



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 08:31 am BST

PDB ID : 5VLL  
Title : Short PCSK9 delta-P' complex with peptide Pep3  
Authors : Eigenbrot, C.; Ultsch, M.  
Deposited on : 2017-04-25  
Resolution : 2.37 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](mailto: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.

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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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

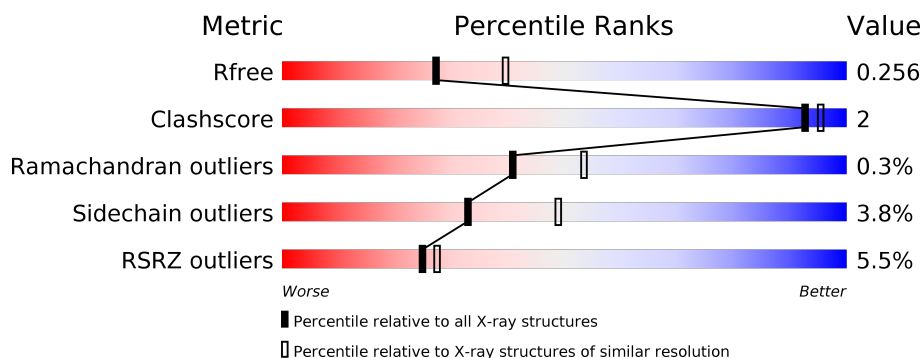
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.37 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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 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	460	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>23%</div> </div> <div>•</div> </div>
2	Y	14	<div> <div>29%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>7%</div> </div> </div>
3	Z	15	<div> <div>13%</div> <div> <div></div> <div>100%</div> </div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3007 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 Proprotein convertase subtilisin/kexin type 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	3	0
			2678	1682	474	509	13			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	167	SER	ARG	engineered mutation	UNP Q8NBP7
A	453	ASN	-	expression tag	UNP Q8NBP7
A	454	SER	-	expression tag	UNP Q8NBP7
A	455	HIS	-	expression tag	UNP Q8NBP7
A	456	HIS	-	expression tag	UNP Q8NBP7
A	457	HIS	-	expression tag	UNP Q8NBP7
A	458	HIS	-	expression tag	UNP Q8NBP7
A	459	HIS	-	expression tag	UNP Q8NBP7
A	460	HIS	-	expression tag	UNP Q8NBP7

- Molecule 2 is a protein called CYS-PHE-ILE-PRO-TRP-ASN-LEU-GLN-ARG-ILE-GLY-L EU-LEU-CYS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	14	Total	C	N	O	S	0	0	0
			116	78	20	16	2			

- Molecule 3 is a protein called ACE-THR-VAL-PHE-THR-SER-TRP-GLU-GLU-TYR-LEU -ASP-TRP-VAL-NH<sub>2</sub>.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Z	15	Total	C	N	O	0	0	1
			123	83	16	24			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

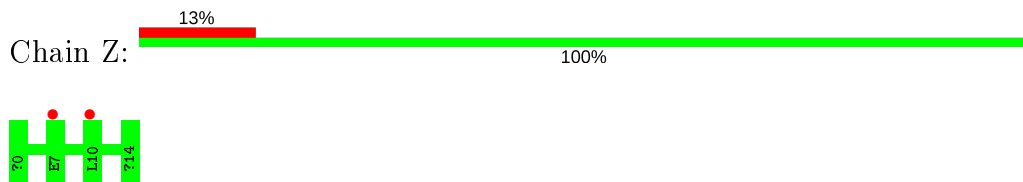
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Ca 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	83	Total 83	O 83	0	0
5	Y	2	Total 2	O 2	0	0
5	Z	4	Total 4	O 4	0	0



- Molecule 1: Proprotein convertase subtilisin/kexin type 9



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.57Å 70.57Å 158.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.34 – 2.37 28.51 – 2.37	Depositor EDS
% Data completeness (in resolution range)	90.8 (29.34-2.37) 91.2 (28.51-2.37)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 2.36Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, $R_{free}$	0.182 , 0.244 0.189 , 0.256	Depositor DCC
$R_{free}$ test set	726 reflections (4.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.0	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 46.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.058 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3007	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% 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: CA, ACE, NH2

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	0.49	0/2733	0.68	0/3710
2	Y	0.48	0/119	0.58	0/161
3	Z	0.44	0/125	0.54	0/173
All	All	0.49	0/2977	0.67	0/4044

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	2678	0	2690	7	0
2	Y	116	0	121	2	0
3	Z	123	0	105	0	0
4	A	1	0	0	0	0
5	A	83	0	0	0	0
5	Y	2	0	0	0	0
5	Z	4	0	0	0	0
All	All	3007	0	2916	9	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 9 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:Y:6:ASN:HD22	2:Y:6:ASN:H	1.51	0.58
1:A:119:LEU:HD12	1:A:303:ARG:HD3	1.90	0.53
1:A:346:VAL:HG22	1:A:366:GLU:HB2	1.96	0.47
1:A:372:SER:HB3	1:A:378:CYS:HB3	1.99	0.44
1:A:185:LEU:HD11	1:A:271:ILE:HD11	2.00	0.43

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	352/460 (76%)	340 (97%)	11 (3%)	1 (0%)	41	53
2	Y	12/14 (86%)	12 (100%)	0	0	100	100
3	Z	13/15 (87%)	13 (100%)	0	0	100	100
All	All	377/489 (77%)	365 (97%)	11 (3%)	1 (0%)	41	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	280	VAL

### 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	290/374 (78%)	280 (97%)	10 (3%)	37	53
2	Y	13/13 (100%)	11 (85%)	2 (15%)	2	3
3	Z	13/13 (100%)	13 (100%)	0	100	100
All	All	316/400 (79%)	304 (96%)	12 (4%)	33	49

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	225	SER
1	A	303	ARG
1	A	414	ARG
1	A	224	ASP
1	A	332	GLU

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

Mol	Chain	Res	Type
2	Y	6	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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 [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<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	355/460 (77%)	0.05	15 (4%) 36 39	30, 43, 60, 103	1 (0%)
2	Y	14/14 (100%)	1.18	4 (28%) 0 0	36, 54, 78, 79	0
3	Z	13/15 (86%)	0.67	2 (15%) 2 2	49, 56, 67, 75	0
All	All	382/489 (78%)	0.11	21 (5%) 25 27	30, 43, 65, 103	1 (0%)

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Y	14	CYS	5.8
2	Y	1	CYS	4.9
1	A	221	SER	4.9
1	A	212	ASP	4.1
1	A	61	THR	4.0

### 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 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CA	A	501	1/1	0.96	0.10	55,55,55,55	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.