



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 9, 2017 – 10:40 PM EST

PDB ID : 5NPO  
Title : Promiscuous Protein Self-Assembly as a Function of Protein Stability  
Authors : Cohen-Khait, R.; Dym, O.; Hamer-Rogotner, S.; Schreiber, G.  
Deposited on : unknown  
Resolution : 1.95 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)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

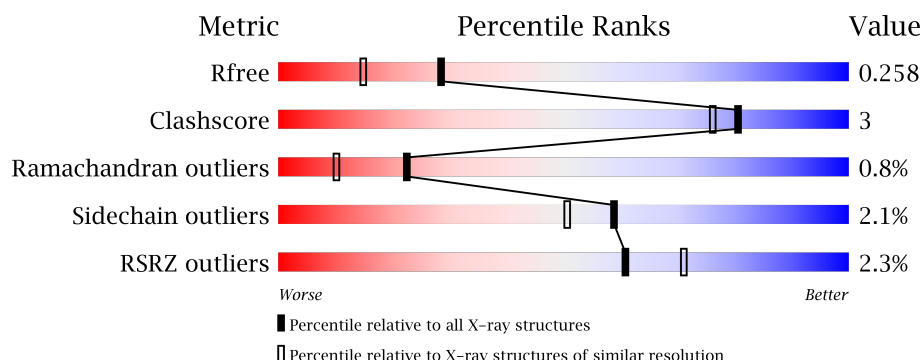
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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))
$R_{free}$	100719	2004 (1.96-1.96)
Clashscore	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)
RSRZ outliers	101464	2018 (1.96-1.96)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	264	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 3%; height: 10px; background-color: red;"></div> <div style="width: 88%; height: 10px; background-color: green;"></div> <div style="width: 9%; height: 10px; background-color: yellow;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> </div> <div> <div style="width: 3%;"></div> <div style="width: 91%;"></div> <div style="width: 8%;"></div> </div> </div>
2	B	265	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 3%; height: 10px; background-color: red;"></div> <div style="width: 71%; height: 10px; background-color: green;"></div> <div style="width: 9%; height: 10px; background-color: yellow;"></div> <div style="width: 16%; height: 10px; background-color: grey;"></div> </div> </div> <div> <div style="width: 3%;"></div> <div style="width: 74%;"></div> <div style="width: 9%;"></div> <div style="width: 16%;"></div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3744 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 Beta-lactamase TEM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2028	1266	360	391	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	-	initiating methionine	UNP P62593
A	84	ILE	VAL	conflict	UNP P62593

- Molecule 2 is a protein called Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	223	Total	C	N	O	S	0	0	0
			1677	1057	294	316	10			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	37	LYS	GLU	engineered mutation	UNP D3INY1
B	42	LYS	ALA	engineered mutation	UNP D3INY1
B	52	ALA	ASN	engineered mutation	UNP D3INY1
B	58	VAL	GLU	engineered mutation	UNP D3INY1
B	120	GLY	ARG	engineered mutation	UNP D3INY1
B	184	VAL	ALA	engineered mutation	UNP D3INY1
B	201	ALA	LEU	engineered mutation	UNP D3INY1
B	263	MET	THR	engineered mutation	UNP D3INY1
B	289	ALA	-	expression tag	UNP D3INY1

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		

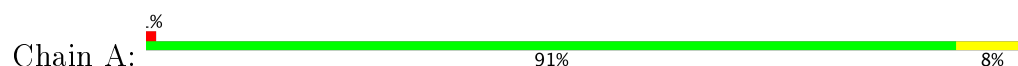
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	28	Total	O	0	0
			28	28		
4	B	10	Total	O	0	0
			10	10		

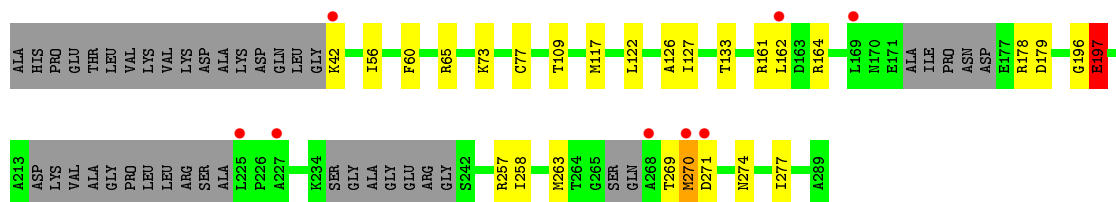
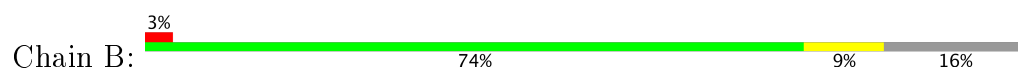
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Beta-lactamase TEM



