



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2018 – 01:42 pm GMT

PDB ID : 2XTJ
Title : The crystal structure of PCSK9 in complex with 1D05 Fab
Authors : Di Marco, S.; Volpari, C.; Carfi, A.
Deposited on : 2010-10-10
Resolution : 2.70 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 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 : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

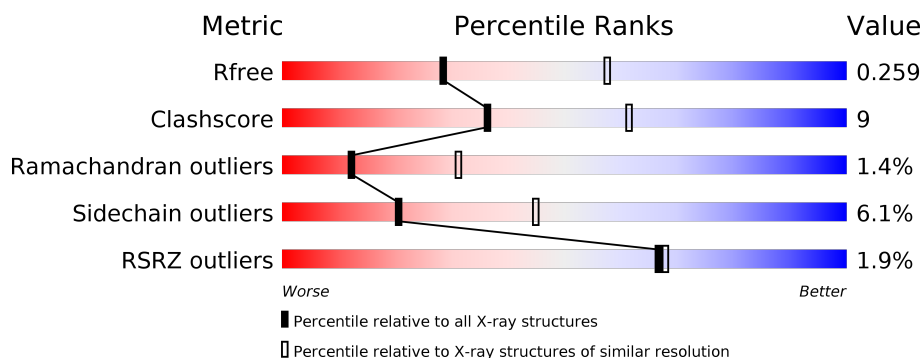
1 Overall quality at a glance

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}	111664	2449 (2.70-2.70)
Clashscore	122126	2756 (2.70-2.70)
Ramachandran outliers	120053	2716 (2.70-2.70)
Sidechain outliers	120020	2716 (2.70-2.70)
RSRZ outliers	108989	2376 (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 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 $\leq 5\%$. 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	312	<div> <div>61%</div> <div>14%</div> <div>22%</div> </div>
2	B	107	<div> <div>76%</div> <div>21%</div> </div>
3	C	106	<div> <div>2%</div> <div>87%</div> <div>8%</div> </div>
4	D	131	<div> <div>79%</div> <div>19%</div> </div>
5	E	124	<div> <div>8%</div> <div>71%</div> <div>10%</div> <div>15%</div> </div>
6	P	114	<div> <div>72%</div> <div>9%</div> <div>19%</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6096 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	242	Total	C	N	O	S	0	1	0
			1772	1100	314	347	11			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	417	LEU	HIS	SEE REMARK 999	UNP Q8NBP7
A	452	ALA	-	expression tag	UNP Q8NBP7
A	453	GLY	-	expression tag	UNP Q8NBP7
A	454	THR	-	expression tag	UNP Q8NBP7
A	455	ALA	-	expression tag	UNP Q8NBP7
A	456	ALA	-	expression tag	UNP Q8NBP7
A	457	ALA	-	expression tag	UNP Q8NBP7
A	458	SER	-	expression tag	UNP Q8NBP7
A	459	HIS	-	expression tag	UNP Q8NBP7
A	460	HIS	-	expression tag	UNP Q8NBP7
A	461	HIS	-	expression tag	UNP Q8NBP7
A	462	HIS	-	expression tag	UNP Q8NBP7
A	463	HIS	-	expression tag	UNP Q8NBP7
A	464	HIS	-	expression tag	UNP Q8NBP7

- Molecule 2 is a protein called FAB FROM A HUMAN MONOCLONAL ANTIBODY, 1D05.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	107	Total	C	N	O	S	0	1	0
			821	511	142	165	3			

- Molecule 3 is a protein called FAB FROM A HUMAN MONOCLONAL ANTIBODY, 1D05.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	105	Total	C	N	O	S	0	0	0
			801	499	134	166	2			

- Molecule 4 is a protein called FAB FROM A HUMAN MONOCLONAL ANTIBODY, 1D05.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	131	Total	C	N	O	S	0	0	0
			1008	636	174	192	6			

- Molecule 5 is a protein called FAB FROM A HUMAN MONOCLONAL ANTIBODY, 1D05.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	0	0
			753	477	123	151	2			

- Molecule 6 is a protein called PROPROTEIN CONVERTASE SUBTILISIN-KEXIN TYPE 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	P	92	Total	C	N	O	S	0	1	0
			741	475	133	131	2			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	39	MET	-	expression tag	UNP Q8NBP7
P	40	LYS	-	expression tag	UNP Q8NBP7
P	41	GLY	-	expression tag	UNP Q8NBP7
P	42	SER	-	expression tag	UNP Q8NBP7
P	43	LYS	-	expression tag	UNP Q8NBP7
P	44	GLY	-	expression tag	UNP Q8NBP7
P	45	SER	-	expression tag	UNP Q8NBP7
P	46	LYS	-	expression tag	UNP Q8NBP7
P	47	GLY	-	expression tag	UNP Q8NBP7
P	48	SER	-	expression tag	UNP Q8NBP7
P	49	LYS	-	expression tag	UNP Q8NBP7
P	50	PRO	-	expression tag	UNP Q8NBP7
P	51	MET	-	expression tag	UNP Q8NBP7
P	52	SER	-	expression tag	UNP Q8NBP7

