



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 3GCX / pdb_00003gcx
Title : PCSK9:EGFA (pH 7.4)
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Deposited on : 2009-02-22
Resolution : 2.70 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 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

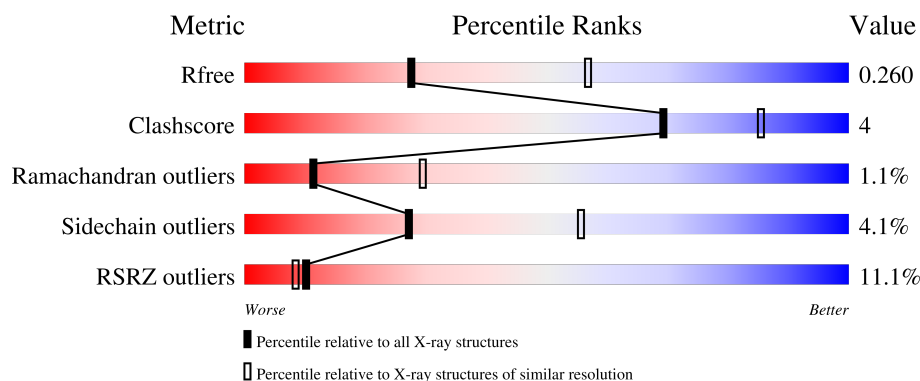
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	100	
2	A	540	
3	E	83	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4277 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	0	0
			740	474	133	131	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	434	Total	C	N	O	S	0	0	0
			3228	2002	588	613	25			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	41	Total	C	N	O	S	0	0	0
			308	183	56	62	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	290	GLY	-	expression tag	UNP P01130
E	291	ALA	-	expression tag	UNP P01130
E	292	MET	-	expression tag	UNP P01130

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	116.05Å 116.05Å 133.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.70 40.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.6 (40.00-2.70) 96.6 (40.00-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.226 , 0.261 0.225 , 0.260	Depositor DCC
R_{free} test set	1270 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	64.0	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4277	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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	0.39	0/757	0.73	0/1023
2	A	0.45	0/3284	0.78	5/4458 (0.1%)
3	E	0.43	0/311	0.66	0/417
All	All	0.43	0/4352	0.76	5/5898 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	529	LEU	CA-C-N	6.36	127.80	119.84
2	A	529	LEU	C-N-CA	6.36	127.80	119.84
2	A	207	ASN	N-CA-C	5.79	117.87	108.26
2	A	208	VAL	CA-C-N	5.42	126.61	119.84
2	A	208	VAL	C-N-CA	5.42	126.61	119.84

There are no chirality outliers.

There are no planarity outliers.

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	3	0
2	A	3228	0	3181	27	0
3	E	308	0	278	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	1	0	0	0	0
All	All	4277	0	4209	30	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 4.

All (30) 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)
2:A:472:THR:HG21	2:A:510:ARG:HH21	1.41	0.83
2:A:449:HIS:HA	2:A:453:TRP:HH2	1.59	0.68
2:A:449:HIS:HA	2:A:453:TRP:CH2	2.30	0.65
2:A:469:ARG:HD2	2:A:515:PHE:HA	1.85	0.58
2:A:426:GLU:HB3	2:A:434:ARG:HG2	1.89	0.54
2:A:395:ILE:HG22	2:A:399:MET:HE2	1.90	0.54
2:A:211:GLU:HB3	2:A:254:ASN:HB2	1.90	0.53
2:A:490:SER:HB2	2:A:520:VAL:HG12	1.90	0.53
2:A:496:ARG:HE	2:A:497:GLY:H	1.55	0.53
1:P:66:ARG:NH1	1:P:67:CYS:O	2.42	0.52
2:A:453:TRP:CD1	2:A:454:GLN:H	2.28	0.52
2:A:185:LEU:HD11	2:A:271:ILE:HD11	1.93	0.51
2:A:330:ALA:O	2:A:333:VAL:HG22	2.11	0.50
2:A:229:HIS:O	2:A:233:VAL:HG23	2.12	0.49
2:A:209:PRO:HG3	2:A:260:THR:HG23	1.94	0.49
2:A:182:VAL:HB	2:A:247:MET:HG2	1.98	0.45
2:A:186:ASP:CG	2:A:187:THR:H	2.26	0.44
2:A:487:SER:HA	2:A:498:GLU:CD	2.43	0.43
2:A:207:ASN:HD22	2:A:207:ASN:HA	1.66	0.43
2:A:403:GLU:HB2	2:A:406:LEU:HG	2.01	0.43
2:A:437:THR:HA	2:A:438:PRO:HD3	1.93	0.42
2:A:472:THR:HG21	2:A:510:ARG:NH2	2.21	0.42
1:P:82:LEU:HD13	1:P:86:THR:HG21	2.02	0.42
1:P:70:ASP:N	1:P:71:PRO:HD2	2.34	0.42
2:A:345:PRO:HD3	2:A:424:ILE:HG23	2.02	0.42
2:A:615:ILE:HD12	2:A:622:VAL:HG22	2.02	0.42
2:A:422:ASP:HA	2:A:439:ASN:CG	2.45	0.41
2:A:530:PRO:HB2	2:A:604:PRO:HG2	2.02	0.41
2:A:455:LEU:HD23	2:A:631:THR:HB	2.03	0.40
2:A:189:ILE:HD13	2:A:200:VAL:HG11	2.03	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	P	90/100 (90%)	88 (98%)	1 (1%)	1 (1%)	11	29
2	A	422/540 (78%)	401 (95%)	16 (4%)	5 (1%)	10	27
3	E	39/83 (47%)	37 (95%)	2 (5%)	0	100	100
All	All	551/723 (76%)	526 (96%)	19 (3%)	6 (1%)	11	29

