



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:13 PM GMT

PDB ID : 2P4E  
Title : Crystal Structure of PCSK9  
Authors : Cunningham, D.; Danley, D.E.; Geoghegan, F.K.; Griffor, M.C.; Hawkins, J.L.; Qiu, X.  
Deposited on : 2007-03-12  
Resolution : 1.98 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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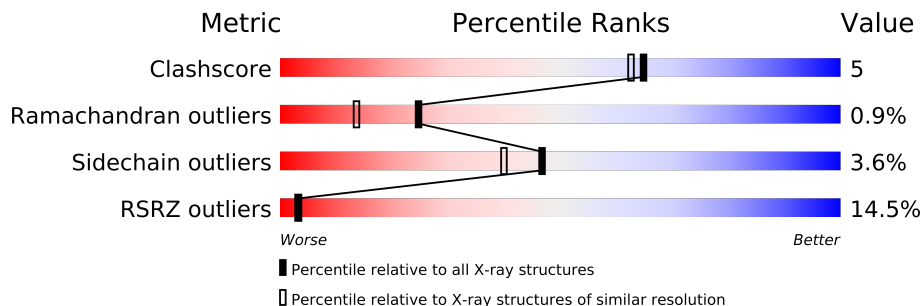
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.98 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))
Clashscore	79885	8091 (2.00-1.96)
Ramachandran outliers	78287	7989 (2.00-1.96)
Sidechain outliers	78261	7987 (2.00-1.96)
RSRZ outliers	66119	6578 (2.00-1.96)

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	692	
1	P	692	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4776 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	1	0
			741	475	134	130	2			
1	A	494	Total	C	N	O	S	0	1	0
			3662	2255	674	701	32			

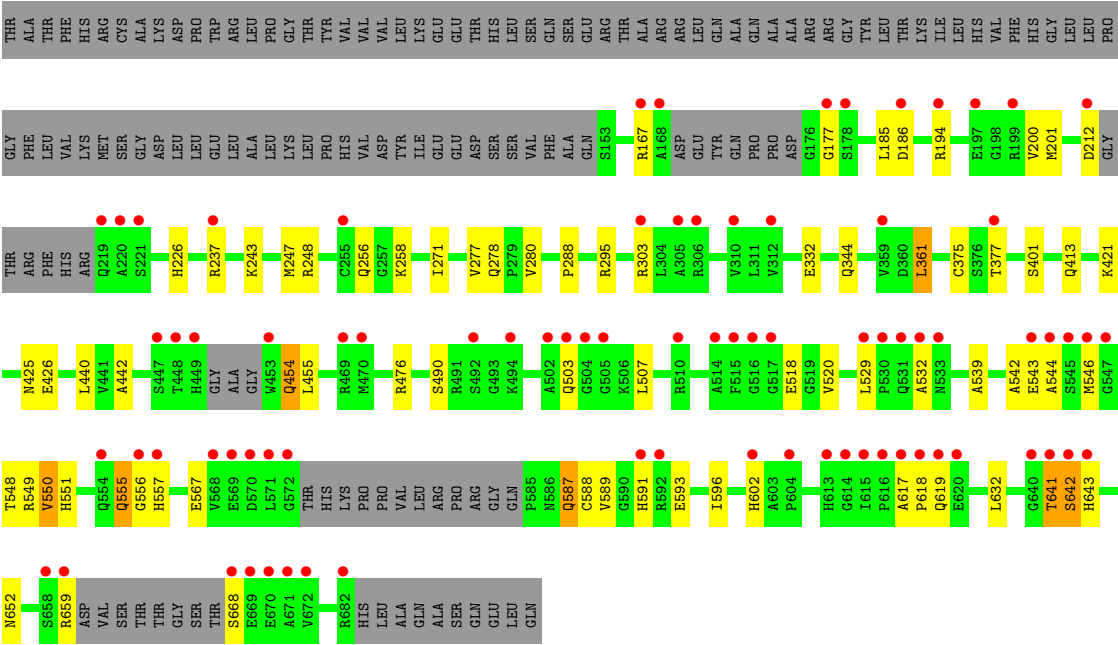
- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	2	Total	Hg	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	281	Total	O	0	0
			281	281		
3	P	90	Total	O	0	0
			90	90		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.81Å 70.67Å 150.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.00 – 1.98 48.16 – 1.98	Depositor EDS
% Data completeness (in resolution range)	97.9 (75.00-1.98) 94.7 (48.16-1.98)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.1	Depositor
R, $R_{free}$	0.200 , 0.250 0.204 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	26.8	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.5	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	0 of 86760 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4776	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.56% 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: HG

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	0.54	0/3734	0.65	0/5070
1	P	0.56	0/765	0.67	0/1034
All	All	0.55	0/4499	0.66	0/6104

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	A	3662	0	3564	44	0
1	P	741	0	751	3	0
2	P	2	0	0	0	0
3	A	281	0	0	2	0
3	P	90	0	0	1	0
All	All	4776	0	4315	45	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 5.

