



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:05 AM UTC

PDB ID : 6YJG / pdb_00006yjc
Title : Crystal structure of MINDY1 mutant-Y114F
Authors : Abdul Rehman, S.A.; Kulathu, Y.
Deposited on : 2020-04-03
Resolution : 3.28 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

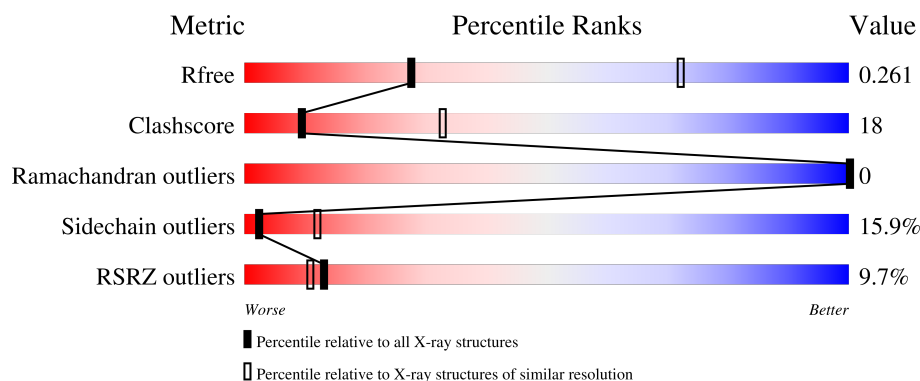
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.28 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	1303 (3.30-3.26)
Clashscore	190562	1354 (3.30-3.26)
Ramachandran outliers	187476	1334 (3.30-3.26)
Sidechain outliers	187428	1333 (3.30-3.26)
RSRZ outliers	180081	1303 (3.30-3.26)

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	289	9% 53% 30% 6% 10%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1984 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.

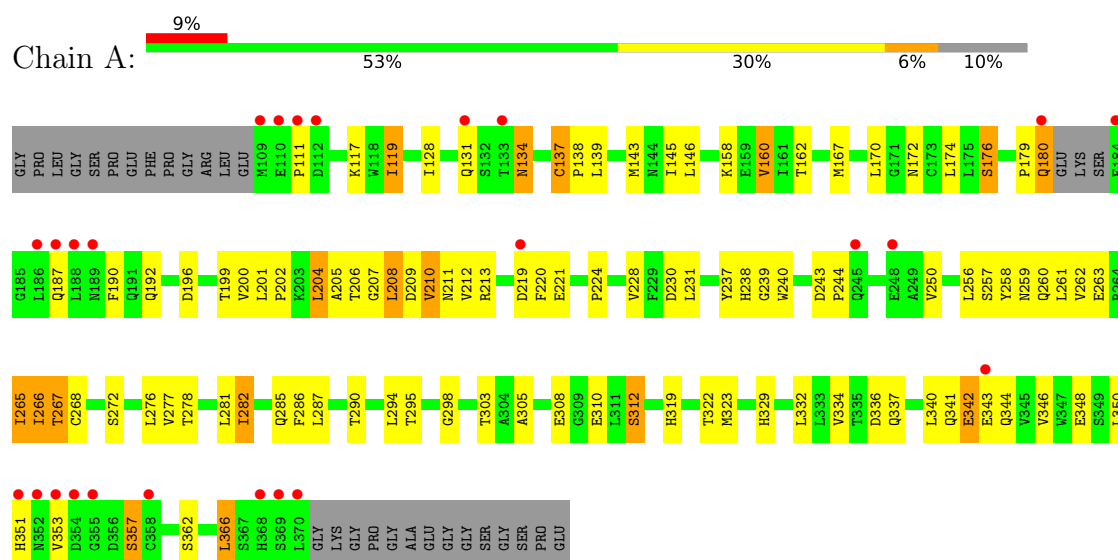
- Molecule 1 is a protein called Ubiquitin carboxyl-terminal hydrolase MINDY1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	259	1984	1271	325	376	12	0	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: Ubiquitin carboxyl-terminal hydrolase MINDY1



