



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2022 – 10:11 am BST

PDB ID : 7NE4
Title : E125A mutant of oligopeptidase B from *S. proteomaculans* with modified hinge region
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Deposited on : 2021-02-03
Resolution : 2.72 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

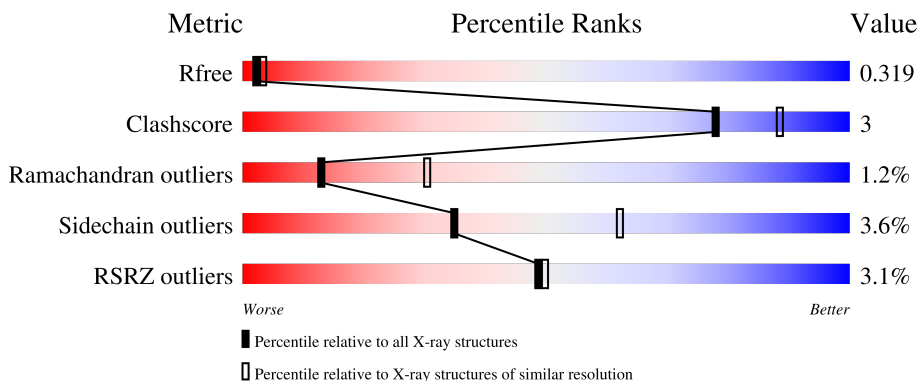
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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 $\leq 5\%$. 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	676	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 5623 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.

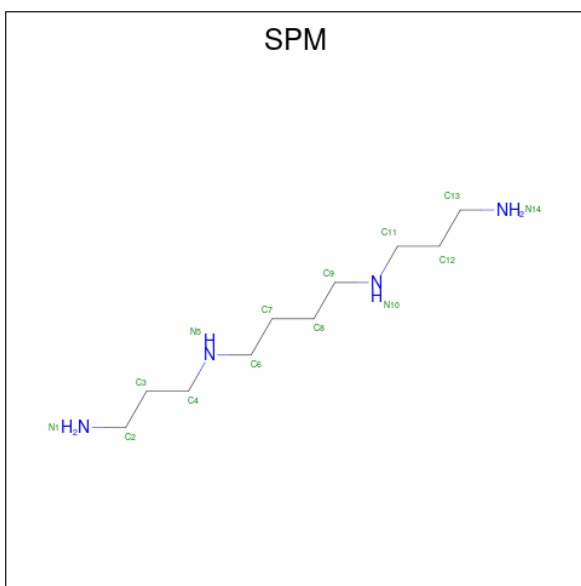
- Molecule 1 is a protein called Oligopeptidase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	676	5531	3514	929	1075	13	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	71	GLU	ILE	engineered mutation	UNP B3VI58
A	72	ASN	PRO	engineered mutation	UNP B3VI58
A	73	LEU	GLN	engineered mutation	UNP B3VI58
A	74	TYR	GLN	engineered mutation	UNP B3VI58
A	75	PHE	GLU	engineered mutation	UNP B3VI58
A	76	GLN	HIS	engineered mutation	UNP B3VI58
A	125	ALA	GLU	engineered mutation	UNP B3VI58

- Molecule 2 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			14	10	4		
2	A	1	Total	C	N	0	0
			14	10	4		
2	A	1	Total	C	N	0	0
			14	10	4		