#### • Molecule 2: Beta-lactamase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.91Å 52.73Å 67.94Å 90.00° 90.59° 90.00°	Depositor
Resolution (Å)	67.94 – 1.95 41.66 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.0 (67.94-1.95) 99.0 (41.66-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.199 , 0.256 0.208 , 0.258	Depositor DCC
$R_{free}$ test set	1634 reflections (4.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.2	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 38.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.028 for h,-k,-l 0.021 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3744	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.09% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.93	0/2062	1.03	10/2791 (0.4%)
2	B	0.84	0/1702	0.95	3/2307 (0.1%)
All	All	0.89	0/3764	0.99	13/5098 (0.3%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	A	176	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	A	61	ARG	NE-CZ-NH2	-6.59	117.01	120.30
1	A	240	ARG	NE-CZ-NH2	6.49	123.55	120.30
2	B	257	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	176	ASP	CB-CG-OD1	6.31	123.98	118.30
1	A	49	LEU	CA-CB-CG	6.02	129.15	115.30
2	B	197	GLU	N-CA-C	5.74	126.49	111.00
2	B	65	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	243	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	A	94	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	85	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	49	LEU	CB-CA-C	-5.05	100.60	110.20

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	2028	0	2036	7	0
2	B	1677	0	1658	18	0
3	B	1	0	0	0	0
4	A	28	0	0	0	0
4	B	10	0	0	0	0
All	All	3744	0	3694	23	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 3.

All (23) 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:109:THR:HG22	2:B:117:MET:CE	2.13	0.77
2:B:269:THR:O	2:B:271:ASP:N	2.19	0.76
2:B:109:THR:HG22	2:B:117:MET:HE3	1.70	0.70
1:A:98:SER:O	1:A:100:ASN:N	2.24	0.70
2:B:270:MET:O	2:B:274:ASN:ND2	2.27	0.67
2:B:109:THR:HG22	2:B:117:MET:HE1	1.82	0.60
1:A:198:LEU:HD23	1:A:198:LEU:O	2.07	0.55
2:B:117:MET:HE3	2:B:122:LEU:CD2	2.39	0.53
2:B:161:ARG:HG3	2:B:161:ARG:O	2.12	0.49
2:B:117:MET:HE3	2:B:122:LEU:HD21	1.95	0.48
1:A:84:ILE:HD13	1:A:91:LEU:HG	1.98	0.45
2:B:77:CYS:HB2	2:B:127:ILE:HD11	1.99	0.45
2:B:162:LEU:HD12	2:B:179:ASP:OD1	2.16	0.45
1:A:148:LEU:HD23	1:A:162:LEU:HD22	1.99	0.45
2:B:269:THR:C	2:B:271:ASP:N	2.71	0.44
2:B:109:THR:HA	2:B:117:MET:HE1	2.00	0.44
2:B:263:MET:CE	2:B:277:ILE:HD11	2.48	0.43
2:B:161:ARG:CG	2:B:161:ARG:O	2.67	0.43
1:A:281:GLY:O	1:A:285:ILE:HG12	2.19	0.43
2:B:109:THR:HG21	2:B:133:THR:HB	2.02	0.42
1:A:62:PRO:HD2	2:B:56:ILE:O	2.19	0.42
1:A:26:HIS:HB2	2:B:60:PHE:CZ	2.54	0.41
2:B:73:LYS:HD3	2:B:126:ALA:O	2.20	0.41

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	261/264 (99%)	252 (97%)	8 (3%)	1 (0%)	38	25
2	B	213/265 (80%)	204 (96%)	6 (3%)	3 (1%)	13	4
All	All	474/529 (90%)	456 (96%)	14 (3%)	4 (1%)	22	10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
2	B	197	GLU
2	B	196	GLY
2	B	270	MET

### 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	217/218 (100%)	214 (99%)	3 (1%)	71	67
2	B	173/216 (80%)	168 (97%)	5 (3%)	48	35
All	All	390/434 (90%)	382 (98%)	8 (2%)	59	50

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ILE
1	A	130	SER

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Mol	Chain	Res	Type
1	A	146	LYS
2	B	42	LYS
2	B	164	ARG
2	B	178	ARG
2	B	197	GLU
2	B	258	ILE

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

Mol	Chain	Res	Type
1	A	175	ASN
2	B	274	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	263/264 (99%)	0.13	3 (1%) 80 86	19, 34, 56, 75	4 (1%)
2	B	223/265 (84%)	0.32	8 (3%) 43 54	22, 41, 65, 90	3 (1%)
All	All	486/529 (91%)	0.22	11 (2%) 61 71	19, 37, 62, 90	7 (1%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	26	HIS	5.2
2	B	268	ALA	4.3
2	B	42	LYS	3.2
2	B	169	LEU	3.1
1	A	113	LEU	3.0
2	B	227	ALA	2.3
2	B	162	LEU	2.3
2	B	271	ASP	2.3
2	B	270	MET	2.1
1	A	227	ALA	2.1
2	B	225	LEU	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	B	300	1/1	0.89	0.32	-	37,37,37,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.