



# Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2025 – 01:08 am BST

PDB ID : 9R2R / pdb\_00009r2r  
Title : De novo designed M7 protein fold  
Authors : Pacesa, M.; Miao, Y.; Georgeon, S.; Schmidt, J.; Correia, B.E.  
Deposited on : 2025-04-30  
Resolution : 2.91 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)

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 Phenix2.0rc1  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

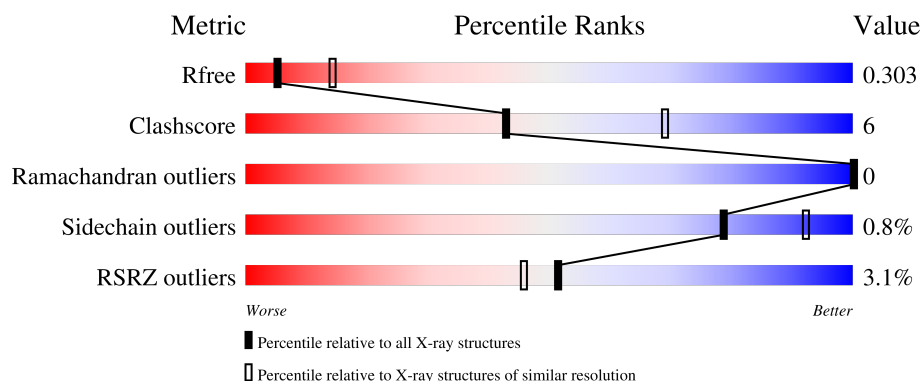
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 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))
$R_{free}$	164625	2797 (2.94-2.90)
Clashscore	180529	3049 (2.94-2.90)
Ramachandran outliers	177936	2981 (2.94-2.90)
Sidechain outliers	177891	2983 (2.94-2.90)
RSRZ outliers	164620	2799 (2.94-2.90)

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  $\geq 3$ , 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	144	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>14%</div> <div>6%</div> </div> </div>
1	B	144	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>16%</div> <div>6%</div> </div> </div>
1	C	144	<div> <div>0%</div> <div> <div></div> <div>74%</div> <div>15%</div> <div>11%</div> </div> </div>
1	D	144	<div> <div>6%</div> <div> <div></div> <div>67%</div> <div>19%</div> <div>14%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4457 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 M7r1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	136	Total	C	N	O	0	0	0
			1150	716	195	239			
1	C	128	Total	C	N	O	0	0	0
			1092	683	182	227			
1	D	124	Total	C	N	O	0	0	0
			1051	665	171	215			
1	B	136	Total	C	N	O	0	0	0
			1157	723	193	241			

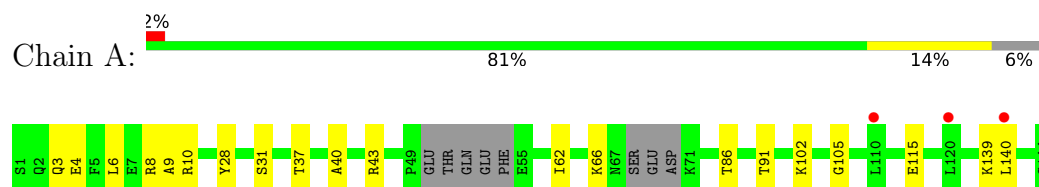
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	O	0	0
			3	3		
2	C	2	Total	O	0	0
			2	2		
2	D	1	Total	O	0	0
			1	1		
2	B	1	Total	O	0	0
			1	1		

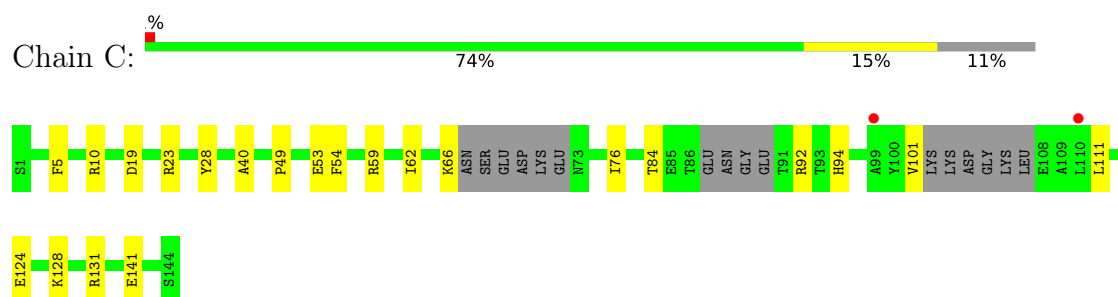
### 3 Residue-property plots [i](#)

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.