All (45) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:344:GLN:HE22	1:A:425:ASN:H	1.17	0.90
1:A:641:THR:HG22	1:A:643:HIS:CE1	2.16	0.80
1:A:548:THR:HG22	1:A:596:ILE:HG22	1.71	0.73
1:A:529:LEU:HG	1:A:532:ALA:HB2	1.78	0.63
1:A:186:ASP:OD2	1:A:288:PRO:HG2	1.98	0.63
1:A:426:GLU:HG2	3:A:855:HOH:O	1.98	0.63
1:A:212:ASP:H	1:A:256:GLN:HE22	1.48	0.62
1:A:588:CYS:HB3	1:A:596:ILE:HD11	1.83	0.61
1:A:588:CYS:CB	1:A:596:ILE:HD11	2.32	0.60
1:A:555:GLN:CD	1:A:556:GLY:H	2.05	0.59
1:A:641:THR:HG22	1:A:643:HIS:HE1	1.68	0.58
1:A:632:LEU:H	1:A:652:ASN:ND2	2.03	0.57
1:P:105:ARG:NH1	3:P:783:HOH:O	2.30	0.57
1:A:185:LEU:HD11	1:A:271:ILE:HD11	1.88	0.56
1:A:256:GLN:NE2	3:A:774:HOH:O	2.37	0.55
1:A:556:GLY:HA3	1:A:602:HIS:CD2	2.42	0.55
1:A:549:ARG:HG2	1:A:589:VAL:HG22	1.90	0.54
1:A:201:MET:HE2	1:A:248:ARG:NH1	2.23	0.54
1:A:454:GLN:HG3	1:A:455:LEU:N	2.23	0.53
1:A:177:GLY:HA2	1:A:401:SER:HB2	1.90	0.52
1:A:476:ARG:HH21	1:A:503:GLN:NE2	2.08	0.52
1:A:617:ALA:O	1:A:619:GLN:N	2.44	0.51
1:A:518:GLU:H	1:A:518:GLU:CD	2.16	0.49
1:P:150:PHE:CE1	1:A:258:LYS:HG2	2.48	0.49
1:A:551:HIS:HB3	1:A:587:GLN:HB2	1.94	0.49
1:P:65:HIS:CE1	1:A:295:ARG:HH11	2.30	0.48
1:A:557:HIS:CE1	1:A:602:HIS:HB2	2.48	0.48
1:A:548:THR:HG22	1:A:596:ILE:CG2	2.43	0.47
1:A:277:VAL:HG12	1:A:278:GLN:HG3	1.98	0.46
1:A:641:THR:CG2	1:A:643:HIS:CE1	2.95	0.46
1:A:237:ARG:O	1:A:243:LYS:HD2	2.16	0.46
1:A:194:ARG:HG3	1:A:377:THR:HG22	1.98	0.45
1:A:201:MET:CE	1:A:248:ARG:NH1	2.81	0.44
1:A:421:LYS:HD3	1:A:440:LEU:CD2	2.48	0.44
1:A:632:LEU:H	1:A:652:ASN:HD22	1.64	0.44
1:A:539:ALA:HB2	1:A:550:VAL:HG13	1.99	0.43
1:A:490:SER:HB2	1:A:520:VAL:HG12	2.00	0.43
1:A:186:ASP:OD1	1:A:226:HIS:ND1	2.40	0.43
1:A:361:LEU:HD22	1:A:442:ALA:HB2	2.00	0.43
1:A:200:VAL:HG22	1:A:247:MET:HB2	2.02	0.42
1:A:542:ALA:HB1	1:A:546:MET:HE2	2.01	0.42
1:A:591:HIS:CD2	1:A:593:GLU:H	2.38	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:476:ARG:HH21	1:A:503:GLN:HE21	1.67	0.40
1:A:539:ALA:CB	1:A:550:VAL:HG13	2.51	0.40
1:A:201:MET:CE	1:A:248:ARG:HH11	2.34	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	483/692 (70%)	459 (95%)	19 (4%)	5 (1%)	22	11
1	P	91/692 (13%)	88 (97%)	3 (3%)	0	100	100
All	All	574/1384 (42%)	547 (95%)	22 (4%)	5 (1%)	25	13

