



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 03:01 PM GMT

PDB ID : 3GCW  
Title : PCSK9:EGFA(H306Y)  
Authors : Kwon, H.J.  
Deposited on : 2009-02-22  
Resolution : 2.70 Å(reported)

This is a full wwPDB validation 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 <http://wwpdb.org/ValidationPDFNotes.html>

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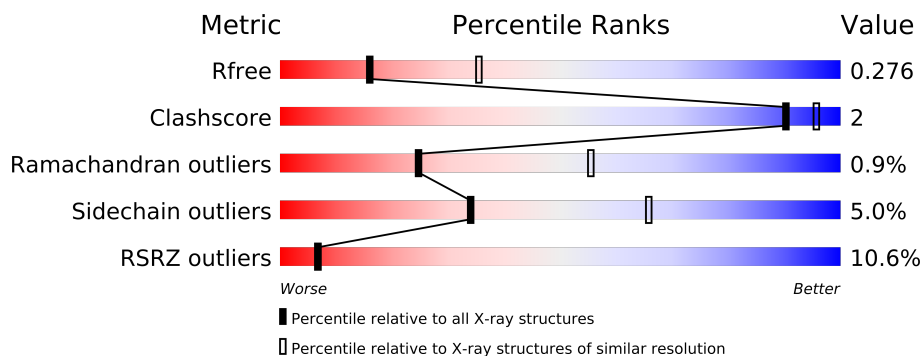
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.70 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))
$R_{free}$	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	P	100	
2	A	540	
3	E	83	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4279 atoms, of which 0 are hydrogen and 0 are deuterium.

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	P	92	Total	C	N	O	S	0	0	0
			740	474	133	131	2			

- Molecule 2 is a protein called Proprotein convertase subtilisin/kexin type 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	434	Total	C	N	O	S	0	0	0
			3228	2002	588	613	25			

- Molecule 3 is a protein called Low-density lipoprotein receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	41	Total	C	N	O	S	0	0	0
			310	186	54	63	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	290	GLY	-	EXPRESSION TAG	UNP P01130
E	291	ALA	-	EXPRESSION TAG	UNP P01130
E	292	MET	-	EXPRESSION TAG	UNP P01130
E	306	TYR	HIS	ENGINEERED	UNP P01130

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

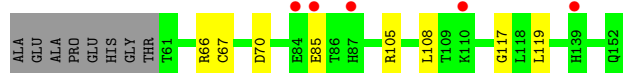
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total	Ca	0	0
			1	1		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

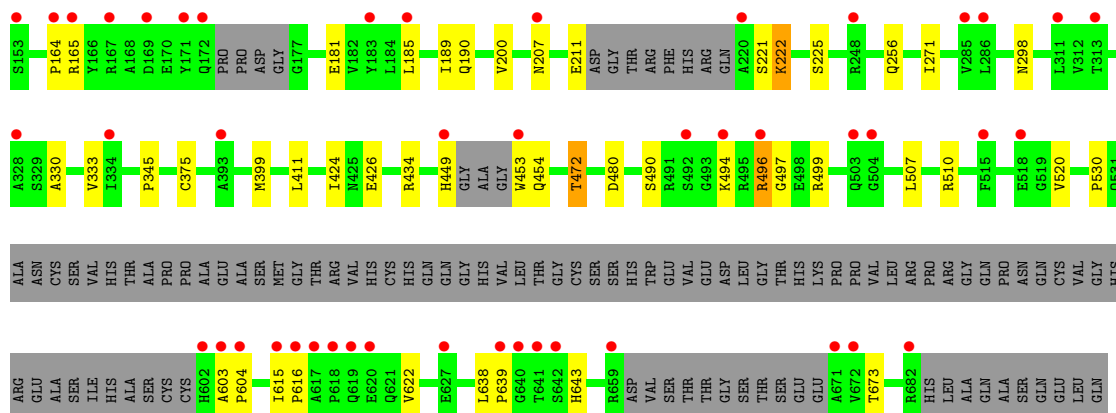
- Molecule 1: Proprotein convertase subtilisin/kexin type 9

Chain P: 



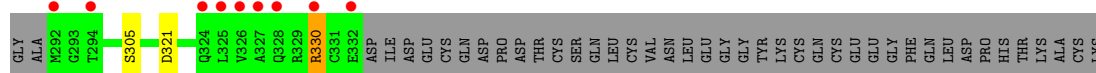
- Molecule 2: Proprotein convertase subtilisin/kexin type 9

Chain A: 



- Molecule 3: Low-density lipoprotein receptor

Chain E: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.66Å 115.66Å 133.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.10 – 2.70 37.04 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.10-2.70) 99.3 (37.04-2.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.03 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, $R_{free}$	0.234 , 0.278 0.234 , 0.276	Depositor DCC
$R_{free}$ test set	1294 reflections (5.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	58.2	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 26.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 25303 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	4279	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.34	0/757	0.49	0/1023
2	A	0.34	0/3284	0.52	0/4458
3	E	0.34	0/313	0.49	0/420
All	All	0.34	0/4354	0.51	0/5901