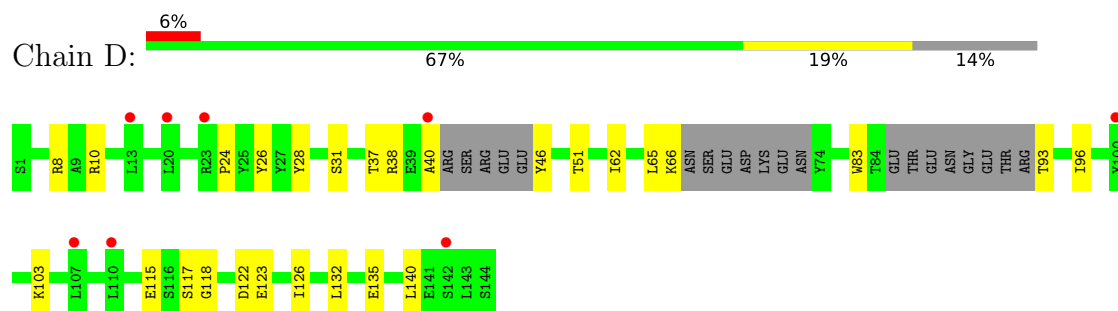
#### • Molecule 1: M7r1



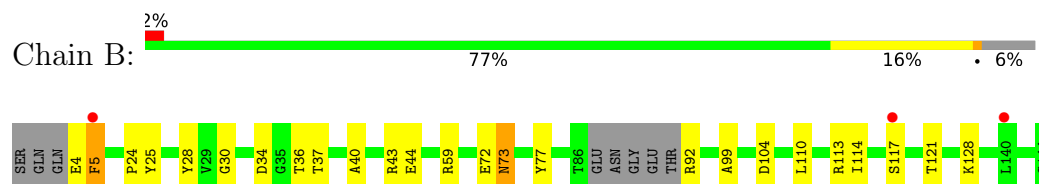
#### • Molecule 1: M7r1



#### • Molecule 1: M7r1



#### • Molecule 1: M7r1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.48Å 88.58Å 65.75Å 90.00° 114.04° 90.00°	Depositor
Resolution (Å)	60.05 – 2.91 60.05 – 2.91	Depositor EDS
% Data completeness (in resolution range)	93.6 (60.05-2.91) 93.8 (60.05-2.91)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.248 , 0.302 0.248 , 0.303	Depositor DCC
$R_{free}$ test set	555 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.1	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 75.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4457	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.10% 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	0.11	0/1168	0.28	0/1570
1	B	0.10	0/1177	0.24	0/1584
1	C	0.10	0/1110	0.24	0/1495
1	D	0.11	0/1069	0.25	0/1438
All	All	0.10	0/4524	0.25	0/6087