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	642	SER
1	A	543	GLU
1	A	618	PRO
1	A	544	ALA
1	A	280	VAL

### 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	394/558 (71%)	378 (96%)	16 (4%)	41	33
1	P	80/558 (14%)	79 (99%)	1 (1%)	80	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	474/1116 (42%)	457 (96%)	17 (4%)	47 40

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	108	LEU
1	A	167	ARG
1	A	303	ARG
1	A	332	GLU
1	A	361	LEU
1	A	375	CYS
1	A	413	GLN
1	A	454	GLN
1	A	507	LEU
1	A	550	VAL
1	A	555	GLN
1	A	567	GLU
1	A	587	GLN
1	A	641	THR
1	A	642	SER
1	A	659	ARG
1	A	668	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	65	HIS
1	P	101	GLN
1	A	219	GLN
1	A	256	GLN
1	A	298	ASN
1	A	344	GLN
1	A	413	GLN
1	A	513	ASN
1	A	537	HIS
1	A	587	GLN
1	A	591	HIS
1	A	602	HIS
1	A	643	HIS
1	A	652	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 2 ligands modelled in this entry, 2 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	494/692 (71%)	1.08	80 (16%) 2 2	15, 30, 58, 71	0
1	P	92/692 (13%)	0.31	5 (5%) 25 26	20, 27, 38, 47	0
All	All	586/1384 (42%)	0.96	85 (14%) 3 3	15, 30, 56, 71	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	615	ILE	13.2
1	A	618	PRO	10.2
1	A	668	SER	9.9
1	A	571	LEU	9.2
1	A	515	PHE	8.9
1	A	219	GLN	8.3
1	A	641	THR	7.9
1	A	572	GLY	7.0
1	A	449	HIS	6.9
1	A	448	THR	6.9
1	A	642	SER	6.3
1	A	617	ALA	6.1
1	A	177	GLY	5.8
1	A	546	MET	5.8
1	A	616	PRO	5.6
1	A	545	SER	5.6
1	A	531	GLN	5.6
1	A	640	GLY	5.1
1	A	505	GLY	5.1
1	A	672	VAL	5.0
1	A	619	GLN	5.0
1	A	570	ASP	4.9
1	A	604	PRO	4.9
1	A	220	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	669	GLU	4.8
1	A	659	ARG	4.7
1	A	453	TRP	4.5
1	A	212	ASP	4.4
1	A	469	ARG	4.3
1	A	670	GLU	4.1
1	A	199	ARG	4.1
1	A	532	ALA	4.0
1	A	569	GLU	3.9
1	A	658	SER	3.9
1	A	543	GLU	3.9
1	A	592	ARG	3.7
1	A	620	GLU	3.5
1	A	514	ALA	3.4
1	A	168	ALA	3.4
1	A	494	LYS	3.4
1	A	544	ALA	3.3
1	A	492	SER	3.3
1	A	671	ALA	3.3
1	A	614	GLY	3.3
1	A	470	MET	3.3
1	A	556	GLY	3.2
1	P	108	LEU	3.2
1	A	516	GLY	3.2
1	A	504	GLY	3.1
1	A	510	ARG	2.9
1	A	359	VAL	2.9
1	A	643	HIS	2.8
1	A	502	ALA	2.8
1	A	503	GLN	2.8
1	A	602	HIS	2.8
1	A	613	HIS	2.8
1	A	312	VAL	2.7
1	A	554	GLN	2.7
1	A	530	PRO	2.7
1	P	104	ARG	2.6
1	A	237	ARG	2.6
1	A	533	ASN	2.5
1	A	178	SER	2.5
1	P	102	ALA	2.4
1	A	591	HIS	2.4
1	A	305	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	568	VAL	2.4
1	P	61	THR	2.3
1	P	105	ARG	2.3
1	A	194	ARG	2.3
1	A	377	THR	2.3
1	A	197	GLU	2.3
1	A	306	ARG	2.2
1	A	221	SER	2.2
1	A	529	LEU	2.2
1	A	517	GLY	2.2
1	A	186	ASP	2.1
1	A	255	CYS	2.1
1	A	310	VAL	2.1
1	A	167	ARG	2.1
1	A	547	GLY	2.1
1	A	557	HIS	2.1
1	A	682	ARG	2.1
1	A	303	ARG	2.0
1	A	447	SER	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
2	HG	P	693	1/1	0.11	-0.35	25,25,25,25	1
2	HG	P	694	1/1	0.08	-1.68	35,35,35,35	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.