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	102.16Å 102.16Å 162.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.21 – 3.28 72.21 – 3.28	Depositor EDS
% Data completeness (in resolution range)	99.9 (72.21-3.28) 99.9 (72.21-3.28)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 3.26Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.205 , 0.246 0.224 , 0.261	Depositor DCC
R_{free} test set	705 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	88.2	Xtriage
Anisotropy	0.651	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 65.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	1984	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.25% 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	1.11	1/2034 (0.0%)	1.60	13/2781 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	210	VAL	C-O	6.20	1.30	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	PRO	N-CA-C	8.34	124.50	113.57
1	A	206	THR	CA-CB-OG1	-6.56	99.76	109.60
1	A	266	ILE	N-CA-C	-6.49	105.42	111.45
1	A	250	VAL	O-C-N	6.29	127.97	121.87
1	A	221	GLU	CB-CA-C	-6.19	100.98	110.26
1	A	192	GLN	N-CA-C	-5.52	105.16	111.07
1	A	221	GLU	N-CA-CB	5.43	118.07	109.71
1	A	278	THR	N-CA-C	-5.29	105.16	111.03
1	A	308	GLU	CB-CA-C	5.22	116.23	109.80
1	A	230	ASP	CA-CB-CG	5.19	117.79	112.60
1	A	265	ILE	O-C-N	5.19	127.11	121.87
1	A	305	ALA	CA-C-O	-5.15	114.52	120.24
1	A	287	LEU	CA-C-O	-5.14	115.40	120.70

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	1984	0	1864	69	0
All	All	1984	0	1864	69	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 18.

All (69) 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:243:ASP:OD1	1:A:244:PRO:HD2	1.36	1.20
1:A:200:VAL:HG11	1:A:224:PRO:CB	1.77	1.14
1:A:180:GLN:HE21	1:A:180:GLN:C	1.63	1.06
1:A:200:VAL:HG11	1:A:224:PRO:HB2	1.39	1.03
1:A:204:LEU:HD11	1:A:228:VAL:HG21	1.42	1.01
1:A:200:VAL:HG11	1:A:224:PRO:HB3	1.49	0.93
1:A:243:ASP:OD1	1:A:244:PRO:CD	2.19	0.91
1:A:158:LYS:HE3	1:A:160:VAL:O	1.89	0.72
1:A:263:GLU:O	1:A:267:THR:HG23	1.90	0.71
1:A:201:LEU:HD23	1:A:201:LEU:O	1.93	0.68
1:A:201:LEU:HD23	1:A:201:LEU:C	2.21	0.66
1:A:143:MET:HE1	1:A:146:LEU:HD12	1.79	0.64
1:A:167:MET:HE3	1:A:205:ALA:HB2	1.80	0.63
1:A:138:PRO:HG3	1:A:208:LEU:HD23	1.82	0.62
1:A:137:CYS:HA	1:A:207:GLY:HA2	1.82	0.60
1:A:342:GLU:HB3	1:A:344:GLN:NE2	2.17	0.59
1:A:257:SER:HB3	1:A:260:GLN:OE1	2.02	0.58
1:A:143:MET:HE3	1:A:170:LEU:HB2	1.84	0.58
1:A:131:GLN:O	1:A:131:GLN:HG3	2.04	0.57
1:A:179:PRO:HA	1:A:190:PHE:CE1	2.40	0.56
1:A:208:LEU:HD11	1:A:210:VAL:HG22	1.87	0.56
1:A:366:LEU:H	1:A:366:LEU:HD22	1.70	0.55
1:A:201:LEU:N	1:A:202:PRO:HD2	2.22	0.55
1:A:257:SER:HB3	1:A:260:GLN:CD	2.31	0.55
1:A:238:HIS:HD2	1:A:240:TRP:H	1.55	0.55
1:A:348:GLU:HG3	1:A:357:SER:HB3	1.88	0.55
1:A:180:GLN:C	1:A:180:GLN:NE2	2.48	0.54
1:A:323:MET:HG3	1:A:332:LEU:HD23	1.90	0.54
1:A:239:GLY:O	1:A:298:GLY:HA3	2.08	0.54
1:A:134:ASN:CG	1:A:319:HIS:NE2	2.67	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:MET:HA	1:A:143:MET:HE2	1.90	0.52
1:A:211:ASN:ND2	1:A:259:ASN:HB2	2.25	0.52
1:A:211:ASN:CG	1:A:259:ASN:HD22	2.18	0.52
1:A:119:ILE:O	1:A:119:ILE:HG13	2.10	0.52
1:A:167:MET:CE	1:A:205:ALA:HB2	2.39	0.52
1:A:286:PHE:O	1:A:290:THR:OG1	2.23	0.52
1:A:200:VAL:CG1	1:A:224:PRO:HB2	2.27	0.52
1:A:238:HIS:CD2	1:A:240:TRP:H	2.29	0.50
1:A:204:LEU:N	1:A:204:LEU:HD23	2.26	0.49
1:A:201:LEU:C	1:A:201:LEU:CD2	2.85	0.49
1:A:337:GLN:O	1:A:340:LEU:HB2	2.12	0.48
1:A:282:ILE:O	1:A:285:GLN:HB3	2.14	0.48
1:A:138:PRO:O	1:A:139:LEU:C	2.55	0.48
1:A:258:TYR:O	1:A:261:LEU:N	2.48	0.47
1:A:334:VAL:O	1:A:334:VAL:HG12	2.15	0.47
1:A:366:LEU:HD22	1:A:366:LEU:N	2.29	0.46
1:A:143:MET:CE	1:A:170:LEU:HB2	2.45	0.46
1:A:210:VAL:CG1	1:A:220:PHE:CD1	2.99	0.46
1:A:208:LEU:HD11	1:A:210:VAL:CG2	2.45	0.46
1:A:237:TYR:HE2	1:A:312:SER:CB	2.29	0.46
1:A:145:ILE:CG1	1:A:322:THR:HG23	2.46	0.46
1:A:143:MET:CE	1:A:146:LEU:HD12	2.45	0.45
1:A:341:GLN:HA	1:A:341:GLN:OE1	2.17	0.45
1:A:366:LEU:H	1:A:366:LEU:CD2	2.30	0.45
1:A:172:ASN:O	1:A:176:SER:HB2	2.18	0.44
1:A:329:HIS:HB3	1:A:351:HIS:CD2	2.53	0.43
1:A:334:VAL:N	1:A:346:VAL:O	2.51	0.43
1:A:213:ARG:CZ	1:A:219:ASP:HB3	2.49	0.42
1:A:196:ASP:O	1:A:200:VAL:HG22	2.19	0.42
1:A:210:VAL:CG1	1:A:220:PHE:HD1	2.33	0.42
1:A:201:LEU:N	1:A:202:PRO:CD	2.83	0.42
1:A:265:ILE:HG22	1:A:266:ILE:HD13	2.02	0.41
1:A:131:GLN:O	1:A:131:GLN:CG	2.67	0.41
1:A:336:ASP:OD2	1:A:337:GLN:N	2.54	0.41
1:A:174:LEU:HD11	1:A:228:VAL:HG13	2.03	0.41
1:A:211:ASN:HD21	1:A:259:ASN:HB2	1.85	0.41
1:A:239:GLY:HA3	1:A:294:LEU:HD13	2.03	0.41
1:A:350:LEU:O	1:A:350:LEU:HG	2.20	0.41
1:A:208:LEU:HD12	1:A:209:ASP:O	2.21	0.40

