



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 04:23 AM GMT

PDB ID : 2W2M  
Title : WT PCSK9-DELTAC BOUND TO WT EGF-A OF LDLR  
Authors : Bottomley, M.J.; Cirillo, A.; Orsatti, L.; Ruggeri, L.; Fisher, T.S.; Santoro, J.C.; Cummings, R.T.; Cubbon, R.M.; Lo Surdo, P.; Calzetta, A.; Noto, A.; Baysarowich, J.; Mattu, M.; Talamo, F.; De Francesco, R.; Sparrow, C.P.; Sitlani, A.; Carfi, A.  
Deposited on : 2008-11-03  
Resolution : 2.40 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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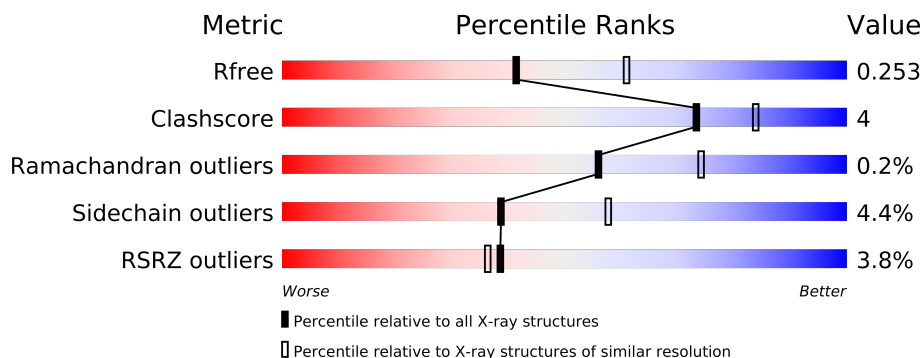
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.40 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	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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	A	312	
2	E	107	
3	P	114	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3408 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	A	277	Total	C	N	O	S	0	3	0
			2054	1281	360	402	11			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	452	ALA	-	EXPRESSION TAG	UNP Q8NBP7
A	453	GLY	-	EXPRESSION TAG	UNP Q8NBP7
A	454	THR	-	EXPRESSION TAG	UNP Q8NBP7
A	455	ALA	-	EXPRESSION TAG	UNP Q8NBP7
A	456	ALA	-	EXPRESSION TAG	UNP Q8NBP7
A	457	ALA	-	EXPRESSION TAG	UNP Q8NBP7
A	458	SER	-	EXPRESSION TAG	UNP Q8NBP7
A	459	HIS	-	EXPRESSION TAG	UNP Q8NBP7
A	460	HIS	-	EXPRESSION TAG	UNP Q8NBP7
A	461	HIS	-	EXPRESSION TAG	UNP Q8NBP7
A	462	HIS	-	EXPRESSION TAG	UNP Q8NBP7
A	463	HIS	-	EXPRESSION TAG	UNP Q8NBP7
A	464	HIS	-	EXPRESSION TAG	UNP Q8NBP7

- Molecule 2 is a protein called LOW-DENSITY LIPOPROTEIN RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	49	Total	C	N	O	S	0	1	0
			373	227	66	73	7			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	266	MET	-	EXPRESSION TAG	UNP P01130
E	267	LYS	-	EXPRESSION TAG	UNP P01130

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Chain	Residue	Modelled	Actual	Comment	Reference
E	268	HIS	-	EXPRESSION TAG	UNP P01130
E	269	HIS	-	EXPRESSION TAG	UNP P01130
E	270	HIS	-	EXPRESSION TAG	UNP P01130
E	271	HIS	-	EXPRESSION TAG	UNP P01130
E	272	HIS	-	EXPRESSION TAG	UNP P01130
E	273	HIS	-	EXPRESSION TAG	UNP P01130
E	274	PRO	-	EXPRESSION TAG	UNP P01130
E	275	MET	-	EXPRESSION TAG	UNP P01130
E	276	SER	-	EXPRESSION TAG	UNP P01130
E	277	ASP	-	EXPRESSION TAG	UNP P01130
E	278	TYR	-	EXPRESSION TAG	UNP P01130
E	279	ASP	-	EXPRESSION TAG	UNP P01130
E	280	ILE	-	EXPRESSION TAG	UNP P01130
E	281	PRO	-	EXPRESSION TAG	UNP P01130
E	282	THR	-	EXPRESSION TAG	UNP P01130
E	283	THR	-	EXPRESSION TAG	UNP P01130
E	284	GLU	-	EXPRESSION TAG	UNP P01130
E	285	ASN	-	EXPRESSION TAG	UNP P01130
E	286	LEU	-	EXPRESSION TAG	UNP P01130
E	287	TYR	-	EXPRESSION TAG	UNP P01130
E	288	PHE	-	EXPRESSION TAG	UNP P01130
E	289	GLN	-	EXPRESSION TAG	UNP P01130
E	290	GLY	-	EXPRESSION TAG	UNP P01130
E	291	ALA	-	EXPRESSION TAG	UNP P01130
E	292	MET	-	EXPRESSION TAG	UNP P01130

