W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 10:27 AM GMT

PDB ID	:	3M0C
Title	:	The X-ray Crystal Structure of PCSK9 in Complex with the LDL receptor
Authors	:	Spraggon, G.; Hampton, E.N.
Deposited on	:	2010-03-02
Resolution	:	7.01 Å(reported)

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

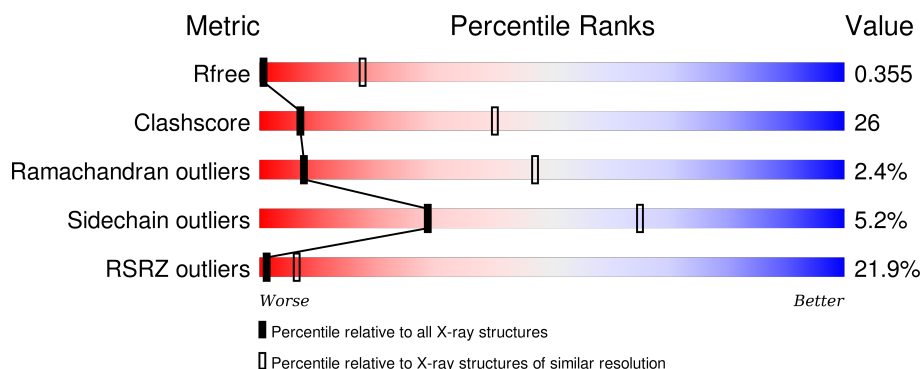|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 7.01 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	Percentile Ranks	Value
Rfree		0.355
Clashscore		26
Ramachandran outliers		2.4%
Sidechain outliers		5.2%
RSRZ outliers		21.9%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1014 (9.50-3.66)
Clashscore	102246	1063 (10.00-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

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. 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 <=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	124	14% 69% 5% 26%
2	B	546	19% 71% 16% • 11%
3	C	791	13% 35% 14% 5% • 46%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7705 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	92	Total 748	C 479	N 136	O 131	S 2	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	486	Total 3618	C 2234	N 668	O 684	S 32	0	1	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	374	TYR	ASP	ENGINEERED	UNP Q8NBP7
B	693	HIS	-	EXPRESSION TAG	UNP Q8NBP7
B	694	HIS	-	EXPRESSION TAG	UNP Q8NBP7
B	695	HIS	-	EXPRESSION TAG	UNP Q8NBP7
B	696	HIS	-	EXPRESSION TAG	UNP Q8NBP7
B	697	HIS	-	EXPRESSION TAG	UNP Q8NBP7
B	698	HIS	-	EXPRESSION TAG	UNP Q8NBP7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	430	Total 3336	C 2079	N 578	O 647	S 32	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	768	HIS	-	EXPRESSION TAG	UNP P01130
C	769	HIS	-	EXPRESSION TAG	UNP P01130
C	770	HIS	-	EXPRESSION TAG	UNP P01130

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Chain	Residue	Modelled	Actual	Comment	Reference
C	771	HIS	-	EXPRESSION TAG	UNP P01130
C	772	HIS	-	EXPRESSION TAG	UNP P01130
C	773	HIS	-	EXPRESSION TAG	UNP P01130

