



wwPDB X-ray Structure Validation Summary Report

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PDB ID : 3P5C
Title : The structure of the LDLR/PCSK9 complex reveals the receptor in an extended conformation
Authors : Lo Surdo, P.; Bottomley, M.J.; Calzetta, A.; Settembre, E.C.; Cirillo, A.; Pandit, S.; Ni, Y.; Hubbard, B.; Sitlani, A.; Carfi, A.
Deposited on : 2010-10-08
Resolution : 4.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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 : 2.36
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) : 2.36

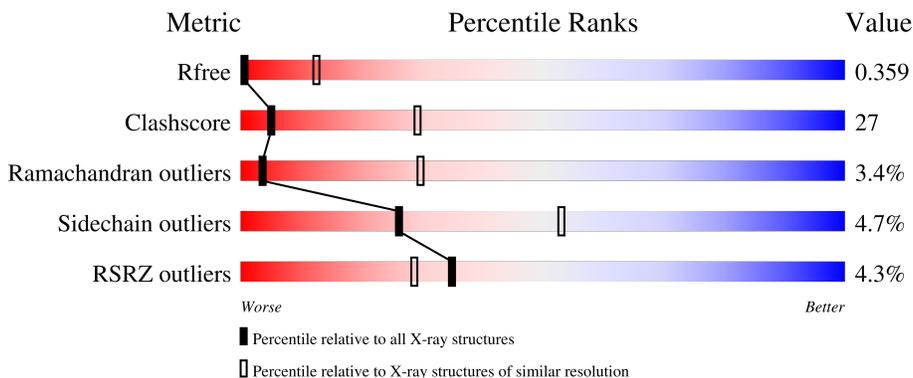
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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}	130704	1005 (4.62-3.78)
Clashscore	141614	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)
Sidechain outliers	138945	1007 (4.62-3.78)
RSRZ outliers	127900	1063 (4.70-3.70)

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 of 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	P	92	 % 88% 11% .
2	A	540	 5% 73% 16% 8% .
3	L	440	 4% 64% 27% 8% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7844 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
			Total	C	N	O	S			
1	P	92	740	474	133	131	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	496	3659	2255	674	698	32	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	440	3441	2143	601	665	32	0	0	0

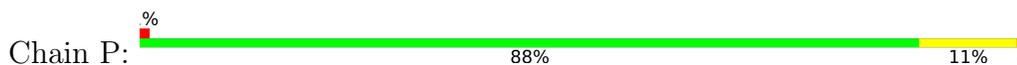
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	L	3	Total	Ca	0	0
			3	3		

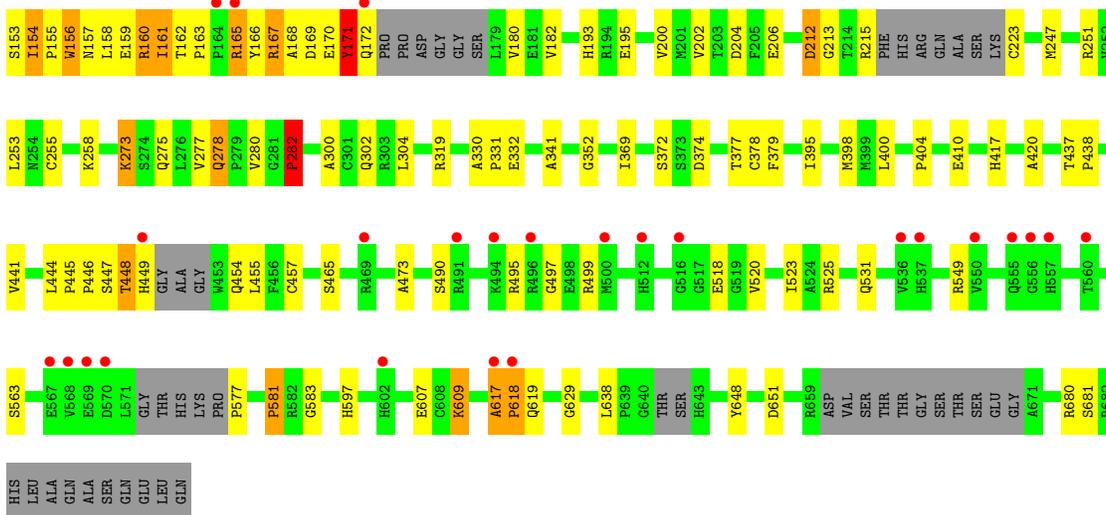
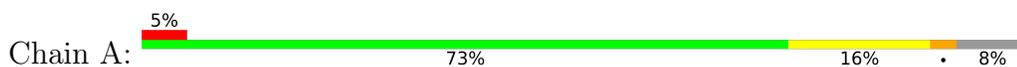
3 Residue-property plots

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

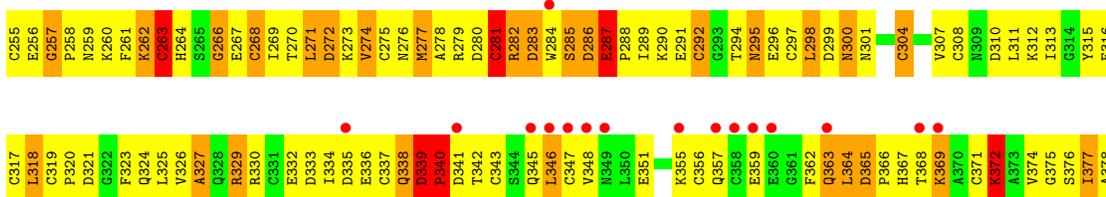
- Molecule 1: Proprotein convertase subtilisin/kexin type 9

