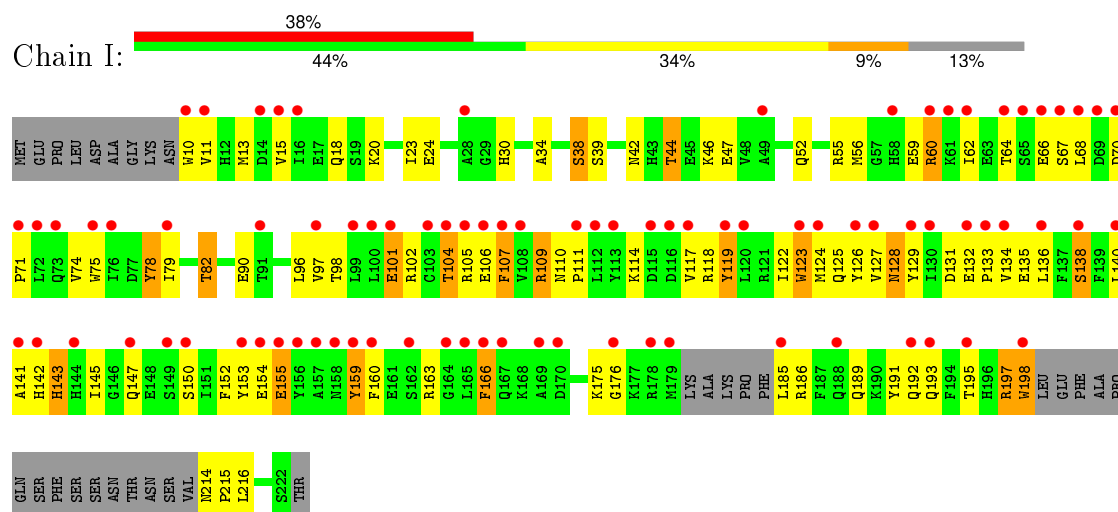
- Molecule 3: MITOTIC SPINDLE CHECKPOINT COMPONENT MAD3



- Molecule 3: MITOTIC SPINDLE CHECKPOINT COMPONENT MAD3



- Molecule 3: MITOTIC SPINDLE CHECKPOINT COMPONENT MAD3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.81Å 286.90Å 72.01Å 90.00° 119.04° 90.00°	Depositor
Resolution (Å)	62.96 – 2.30 62.96 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (62.96-2.30) 99.8 (62.96-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.29Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.221 , 0.267 0.209 , 0.257	Depositor DCC
R_{free} test set	1968 reflections (1.78%)	DCC
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.6	EDS
Estimated twinning fraction	0.002 for -h-l,k,h 0.002 for l,k,-h-l 0.024 for h,-k,-h-l 0.022 for -h-l,-k,l 0.024 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 110586 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16896	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.36	0/2559	0.54	0/3492
1	D	0.34	0/2465	0.56	0/3366
1	G	0.28	0/2458	0.49	0/3361
2	B	0.36	0/1494	0.50	0/2016
2	E	0.27	0/1394	0.43	0/1895
2	H	0.29	0/1502	0.46	0/2032
3	C	0.35	0/1847	0.46	0/2495
3	F	0.34	0/1625	0.48	0/2198
3	I	0.27	0/1614	0.44	0/2187
All	All	0.32	0/16958	0.50	0/23042

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
3	I	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	I	107	PHE	Peptide

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	2499	0	2393	33	0
1	D	2406	0	2290	46	0
1	G	2400	0	2269	76	0
2	B	1469	0	1476	23	0
2	E	1369	0	1312	83	0
2	H	1477	0	1462	48	0
3	C	1799	0	1718	27	0
3	F	1585	0	1472	41	0
3	I	1574	0	1434	88	0
4	A	114	0	0	3	0
4	B	33	0	0	0	0
4	C	33	0	0	0	0
4	D	61	0	0	3	0
4	E	1	0	0	0	0
4	F	48	0	0	0	0
4	G	21	0	0	0	0
4	H	6	0	0	0	0
4	I	1	0	0	0	0
All	All	16896	0	15826	436	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 13.

The worst 5 of 436 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:466:TYR:O	1:A:467:ASP:HB3	1.49	1.08
3:C:222:SER:O	3:C:223:THR:HB	1.54	1.05
1:G:177:ILE:HD11	1:G:458:GLU:HA	1.42	0.99
1:D:164:PHE:HE1	1:D:432:ILE:HD11	1.25	0.97
3:I:122:ILE:HG22	3:I:126:TYR:CE1	2.01	0.95

There are no symmetry-related clashes.

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	322/401 (80%)	318 (99%)	4 (1%)	0	100	100
1	D	310/401 (77%)	303 (98%)	7 (2%)	0	100	100
1	G	313/401 (78%)	306 (98%)	7 (2%)	0	100	100
2	B	176/203 (87%)	176 (100%)	0	0	100	100
2	E	171/203 (84%)	169 (99%)	2 (1%)	0	100	100
2	H	179/203 (88%)	178 (99%)	1 (1%)	0	100	100
3	C	213/223 (96%)	213 (100%)	0	0	100	100
3	F	192/223 (86%)	191 (100%)	1 (0%)	0	100	100
3	I	187/223 (84%)	185 (99%)	2 (1%)	0	100	100
All	All	2063/2481 (83%)	2039 (99%)	24 (1%)	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	269/340 (79%)	260 (97%)	9 (3%)	45	61
1	D	259/340 (76%)	248 (96%)	11 (4%)	36	49
1	G	255/340 (75%)	244 (96%)	11 (4%)	35	47
2	B	166/187 (89%)	157 (95%)	9 (5%)	27	36
2	E	145/187 (78%)	134 (92%)	11 (8%)	16	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	160/187 (86%)	147 (92%)	13 (8%)	15	18
3	C	196/203 (97%)	184 (94%)	12 (6%)	23	30
3	F	163/203 (80%)	154 (94%)	9 (6%)	27	36
3	I	162/203 (80%)	134 (83%)	28 (17%)	2	2
All	All	1775/2190 (81%)	1662 (94%)	113 (6%)	22	28

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	194	ASP
1	G	177	ILE
3	I	143	HIS
3	F	13	MET
3	F	185	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	70	GLN
3	I	128	ASN
2	H	70	GLN
1	A	429	GLN
2	H	117	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 ⓘ

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	326/401 (81%)	0.50	4 (1%) 81 85	17, 33, 64, 116	0
1	D	314/401 (78%)	0.64	14 (4%) 37 46	19, 42, 84, 116	0
1	G	317/401 (79%)	1.23	61 (19%) 2 2	43, 72, 103, 124	0
2	B	180/203 (88%)	0.45	1 (0%) 90 93	25, 44, 69, 109	0
2	E	175/203 (86%)	1.69	66 (37%) 0 0	40, 85, 127, 150	0
2	H	185/203 (91%)	1.54	54 (29%) 1 1	47, 70, 117, 139	0
3	C	215/223 (96%)	0.53	5 (2%) 64 72	19, 46, 81, 118	0
3	F	196/223 (87%)	0.75	17 (8%) 13 18	21, 53, 115, 149	0
3	I	193/223 (86%)	2.11	85 (44%) 0 0	40, 97, 133, 147	0
All	All	2101/2481 (84%)	0.99	307 (14%) 3 5	17, 56, 111, 150	0

The worst 5 of 307 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	151	PHE	9.7
3	I	117	VAL	8.8
3	I	141	ALA	8.6
3	I	158	ASN	8.3
2	E	153	VAL	8.3

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.