



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2026 – 04:22 pm BST

PDB ID : 9R7K / pdb\_00009r7k  
Title : De novo designed enzyme for the Morita-Baylis-Hillman reaction (MBH61)  
Authors : Tripp, A.; Bijelic, A.; Fischer, C.; Moser, M.; Oberdorfer, G.  
Deposited on : 2025-05-14  
Resolution : 2.95 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](mailto:validation@mail.wwpdb.org)

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<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>.

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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

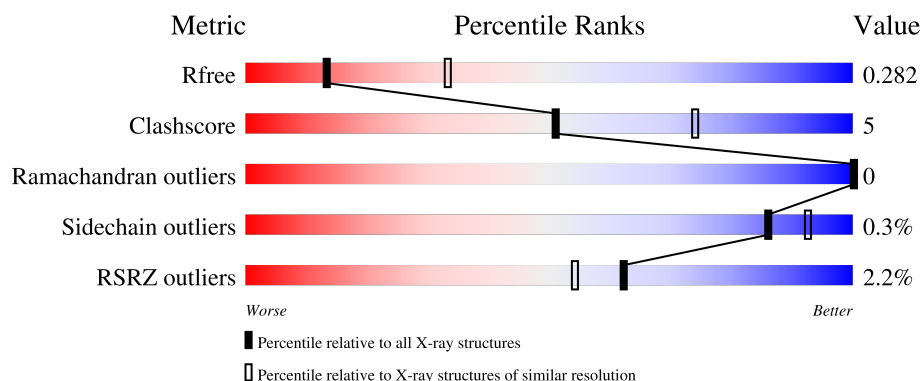
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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  $\geq 3$ , 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	221	<div> <div>3%</div> <div>82%</div> <div>10%</div> <div>7%</div> </div>
1	B	221	<div> <div>2%</div> <div>78%</div> <div>15%</div> <div>7%</div> </div>
1	C	221	<div> <div>0%</div> <div>84%</div> <div>9%</div> <div>7%</div> </div>
1	D	221	<div> <div>2%</div> <div>81%</div> <div>12%</div> <div>7%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6257 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 De novo designed enzyme for the Morita-Baylis-Hillman reaction (MBH61).

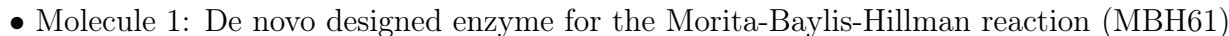
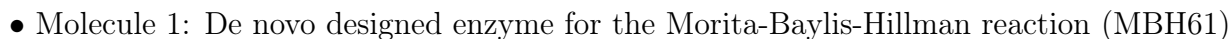
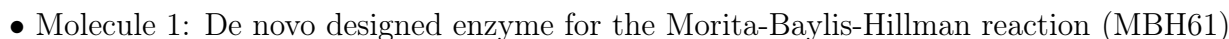
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	0	1	0
			1538	973	274	291			
1	B	206	Total	C	N	O	0	0	0
			1576	997	282	297			
1	C	205	Total	C	N	O	0	0	0
			1557	985	277	295			
1	D	205	Total	C	N	O	0	0	0
			1566	991	279	296			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	8	Total	O	0	0
			8	8		
2	B	6	Total	O	0	0
			6	6		
2	C	2	Total	O	0	0
			2	2		
2	D	4	Total	O	0	0
			4	4		



- Molecule 1: De novo designed enzyme for the Morita-Baylis-Hillman reaction (MBH61)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.67Å 89.11Å 184.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.29 – 2.95 48.29 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.29-2.95) 99.9 (48.29-2.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 2.48Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, $R_{free}$	0.227 , 0.288 0.223 , 0.282	Depositor DCC
$R_{free}$ test set	1650 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.1	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 36.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6257	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.41% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.43	0/1561	0.66	0/2124
1	B	0.46	0/1600	0.64	0/2172
1	C	0.43	0/1581	0.63	0/2148
1	D	0.40	0/1591	0.62	0/2162
All	All	0.43	0/6333	0.64	0/8606

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	79	ARG	Sidechain

### 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	1538	0	1524	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1576	0	1588	21	0
1	C	1557	0	1555	12	0
1	D	1566	0	1562	20	0
2	A	8	0	0	1	0
2	B	6	0	0	0	0
2	C	2	0	0	0	0
2	D	4	0	0	0	0
All	All	6257	0	6229	65	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 5.

