



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 12:43 am BST

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

MolProbity	:	4.02b-467
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

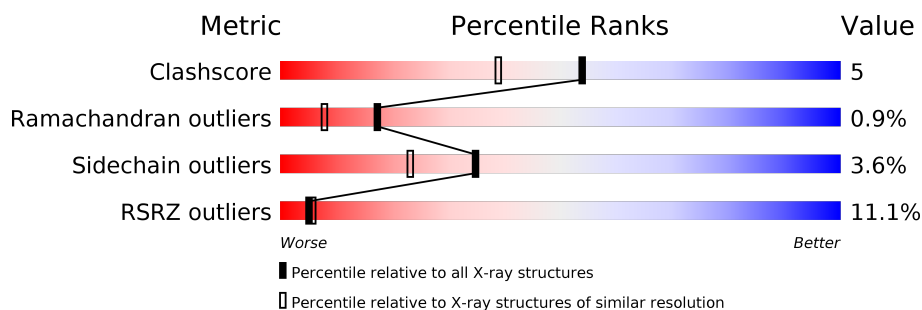
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (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 ≥ 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	692	<div> <div>9%</div> <div>61%</div> <div>10%</div> <div>29%</div> </div>
1	P	692	<div> <div>13%</div> <div>87%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4776 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	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).

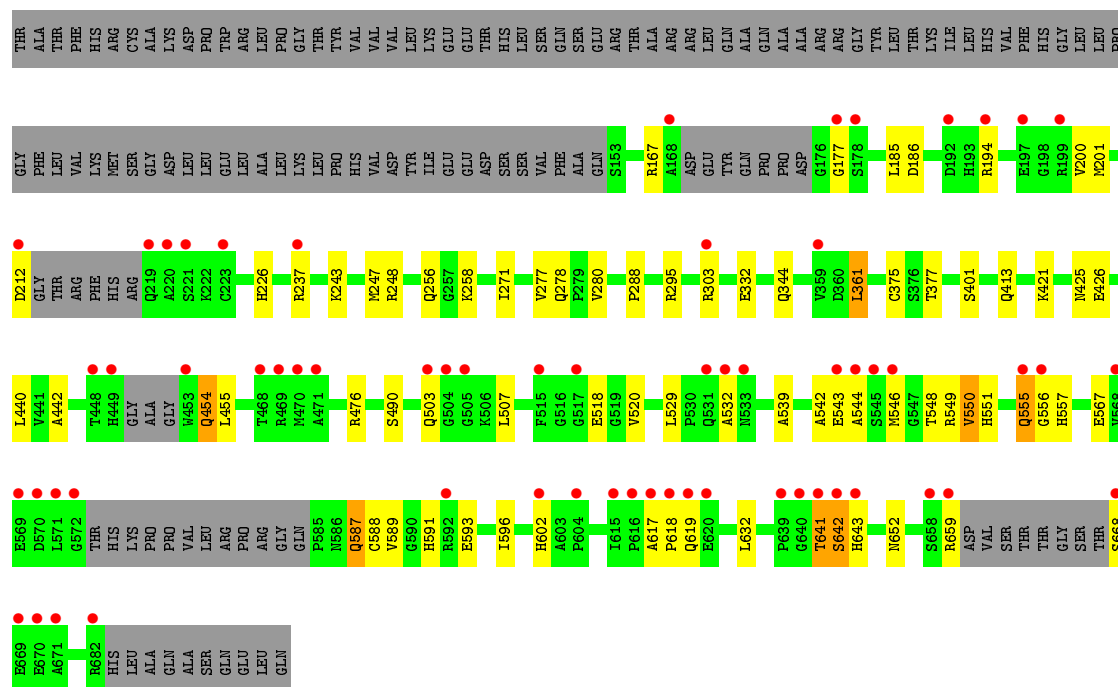
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	2	Total	Hg	0	0
			2	2		

- Molecule 3 is water.