- Molecule 3 is a protein called PROPROTEIN CONVERTASE SUBTILISIN/KEXIN TYPE 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	92	Total	C	N	O	S	0	4	0
			763	491	138	132	2			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	39	MET	-	EXPRESSION TAG	UNP Q8NBP7
P	40	LYS	-	EXPRESSION TAG	UNP Q8NBP7
P	41	GLY	-	EXPRESSION TAG	UNP Q8NBP7
P	42	SER	-	EXPRESSION TAG	UNP Q8NBP7
P	43	LYS	-	EXPRESSION TAG	UNP Q8NBP7
P	44	GLY	-	EXPRESSION TAG	UNP Q8NBP7

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Chain	Residue	Modelled	Actual	Comment	Reference
P	45	SER	-	EXPRESSION TAG	UNP Q8NBP7
P	46	LYS	-	EXPRESSION TAG	UNP Q8NBP7
P	47	GLY	-	EXPRESSION TAG	UNP Q8NBP7
P	48	SER	-	EXPRESSION TAG	UNP Q8NBP7
P	49	LYS	-	EXPRESSION TAG	UNP Q8NBP7
P	50	PRO	-	EXPRESSION TAG	UNP Q8NBP7
P	51	MET	-	EXPRESSION TAG	UNP Q8NBP7
P	52	SER	-	EXPRESSION TAG	UNP Q8NBP7

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	E	2	Total Ca 2 2	0	0

- Molecule 5 is water.

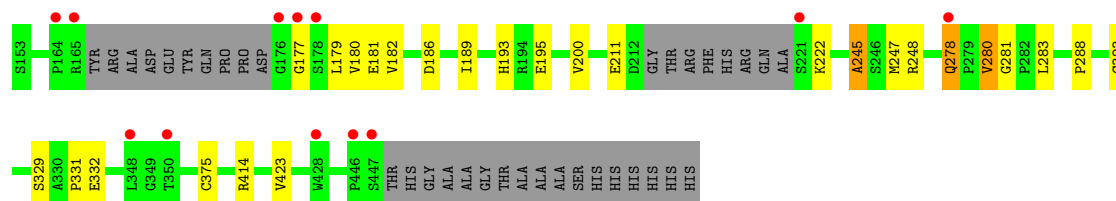
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	117	Total O 117 117	0	0
5	E	41	Total O 41 41	0	0
5	P	57	Total O 57 57	0	0

### 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.

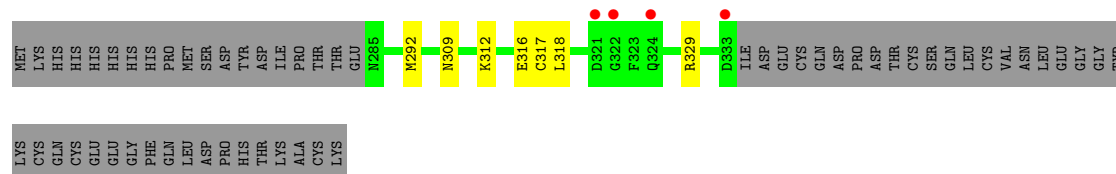
#### • Molecule 1: PROPROTEIN CONVERTASE SUBTILISIN/KEXIN TYPE 9

Chain A: 



#### • Molecule 2: LOW-DENSITY LIPOPROTEIN RECEPTOR

Chain E: 



#### • Molecule 3: PROPROTEIN CONVERTASE SUBTILISIN/KEXIN TYPE 9

Chain P: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.00Å 83.00Å 211.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 2.40 45.11 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.00-2.40) 99.9 (45.11-2.40)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.215 , 0.254 0.213 , 0.253	Depositor DCC
$R_{free}$ test set	1512 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.2	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 31.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 29811 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3408	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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	A	0.38	0/2096	0.54	0/2853
2	E	0.51	0/381	0.55	0/512
3	P	0.38	0/792	0.58	1/1067 (0.1%)
All	All	0.40	0/3269	0.55	1/4432 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	133	LEU	CA-CB-CG	5.07	126.97	115.30

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	A	2054	0	2040	15	0
2	E	373	0	335	6	0
3	P	763	0	794	6	0
4	A	1	0	0	0	0
4	E	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	117	0	0	0	0
5	E	41	0	0	1	0
5	P	57	0	0	0	0
All	All	3408	0	3169	27	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 4.