All (65) 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:B:58:ARG:O	1:B:62:LEU:HD22	1.70	0.92
1:C:150:LEU:HD22	1:C:176:GLU:HG2	1.68	0.75
1:D:14:GLU:HG2	1:D:197:ARG:HH12	1.50	0.74
1:A:58:ARG:HG3	1:D:58:ARG:HG3	1.74	0.69
1:D:99:GLN:O	1:D:103:GLU:HG3	1.97	0.65
1:D:119:PHE:HE2	1:D:159:VAL:HG13	1.62	0.64
1:B:191:ALA:O	1:B:195:ARG:HG2	1.98	0.64
1:D:166:ARG:O	1:D:170:GLU:HG3	1.97	0.64
1:A:198:LEU:HD12	1:A:199:PRO:HD2	1.79	0.63
1:A:141:THR:HG23	1:A:144:ALA:H	1.63	0.62
1:B:20:LEU:HD21	1:B:92:LYS:HE2	1.81	0.61
1:C:4:LEU:O	1:C:8:ILE:HG13	2.00	0.60
1:B:193:ALA:O	1:B:197:ARG:HG3	2.01	0.59
1:B:79:ARG:HD2	1:B:87:ARG:HH21	1.67	0.58
1:C:99:GLN:O	1:C:103:GLU:HG3	2.04	0.57
1:D:79:ARG:NE	1:D:87:ARG:HH21	2.04	0.56
1:B:113:VAL:HG21	1:B:122:TYR:HD1	1.70	0.56
1:D:119:PHE:CE2	1:D:159:VAL:HG13	2.41	0.56
1:B:150:LEU:HD22	1:B:176:GLU:HG3	1.87	0.55
1:A:175:HIS:O	1:A:179:VAL:HG23	2.07	0.54
1:D:14:GLU:HG2	1:D:197:ARG:NH1	2.20	0.54
1:A:20:LEU:HD13	1:A:89:ARG:HG3	1.91	0.53
1:D:128:TYR:CZ	1:D:159:VAL:HG21	2.44	0.52
1:D:155:ASP:OD1	1:D:158:LYS:HE2	2.09	0.52
1:A:61:ALA:HB1	1:A:172:LEU:HG	1.92	0.52
1:D:79:ARG:HE	1:D:87:ARG:HH21	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:VAL:CG2	1:C:126:GLN:HG3	2.42	0.50
1:D:31:GLN:HB2	1:D:101:VAL:HG21	1.94	0.50
1:A:150:LEU:HD22	1:A:176:GLU:HG2	1.94	0.50
1:B:118:ILE:HD13	1:C:127:ARG:CZ	2.42	0.49
1:B:-5:LEU:O	1:B:-4:TYR:HB2	2.12	0.49
1:A:99:GLN:O	1:A:103:GLU:HG3	2.13	0.49
1:A:198:LEU:O	1:A:199:PRO:C	2.55	0.49
1:B:162:GLY:O	1:B:166:ARG:HG3	2.13	0.49
1:B:175:HIS:O	1:B:179:VAL:HG23	2.13	0.48
1:D:4:LEU:O	1:D:8:ILE:HG13	2.14	0.48
1:B:150:LEU:HD13	1:B:180:ARG:NH2	2.28	0.47
1:B:95:GLU:HG2	1:B:130:LEU:HD21	1.96	0.47
1:D:79:ARG:HD3	1:D:87:ARG:HH21	1.80	0.47
1:D:71:VAL:HG21	1:D:133:GLU:HG2	1.96	0.47
1:A:184:ARG:HD2	2:A:301:HOH:O	2.14	0.47
1:B:113:VAL:HG21	1:B:122:TYR:CD1	2.49	0.46
1:A:92:LYS:HE3	1:A:92:LYS:HB2	1.82	0.46
1:B:118:ILE:HD13	1:C:127:ARG:NH2	2.30	0.46
1:D:79:ARG:CD	1:D:87:ARG:HH21	2.27	0.46
1:B:4:LEU:O	1:B:8:ILE:HG13	2.16	0.45
1:B:99:GLN:O	1:B:103:GLU:HG3	2.17	0.45
1:C:100:TYR:CD1	1:C:100:TYR:C	2.95	0.45
1:A:100:TYR:C	1:A:100:TYR:CD1	2.95	0.45
1:A:89:ARG:O	1:A:93:VAL:HG23	2.17	0.44
1:B:61:ALA:HB1	1:B:172:LEU:HD22	1.99	0.44
1:D:102:ILE:HG12	1:D:123:ALA:HA	1.99	0.44
1:B:100:TYR:C	1:B:100:TYR:CD1	2.96	0.44
1:B:41:HIS:HB3	1:B:45:GLU:HG3	2.00	0.43
1:D:134:LEU:HA	1:D:134:LEU:HD23	1.80	0.43
1:C:128:TYR:CE2	1:C:159:VAL:HG21	2.54	0.43
1:A:42:THR:OG1	1:A:45:GLU:HG2	2.20	0.42
1:B:105:SER:OG	1:B:122:TYR:HB3	2.20	0.42
1:C:42:THR:OG1	1:C:45:GLU:HG2	2.20	0.42
1:A:178:GLU:OE2	1:D:55:LYS:HD2	2.19	0.42
1:D:42:THR:OG1	1:D:45:GLU:HG2	2.20	0.41
1:C:160:TYR:HB3	1:C:165:HIS:CG	2.56	0.41
1:C:31:GLN:CB	1:C:101:VAL:HG11	2.51	0.40
1:A:41:HIS:HB3	1:A:45:GLU:HG3	2.03	0.40
1:C:91:ARG:NH2	1:C:138:ASP:OD1	2.54	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	204/221 (92%)	200 (98%)	4 (2%)	0	100	100
1	B	204/221 (92%)	200 (98%)	4 (2%)	0	100	100
1	C	203/221 (92%)	198 (98%)	5 (2%)	0	100	100
1	D	203/221 (92%)	199 (98%)	4 (2%)	0	100	100
All	All	814/884 (92%)	797 (98%)	17 (2%)	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	A	141/164 (86%)	140 (99%)	1 (1%)	76	87
1	B	149/164 (91%)	148 (99%)	1 (1%)	76	87
1	C	146/164 (89%)	146 (100%)	0	100	100
1	D	147/164 (90%)	147 (100%)	0	100	100
All	All	583/656 (89%)	581 (100%)	2 (0%)	86	92

