



wwPDB X-ray Structure Validation Summary Report i

Mar 1, 2014 – 01:48 AM GMT

PDB ID : 2I3T
Title : Bub3 complex with Mad3 (BubR1) GLEBS motif
Authors : Larsen, N.A.; Harrison, S.C.
Deposited on : 2006-08-20
Resolution : 2.80 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

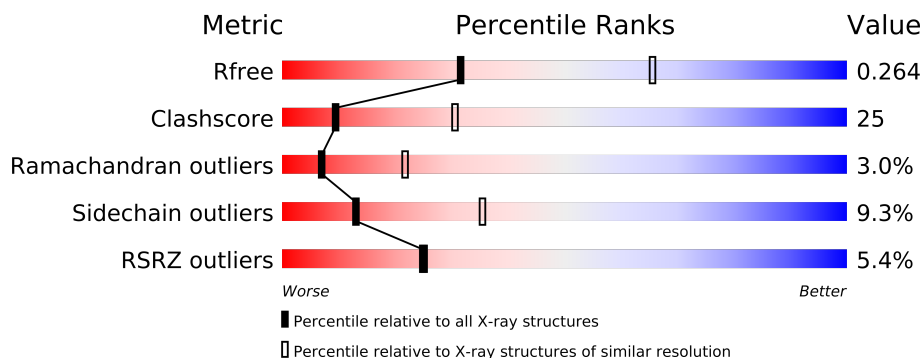
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	341	
1	C	341	
1	E	341	
1	G	341	
2	B	54	
2	D	54	
2	F	54	
2	H	54	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11816 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Cell cycle arrest protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2645	1677	443	512	13			
1	C	334	Total	C	N	O	S	0	0	0
			2645	1677	443	512	13			
1	E	334	Total	C	N	O	S	0	0	0
			2645	1677	443	512	13			
1	G	334	Total	C	N	O	S	0	0	0
			2645	1677	443	512	13			

- Molecule 2 is a protein called Spindle assembly checkpoint component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	35	Total	C	N	O	S	0	0	0
			294	191	47	53	3			
2	D	43	Total	C	N	O	S	0	0	0
			354	224	59	68	3			
2	F	35	Total	C	N	O	S	0	0	0
			294	191	47	53	3			
2	H	35	Total	C	N	O	S	0	0	0
			294	191	47	53	3			

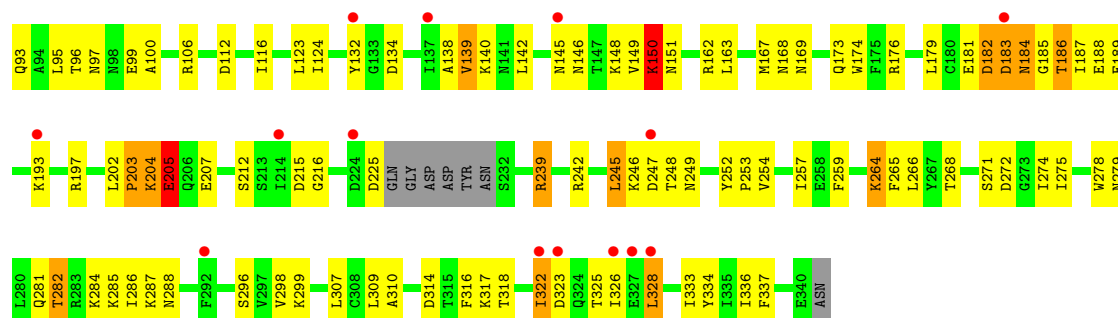
There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	353	MET	-	INITIATING METHIONINE	UNP P47074
B	401	HIS	-	EXPRESSION TAG	UNP P47074
B	402	HIS	-	EXPRESSION TAG	UNP P47074
B	403	HIS	-	EXPRESSION TAG	UNP P47074
B	404	HIS	-	EXPRESSION TAG	UNP P47074
B	405	HIS	-	EXPRESSION TAG	UNP P47074
B	406	HIS	-	EXPRESSION TAG	UNP P47074
D	353	MET	-	INITIATING METHIONINE	UNP P47074

