Full wwPDB X-ray Structure Validation Report (i)

Apr 21, 2024 – 03:43 pm BST

PDB ID	:	7AI1
Title	:	Crystal structure of human MDM2-G443T RING domain homodimer bound to UbcH5B-Ub (Crystal form 2)
Authors	:	Magnussen, H.M.; Huang, D.T.
Deposited on	:	2020-09-25
Resolution	:	2.07 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 (i) 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 (i)) were used in the production of this report:

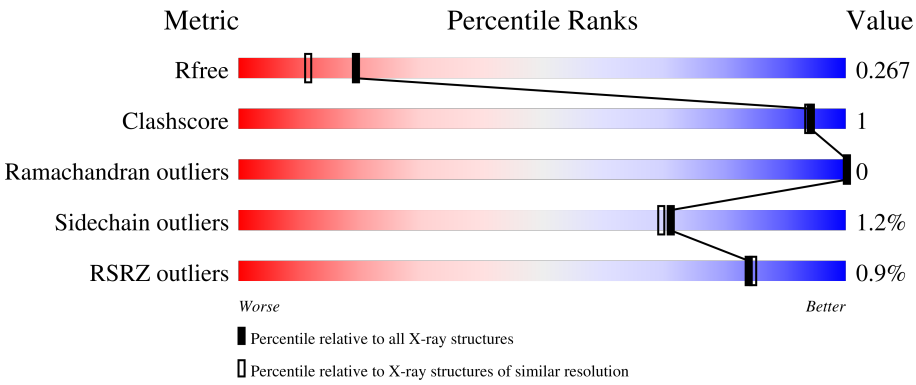
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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 <=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	AAA	75	% 79% • 17%
1	DDD	75	% 75% 5% • 19%
2	BBB	147	% 93% 7% •
2	EEE	147	% 97% • •
3	CCC	81	90% 5% 5%

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Mol	Chain	Length	Quality of chain
3	FFF	81	94% • 5%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 9348 atoms, of which 4584 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 E3 ubiquitin-protein ligase Mdm2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	AAA	62	1015	312	528	89	77	9	30	1	0
1	DDD	61	970	299	501	86	75	9	29	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	417	GLY	-	expression tag	UNP Q00987
AAA	418	SER	-	expression tag	UNP Q00987
AAA	443	THR	GLY	engineered mutation	UNP Q00987
DDD	417	GLY	-	expression tag	UNP Q00987
DDD	418	SER	-	expression tag	UNP Q00987
DDD	443	THR	GLY	engineered mutation	UNP Q00987

- Molecule 2 is a protein called Ubiquitin-conjugating enzyme E2 D2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	BBB	146	2310	746	1152	197	209	6	62	0	0
2	EEE	146	2277	740	1131	195	205	6	66	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	22	ARG	SER	engineered mutation	UNP P62837
BBB	85	LYS	CYS	engineered mutation	UNP P62837
EEE	22	ARG	SER	engineered mutation	UNP P62837
EEE	85	LYS	CYS	engineered mutation	UNP P62837

- Molecule 3 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	CCC	77	1232	380	627	105	119	1	32	1	0
			Total	C	H	N	O	S			
3	FFF	77	1240	381	633	106	119	1	30	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CCC	-4	GLY	-	expression tag	UNP P0CG47
CCC	-3	SER	-	expression tag	UNP P0CG47
CCC	0	SER	-	insertion	UNP P0CG47
FFF	-4	GLY	-	expression tag	UNP P0CG47
FFF	-3	SER	-	expression tag	UNP P0CG47
FFF	0	SER	-	insertion	UNP P0CG47