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

Mol	Chain	Res	Type
1	A	199	PRO
1	B	79	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	HIS
1	B	-2	GLN
1	B	126	GLN
1	C	32	GLN
1	C	126	GLN
1	C	165	HIS
1	D	-2	GLN

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	205/221 (92%)	-0.07	6 (2%) 53 46	13, 41, 67, 86	1 (0%)
1	B	206/221 (93%)	-0.01	4 (1%) 66 58	18, 41, 67, 98	0
1	C	205/221 (92%)	-0.06	3 (1%) 72 65	24, 42, 64, 106	0
1	D	205/221 (92%)	0.13	5 (2%) 59 51	24, 52, 81, 111	0
All	All	821/884 (92%)	-0.00	18 (2%) 62 54	13, 43, 73, 111	1 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-6	ASN	4.4
1	B	199	PRO	4.3
1	D	199	PRO	3.4
1	A	-5	LEU	3.1
1	A	79[A]	ARG	2.8
1	A	57	PRO	2.8
1	D	-5	LEU	2.7
1	D	163	PRO	2.6
1	C	-4	TYR	2.6
1	D	-4	TYR	2.5
1	A	141	THR	2.5
1	C	197	ARG	2.4
1	C	199	PRO	2.4
1	B	163	PRO	2.2
1	B	31	GLN	2.2
1	A	199	PRO	2.1
1	D	161	LYS	2.1
1	A	197	ARG	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.