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	616	PRO
2	A	209	PRO
1	P	117	GLY
2	A	164	PRO
2	A	530	PRO
2	A	639	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	P	79/84 (94%)	76 (96%)	3 (4%)	29	58
2	A	345/431 (80%)	329 (95%)	16 (5%)	24	51
3	E	35/71 (49%)	35 (100%)	0	100	100
All	All	459/586 (78%)	440 (96%)	19 (4%)	27	56

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	85	GLU
1	P	105	ARG
1	P	108	LEU
2	A	159	GLU
2	A	165	ARG
2	A	179	LEU
2	A	181	GLU
2	A	207	ASN
2	A	211	GLU
2	A	222	LYS
2	A	256	GLN
2	A	283	LEU
2	A	339	THR
2	A	387	GLN
2	A	432	ASP
2	A	472	THR
2	A	496	ARG
2	A	507	LEU
2	A	619	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	190	GLN
2	A	207	ASN
2	A	229	HIS
2	A	298	ASN
3	E	300	ASN
3	E	306	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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	P	92/100 (92%)	0.62	4 (4%) 40 36	47, 58, 67, 69	0
2	A	434/540 (80%)	0.84	57 (13%) 7 6	51, 58, 71, 93	0
3	E	41/83 (49%)	1.10	2 (4%) 35 31	56, 59, 62, 64	0
All	All	567/723 (78%)	0.82	63 (11%) 10 8	47, 58, 68, 93	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	220	ALA	4.8
2	A	171	TYR	4.3
2	A	221	SER	4.2
2	A	671	ALA	4.1
2	A	641	THR	4.0
2	A	211	GLU	3.8
2	A	192	ASP	3.7
2	A	618	PRO	3.7
2	A	449	HIS	3.5
2	A	617	ALA	3.5
1	P	85	GLU	3.5
2	A	172	GLN	3.4
2	A	642	SER	3.3
3	E	292	MET	3.3
2	A	509	CYS	3.2
2	A	177	GLY	3.1
2	A	223	CYS	3.1
2	A	208	VAL	3.1
2	A	209	PRO	3.1
2	A	504	GLY	3.0
2	A	168	ALA	3.0
2	A	165	ARG	3.0
2	A	496	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
2	A	619	GLN	2.9
2	A	639	PRO	2.9
2	A	166	TYR	2.8
2	A	186	ASP	2.8
2	A	323	CYS	2.7
2	A	506	LYS	2.7
2	A	207	ASN	2.7
2	A	505	GLY	2.7
2	A	511	ALA	2.6
2	A	445	PRO	2.6
2	A	651	ASP	2.6
1	P	116	HIS	2.6
2	A	453	TRP	2.5
1	P	84	GLU	2.5
2	A	430	PRO	2.5
2	A	468	THR	2.4
2	A	153	SER	2.4
2	A	508	VAL	2.4
2	A	659	ARG	2.4
2	A	512	HIS	2.4
2	A	531	GLN	2.4
2	A	643	HIS	2.4
2	A	474	ILE	2.3
2	A	159	GLU	2.3
2	A	205	PHE	2.3
2	A	163	PRO	2.3
1	P	117	GLY	2.3
2	A	471	ALA	2.3
2	A	627	GLU	2.2
3	E	328	GLN	2.2
2	A	473	ALA	2.1
2	A	306	ARG	2.1
2	A	206	GLU	2.0
2	A	332	GLU	2.0
2	A	178	SER	2.0
2	A	602	HIS	2.0
2	A	520	VAL	2.0
2	A	626	CYS	2.0
2	A	494	LYS	2.0
2	A	277	VAL	2.0

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	CA	E	1	1/1	0.89	0.09	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.