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	255/289 (88%)	229 (90%)	26 (10%)	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	214/253 (85%)	180 (84%)	34 (16%)	2	12

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	LYS
1	A	119	ILE
1	A	128	ILE
1	A	134	ASN
1	A	137	CYS
1	A	160	VAL
1	A	162	THR
1	A	176	SER
1	A	180	GLN
1	A	187	GLN
1	A	199	THR
1	A	204	LEU
1	A	208	LEU

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Mol	Chain	Res	Type
1	A	212	VAL
1	A	231	LEU
1	A	256	LEU
1	A	262	VAL
1	A	267	THR
1	A	268	CYS
1	A	272	SER
1	A	276	LEU
1	A	277	VAL
1	A	281	LEU
1	A	282	ILE
1	A	295	THR
1	A	303	THR
1	A	310	GLU
1	A	312	SER
1	A	342	GLU
1	A	343	GLU
1	A	353	VAL
1	A	357	SER
1	A	362	SER
1	A	366	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	A	180	GLN
1	A	187	GLN
1	A	238	HIS
1	A	259	ASN
1	A	275	ASN
1	A	317	ASN
1	A	329	HIS
1	A	337	GLN
1	A	352	ASN

5.3.3 RNA ⓘ

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	259/289 (89%)	0.37	25 (9%) 13 11	63, 90, 135, 192	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	112	ASP	5.8
1	A	133	THR	5.0
1	A	352	ASN	4.7
1	A	109	MET	4.2
1	A	245	GLN	4.2
1	A	189	ASN	4.1
1	A	188	LEU	4.1
1	A	111	PRO	3.6
1	A	351	HIS	3.2
1	A	110	GLU	2.9
1	A	184	GLU	2.8
1	A	131	GLN	2.6
1	A	368	HIS	2.5
1	A	248	GLU	2.5
1	A	370	LEU	2.5
1	A	187	GLN	2.5
1	A	353	VAL	2.5
1	A	358	CYS	2.4
1	A	354	ASP	2.4
1	A	186	LEU	2.4
1	A	180	GLN	2.3
1	A	355	GLY	2.3
1	A	219	ASP	2.2
1	A	343	GLU	2.1
1	A	369	SER	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.