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

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	3	Total 3	Ca 3	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.
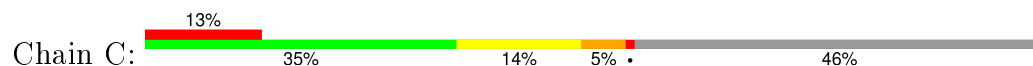
- Molecule 1: Proprotein convertase subtilisin/kexin type 9
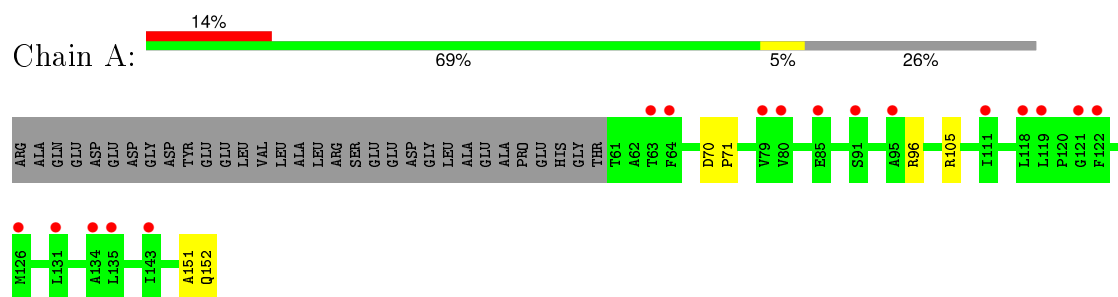
- Molecule 2: Proprotein convertase subtilisin/kexin type 9
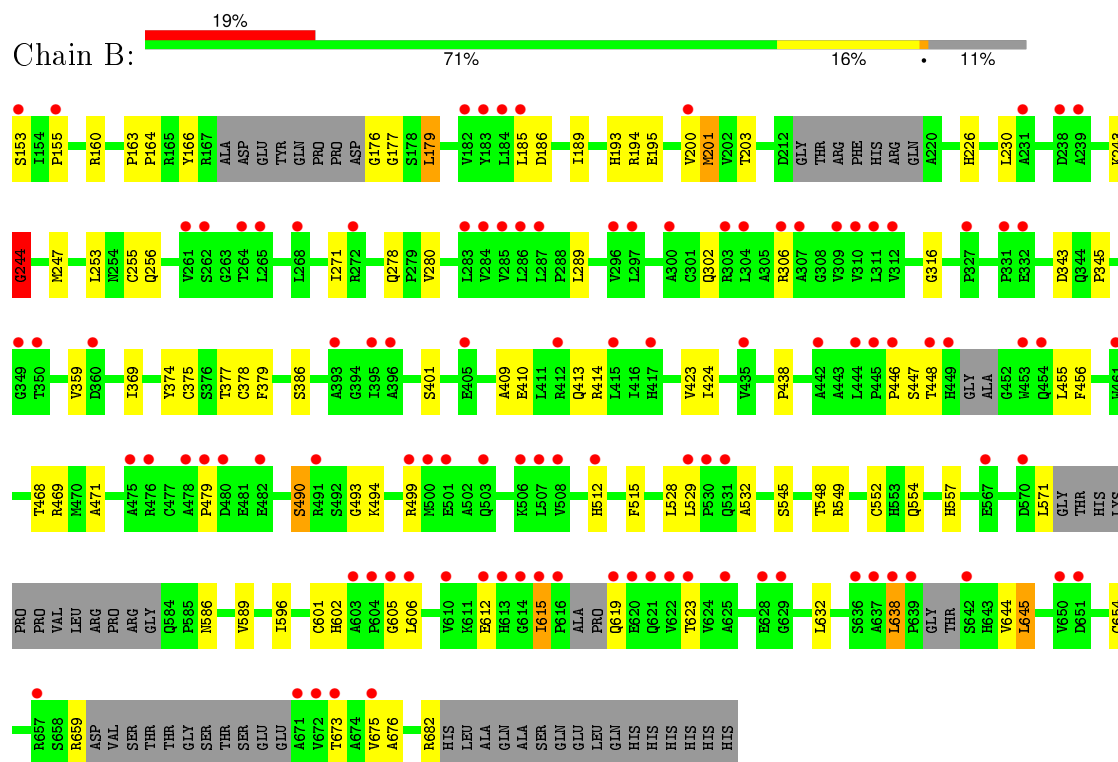
- Molecule 3: Low-density lipoprotein receptor

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	322.91Å 322.91Å 76.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	279.64 – 7.01 279.64 – 7.01	Depositor EDS
% Data completeness (in resolution range)	82.2 (279.64-7.01) 97.6 (279.64-7.01)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 6.74Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.341 , 0.362 0.338 , 0.355	Depositor DCC
R_{free} test set	337 reflections (4.63%)	DCC
Wilson B-factor (Å^2)	247.1	Xtriage
Anisotropy	0.739	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 198.7	EDS
Estimated twinning fraction	0.189 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.28, < L^2 > = 0.12$	Xtriage
Outliers	0 of 7313 reflections	Xtriage
F_o,F_c correlation	0.72	EDS
Total number of atoms	7705	wwPDB-VP
Average B, all atoms (Å^2)	182.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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

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	0.80	0/768	0.77	0/1037
2	B	0.73	3/3687 (0.1%)	0.75	1/5003 (0.0%)
3	C	0.65	3/3405 (0.1%)	1.09	21/4628 (0.5%)
All	All	0.70	6/7860 (0.1%)	0.91	22/10668 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
3	C	0	2
All	All	0	4