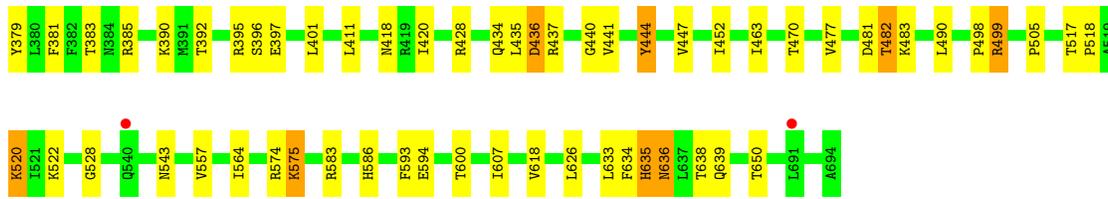


- Molecule 2: Proprotein convertase subtilisin/kexin type 9



- Molecule 3: Low density lipoprotein receptor variant





4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	320.89Å 320.89Å 77.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 4.20 39.71 – 4.20	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.00-4.20) 98.5 (39.71-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 4.13Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.325 , 0.348 0.331 , 0.359	Depositor DCC
R_{free} test set	1660 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	144.4	Xtrriage
Anisotropy	0.227	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 113.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	0.116 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	7844	wwPDB-VP
Average B, all atoms (Å ²)	161.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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 [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	P	0.35	0/757	0.48	0/1023
2	A	0.38	1/3724 (0.0%)	0.54	3/5059 (0.1%)
3	L	0.55	3/3514 (0.1%)	0.77	12/4771 (0.3%)
All	All	0.46	4/7995 (0.1%)	0.65	15/10853 (0.1%)

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
3	L	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	257	GLY	C-O	9.40	1.38	1.23
2	A	171	TYR	N-CA	5.50	1.57	1.46
3	L	440	GLY	C-O	5.08	1.31	1.23
3	L	258	PRO	N-CD	5.02	1.54	1.47

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	282	PRO	CA-N-CD	-10.82	96.34	111.50
3	L	436	ASP	C-N-CA	8.77	143.62	121.70
3	L	281	CYS	N-CA-C	-6.19	94.28	111.00
3	L	444	TYR	CB-CG-CD1	-6.11	117.33	121.00
3	L	272	ASP	N-CA-C	-6.00	94.79	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	L	257	GLY	Mainchain
3	L	375	GLY	Mainchain

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	P	740	0	750	11	0
2	A	3659	0	3537	113	19
3	L	3441	0	3321	303	20
4	A	1	0	0	0	0
4	L	3	0	0	0	0
All	All	7844	0	7608	417	20

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 27.

The worst 5 of 417 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:L:274:VAL:CG2	3:L:312:LYS:HD3	1.25	1.67
2:A:166:TYR:CE2	2:A:168:ALA:HB2	1.27	1.62
2:A:166:TYR:HE2	2:A:168:ALA:CB	1.17	1.54
3:L:274:VAL:HG11	3:L:312:LYS:CG	1.32	1.50
3:L:374:VAL:HG11	3:L:418:ASN:CB	1.43	1.48

The worst 5 of 20 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:A:160:ARG:NE	3:L:279:ARG:CZ[2_564]	1.19	1.01
2:A:159:GLU:OE2	3:L:284:TRP:CZ3[2_564]	1.27	0.93
2:A:160:ARG:CD	3:L:279:ARG:NH2[2_564]	1.50	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:160:ARG:NE	3:L:279:ARG:NE[2_564]	1.58	0.62
2:A:417:HIS:NE2	3:L:277:MET:CE[2_564]	1.58	0.62

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	P	90/92 (98%)	86 (96%)	4 (4%)	0	100	100
2	A	482/540 (89%)	435 (90%)	35 (7%)	12 (2%)	5	35
3	L	438/440 (100%)	351 (80%)	65 (15%)	22 (5%)	2	23
All	All	1010/1072 (94%)	872 (86%)	104 (10%)	34 (3%)	3	30

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	282	PRO
2	A	448	THR
2	A	581	PRO
2	A	618	PRO
3	L	271	LEU

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	P	79/79 (100%)	78 (99%)	1 (1%)	69	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	388/430 (90%)	375 (97%)	13 (3%)	37	61
3	L	388/388 (100%)	362 (93%)	26 (7%)	16	43
All	All	855/897 (95%)	815 (95%)	40 (5%)	26	53

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	363	GLN
3	L	499	ARG
3	L	364	LEU
3	L	372	LYS
3	L	575	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
3	L	439	HIS
3	L	586	HIS
3	L	636	ASN
3	L	635	HIS
3	L	264	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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	P	92/92 (100%)	0.02	1 (1%) 80 72	80, 150, 197, 200	0
2	A	496/540 (91%)	0.27	25 (5%) 28 24	77, 171, 200, 200	0
3	L	440/440 (100%)	0.22	18 (4%) 37 30	67, 164, 200, 200	0
All	All	1028/1072 (95%)	0.22	44 (4%) 35 29	67, 166, 200, 200	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	164	PRO	4.9
3	L	359	GLU	4.6
3	L	346	LEU	4.4
3	L	357	GLN	4.3
3	L	349	ASN	3.8

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 monosaccharides 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
4	CA	L	3	1/1	0.30	0.12	155,155,155,155	0
4	CA	L	1	1/1	0.74	0.19	155,155,155,155	0
4	CA	A	4	1/1	0.85	0.43	155,155,155,155	0
4	CA	L	2	1/1	0.88	0.15	155,155,155,155	0

6.5 Other polymers [i](#)

There are no such residues in this entry.