

wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2021 – 12:13 PM EDT

PDB ID : 1A2Q

Title : SUBTILISIN BPN' MUTANT 7186

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Deposited on : 1998-01-08

Resolution : 1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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) : NOT EXECUTED EDS : NOT EXECUTED

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

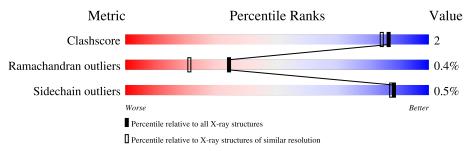
Validation Pipeline (wwPDB-VP) : 2.23.2

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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain	
1	A	275	89%	11%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2153 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		
1	A	275	Total 1957	C 1214	N 336	O 399	P 1	S 7	0	4	0

There are 5 discrepancies between the modelled and reference sequences:

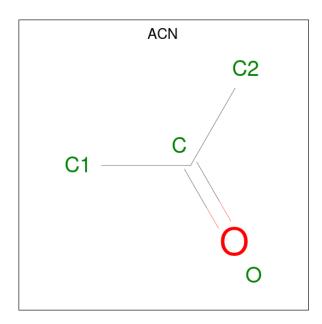
Chain	Residue	Modelled	Actual	Comment	Reference
A	22	CYS	THR	engineered mutation	UNP P00782
A	87	CYS	SER	engineered mutation	UNP P00782
A	169	ALA	GLY	engineered mutation	UNP P00782
A	218	SER	ASN	engineered mutation	UNP P00782
A	221	MIS	SER	modified residue	UNP P00782

• Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Ca 2 2	0	0

• Molecule 3 is ACETONE (three-letter code: ACN) (formula: C₃H₆O).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 3 1	0	0
3	A	1	Total C O 4 3 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	186	Total O 186 186	0	0

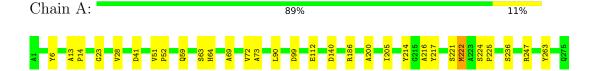


3 Residue-property plots (i)

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.

Note EDS was not executed.

• Molecule 1: SUBTILISIN BPN'





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source	
Space group	P 1 21 1	Depositor	
Cell constants	41.64Å 79.45Å 37.26Å	Depositor	
a, b, c, α , β , γ	90.00° 114.53° 90.00°	Depositor	
Resolution (Å)	10.00 - 1.80	Depositor	
% Data completeness	(Not available) (10.00-1.80)	Depositor	
(in resolution range)	(10.00 1.00)		
R_{merge}	(Not available)	Depositor	
R_{sym}	(Not available)	Depositor	
Refinement program	PROFFT, PROLSQ	Depositor	
R, R_{free}	0.145 , (Not available)	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	2153	wwPDB-VP	
Average B, all atoms (Å ²)	10.0	wwPDB-VP	



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: CA, ACN, MIS

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	Bo	ond angles
Mol	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	1.10	0/1991	1.39	18/2715 (0.7%)

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	186	ARG	NE-CZ-NH2	-7.97	116.32	120.30
1	A	247	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	A	140	ASP	CB-CG-OD1	6.67	124.30	118.30
1	A	247	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	A	41	ASP	CB-CG-OD1	6.20	123.88	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	A	1957	0	1917	8	0
2	A	2	0	0	0	0
3	A	8	0	12	0	0
4	A	186	0	0	0	0
All	All	2153	0	1929	8	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 2.

The worst 5 of 8 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:224:SER:N	1:A:225:PRO:HD2	2.31	0.46
1:A:23:GLY:HA2	1:A:236:SER:HB3	2.00	0.42
1:A:69:ALA:HB1	1:A:90:LEU:HD21	2.02	0.42
1:A:28:VAL:HG11	1:A:72:VAL:HG11	2.02	0.41
1:A:13:ALA:N	1:A:14:PRO:CD	2.83	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	276/275 (100%)	267 (97%)	8 (3%)	1 (0%)	34	21

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	SER

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	207/204 (102%)	206 (100%)	1 (0%)	88 87		

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

Mol	Chain	Res	Type		
1	A	222	MET		

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	Chain	Res	Link	Во	ond leng	ths	В	ond ang	les
			nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
1	MIS	A	221	1	11,12,13	1.57	4 (36%)	10,16,18	2.08	4 (40%)	

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MIS	A	221	1	-	2/10/13/15	-

All (4) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(A)	$Ideal(\AA)$
1	A	221	MIS	P-O2P	-2.51	1.42	1.50
1	A	221	MIS	P-O3P	-2.39	1.54	1.60
1	A	221	MIS	O3P-C1	2.26	1.54	1.46
1	A	221	MIS	P-O1P	-2.20	1.45	1.55

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	221	MIS	O3P-P-O2P	3.77	123.60	109.47
1	A	221	MIS	C3-C1-C2	-3.31	95.88	113.47
1	A	221	MIS	O1P-P-O3P	-3.03	94.82	106.78
1	A	221	MIS	O1P-P-O2P	-2.20	101.36	112.24

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	221	MIS	CA-CB-OG-P
1	A	221	MIS	CB-OG-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	Ros	Link	Bond lengths			Bond angles		
			nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
3	ACN	A	290	-	3,3,3	0.45	0	3,3,3	0.70	0



	Mol	Type	ype Chain Res Link		Link	В	ond leng	gths	Bond angles		
	MIOI	туре	Chain	nes	LINK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
Ī	3	ACN	A	291	-	3,3,3	0.43	0	3,3,3	0.67	0

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)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

