



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:47 PM UTC

PDB ID : 6BDB / pdb_00006bdb
Title : I-OnuI K227Y, D236A bound to A3G substrate (pre-cleavage complex)
Authors : Brown, C.; Zhang, K.; McMurrrough, T.A.; Laforet, M.; Gloor, G.B.; Edgell, D.R.; Junop, M.
Deposited on : 2017-10-22
Resolution : 1.50 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

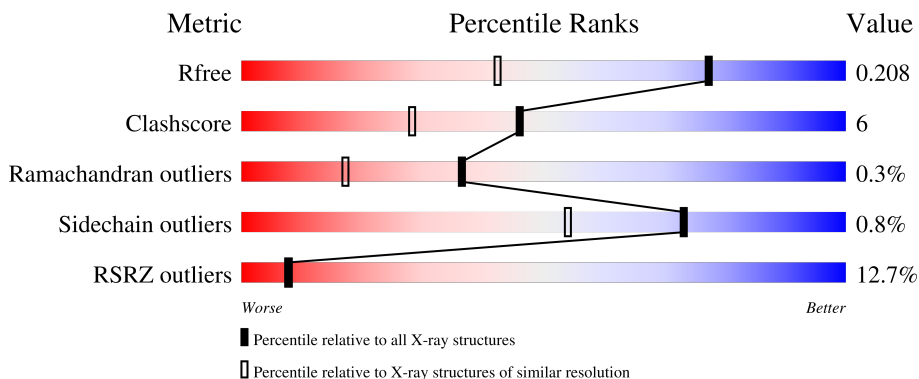
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


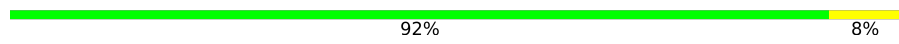

The reported resolution of this entry is 1.50 Å.

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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	307	
2	B	26	
3	C	26	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3983 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 Ribosomal protein 3/homing endonuclease-like protein fusion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	295	2340	1518	388	425	9	0	2	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q4VWW5
A	-2	PRO	-	expression tag	UNP Q4VWW5
A	-1	LEU	-	expression tag	UNP Q4VWW5
A	0	GLY	-	expression tag	UNP Q4VWW5
A	7	GLU	ARG	conflict	UNP Q4VWW5
A	227	TYR	LYS	engineered mutation	UNP Q4VWW5
A	236	ALA	ASP	engineered mutation	UNP Q4VWW5

- Molecule 2 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	26	513	250	77	161	25	0	0	0

- Molecule 3 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	26	547	259	116	147	25	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	342	Total	O	0	0
			342	342		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	125	Total 125	O 125	0	0
4	C	116	Total 116	O 116	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	43.37Å 67.19Å 169.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.02 – 1.50 42.02 – 1.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (42.02-1.50) 100.0 (42.02-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 1.50Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.185 , 0.206 0.192 , 0.208	Depositor DCC
R_{free} test set	4055 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	17.8	Xtrriage
Anisotropy	0.487	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3983	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.01% 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	0.63	2/2388 (0.1%)	0.88	4/3221 (0.1%)
2	B	0.43	0/569	0.75	0/873
3	C	0.48	0/619	0.70	0/957
All	All	0.58	2/3576 (0.1%)	0.83	4/5051 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	ILE	C-O	-5.94	1.17	1.24
1	A	301	ARG	C-O	-5.24	1.17	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	SER	CA-C-N	-6.29	112.26	122.26
1	A	230	SER	C-N-CA	-6.29	112.26	122.26
1	A	153	ILE	N-CA-C	5.46	115.51	107.15
1	A	44	GLY	N-CA-C	5.43	119.07	111.19

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	2340	0	2351	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	513	0	299	2	0
3	C	547	0	292	2	0
4	A	342	0	0	10	0
4	B	125	0	0	2	0
4	C	116	0	0	1	0
All	All	3983	0	2942	37	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 6.

