



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:03 AM UTC

PDB ID : 7MCD / pdb_00007mcd
Title : Crystal structure of an AI-designed TIM-barrel F15C
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Deposited on : 2021-04-02
Resolution : 1.90 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
Xtrriage (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

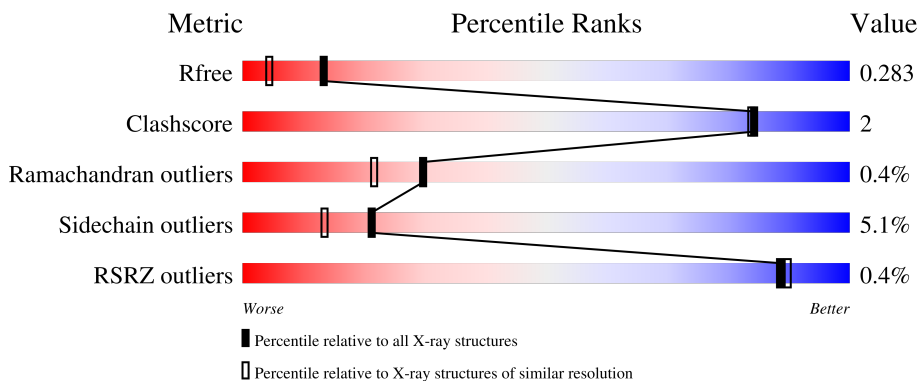
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	184	 89% 9% ...
1	B	184	 88% 8% ...
1	C	184	 90% 8% ...
1	D	184	 92% 7% ...

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5828 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 AI-designed TIM-barrel F15C.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	183	1424	905	239	280	0	0	0
1	B	181	1409	897	236	275	1	0	0
1	C	183	1427	908	239	279	1	0	0
1	D	183	1424	905	239	280	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	29	Total	O	0	2
			31	31		
2	B	28	Total	O	0	1
			29	29		
2	C	51	Total	O	0	0
			51	51		
2	D	32	Total	O	0	1
			33	33		

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.

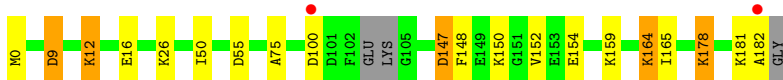
- Molecule 1: AI-designed TIM-barrel F15C

Chain A:  89% 9% ...




- Molecule 1: AI-designed TIM-barrel F15C

Chain B:  88% 8% ..




- Molecule 1: AI-designed TIM-barrel F15C

Chain C:  90% 8% ..



- Molecule 1: AI-designed TIM-barrel F15C

Chain D:  92% 7% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.23Å 103.57Å 80.94Å 90.00° 90.39° 90.00°	Depositor
Resolution (Å)	38.93 – 1.90 38.93 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (38.93-1.90) 99.2 (38.93-1.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 1.89Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.177 , 0.257 (Not available) , 0.283	Depositor DCC
R_{free} test set	2849 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtrriage
Anisotropy	1.310	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	0.007 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5828	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.8719e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	1.07	0/1439	1.48	1/1918 (0.1%)
1	B	1.02	0/1423	1.46	0/1897
1	C	1.05	0/1442	1.41	2/1923 (0.1%)
1	D	1.07	0/1439	1.48	2/1918 (0.1%)
All	All	1.05	0/5743	1.46	5/7656 (0.1%)

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
1	D	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	71	ALA	CA-C-N	5.67	128.13	120.65
1	C	71	ALA	C-N-CA	5.67	128.13	120.65
1	A	26	LYS	CB-CA-C	5.45	119.94	110.79
1	D	159	LYS	CA-C-N	5.16	127.15	120.44
1	D	159	LYS	C-N-CA	5.16	127.15	120.44

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	117	ALA	Peptide

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	1424	0	1489	7	0
1	B	1409	0	1475	10	0
1	C	1427	0	1495	7	0
1	D	1424	0	1489	4	0
2	A	31	0	0	0	0
2	B	29	0	0	0	0
2	C	51	0	0	0	0
2	D	33	0	0	0	0
All	All	5828	0	5948	27	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 2.

