Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2021 – 05:10 AM EDT

PDB ID	:	3BGO
Title	:	Azide complex of Engineered Subtilisin SUBT_BACAM
Authors	:	Gallagher, D.T.; Bryan, P.N.
Deposited on	:	2007-11-27
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 following versions of software and data (see references (i)) were used in the production of this report:

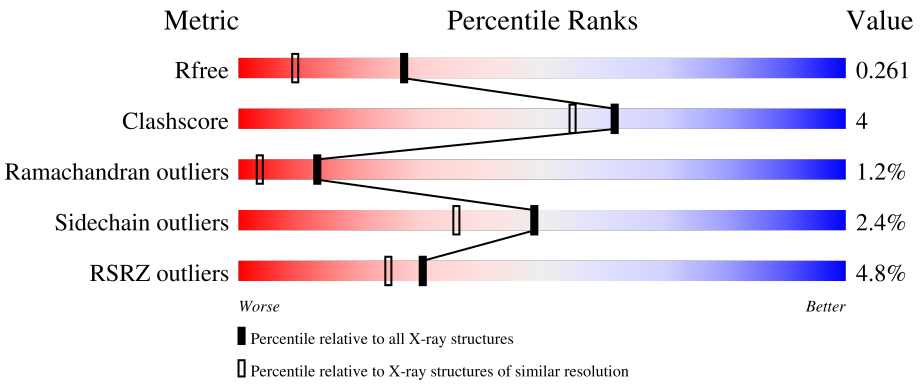
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
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	P	80	2% 82% 6% 11%
2	S	266	5% 87% 9% • • •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2694 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 Subtilisin BPN'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	P	71	558	357	91	108	2	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	2	MET	-	expression tag	UNP P00782
P	3	GLY	-	expression tag	UNP P00782
P	19	GLY	THR	SEE REMARK 999	UNP P00782
P	20	PHE	MET	SEE REMARK 999	UNP P00782
P	21	LYS	SER	SEE REMARK 999	UNP P00782
P	22	SER	THR	SEE REMARK 999	UNP P00782
P	23	CYS	MET	SEE REMARK 999	UNP P00782
P	?	-	SER	SEE REMARK 999	UNP P00782
P	?	-	ALA	SEE REMARK 999	UNP P00782
P	27	GLU	LYS	engineered mutation	UNP P00782
P	37	LEU	VAL	engineered mutation	UNP P00782
P	40	CYS	GLN	engineered mutation	UNP P00782
P	57	GLU	LYS	engineered mutation	UNP P00782
P	72	LYS	HIS	engineered mutation	UNP P00782
P	73	LEU	VAL	engineered mutation	UNP P00782
P	74	TYR	ALA	engineered mutation	UNP P00782
P	75	ARG	HIS	engineered mutation	UNP P00782
P	77	LEU	TYR	engineered mutation	UNP P00782
P	78	SER	-	expression tag	UNP P00782
P	79	ALA	-	expression tag	UNP P00782
P	80	THR	-	expression tag	UNP P00782
P	81	SER	-	expression tag	UNP P00782

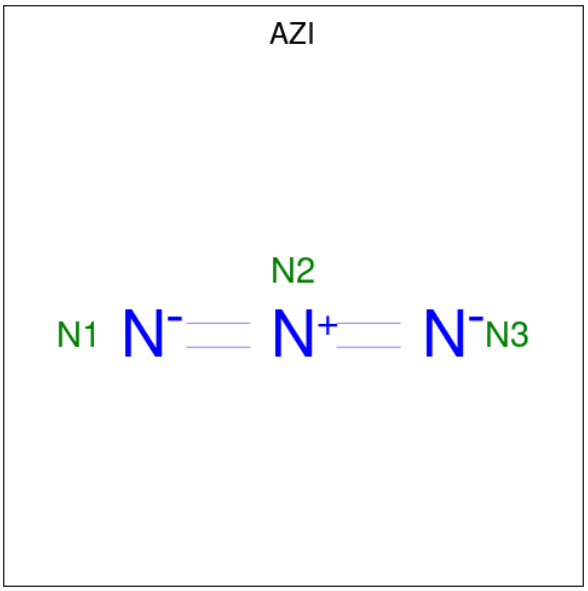
- Molecule 2 is a protein called Subtilisin BPN'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	S	263	1836	1145	316	370	5	0	0	0