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

- Molecule 1: Proprotein convertase subtilisin/kexin type 9





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.1	Depositor
R, R_{free}	0.200 , 0.250 0.203 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4776	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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

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 Too-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 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	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

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 5.

All (45) 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: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:186:ASP:OD2	1:A:288:PRO:HG2	1.98	0.63
1:A:529:LEU:HG	1:A:532:ALA:HB2	1.78	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:237:ARG:O	1:A:243:LYS:HD2	2.16	0.46
1:A:641:THR:CG2	1:A:643:HIS:CE1	2.95	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	Interatomic distance (Å)	Clash overlap (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 [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	483/692 (70%)	459 (95%)	19 (4%)	5 (1%)	15	6
1	P	91/692 (13%)	88 (97%)	3 (3%)	0	100	100
All	All	574/1384 (42%)	547 (95%)	22 (4%)	5 (1%)	17	8

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 [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	394/558 (71%)	378 (96%)	16 (4%)	30	18
1	P	80/558 (14%)	79 (99%)	1 (1%)	69	64
All	All	474/1116 (42%)	457 (96%)	17 (4%)	35	23

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

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Mol	Chain	Res	Type
1	A	652	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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.

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 ⓘ

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, 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	494/692 (71%)	0.90	62 (12%) 3 4	15, 30, 58, 71	0
1	P	92/692 (13%)	0.17	3 (3%) 46 49	20, 27, 38, 47	0
All	All	586/1384 (42%)	0.78	65 (11%) 5 6	15, 30, 56, 71	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	618	PRO	9.2
1	A	617	ALA	7.2
1	A	515	PHE	6.8
1	A	545	SER	6.7
1	A	546	MET	6.6
1	A	641	THR	6.6
1	A	668	SER	6.5
1	A	640	GLY	6.3
1	A	571	LEU	6.1
1	A	556	GLY	6.1
1	A	615	ILE	6.1
1	A	642	SER	5.9
1	A	569	GLU	5.9
1	A	671	ALA	5.5
1	A	177	GLY	5.5
1	A	449	HIS	5.1
1	A	543	GLU	5.1
1	A	669	GLU	4.8
1	A	219	GLN	4.7
1	A	469	ARG	4.6
1	A	659	ARG	4.5
1	A	470	MET	4.2
1	A	504	GLY	4.1
1	A	570	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	616	PRO	4.1
1	A	544	ALA	4.0
1	A	212	ASP	4.0
1	A	568	VAL	3.8
1	A	619	GLN	3.6
1	A	453	TRP	3.6
1	A	468	THR	3.6
1	A	604	PRO	3.5
1	A	503	GLN	3.5
1	A	531	GLN	3.4
1	A	220	ALA	3.4
1	A	448	THR	3.3
1	A	620	GLU	3.3
1	A	670	GLU	3.3
1	A	471	ALA	3.2
1	A	517	GLY	3.0
1	A	237	ARG	3.0
1	A	592	ARG	3.0
1	A	192	ASP	3.0
1	A	572	GLY	2.9
1	A	303	ARG	2.9
1	A	505	GLY	2.9
1	A	194	ARG	2.8
1	A	199	ARG	2.7
1	A	221	SER	2.7
1	P	104	ARG	2.6
1	A	555	GLN	2.5
1	A	602	HIS	2.4
1	P	61	THR	2.4
1	A	658	SER	2.4
1	A	639	PRO	2.3
1	A	532	ALA	2.3
1	A	682	ARG	2.3
1	A	359	VAL	2.2
1	A	178	SER	2.2
1	A	643	HIS	2.2
1	A	197	GLU	2.2
1	P	108	LEU	2.2
1	A	223	CYS	2.2
1	A	533	ASN	2.1
1	A	168	ALA	2.1

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, 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(\AA^2)	Q<0.9
2	HG	P	694	1/1	0.99	0.09	35,35,35,35	1
2	HG	P	693	1/1	1.00	0.13	25,25,25,25	1

6.5 Other polymers [i](#)

There are no such residues in this entry.