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0

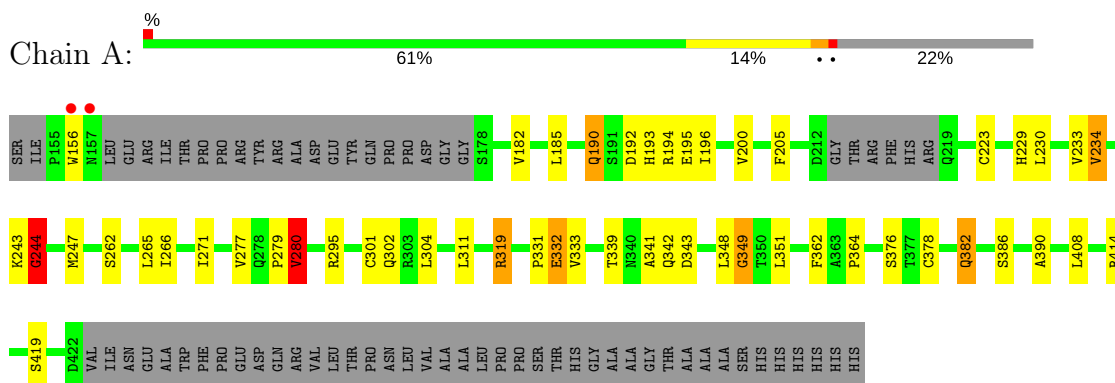
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	61	Total O 61 61	0	0
8	B	30	Total O 30 30	0	0
8	C	12	Total O 12 12	0	0
8	D	48	Total O 48 48	0	0
8	E	11	Total O 11 11	0	0
8	P	37	Total O 37 37	0	0

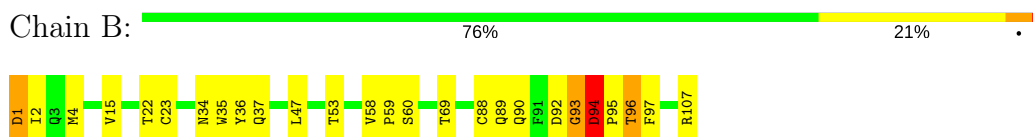
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

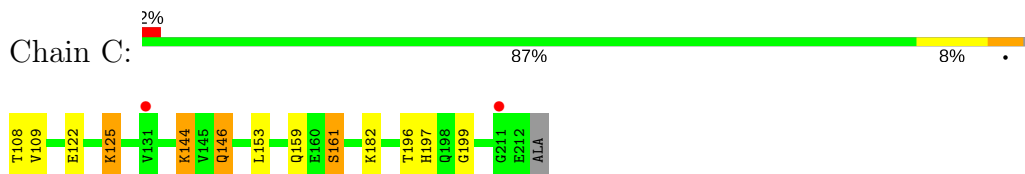
- Molecule 1: PROPROTEIN CONVERTASE SUBTILISIN/KEXIN TYPE 9



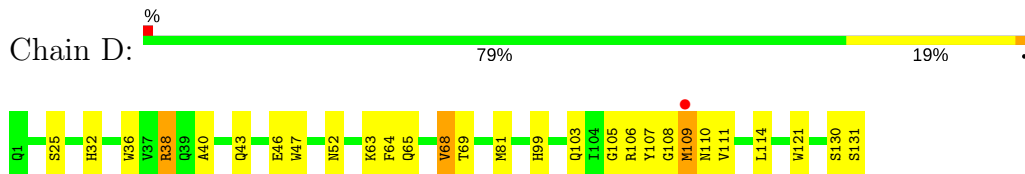
- Molecule 2: FAB FROM A HUMAN MONOCLONAL ANTIBODY, 1D05