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	2	LYS	GLN	engineered mutation	UNP P00782
S	3	CYS	SER	engineered mutation	UNP P00782
S	5	SER	PRO	engineered mutation	UNP P00782
S	9	ALA	SER	engineered mutation	UNP P00782
S	31	LEU	ILE	engineered mutation	UNP P00782
S	32	ALA	ASP	engineered mutation	UNP P00782
S	43	ASN	LYS	engineered mutation	UNP P00782
S	50	PHE	MET	engineered mutation	UNP P00782
S	?	-	VAL	deletion	UNP P00782
S	?	-	ALA	deletion	UNP P00782
S	?	-	ALA	deletion	UNP P00782
S	?	-	LEU	deletion	UNP P00782
S	?	-	ASN	deletion	UNP P00782
S	?	-	ASN	deletion	UNP P00782
S	?	-	SER	deletion	UNP P00782
S	?	-	ILE	deletion	UNP P00782
S	?	-	GLY	deletion	UNP P00782
S	74	ALA	GLY	engineered mutation	UNP P00782
S	104	ALA	TYR	engineered mutation	UNP P00782
S	128	SER	GLY	engineered mutation	UNP P00782
S	156	SER	GLU	engineered mutation	UNP P00782
S	166	SER	GLY	engineered mutation	UNP P00782
S	169	ALA	GLY	engineered mutation	UNP P00782
S	188	PRO	SER	engineered mutation	UNP P00782
S	206	CYS	GLN	engineered mutation	UNP P00782
S	212	GLY	ASN	engineered mutation	UNP P00782
S	217	LEU	TYR	engineered mutation	UNP P00782
S	218	SER	ASN	engineered mutation	UNP P00782
S	221	ALA	SER	engineered mutation	UNP P00782
S	254	ALA	THR	engineered mutation	UNP P00782
S	271	GLU	GLN	engineered mutation	UNP P00782

- Molecule 3 is AZIDE ION (three-letter code: AZI) (formula: N_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	S	1	Total N 3 3	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	S	4	Total Zn 4 4	0	0

- Molecule 5 is water.

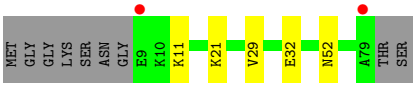
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	P	70	Total O 70 70	0	0
5	S	223	Total O 223 223	0	0

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.

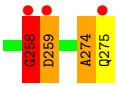
- Molecule 1: Subtilisin BPN'

Chain P:



- Molecule 2: Subtilisin BPN'

Chain S:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	44.29Å 72.84Å 95.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.80 15.87 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (8.00-1.80) 99.8 (15.87-1.80)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.62 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.205 , 0.262 0.212 , 0.261	Depositor DCC
R_{free} test set	1477 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	23.9	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 51.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2694	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN, AZI

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	P	0.87	0/565	0.75	0/751
2	S	0.90	1/1873 (0.1%)	0.89	9/2561 (0.4%)
All	All	0.90	1/2438 (0.0%)	0.86	9/3312 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	275	GLN	CA-C	5.12	1.66	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	274	ALA	CA-C-N	7.73	134.21	117.20
2	S	274	ALA	O-C-N	-7.40	110.87	122.70
2	S	275	GLN	N-CA-C	6.54	128.66	111.00
2	S	274	ALA	N-CA-C	6.32	128.07	111.00
2	S	126	LEU	CB-CG-CD1	5.50	120.34	111.00
2	S	258	GLY	O-C-N	5.33	131.22	122.70
2	S	126	LEU	CA-CB-CG	5.28	127.45	115.30
2	S	74	ALA	C-N-CA	5.21	134.71	121.70
2	S	120	ASP	CB-CG-OD1	-5.02	113.78	118.30