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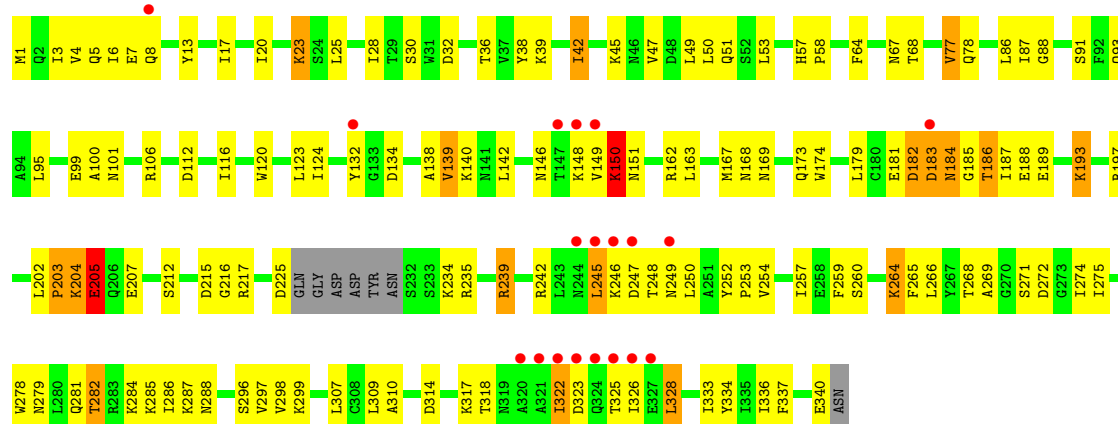
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Chain	Residue	Modelled	Actual	Comment	Reference
D	401	HIS	-	EXPRESSION TAG	UNP P47074
D	402	HIS	-	EXPRESSION TAG	UNP P47074
D	403	HIS	-	EXPRESSION TAG	UNP P47074
D	404	HIS	-	EXPRESSION TAG	UNP P47074
D	405	HIS	-	EXPRESSION TAG	UNP P47074
D	406	HIS	-	EXPRESSION TAG	UNP P47074
F	353	MET	-	INITIATING METHIONINE	UNP P47074
F	401	HIS	-	EXPRESSION TAG	UNP P47074
F	402	HIS	-	EXPRESSION TAG	UNP P47074
F	403	HIS	-	EXPRESSION TAG	UNP P47074
F	404	HIS	-	EXPRESSION TAG	UNP P47074
F	405	HIS	-	EXPRESSION TAG	UNP P47074
F	406	HIS	-	EXPRESSION TAG	UNP P47074
H	353	MET	-	INITIATING METHIONINE	UNP P47074
H	401	HIS	-	EXPRESSION TAG	UNP P47074
H	402	HIS	-	EXPRESSION TAG	UNP P47074
H	403	HIS	-	EXPRESSION TAG	UNP P47074
H	404	HIS	-	EXPRESSION TAG	UNP P47074
H	405	HIS	-	EXPRESSION TAG	UNP P47074
H	406	HIS	-	EXPRESSION TAG	UNP P47074



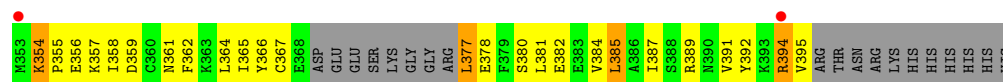
- Molecule 1: Cell cycle arrest protein

Chain G:



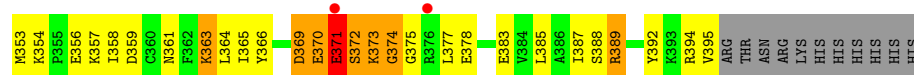
- Molecule 2: Spindle assembly checkpoint component

Chain B:



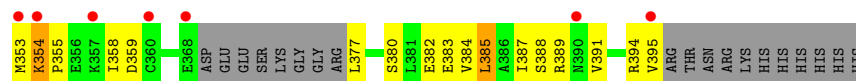
- Molecule 2: Spindle assembly checkpoint component

Chain D:



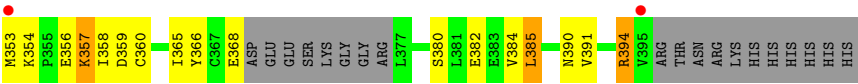
- Molecule 2: Spindle assembly checkpoint component

Chain F:



- Molecule 2: Spindle assembly checkpoint component

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.35Å 173.34Å 90.02Å 90.00° 95.30° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 49.04 – 2.69	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.80) 89.8 (49.04-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.238 , 0.267 0.236 , 0.264	Depositor DCC
R_{free} test set	1813 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	52.8	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 38784 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11816	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.43	0/2690	1.02	3/3640 (0.1%)
1	C	0.43	0/2690	0.72	3/3640 (0.1%)
1	E	0.43	0/2690	0.72	3/3640 (0.1%)
1	G	0.42	0/2690	0.72	3/3640 (0.1%)
2	B	0.53	0/297	0.70	0/395
2	D	0.47	0/358	0.73	0/476
2	F	0.51	0/297	0.81	0/395
2	H	0.55	0/297	0.79	0/395
All	All	0.43	0/12009	0.80	12/16221 (0.1%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	ARG	NE-CZ-NH1	-30.35	105.13	120.30
1	A	239	ARG	NE-CZ-NH2	29.07	134.83	120.30
1	A	239	ARG	CD-NE-CZ	17.96	148.74	123.60
1	C	239	ARG	NE-CZ-NH2	-10.62	114.99	120.30
1	E	239	ARG	NE-CZ-NH2	-10.03	115.29	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2645	0	2638	143	0
1	C	2645	0	2638	128	0
1	E	2645	0	2638	134	0
1	G	2645	0	2638	148	0
2	B	294	0	303	26	0
2	D	354	0	357	36	0
2	F	294	0	303	13	0
2	H	294	0	303	18	0
All	All	11816	0	11818	582	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 25.

The worst 5 of 582 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:148:LYS:HD3	1:E:149:VAL:H	1.12	1.15
1:A:148:LYS:HD3	1:A:149:VAL:H	1.12	1.13
1:C:148:LYS:HD3	1:C:149:VAL:H	1.12	1.13
1:G:139:VAL:HG11	1:G:179:LEU:HD13	1.30	1.12
1:C:139:VAL:HG11	1:C:179:LEU:HD13	1.32	1.11

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	330/341 (97%)	294 (89%)	27 (8%)	9 (3%)	8	25
1	C	330/341 (97%)	295 (89%)	26 (8%)	9 (3%)	8	25
1	E	330/341 (97%)	296 (90%)	25 (8%)	9 (3%)	8	25
1	G	330/341 (97%)	293 (89%)	28 (8%)	9 (3%)	8	25
2	B	31/54 (57%)	26 (84%)	3 (10%)	2 (6%)	2	5
2	D	41/54 (76%)	28 (68%)	8 (20%)	5 (12%)	1	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	31/54 (57%)	26 (84%)	5 (16%)	0	100	100
2	H	31/54 (57%)	28 (90%)	2 (6%)	1 (3%)	6	20
All	All	1454/1580 (92%)	1286 (88%)	124 (8%)	44 (3%)	7	22

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	ASP
1	A	204	LYS
2	B	394	ARG
1	C	183	ASP
1	C	204	LYS

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	299/305 (98%)	273 (91%)	26 (9%)	15	39
1	C	299/305 (98%)	273 (91%)	26 (9%)	15	39
1	E	299/305 (98%)	273 (91%)	26 (9%)	15	39
1	G	299/305 (98%)	273 (91%)	26 (9%)	15	39
2	B	34/51 (67%)	31 (91%)	3 (9%)	14	38
2	D	40/51 (78%)	34 (85%)	6 (15%)	4	12
2	F	34/51 (67%)	29 (85%)	5 (15%)	4	13
2	H	34/51 (67%)	28 (82%)	6 (18%)	3	8
All	All	1338/1424 (94%)	1214 (91%)	124 (9%)	13	35

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	370	GLU
1	E	132	TYR
1	G	309	LEU
2	D	371	GLU

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Mol	Chain	Res	Type
1	E	8	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	361	ASN
1	E	151	ASN
1	G	249	ASN
1	E	93	GLN
1	E	173	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	334/341 (97%)	0.17	14 (4%) 35 35	33, 53, 90, 104	0
1	C	334/341 (97%)	0.26	18 (5%) 25 25	34, 53, 89, 104	0
1	E	334/341 (97%)	0.25	16 (4%) 29 30	35, 55, 90, 103	0
1	G	334/341 (97%)	0.32	19 (5%) 23 23	36, 54, 89, 104	0
2	B	35/54 (64%)	0.53	2 (5%) 23 23	50, 66, 94, 108	0
2	D	43/54 (79%)	0.45	2 (4%) 30 30	51, 64, 108, 112	0
2	F	35/54 (64%)	1.09	7 (20%) 2 1	46, 61, 103, 114	0
2	H	35/54 (64%)	0.13	2 (5%) 23 23	39, 50, 69, 87	0
All	All	1484/1580 (93%)	0.28	80 (5%) 25 25	33, 55, 92, 114	0

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	353	MET	10.3
2	B	353	MET	8.7
1	G	323	ASP	6.2
1	C	326	ILE	6.0
1	E	326	ILE	5.7

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.