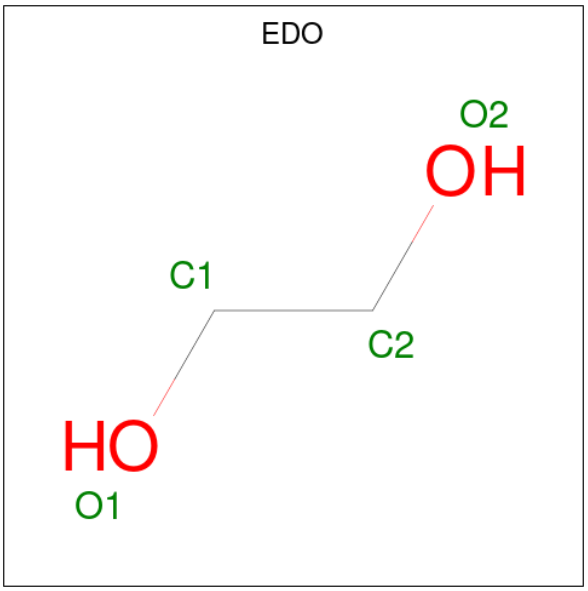
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	AAA	1	1	1	0	0
			Total	Cl		
4	DDD	1	1	1	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
5	AAA	2	2	2	0	0
			Total	Zn		
5	DDD	2	2	2	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
6	BBB	1	10	2	6	2	1	0
			Total	C	H	O		
6	BBB	1	10	2	6	2	1	0

- Molecule 7 is water.

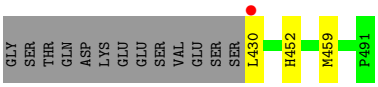
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	AAA	41	41	41	0	0
			Total	O		
7	BBB	77	77	77	0	0
			Total	O		
7	CCC	40	40	40	0	0
			Total	O		
7	DDD	31	31	31	0	0
			Total	O		
7	EEE	42	42	42	0	0
			Total	O		
7	FFF	47	47	47	0	0

3 Residue-property plots (i)

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

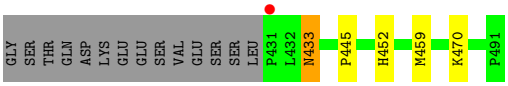
• Molecule 1: E3 ubiquitin-protein ligase Mdm2

Chain AAA:



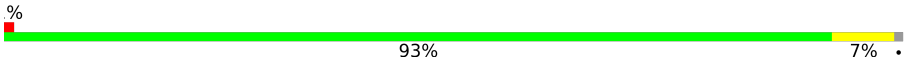
• Molecule 1: E3 ubiquitin-protein ligase Mdm2

Chain DDD:



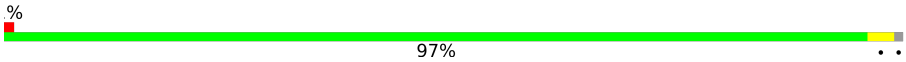
• Molecule 2: Ubiquitin-conjugating enzyme E2 D2

Chain BBB:



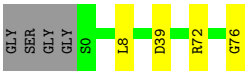
• Molecule 2: Ubiquitin-conjugating enzyme E2 D2

Chain EEE:



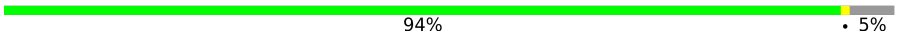
• Molecule 3: Polyubiquitin-B

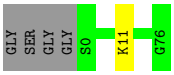
Chain CCC:



• Molecule 3: Polyubiquitin-B

Chain FFF:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	56.27Å 80.69Å 135.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.48 – 2.07 69.38 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.5 (69.48-2.07) 99.5 (69.38-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.212 , 0.266 0.220 , 0.267	Depositor DCC
R_{free} test set	1887 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	27.2	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 37.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9348	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, CL, ZN

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	AAA	0.65	0/501	0.83	0/675
1	DDD	0.67	0/480	0.80	0/647
2	BBB	0.69	0/1193	0.80	0/1627
2	EEE	0.65	0/1182	0.76	0/1615
3	CCC	0.69	0/614	0.80	0/827
3	FFF	0.68	0/613	0.79	0/824
All	All	0.67	0/4583	0.79	0/6215

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 (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	AAA	487	528	520	1	0
1	DDD	469	501	491	3	0
2	BBB	1158	1152	1138	6	0
2	EEE	1146	1131	1109	2	0
3	CCC	605	627	625	3	0
3	FFF	607	633	634	1	0
4	AAA	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	DDD	1	0	0	0	0
5	AAA	2	0	0	0	0
5	DDD	2	0	0	0	0
6	BBB	8	12	12	0	0
7	AAA	41	0	0	0	0
7	BBB	77	0	0	0	0
7	CCC	40	0	0	0	0
7	DDD	31	0	0	0	0
7	EEE	42	0	0	0	0
7	FFF	47	0	0	0	0
All	All	4764	4584	4529	12	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 1.