All (37) 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:192:LEU:HD11	1:A:287:LEU:HD22	1.55	0.85
1:A:22:GLU:OE2	4:A:402:HOH:O	1.97	0.81
1:A:186:ILE:HD12	1:A:195:GLN:CD	2.10	0.75
1:A:52:LYS:HD3	1:A:303:PHE:CZ	2.22	0.75
1:A:154:ILE:HD12	1:A:154:ILE:C	2.15	0.72
3:C:21:DG:OP1	4:C:101:HOH:O	2.08	0.71
1:A:105:GLY:HA2	1:A:108:MET:HE2	1.74	0.70
1:A:186:ILE:HB	1:A:195:GLN:HB3	1.75	0.69
1:A:7:GLU:N	4:A:405:HOH:O	2.31	0.62
1:A:186:ILE:O	1:A:194:VAL:HA	2.01	0.61
1:A:186:ILE:HD12	1:A:195:GLN:OE1	2.01	0.60
1:A:186:ILE:CD1	1:A:195:GLN:OE1	2.49	0.60
1:A:151:PRO:HD2	4:A:413:HOH:O	2.05	0.56
1:A:148:LYS:N	4:A:407:HOH:O	2.40	0.54
1:A:279:LYS:NZ	4:A:408:HOH:O	2.41	0.53
1:A:192:LEU:CD1	1:A:287:LEU:HD22	2.32	0.53
1:A:192:LEU:O	1:A:192:LEU:HD12	2.09	0.52
1:A:130:GLU:OE1	1:A:133:ARG:NH2	2.43	0.51
2:B:15:DG:OP1	4:B:101:HOH:O	2.20	0.50
1:A:64:TRP:HB3	1:A:66:VAL:HG22	1.95	0.47
1:A:154:ILE:C	1:A:154:ILE:CD1	2.86	0.47
1:A:128:ILE:O	1:A:132:VAL:HG23	2.15	0.47
1:A:151:PRO:CD	4:A:413:HOH:O	2.62	0.46
1:A:186:ILE:HD13	1:A:195:GLN:OE1	2.16	0.46
1:A:192:LEU:HD12	1:A:192:LEU:C	2.40	0.46
1:A:289:GLU:OE1	4:A:403:HOH:O	2.20	0.44
1:A:194:VAL:O	1:A:194:VAL:HG13	2.17	0.44
1:A:231:GLU:N	1:A:231:GLU:OE1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ASN:HB3	4:A:596:HOH:O	2.17	0.44
3:C:23:DA:H2''	3:C:24:DA:H8	1.83	0.44
1:A:225:LYS:HD3	1:A:238:VAL:HG21	2.00	0.43
1:A:192:LEU:CD1	1:A:192:LEU:C	2.92	0.43
1:A:151:PRO:N	4:A:413:HOH:O	2.52	0.42
1:A:150:PHE:HA	4:A:413:HOH:O	2.19	0.42
2:B:23:DA:H4'	4:B:205:HOH:O	2.20	0.41
1:A:52:LYS:HD3	1:A:303:PHE:CE1	2.54	0.41
1:A:154:ILE:HD12	1:A:155:SER:N	2.35	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	293/307 (95%)	280 (96%)	12 (4%)	1 (0%)	36 17

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	LYS

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	A	255/276 (92%)	253 (99%)	2 (1%)	73 54

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	LEU
1	A	261	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	296	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	295/307 (96%)	0.71	43 (14%) 6 6	12, 22, 49, 65	2 (0%)
2	B	26/26 (100%)	0.17	0 100 100	14, 28, 37, 45	0
3	C	26/26 (100%)	0.23	1 (3%) 44 48	15, 23, 48, 53	0
All	All	347/359 (96%)	0.63	44 (12%) 8 8	12, 23, 48, 65	2 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	303	PHE	7.0
1	A	154	ILE	5.7
1	A	186	ILE	5.7
1	A	155	SER	4.6
1	A	153	ILE	4.6
1	A	192	LEU	4.2
1	A	33	ASN	4.0
1	A	189	LYS	3.7
1	A	39	TYR	3.7
1	A	190	SER	3.6
1	A	230	SER	3.6
1	A	37	VAL	3.5
1	A	147	LYS	3.3
1	A	140	TRP	3.3
1	A	125	ILE	3.2
1	A	193	GLY	3.2
1	A	150	PHE	3.1
1	A	188	SER	3.1
1	A	287	LEU	3.0
1	A	151	PRO	2.8
1	A	149	ALA	2.6
1	A	295	LEU	2.6
1	A	115[A]	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	194	VAL	2.5
1	A	283	THR	2.5
1	A	123	LEU	2.5
1	A	124	LYS	2.5
1	A	285	SER	2.4
1	A	29	ILE	2.4
1	A	31	ASN	2.4
1	A	132	VAL	2.3
1	A	127	GLY	2.3
1	A	191	LYS	2.3
1	A	9	SER	2.2
1	A	126	ASN	2.2
1	A	158	ARG	2.1
1	A	159	SER	2.1
1	A	49	LEU	2.1
1	A	41	THR	2.1
3	C	26	DG	2.1
1	A	296	ASN	2.1
1	A	144	ASP	2.1
1	A	288	ASP	2.0
1	A	8	GLU	2.0

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.