



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2023 – 08:47 AM EDT

PDB ID : 8CWZ  
Title : Accurate computational design of genetically encoded 3D protein crystals  
Authors : Bera, A.K.; Li, Z.; Baker, D.  
Deposited on : 2022-05-19  
Resolution : 5.53 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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

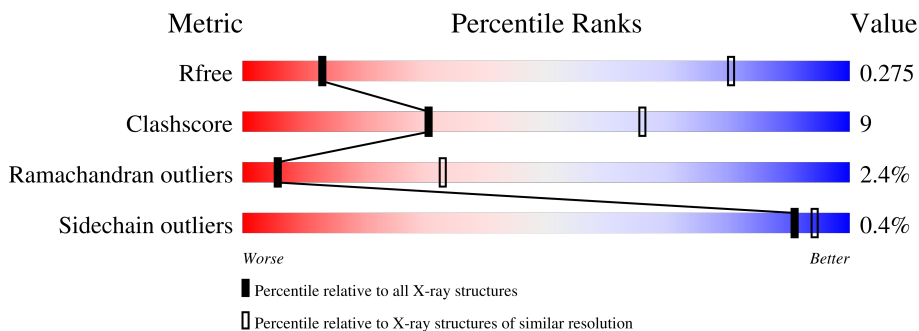
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 5.53 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))
$R_{free}$	130704	1000 (7.20-3.84)
Clashscore	141614	1011 (7.12-3.90)
Ramachandran outliers	138981	1015 (7.20-3.82)
Sidechain outliers	138945	1191 (7.20-3.80)

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	148	
2	B	216	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2562 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 I432-1-X3 Chain A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	135	1038	669	169	199	1	0	0	0


- Molecule 2 is a protein called I432-1-X3 Chain B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	203	1524	992	251	271	10	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. 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. 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: I432-1-X3 Chain A

Chain A:  82% 9% 9%



- Molecule 2: I432-1-X3 Chain B

Chain B:  65% 27% 6%



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	239.29Å 239.29Å 239.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	169.21 – 5.53 169.21 – 5.53	Depositor EDS
% Data completeness (in resolution range)	85.5 (169.21-5.53) 85.6 (169.21-5.53)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.65 (at 5.42Å)	Xtrriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, $R_{free}$	0.232 , 0.274 0.232 , 0.275	Depositor DCC
$R_{free}$ test set	351 reflections (10.26%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	301.9	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 291.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	2562	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	309.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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	0.25	0/1050	0.44	0/1416
2	B	0.29	0/1554	0.51	0/2098
All	All	0.27	0/2604	0.48	0/3514

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
2	B	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	41	PHE	Peptide
2	B	74	CYS	Peptide
2	B	89	HIS	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	1038	0	1093	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1524	0	1590	38	0
All	All	2562	0	2683	48	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 9.

All (48) 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)
2:B:111:THR:HG1	2:B:113:THR:HG1	1.21	0.85
2:B:69:THR:OG1	2:B:73:GLN:NE2	2.11	0.82
2:B:88:PRO:O	2:B:90:LEU:N	2.22	0.72
1:A:19:ARG:HD3	1:A:22:LEU:HD22	1.71	0.72
2:B:73:GLN:HA	2:B:76:LYS:HD3	1.73	0.71
2:B:183:THR:O	2:B:185:GLU:N	2.28	0.67
2:B:73:GLN:OE1	2:B:73:GLN:N	2.31	0.63
2:B:89:HIS:H	2:B:108:GLY:N	1.96	0.63
2:B:8:HIS:O	2:B:10:ILE:N	2.31	0.62
2:B:72:ARG:O	2:B:75:LYS:HG2	1.99	0.62
2:B:96:GLU:HA	2:B:99:LYS:HB3	1.80	0.62
2:B:93:GLU:O	2:B:97:PHE:N	2.31	0.60
2:B:89:HIS:H	2:B:108:GLY:H	1.48	0.60
2:B:68:VAL:HB	2:B:87:SER:HB3	1.83	0.59
1:A:27:TYR:CE2	1:A:47:VAL:HG21	2.40	0.57
2:B:65:ALA:HB3	2:B:85:ILE:HG22	1.87	0.56
2:B:19:VAL:HG13	2:B:49:VAL:HG22	1.86	0.56
2:B:190:LEU:HA	2:B:193:LEU:HD12	1.90	0.54
2:B:109:VAL:HG13	2:B:114:GLU:HB2	1.91	0.53
2:B:69:THR:H	2:B:73:GLN:NE2	2.06	0.53
1:A:19:ARG:HB3	1:A:22:LEU:HB2	1.90	0.53
2:B:166:PHE:HA	2:B:170:VAL:HG22	1.90	0.52
2:B:132:GLU:HB3	2:B:156:GLY:HA3	1.92	0.52
2:B:69:THR:HA	2:B:90:LEU:HD21	1.94	0.50
2:B:30:PHE:HB2	2:B:37:ILE:HD11	1.94	0.49
2:B:15:ARG:HG2	2:B:40:THR:OG1	2.12	0.48
2:B:86:VAL:HG12	2:B:106:MET:HB3	1.96	0.48
2:B:39:ILE:N	2:B:64:GLY:O	2.40	0.47
1:A:21:SER:HA	1:A:51:LEU:HD11	1.97	0.47
2:B:5:PHE:O	2:B:7:LYS:N	2.48	0.47
2:B:192:VAL:HA	2:B:195:VAL:HG12	1.97	0.47
2:B:89:HIS:CE1	2:B:90:LEU:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:LEU:HD21	2:B:149:VAL:HG11	1.98	0.45
2:B:89:HIS:N	2:B:108:GLY:H	2.13	0.45
2:B:39:ILE:HG13	2:B:50:ILE:HG12	1.99	0.43
1:A:17:LEU:C	1:A:19:ARG:H	2.22	0.43
2:B:11:VAL:HG22	2:B:36:LEU:HD13	2.00	0.43
2:B:28:ALA:HB1	2:B:188:GLU:HB2	2.00	0.42
2:B:110:MET:N	2:B:114:GLU:OE1	2.45	0.42
1:A:27:TYR:HE2	1:A:47:VAL:HG21	1.84	0.42
2:B:118:ALA:O	2:B:121:LEU:HB2	2.19	0.42
1:A:9:MET:HA	1:A:12:LEU:HD12	2.01	0.42
2:B:8:HIS:O	2:B:36:LEU:HD12	2.18	0.42
2:B:30:PHE:HA	2:B:34:VAL:O	2.19	0.41
1:A:17:LEU:O	1:A:19:ARG:N	2.54	0.41
1:A:76:LYS:HD2	1:A:107:GLU:CD	2.41	0.41
1:A:48:LEU:O	1:A:52:LYS:N	2.54	0.41
2:B:93:GLU:O	2:B:97:PHE:HB2	2.21	0.41

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	133/148 (90%)	121 (91%)	12 (9%)	0	100	100
2	B	201/216 (93%)	168 (84%)	25 (12%)	8 (4%)	3	23
All	All	334/364 (92%)	289 (86%)	37 (11%)	8 (2%)	6	33

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	6	LYS
2	B	89	HIS

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Mol	Chain	Res	Type
2	B	9	LYS
2	B	185	GLU
2	B	5	PHE
2	B	77	ALA
2	B	91	ASP
2	B	184	PRO

### 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	104/115 (90%)	104 (100%)	0	100	100
2	B	163/177 (92%)	162 (99%)	1 (1%)	86	91
All	All	267/292 (91%)	266 (100%)	1 (0%)	91	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	41	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	73	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 monosaccharides 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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.