All (12) 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:AAA:430:LEU:HD23	1:DDD:445:PRO:HB3	1.93	0.50
3:CCC:39:ASP:O	3:CCC:72[A]:ARG:HD2	2.12	0.49
2:BBB:6:ILE:HG22	2:BBB:30:MET:CE	2.44	0.48
2:BBB:75:HIS:CE1	2:BBB:113:PRO:HB3	2.50	0.47
1:DDD:433:ASN:ND2	1:DDD:433:ASN:H	2.13	0.46
2:BBB:97:LEU:HD23	3:CCC:8:LEU:HD11	1.99	0.45
1:DDD:433:ASN:OD1	3:FFF:11:LYS:HG3	2.19	0.43
2:EEE:36:THR:HA	2:EEE:50:PHE:O	2.18	0.43
2:BBB:36:THR:HA	2:BBB:50:PHE:O	2.20	0.42
2:EEE:75:HIS:CE1	2:EEE:113:PRO:HB3	2.55	0.41
2:BBB:117:ASP:O	3:CCC:76:GLY:HA2	2.20	0.40
2:BBB:120:VAL:HG11	2:BBB:123:ILE:HD12	2.04	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	AAA	61/75 (81%)	56 (92%)	5 (8%)	0	100	100
1	DDD	59/75 (79%)	54 (92%)	5 (8%)	0	100	100
2	BBB	144/147 (98%)	141 (98%)	3 (2%)	0	100	100
2	EEE	144/147 (98%)	141 (98%)	3 (2%)	0	100	100
3	CCC	76/81 (94%)	72 (95%)	4 (5%)	0	100	100
3	FFF	75/81 (93%)	74 (99%)	1 (1%)	0	100	100
All	All	559/606 (92%)	538 (96%)	21 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	57/68 (84%)	55 (96%)	2 (4%)	36	29
1	DDD	54/68 (79%)	50 (93%)	4 (7%)	13	6
2	BBB	126/131 (96%)	126 (100%)	0	100	100
2	EEE	122/131 (93%)	122 (100%)	0	100	100
3	CCC	68/70 (97%)	68 (100%)	0	100	100
3	FFF	69/70 (99%)	69 (100%)	0	100	100
All	All	496/538 (92%)	490 (99%)	6 (1%)	71	69

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	452	HIS
1	AAA	459	MET
1	DDD	433	ASN
1	DDD	452	HIS

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Mol	Chain	Res	Type
1	DDD	459	MET
1	DDD	470	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	EDO	BBB	201	-	3,3,3	0.16	0	2,2,2	0.08	0
6	EDO	BBB	202	-	3,3,3	0.25	0	2,2,2	0.31	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	BBB	201	-	-	0/1/1/1	-
6	EDO	BBB	202	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	AAA	62/75 (82%)	-0.05	1 (1%)	72	73	18, 24, 39, 46	0
1	DDD	61/75 (81%)	-0.05	1 (1%)	72	73	19, 26, 47, 60	0
2	BBB	146/147 (99%)	0.12	1 (0%)	87	88	18, 31, 56, 70	0
2	EEE	146/147 (99%)	0.28	2 (1%)	75	76	21, 41, 67, 76	0
3	CCC	77/81 (95%)	-0.04	0	100	100	20, 31, 51, 62	0
3	FFF	77/81 (95%)	0.02	0	100	100	19, 34, 53, 60	0
All	All	569/606 (93%)	0.09	5 (0%)	84	85	18, 33, 59, 76	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	431	PRO	2.9
2	EEE	129	THR	2.5
2	BBB	129	THR	2.3
2	EEE	20	GLN	2.2
1	AAA	430	LEU	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	BBB	202	4/4	0.91	0.14	34,35,37,38	1
6	EDO	BBB	201	4/4	0.98	0.11	27,29,29,29	1
4	CL	AAA	501	1/1	0.98	0.08	30,30,30,30	0
4	CL	DDD	501	1/1	0.99	0.06	33,33,33,33	0
5	ZN	DDD	502	1/1	0.99	0.11	32,32,32,32	0
5	ZN	DDD	503	1/1	1.00	0.14	20,20,20,20	0
5	ZN	AAA	503	1/1	1.00	0.13	20,20,20,20	0
5	ZN	AAA	502	1/1	1.00	0.13	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.