All (27) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:P:69[B]:LYS:HG3	3:P:71:PRO:HD2	1.73	0.70
2:E:316:GLU:HG3	2:E:318:LEU:CD1	2.26	0.66
1:A:177:GLY:HA3	1:A:245:ALA:HA	1.79	0.64
1:A:186:ASP:OD2	1:A:288:PRO:HG2	2.02	0.60
3:P:98:LEU:HB2	3:P:137:LEU:HD11	1.86	0.57
1:A:278:GLN:HG2	1:A:278:GLN:O	2.05	0.57
1:A:200:VAL:HG22	1:A:247:MET:HB2	1.88	0.55
2:E:316:GLU:HG3	2:E:318:LEU:HD11	1.87	0.55
1:A:193:HIS:HD2	1:A:195:GLU:H	1.53	0.54
1:A:278:GLN:O	1:A:278:GLN:CG	2.59	0.51
1:A:280:VAL:HG23	1:A:281:GLY:H	1.75	0.50
1:A:323:CYS:HA	1:A:329:SER:HB3	1.94	0.49
1:A:181:GLU:CD	1:A:248:ARG:HE	2.16	0.49
3:P:133:LEU:C	3:P:133:LEU:HD23	2.36	0.46
3:P:70:ASP:HB3	3:P:71:PRO:HD3	1.98	0.46
3:P:88:LEU:HD13	3:P:116:HIS:HB3	1.99	0.45
1:A:182:VAL:HB	1:A:247:MET:HG2	1.98	0.44
1:A:331:PRO:O	1:A:332:GLU:HB2	2.18	0.43
1:A:177:GLY:HA2	1:A:180:VAL:HB	2.00	0.43
1:A:331:PRO:O	1:A:332:GLU:CB	2.67	0.42
2:E:317:CYS:C	2:E:318:LEU:HD12	2.40	0.42
1:A:189:ILE:HD13	1:A:200:VAL:HG11	2.02	0.41
2:E:292:MET:CE	2:E:312:LYS:HE2	2.50	0.41
2:E:329:ARG:NH1	5:E:2040:HOH:O	2.52	0.41
3:P:118:LEU:HD23	3:P:118:LEU:HA	1.93	0.41
1:A:193:HIS:CD2	1:A:195:GLU:H	2.37	0.40
2:E:309:ASN:HB3	2:E:316:GLU:HG2	2.04	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	274/312 (88%)	262 (96%)	11 (4%)	1 (0%)	43	61
2	E	48/107 (45%)	44 (92%)	4 (8%)	0	100	100
3	P	94/114 (82%)	90 (96%)	4 (4%)	0	100	100
All	All	416/533 (78%)	396 (95%)	19 (5%)	1 (0%)	56	74

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	245	ALA

### 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	A	224/247 (91%)	215 (96%)	9 (4%)	42	63
2	E	40/95 (42%)	40 (100%)	0	100	100
3	P	83/95 (87%)	77 (93%)	6 (7%)	21	31
All	All	347/437 (79%)	332 (96%)	15 (4%)	39	59

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	LEU
1	A	211	GLU
1	A	222	LYS
1	A	278	GLN
1	A	280	VAL

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Mol	Chain	Res	Type
1	A	283	LEU
1	A	375	CYS
1	A	414	ARG
1	A	423	VAL
3	P	61	THR
3	P	97	ARG
3	P	98	LEU
3	P	108	LEU
3	P	119	LEU
3	P	133	LEU

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

Mol	Chain	Res	Type
1	A	193	HIS
1	A	278	GLN
2	E	309	ASN
3	P	99	GLN

### 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 3 ligands modelled in this entry, 3 are 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	A	277/312 (88%)	0.03	12 (4%) 34 32	16, 24, 38, 50	0
2	E	49/107 (45%)	-0.01	4 (8%) 12 10	24, 27, 39, 41	0
3	P	92/114 (80%)	-0.43	0 100 100	15, 24, 31, 35	0
All	All	418/533 (78%)	-0.08	16 (3%) 38 36	15, 25, 38, 50	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	178	SER	8.4
1	A	447	SER	6.1
1	A	221	SER	4.5
1	A	446	PRO	3.3
1	A	164	PRO	3.1
1	A	165	ARG	3.1
1	A	176	GLY	3.1
2	E	322	GLY	2.8
1	A	278	GLN	2.6
1	A	428	TRP	2.3
1	A	348	LEU	2.2
2	E	321	ASP	2.2
1	A	350	THR	2.1
2	E	333	ASP	2.1
2	E	324[A]	GLN	2.1
1	A	177	GLY	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	A	1448	1/1	0.11	-0.86	61,61,61,61	0
4	CA	E	1334	1/1	0.09	-1.41	30,30,30,30	0
4	CA	E	1335	1/1	0.04	-19.83	92,92,92,92	0

### 6.5 Other polymers

There are no such residues in this entry.