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	487	ARG	CD-NE	-17.20	1.17	1.46
3	C	444	TYR	N-CA	-17.05	1.12	1.46
3	C	343	CYS	CB-SG	-8.72	1.67	1.82
2	B	654	CYS	CB-SG	-6.39	1.71	1.82
2	B	255	CYS	C-N	-5.59	1.21	1.34

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	428	ARG	NE-CZ-NH2	-9.01	115.80	120.30
3	C	518	PRO	N-CA-CB	8.64	113.67	103.30
3	C	517	THR	CA-C-O	-8.61	102.01	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	346	LEU	N-CA-C	7.29	130.68	111.00
3	C	444	TYR	N-CA-CB	6.68	122.63	110.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	244	GLY	Peptide
2	B	494	LYS	Peptide
3	C	517	THR	Mainchain,Peptide

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	748	0	763	5	2
2	B	3618	0	3529	93	6
3	C	3336	0	3186	326	8
4	C	3	0	0	0	0
All	All	7705	0	7478	399	8

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 26.

The worst 5 of 399 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)
3:C:527:ASN:HA	3:C:661:LEU:CD1	1.32	1.52
3:C:340:PRO:O	3:C:342:THR:N	1.58	1.35
3:C:339:ASP:HA	3:C:340:PRO:O	1.35	1.25
3:C:323:PHE:CZ	3:C:351:GLU:OE2	1.94	1.21
3:C:339:ASP:OD1	3:C:342:THR:HG21	1.41	1.20

The worst 5 of 8 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:PRO:CA	3:C:284:TRP:CA[3_655]	1.95	0.25
2:B:164:PRO:CA	3:C:284:TRP:CB[3_655]	1.98	0.22
2:B:164:PRO:CB	3:C:286:ASP:O[3_655]	2.01	0.19
1:A:105[A]:ARG:CZ	3:C:530:ASP:OD1[4_545]	2.07	0.13
2:B:164:PRO:C	3:C:284:TRP:CB[3_655]	2.08	0.12

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	91/124 (73%)	90 (99%)	1 (1%)	0	100	100
2	B	471/546 (86%)	459 (98%)	9 (2%)	3 (1%)	30	74
3	C	426/791 (54%)	362 (85%)	43 (10%)	21 (5%)	3	31
All	All	988/1461 (68%)	911 (92%)	53 (5%)	24 (2%)	7	47

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	257	GLY
3	C	271	LEU
3	C	287	GLU
3	C	291	GLU
3	C	340	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	A	80/104 (77%)	79 (99%)	1 (1%)	76	89
2	B	389/437 (89%)	378 (97%)	11 (3%)	51	78
3	C	374/691 (54%)	342 (91%)	32 (9%)	13	47
All	All	843/1232 (68%)	799 (95%)	44 (5%)	29	65

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	317	CYS
3	C	339	ASP
3	C	612	ARG
3	C	318	LEU
3	C	336	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	264	HIS
3	C	309	ASN
3	C	543	ASN
2	B	619	GLN
3	C	453	GLN

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 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.

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, 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	92/124 (74%)	0.93	17 (18%)	2	7	106, 181, 209, 231	0
2	B	486/546 (89%)	0.87	105 (21%)	1	6	81, 178, 253, 349	0
3	C	430/791 (54%)	1.17	99 (23%)	1	6	79, 170, 278, 322	1 (0%)
All	All	1008/1461 (68%)	1.00	221 (21%)	1	6	79, 176, 268, 349	1 (0%)

The worst 5 of 221 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	642	GLY	10.8
3	C	649	THR	9.8
3	C	648	ARG	8.3
3	C	412	ASP	8.2
3	C	641	ARG	7.8

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. 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, 95th percentile and maximum values of B factors

wwPDB X-ray Structure Validation Summary Report

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	LLDF	B-factors($Å^2$)	Q<0.9
4	CA	C	1002	1/1	0.73	0.35	-0.32	153,153,153,153	0
4	CA	C	1003	1/1	0.94	0.25	-0.89	170,170,170,170	0
4	CA	C	1001	1/1	0.87	0.32	-1.14	136,136,136,136	0

6.5 Other polymers (i)

There are no such residues in this entry.