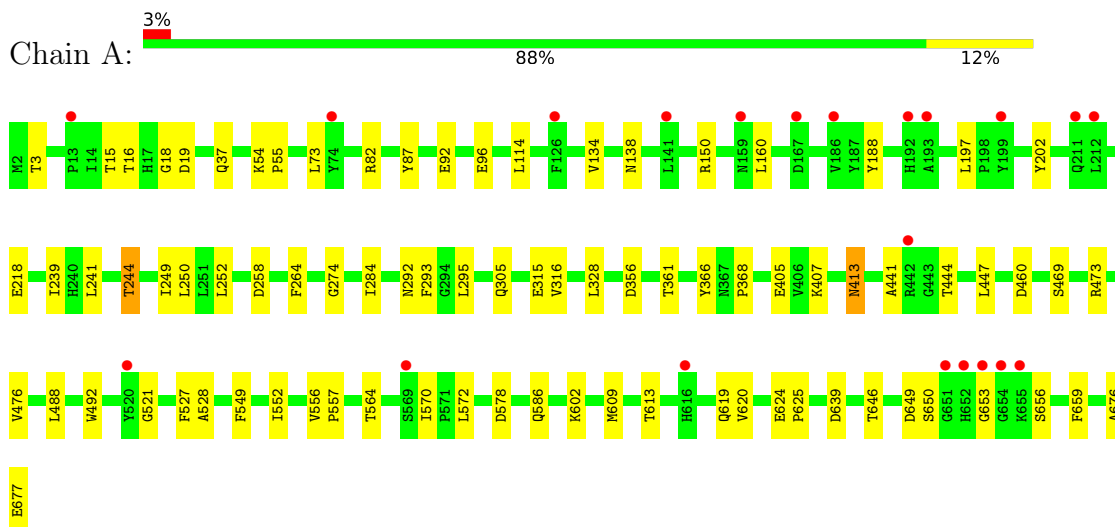
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total	O	0	0
			50	50		

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: Oligopeptidase B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.84Å 98.56Å 108.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.85 – 2.72 44.85 – 2.72	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.85-2.72) 100.0 (44.85-2.72)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.60 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.250 , 0.306 0.267 , 0.319	Depositor DCC
R_{free} test set	1023 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	5623	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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: SPM

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	0.35	0/5676	0.58	0/7716

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	A	5531	0	5246	32	0
2	A	42	0	78	0	0
3	A	50	0	0	0	0
All	All	5623	0	5324	32	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 (32) 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)
1:A:613:THR:HG23	1:A:646:THR:HG23	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:LEU:HD12	1:A:476:VAL:HB	1.78	0.64
1:A:366:TYR:CE2	1:A:368:PRO:HG3	2.33	0.63
1:A:624:GLU:HB2	1:A:625:PRO:HD3	1.85	0.57
1:A:295:LEU:CD2	1:A:328:LEU:HD21	2.38	0.53
1:A:315:GLU:HG2	1:A:316:VAL:HG23	1.92	0.52
1:A:249:ILE:HD11	1:A:274:GLY:HA2	1.94	0.50
1:A:441:ALA:O	1:A:444:THR:HG22	2.12	0.49
1:A:556:VAL:HB	1:A:620:VAL:HG13	1.94	0.49
1:A:413:ASN:HD22	1:A:413:ASN:N	2.11	0.49
1:A:488:LEU:HD12	1:A:492:TRP:CZ3	2.50	0.47
1:A:73:LEU:HD11	1:A:659:PHE:HZ	1.79	0.46
1:A:447:LEU:HD13	1:A:521:GLY:HA3	1.98	0.45
1:A:295:LEU:HD23	1:A:328:LEU:HD21	1.97	0.45
1:A:361:THR:OG1	1:A:460:ASP:HB3	2.17	0.44
1:A:284:ILE:N	1:A:284:ILE:HD12	2.32	0.44
1:A:564:THR:HG23	1:A:570:ILE:HD13	1.98	0.44
1:A:527:PHE:CZ	1:A:676:ALA:HB2	2.55	0.42
1:A:469:SER:O	1:A:473:ARG:NH1	2.50	0.42
1:A:188:TYR:CZ	1:A:202:TYR:HB2	2.55	0.42
1:A:134:VAL:CG1	1:A:138:ASN:HA	2.50	0.42
1:A:96:GLU:O	1:A:656:SER:HA	2.20	0.41
1:A:528:ALA:HB2	1:A:549:PHE:CE1	2.54	0.41
1:A:552:ILE:HG21	1:A:609:MET:HE3	2.01	0.41
1:A:54:LYS:N	1:A:55:PRO:CD	2.84	0.41
1:A:239:ILE:HD11	1:A:252:LEU:HD11	2.02	0.41
1:A:488:LEU:HD12	1:A:492:TRP:CE3	2.56	0.41
1:A:557:PRO:HD2	1:A:625:PRO:HG3	2.03	0.41
1:A:244:THR:CG2	1:A:578:ASP:HB2	2.51	0.41
1:A:292:ASN:O	1:A:293:PHE:HB2	2.20	0.40
1:A:87:TYR:CE2	1:A:114:LEU:HD11	2.56	0.40
1:A:405:GLU:OE2	1:A:407:LYS:NZ	2.51	0.40