All (27) 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:C:23:HIS:O	1:C:26:LYS:HE2	1.80	0.81
1:B:164:LYS:HG2	1:B:165:ILE:HG13	1.69	0.74
1:D:49:LEU:HD12	1:D:71:ALA:HB1	1.82	0.60
1:A:95:LEU:HD12	1:A:117:ALA:HB1	1.90	0.53
1:B:164:LYS:HB2	1:D:118:LYS:HG3	1.90	0.53
1:A:149:GLU:H	1:A:149:GLU:CD	2.16	0.53
1:C:4:ILE:HG12	1:C:29:ALA:HB3	1.91	0.52
1:B:148:PHE:HZ	1:B:178:LYS:HB3	1.76	0.51
1:D:104:LYS:O	1:D:108:GLU:HG2	2.13	0.48
1:B:50:ILE:HG12	1:B:75:ALA:HB3	1.96	0.48
1:B:147:ASP:OD1	1:B:147:ASP:C	2.56	0.48
1:A:4:ILE:HG12	1:A:29:ALA:HB3	1.96	0.47
1:B:12:LYS:HE3	1:B:12:LYS:HA	1.96	0.47
1:B:9:ASP:OD1	1:B:12:LYS:HB2	2.14	0.47
1:A:26:LYS:HG2	1:A:27:ILE:HG13	1.96	0.47
1:B:150:LYS:O	1:B:154:GLU:HG2	2.14	0.46
1:B:12:LYS:HE2	1:B:16:GLU:OE2	2.15	0.46
1:C:96:ILE:HG12	1:C:121:ALA:HB3	1.97	0.45
1:B:152:VAL:HG13	1:B:182:ALA:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:LEU:HD12	1:C:71:ALA:HB1	2.00	0.43
1:C:50:ILE:HG12	1:C:75:ALA:HB3	2.02	0.42
1:C:1:ASP:HA	1:C:166:ILE:O	2.20	0.42
1:A:125:LYS:HE2	1:A:146:ASP:OD2	2.19	0.42
1:C:95:LEU:HD12	1:C:117:ALA:HB1	2.01	0.42
1:A:142:ILE:HG12	1:A:167:ALA:HB3	2.02	0.41
1:D:49:LEU:HD12	1:D:71:ALA:CB	2.49	0.40
1:A:50:ILE:HG12	1:A:75:ALA:HB3	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	A	181/184 (98%)	177 (98%)	4 (2%)	0	100	100
1	B	177/184 (96%)	173 (98%)	3 (2%)	1 (1%)	21	13
1	C	181/184 (98%)	178 (98%)	3 (2%)	0	100	100
1	D	181/184 (98%)	178 (98%)	1 (1%)	2 (1%)	11	4
All	All	720/736 (98%)	706 (98%)	11 (2%)	3 (0%)	30	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	118	LYS
1	B	100	ASP
1	D	164	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	148/149 (99%)	140 (95%)	8 (5%)	20	12
1	B	147/149 (99%)	137 (93%)	10 (7%)	14	7
1	C	149/149 (100%)	143 (96%)	6 (4%)	28	20
1	D	148/149 (99%)	142 (96%)	6 (4%)	27	19
All	All	592/596 (99%)	562 (95%)	30 (5%)	21	13

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LYS
1	A	108	GLU
1	A	147	ASP
1	A	149	GLU
1	A	150	LYS
1	A	153	GLU
1	A	178	LYS
1	A	181	LYS
1	B	0	MET
1	B	9	ASP
1	B	12	LYS
1	B	26	LYS
1	B	55	ASP
1	B	147	ASP
1	B	159	LYS
1	B	164	LYS
1	B	178	LYS
1	B	181	LYS
1	C	1	ASP
1	C	26	LYS
1	C	55	ASP
1	C	101	ASP
1	C	160	ARG
1	C	181	LYS

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Mol	Chain	Res	Type
1	D	11	GLU
1	D	26	LYS
1	D	55	ASP
1	D	82	GLU
1	D	110	LYS
1	D	147	ASP

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	23	HIS
1	B	115	HIS

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 [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	A	183/184 (99%)	-0.09	0 100 100	28, 49, 79, 103	0
1	B	181/184 (98%)	-0.04	2 (1%) 78 80	28, 53, 81, 93	0
1	C	183/184 (99%)	-0.19	1 (0%) 87 89	27, 45, 73, 93	0
1	D	183/184 (99%)	-0.11	0 100 100	29, 50, 82, 92	0
All	All	730/736 (99%)	-0.11	3 (0%) 88 90	27, 49, 79, 103	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	182	ALA	3.1
1	B	100	ASP	2.2
1	C	181	LYS	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.