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	A	1150	0	1104	13	0
1	B	1157	0	1104	15	0
1	C	1092	0	1036	12	0
1	D	1051	0	1011	16	0
2	A	3	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
All	All	4457	0	4255	53	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 (53) 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:28:TYR:HB3	1:C:40:ALA:HB3	1.71	0.73
1:A:28:TYR:HB3	1:A:40:ALA:HB3	1.78	0.64
1:D:28:TYR:HB3	1:D:40:ALA:HB3	1.83	0.60
1:C:10:ARG:HH21	1:C:141:GLU:HA	1.68	0.57
1:A:10:ARG:HG3	1:A:140:LEU:HD23	1.88	0.56
1:D:26:TYR:HD1	1:D:115:GLU:HG2	1.71	0.55
1:C:131:ARG:HH12	1:D:135:GLU:HG2	1.73	0.54
1:A:4:GLU:O	1:A:8:ARG:HG2	2.07	0.53
1:A:62:ILE:O	1:A:66:LYS:HG2	2.07	0.53
1:C:19:ASP:HB3	1:C:23:ARG:HG2	1.92	0.51
1:C:59:ARG:HH11	1:C:59:ARG:HB3	1.73	0.50
1:D:10:ARG:HG3	1:D:140:LEU:HD23	1.94	0.50
1:B:28:TYR:HD1	1:B:113:ARG:HG2	1.76	0.50
1:B:25:TYR:HE1	1:B:114:ILE:HG22	1.75	0.49
1:A:31:SER:HB2	1:A:37:THR:HG22	1.94	0.49
1:B:92:ARG:NH2	1:B:121:THR:H	2.11	0.49
1:B:34:ASP:HB2	1:B:36:THR:HG23	1.97	0.47
1:D:24:PRO:HD3	1:D:118:GLY:HA2	1.97	0.47
1:D:83:TRP:O	1:D:93:THR:HA	2.15	0.47
1:D:26:TYR:CD1	1:D:115:GLU:HG2	2.50	0.47
1:B:5:PHE:HE1	1:B:110:LEU:HD22	1.78	0.47
1:D:65:LEU:HD11	1:D:103:LYS:HD3	1.97	0.46
1:A:9:ALA:HB3	1:A:140:LEU:HD21	1.96	0.46
1:A:86:THR:HB	1:A:91:THR:HG22	1.98	0.46
1:A:139:LYS:HZ2	1:B:128:LYS:HD2	1.79	0.46
1:A:3:GLN:HA	1:A:6:LEU:HD12	1.98	0.45
1:C:49:PRO:O	1:C:53:GLU:HG2	2.16	0.45
1:B:28:TYR:HB3	1:B:40:ALA:HB3	1.97	0.45
1:D:96:ILE:HD12	1:D:132:LEU:HD23	1.99	0.45
1:B:73:ASN:HB3	1:B:104:ASP:HA	1.98	0.45
1:D:123:GLU:HA	1:D:126:ILE:HD12	1.98	0.44
1:A:86:THR:OG1	1:B:72:GLU:HA	2.17	0.44
1:A:43:ARG:HH21	1:A:115:GLU:HG2	1.83	0.43
1:C:62:ILE:O	1:C:66:LYS:HG2	2.18	0.43
1:B:30:GLY:O	1:B:37:THR:HA	2.18	0.43
1:C:92:ARG:HB3	1:C:94:HIS:HE1	1.84	0.43
1:D:38:ARG:HD3	1:D:51:THR:HG22	2.00	0.43
1:C:54:PHE:HD2	1:C:111:LEU:HD13	1.84	0.43
1:B:77:TYR:O	1:B:99:ALA:HA	2.20	0.42
1:A:139:LYS:HE3	1:A:139:LYS:HB3	1.84	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:GLU:HG2	1:C:128:LYS:HE3	2.02	0.42
1:D:62:ILE:O	1:D:66:LYS:HG2	2.20	0.42
1:B:4:GLU:HG2	1:B:5:PHE:H	1.84	0.42
1:D:8:ARG:HD3	1:D:8:ARG:HA	1.82	0.42
1:A:102:LYS:HE2	1:A:105:GLY:HA2	2.02	0.42
1:B:59:ARG:HH11	1:B:59:ARG:HA	1.85	0.42
1:D:24:PRO:HB3	1:D:117:SER:C	2.45	0.41
1:C:76:ILE:HG23	1:C:101:VAL:HG22	2.02	0.41
1:D:122:ASP:O	1:D:126:ILE:HG13	2.21	0.40
1:D:31:SER:HB2	1:D:37:THR:HG22	2.02	0.40
1:C:84:THR:HA	1:C:92:ARG:O	2.21	0.40
1:B:43:ARG:HD2	1:B:44:GLU:N	2.37	0.40
1:B:24:PRO:HB3	1:B:117:SER:C	2.47	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	130/144 (90%)	126 (97%)	4 (3%)	0	100	100
1	B	132/144 (92%)	129 (98%)	3 (2%)	0	100	100
1	C	120/144 (83%)	117 (98%)	3 (2%)	0	100	100
1	D	116/144 (81%)	110 (95%)	6 (5%)	0	100	100
All	All	498/576 (86%)	482 (97%)	16 (3%)	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	125/133 (94%)	125 (100%)	0	100	100
1	B	126/133 (95%)	124 (98%)	2 (2%)	58	83
1	C	119/133 (90%)	118 (99%)	1 (1%)	79	92
1	D	114/133 (86%)	113 (99%)	1 (1%)	75	91
All	All	484/532 (91%)	480 (99%)	4 (1%)	79	92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	5	PHE
1	D	46	TYR
1	B	5	PHE
1	B	73	ASN

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

Mol	Chain	Res	Type
1	D	52	GLN
1	B	67	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	136/144 (94%)	0.21	3 (2%) 62 56	48, 82, 143, 202	0
1	B	136/144 (94%)	0.18	3 (2%) 62 56	44, 75, 149, 246	0
1	C	128/144 (88%)	0.22	2 (1%) 70 65	49, 92, 158, 197	0
1	D	124/144 (86%)	0.40	8 (6%) 26 22	58, 107, 172, 229	0
All	All	524/576 (90%)	0.25	16 (3%) 51 46	44, 90, 161, 246	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	20	LEU	3.1
1	C	99	ALA	2.8
1	D	13	LEU	2.8
1	B	140	LEU	2.6
1	B	5	PHE	2.4
1	B	117	SER	2.4
1	D	107	LEU	2.4
1	A	110	LEU	2.4
1	A	120	LEU	2.4
1	A	140	LEU	2.3
1	D	23	ARG	2.3
1	C	110	LEU	2.1
1	D	110	LEU	2.1
1	D	100	TYR	2.1
1	D	40	ALA	2.1
1	D	142	SER	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 monosaccharides 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.