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	674/676 (100%)	623 (92%)	43 (6%)	8 (1%)	13	30

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	650	SER
1	A	15	THR
1	A	258	ASP
1	A	649	ASP
1	A	18	GLY
1	A	264	PHE
1	A	572	LEU
1	A	653	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	A	589/589 (100%)	568 (96%)	21 (4%)	35	62

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	16	THR
1	A	19	ASP
1	A	37	GLN
1	A	82	ARG
1	A	92	GLU
1	A	150	ARG
1	A	160	LEU
1	A	197	LEU
1	A	218	GLU
1	A	241	LEU

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Mol	Chain	Res	Type
1	A	244	THR
1	A	250	LEU
1	A	305	GLN
1	A	356	ASP
1	A	413	ASN
1	A	586	GLN
1	A	602	LYS
1	A	619	GLN
1	A	639	ASP
1	A	677	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	139	GLN
1	A	413	ASN
1	A	481	HIS
1	A	586	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](#)

3 ligands are 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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SPM	A	702	-	13,13,13	0.16	0	12,12,12	0.18	0
2	SPM	A	703	-	13,13,13	0.16	0	12,12,12	0.14	0
2	SPM	A	701	-	13,13,13	0.15	0	12,12,12	0.20	0

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
2	SPM	A	702	-	-	5/11/11/11	-
2	SPM	A	703	-	-	6/11/11/11	-
2	SPM	A	701	-	-	6/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	703	SPM	N10-C11-C12-C13
2	A	702	SPM	N5-C6-C7-C8
2	A	703	SPM	C7-C8-C9-N10
2	A	703	SPM	N5-C6-C7-C8
2	A	702	SPM	C12-C11-N10-C9
2	A	701	SPM	C2-C3-C4-N5
2	A	701	SPM	C6-C7-C8-C9
2	A	701	SPM	C8-C9-N10-C11
2	A	701	SPM	N10-C11-C12-C13
2	A	701	SPM	N5-C6-C7-C8
2	A	702	SPM	C6-C7-C8-C9
2	A	701	SPM	C12-C11-N10-C9
2	A	703	SPM	C8-C9-N10-C11
2	A	702	SPM	C2-C3-C4-N5
2	A	703	SPM	C12-C11-N10-C9

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Mol	Chain	Res	Type	Atoms
2	A	703	SPM	C6-C7-C8-C9
2	A	702	SPM	C8-C9-N10-C11

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	A	676/676 (100%)	0.39	21 (3%) 49 50	19, 28, 40, 65	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	651	GLY	4.4
1	A	74	TYR	3.9
1	A	652	HIS	3.7
1	A	654	GLY	3.6
1	A	13	PRO	3.5
1	A	212	LEU	3.0
1	A	442	ARG	3.0
1	A	192	HIS	3.0
1	A	167	ASP	2.3
1	A	211	GLN	2.2
1	A	520	TYR	2.2
1	A	199	TYR	2.2
1	A	186	VAL	2.2
1	A	655	LYS	2.1
1	A	569	SER	2.1
1	A	141	LEU	2.1
1	A	126	PHE	2.1
1	A	653	GLY	2.1
1	A	616	HIS	2.1
1	A	159	ASN	2.1
1	A	193	ALA	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
2	SPM	A	703	14/14	0.79	0.34	48,48,49,49	0
2	SPM	A	702	14/14	0.83	0.26	55,55,56,56	0
2	SPM	A	701	14/14	0.85	0.30	47,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.