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	P	558	0	573	3	0
2	S	1836	0	1805	18	0
3	S	3	0	0	0	0
4	S	4	0	0	0	0
5	P	70	0	0	2	0
5	S	223	0	0	1	0
All	All	2694	0	2378	21	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 (21) 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:S:258:GLY:O	2:S:259:ASP:HB2	1.71	0.91
2:S:63:SER:OG	2:S:210:PRO:HD2	1.76	0.85
2:S:62:ASN:O	2:S:63:SER:HB2	1.96	0.65
2:S:258:GLY:O	2:S:259:ASP:CB	2.45	0.64
2:S:63:SER:OG	2:S:210:PRO:CD	2.48	0.61
2:S:19:GLN:HE22	2:S:237:LYS:HZ2	1.48	0.60
1:P:29:VAL:O	1:P:32:GLU:HG2	2.03	0.59
2:S:4:VAL:N	2:S:214:TYR:HH	2.01	0.59
2:S:125:SER:HB3	2:S:221:ALA:HB1	1.89	0.54
2:S:125:SER:HB3	2:S:221:ALA:CB	2.41	0.51
1:P:52:ASN:ND2	5:P:464:HOH:O	2.43	0.50
1:P:11:LYS:HE2	5:S:547:HOH:O	2.12	0.49
2:S:238:HIS:HE2	2:S:274:ALA:C	2.18	0.47
2:S:62:ASN:O	2:S:63:SER:CB	2.61	0.45
2:S:67:HIS:CD2	2:S:207:SER:HB3	2.52	0.44
5:P:600:HOH:O	2:S:113:TRP:HA	2.19	0.42
2:S:29:ALA:HB2	2:S:119:MET:HG3	2.02	0.41
2:S:64:HIS:HE1	2:S:96:LEU:HD12	1.86	0.41
2:S:32:ALA:HB1	2:S:64:HIS:CE1	2.56	0.40
2:S:67:HIS:HA	2:S:208:THR:O	2.22	0.40
2:S:13:ALA:N	2:S:14:PRO:CD	2.85	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	P	69/80 (86%)	68 (99%)	1 (1%)	0	100	100
2	S	261/266 (98%)	248 (95%)	9 (3%)	4 (2%)	10	2
All	All	330/346 (95%)	316 (96%)	10 (3%)	4 (1%)	13	3

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S	41	ASP
2	S	259	ASP
2	S	63	SER
2	S	258	GLY

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	P	59/65 (91%)	58 (98%)	1 (2%)	60	51
2	S	193/195 (99%)	188 (97%)	5 (3%)	46	32
All	All	252/260 (97%)	246 (98%)	6 (2%)	49	36

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	21	LYS
2	S	63	SER

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Mol	Chain	Res	Type
2	S	64	HIS
2	S	126	LEU
2	S	217	LEU
2	S	222	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	S	19	GLN
2	S	59	GLN
2	S	61	ASN
2	S	252	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)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	AZI	S	277	-	0,2,2	-	-	0,1,1	-	-

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 (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, 95th 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^2)	Q<0.9
1	P	71/80 (88%)	0.18	2 (2%)	53	47	17, 22, 32, 45	0
2	S	263/266 (98%)	0.23	14 (5%)	26	21	13, 20, 34, 48	0
All	All	334/346 (96%)	0.22	16 (4%)	30	25	13, 21, 34, 48	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	S	4	VAL	17.2
2	S	40	PRO	9.5
1	P	9	GLU	6.4
2	S	258	GLY	5.9
2	S	41	ASP	5.1
2	S	275	GLN	5.0
2	S	5	SER	4.3
2	S	259	ASP	3.1
2	S	214	TYR	2.6
1	P	79	ALA	2.5
2	S	211	GLY	2.4
2	S	161	SER	2.3
2	S	43	ASN	2.3
2	S	37	SER	2.1
2	S	160	GLY	2.0
2	S	25	ASN	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)

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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å^2)	Q<0.9
3	AZI	S	277	3/3	0.73	0.27	25,25,32,36	0
4	ZN	S	278	1/1	0.95	0.17	43,43,43,43	0
4	ZN	S	281	1/1	0.96	0.05	27,27,27,27	0
4	ZN	S	280	1/1	0.98	0.08	41,41,41,41	0
4	ZN	S	279	1/1	1.00	0.03	22,22,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.