

Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 12:56 PM EDT

PDB ID	:	2NU3
Title	:	Accommodation of positively-charged residues in a hydrophobic specificity
		pocket: Crystal structures of SGPB in complex with OMTKY3 variants Lys18I
		and Arg18I
Authors	:	Bateman, K.S.; Anderson, S.; Lu, W.; Qasim, M.A.; Huang, K.; Laskowski
		Jr., M.; James, M.N.G.
Deposited on		
Resolution	:	1.80 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 (i) 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 (1)) were used in the production of this report:

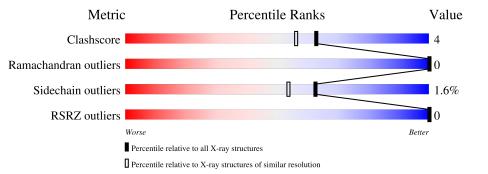
MolProbity Xtriage (Phenix) EDS	: :	1.13 2.35
Refmac	:	20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158
Ideal geometry (proteins)	:	0
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)		

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 >=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 <=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	Е	185	93%	7%
2	Ι	51	86%	12% ·



2NU3

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1850 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 Streptogrisin B, Proteinase B.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Е	185	Total 1311	C 800	N 228	0 277	S 6	0	1	0

• Molecule 2 is a protein called Ovomucoid.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	Ι	51	Total 388	C 238	N 66	O 78	S 6	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ι	18	LYS	LEU	engineered mutation	UNP P68390

• Molecule 3 is water.

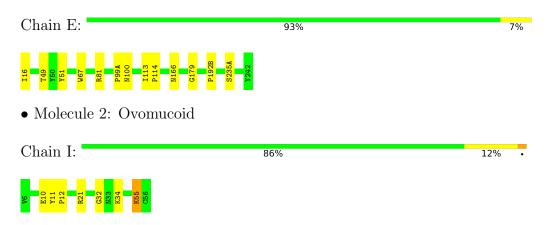
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Е	116	Total O 116 116	0	0
3	Ι	35	Total O 35 35	0	0



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 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: Streptogrisin B, Proteinase B





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	45.35Å 54.52 Å 45.65 Å	Deperitor
a, b, c, α , β , γ	90.00° 119.20° 90.00°	Depositor
Resolution (Å)	20.00 - 1.80	Depositor
Resolution (A)	39.85 - 1.79	EDS
% Data completeness	(Not available) $(20.00-1.80)$	Depositor
(in resolution range)	92.8 (39.85 - 1.79)	EDS
R _{merge}	0.06	Depositor
$\frac{R_{sym}}{< I/\sigma(I) > 1}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.98 (at 1.78 Å)	Xtriage
Refinement program	TNT	Depositor
D D	0.148 , (Not available)	Depositor
R, R_{free}	0.141 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor $(Å^2)$	12.6	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32, 57.8	EDS
L-test for twinning ²	$< L >=0.48, < L^2>=0.31$	Xtriage
	0.008 for -h-l,k,h	
	0.008 for l,k,-h-l	
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
	0.030 for -h-l,-k,l	
	0.037 for l,-k,h	
F_o, F_c correlation	0.97	EDS
Total number of atoms	1850	wwPDB-VP
Average B, all atoms $(Å^2)$	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.85% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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	Mol Chain		lengths	Bond angles		
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	Ε	0.65	0/1340	0.69	0/1826	
2	Ι	0.61	0/396	0.66	0/533	
All	All	0.64	0/1736	0.69	0/2359	

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	Е	1311	0	1228	9	0
2	Ι	388	0	360	6	0
3	Е	116	0	0	1	0
3	Ι	35	0	0	0	0
All	All	1850	0	1588	14	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 4.

All (14) 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:I:11:TYR:HB3	2:I:12:PRO:HA	1.70	0.73	



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
1:E:166:ASN:HD22	1:E:179:GLY:HA2	1.60	0.66	
1:E:49:THR:HG22	1:E:51:TYR:CE1	2.39	0.57	
1:E:166:ASN:ND2	1:E:179:GLY:HA2	2.22	0.55	
1:E:67:TRP:CD2	1:E:81:ARG:HG3	2.43	0.54	
2:I:21:ARG:HB3	2:I:21:ARG:CZ	2.39	0.51	
2:I:10:GLU:HG2	2:I:10:GLU:O	2.11	0.50	
2:I:11:TYR:CB	2:I:12:PRO:HA	2.40	0.50	
1:E:16:ILE:N	3:E:345:HOH:O	2.45	0.48	
1:E:99(A):PRO:O	1:E:100:ASN:HB2	2.17	0.45	
2:I:55:LYS:HB2	2:I:55:LYS:HE3	1.36	0.43	
1:E:166:ASN:HA	1:E:179:GLY:HA2	2.01	0.41	
1:E:113:ILE:HA	1:E:114:PRO:HD3	1.92	0.40	
1:E:192(B):PRO:CB	2:I:32:GLY:HA3	2.52	0.40	

Continued from previous page...

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	Favoured Allowed Outliers Pe		Percentiles
1	Ε	184/185~(100%)	175~(95%)	9~(5%)	0	100 100
2	Ι	49/51~(96%)	48 (98%)	1 (2%)	0	100 100
All	All	233/236~(99%)	223~(96%)	10 (4%)	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.



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ε	139/138 (101%)	138 (99%)	1 (1%)	84 81	
2	Ι	45/45~(100%)	43 (96%)	2(4%)	28 14	
All	All	184/183~(100%)	181 (98%)	3(2%)	62 54	

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Ε	235(A)	SER
2	Ι	34	LYS
2	Ι	55	LYS

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

Mol	Chain	Res	Type
1	Ε	166	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 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 (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^{th} 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	$\langle RSRZ \rangle$	#	#RSRZ>2		$OWAB(Å^2)$	Q<0.9
1	Ε	185/185~(100%)	-0.89	0	100	100	6, 13, 29, 38	0
2	Ι	51/51~(100%)	-0.78	0	100	100	8, 14, 36, 53	0
All	All	236/236~(100%)	-0.87	0	100	100	6, 13, 33, 53	0

There are no RSRZ outliers to report.

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.