- Molecule 3: FAB FROM A HUMAN MONOCLONAL ANTIBODY, 1D05

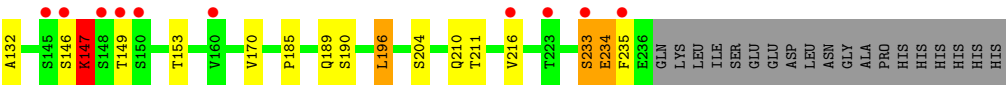


- Molecule 4: FAB FROM A HUMAN MONOCLONAL ANTIBODY, 1D05

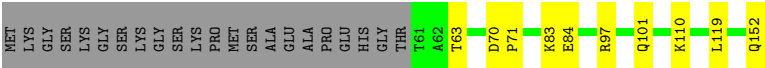


- Molecule 5: FAB FROM A HUMAN MONOCLONAL ANTIBODY, 1D05





● Molecule 6: 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	66.59Å 67.83Å 250.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.70 65.48 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.00-2.70) 100.0 (65.48-2.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.259 0.199 , 0.259	Depositor DCC
R_{free} test set	1630 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.039 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6096	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: 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	0.54	0/1795	0.70	0/2435
2	B	0.53	0/837	0.67	0/1132
3	C	0.43	0/817	0.57	0/1111
4	D	0.55	0/1030	0.71	0/1394
5	E	0.46	0/772	0.65	1/1057 (0.1%)
6	P	0.52	0/761	0.63	0/1028
All	All	0.52	0/6012	0.67	1/8157 (0.0%)

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
1	A	0	1
2	B	0	1
4	D	0	2
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	196	LEU	CA-CB-CG	5.71	128.44	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	244	GLY	Peptide
2	B	93	GLY	Peptide
4	D	107	TYR	Peptide
4	D	121	TRP	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	1772	0	1761	33	0
2	B	821	0	801	25	0
3	C	801	0	765	12	0
4	D	1008	0	983	23	0
5	E	753	0	740	15	0
6	P	741	0	750	3	0
7	A	1	0	0	0	0
8	A	61	0	0	1	0
8	B	30	0	0	0	0
8	C	12	0	0	1	0
8	D	48	0	0	4	0
8	E	11	0	0	0	0
8	P	37	0	0	0	0
All	All	6096	0	5800	101	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 9.

The worst 5 of 101 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)
5:E:146:SER:HB2	5:E:147:LYS:HB2	1.36	1.07
2:B:34:ASN:HD22	2:B:89:GLN:NE2	1.67	0.92
4:D:103:GLN:HE21	4:D:105:GLY:H	1.19	0.87
2:B:4:MET:HE1	2:B:90:GLN:HG2	1.60	0.83
2:B:36:TYR:HE2	2:B:89:GLN:HG2	1.47	0.79

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	237/312 (76%)	221 (93%)	11 (5%)	5 (2%)	8	20
2	B	106/107 (99%)	97 (92%)	8 (8%)	1 (1%)	19	44
3	C	103/106 (97%)	101 (98%)	2 (2%)	0	100	100
4	D	129/131 (98%)	124 (96%)	3 (2%)	2 (2%)	11	27
5	E	103/124 (83%)	94 (91%)	6 (6%)	3 (3%)	5	12
6	P	91/114 (80%)	89 (98%)	2 (2%)	0	100	100
All	All	769/894 (86%)	726 (94%)	32 (4%)	11 (1%)	12	31

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	280	VAL
5	E	147	LYS
5	E	235	PHE
1	A	244	GLY
1	A	349	GLY

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	190/247 (77%)	178 (94%)	12 (6%)	20	44
2	B	92/91 (101%)	84 (91%)	8 (9%)	11	26
3	C	92/94 (98%)	86 (94%)	6 (6%)	19	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	106/106 (100%)	103 (97%)	3 (3%)	47	77
5	E	88/108 (82%)	82 (93%)	6 (7%)	17	40
6	P	79/95 (83%)	74 (94%)	5 (6%)	20	44
All	All	647/741 (87%)	607 (94%)	40 (6%)	20	44

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

Mol	Chain	Res	Type
2	B	94	ASP
3	C	144	LYS
6	P	83	LYS
3	C	109	VAL
3	C	146	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	123	GLN
3	C	159	GLN
4	D	103	GLN
2	B	89	GLN
5	E	210	GLN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

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 [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	242/312 (77%)	0.14	2 (0%) 86 87	11, 24, 52, 80	0
2	B	107/107 (100%)	0.09	0 100 100	17, 31, 42, 47	0
3	C	105/106 (99%)	0.57	2 (1%) 66 68	40, 49, 57, 62	0
4	D	131/131 (100%)	0.17	1 (0%) 86 87	16, 27, 38, 44	0
5	E	105/124 (84%)	0.79	10 (9%) 8 6	37, 49, 69, 82	0
6	P	92/114 (80%)	0.01	0 100 100	18, 26, 37, 43	0
All	All	782/894 (87%)	0.27	15 (1%) 66 68	11, 31, 56, 82	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	235	PHE	4.4
5	E	146	SER	4.3
5	E	148	SER	3.9
5	E	149	THR	3.8
3	C	211	GLY	2.7

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

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
7	CA	A	1423	1/1	0.88	0.12	62,62,62,62	0

6.5 Other polymers

There are no such residues in this entry.