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	740	0	750	1	0
2	A	3228	0	3181	16	0
3	E	310	0	280	1	0
4	E	1	0	0	0	0
All	All	4279	0	4211	18	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (18) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:449:HIS:HA	2:A:453:TRP:CH2	2.22	0.75
2:A:211:GLU:HB2	2:A:256:GLN:HE21	1.57	0.70
2:A:330:ALA:O	2:A:333:VAL:HG22	1.99	0.61
2:A:185:LEU:HD11	2:A:271:ILE:HD11	1.86	0.57
2:A:490:SER:HB2	2:A:520:VAL:HG12	1.88	0.55
3:E:305:SER:OG	3:E:330:ARG:HA	2.09	0.53
1:P:66:ARG:NH1	1:P:67:CYS:O	2.42	0.49
2:A:426:GLU:HB3	2:A:434:ARG:HG2	1.98	0.46
2:A:496:ARG:HE	2:A:497:GLY:H	1.64	0.44
2:A:615:ILE:HD12	2:A:622:VAL:HG22	2.00	0.43
2:A:603:ALA:HA	2:A:604:PRO:HD3	1.84	0.43
2:A:345:PRO:HD3	2:A:424:ILE:HG23	2.01	0.43
2:A:638:LEU:HB2	2:A:673:THR:HB	2.01	0.42
2:A:472:THR:HG21	2:A:510:ARG:NH2	2.35	0.42
2:A:222:LYS:HE2	2:A:222:LYS:HA	2.02	0.41
2:A:189:ILE:HD13	2:A:200:VAL:HG11	2.03	0.41
2:A:399:MET:HE3	2:A:411:LEU:HG	2.03	0.41
2:A:453:TRP:HD1	2:A:454:GLN:H	1.69	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	P	90/100 (90%)	88 (98%)	1 (1%)	1 (1%)	21	49
2	A	422/540 (78%)	401 (95%)	17 (4%)	4 (1%)	25	55
3	E	39/83 (47%)	37 (95%)	2 (5%)	0	100	100
All	All	551/723 (76%)	526 (96%)	20 (4%)	5 (1%)	25	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	616	PRO
2	A	639	PRO
2	A	164	PRO
1	P	117	GLY
2	A	530	PRO

### 5.3.2 Protein sidechains ⓘ

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	79/84 (94%)	74 (94%)	5 (6%)	25	53
2	A	345/431 (80%)	329 (95%)	16 (5%)	37	70
3	E	35/71 (49%)	33 (94%)	2 (6%)	29	58
All	All	459/586 (78%)	436 (95%)	23 (5%)	34	66

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	70	ASP
1	P	85	GLU
1	P	105	ARG
1	P	108	LEU
1	P	119	LEU
2	A	165	ARG
2	A	181	GLU
2	A	190	GLN
2	A	207	ASN
2	A	221	SER
2	A	222	LYS
2	A	225	SER
2	A	298	ASN
2	A	375	CYS
2	A	472	THR
2	A	480	ASP
2	A	494	LYS
2	A	496	ARG
2	A	499	ARG

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Mol	Chain	Res	Type
2	A	507	LEU
2	A	643	HIS
3	E	321	ASP
3	E	330	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	101	GLN
2	A	207	ASN
2	A	256	GLN
2	A	298	ASN
2	A	342	GLN
2	A	619	GLN
3	E	300	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	P	92/100 (92%)	0.31	5 (5%) 25 27	45, 54, 64, 67	0
2	A	434/540 (80%)	0.79	46 (10%) 7 7	47, 54, 68, 88	0
3	E	41/83 (49%)	0.93	9 (21%) 1 1	51, 55, 62, 66	0
All	All	567/723 (78%)	0.72	60 (10%) 7 7	45, 55, 66, 88	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	292	MET	7.1
2	A	641	THR	6.9
2	A	153	SER	6.2
2	A	603	ALA	5.8
2	A	220	ALA	5.1
2	A	504	GLY	5.0
2	A	602	HIS	4.8
2	A	616	PRO	4.6
2	A	640	GLY	4.5
2	A	617	ALA	4.4
2	A	620	GLU	4.1
3	E	328	GLN	4.0
2	A	515	PHE	3.5
3	E	330	ARG	3.4
2	A	615	ILE	3.4
2	A	672	VAL	3.2
2	A	619	GLN	3.2
1	P	85	GLU	3.1
2	A	618	PRO	3.1
3	E	332	GLU	3.1
2	A	449	HIS	3.1
2	A	164	PRO	3.0
2	A	682	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
3	E	327	ALA	2.9
2	A	518	GLU	2.9
2	A	671	ALA	2.9
2	A	659	ARG	2.8
2	A	496	ARG	2.7
2	A	172	GLN	2.7
2	A	207	ASN	2.6
2	A	167	ARG	2.6
3	E	326	VAL	2.5
1	P	110	LYS	2.4
2	A	311	LEU	2.4
2	A	642	SER	2.4
2	A	285	VAL	2.3
1	P	87	HIS	2.3
2	A	169	ASP	2.3
2	A	453	TRP	2.3
2	A	165	ARG	2.3
2	A	328	ALA	2.3
2	A	171	TYR	2.3
1	P	84	GLU	2.3
2	A	627	GLU	2.3
2	A	286	LEU	2.3
3	E	294	THR	2.3
2	A	334	ILE	2.2
2	A	393	ALA	2.2
3	E	325	LEU	2.2
3	E	324	GLN	2.2
2	A	503	GLN	2.1
2	A	183	TYR	2.1
2	A	248	ARG	2.1
2	A	492	SER	2.1
2	A	494	LYS	2.1
2	A	604	PRO	2.1
1	P	139	HIS	2.0
2	A	313	THR	2.0
2	A	185	LEU	2.0
2	A	639	PRO	2.0

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

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

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	CA	E	1	1/1	0.08	-1.26	48,48,48,48	0

### 6.5 Other polymers

There are no such residues in this entry.