



## wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Feb 19, 2018 – 12:33 AM EST

PDB ID : 6FCZ  
EMDB ID: : EMD-4232  
Title : Model of gC1q-Fc complex based on 7A EM map  
Authors : Ugurlar, D.; Howes, S.C.; de Kreuk, B.J.K.; de Jong, R.N.; Beurskens, F.J.;  
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Deposited on : 2017-12-21  
Resolution : 10.00 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

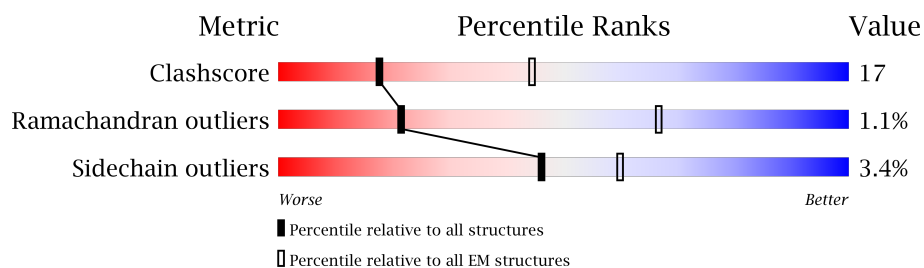
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 10.00 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	133	
2	B	132	
3	C	129	
4	H	216	
4	K	216	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6710 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Complement C1q subcomponent subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	133	Total	C	N	O	S	0	0
			1052	671	181	195	5		

- Molecule 2 is a protein called Complement C1q subcomponent subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	132	Total	C	N	O	S	0	0
			1053	665	186	195	7		

- Molecule 3 is a protein called Complement C1q subcomponent subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	129	Total	C	N	O	S	0	0
			1010	649	169	188	4		

- Molecule 4 is a protein called Immunoglobulin gamma-1 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	216	Total	C	N	O	S	0	0
			1721	1096	289	330	6		
4	K	210	Total	C	N	O	S	0	0
			1676	1067	282	321	6		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	A	75	Total	O	0
			75	75	
5	B	43	Total	O	0
			43	43	
5	C	76	Total	O	0
			76	76	

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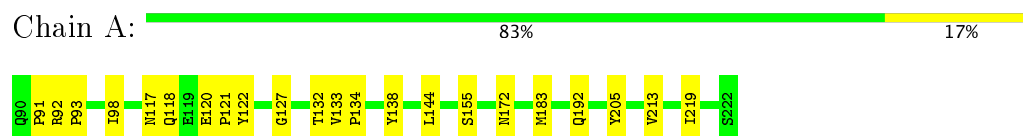
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Mol	Chain	Residues	Atoms		AltConf
5	H	2	Total	O	0
			2	2	
5	K	2	Total	O	0
			2	2	

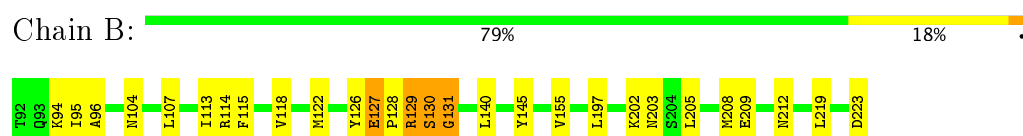
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

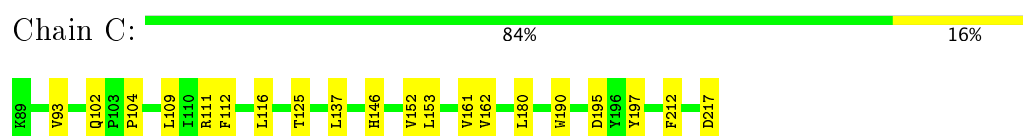
- Molecule 1: Complement C1q subcomponent subunit A



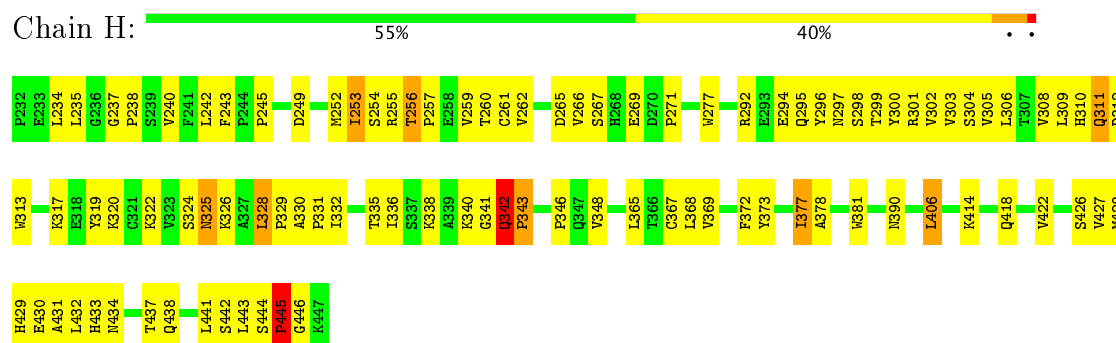
- Molecule 2: Complement C1q subcomponent subunit B



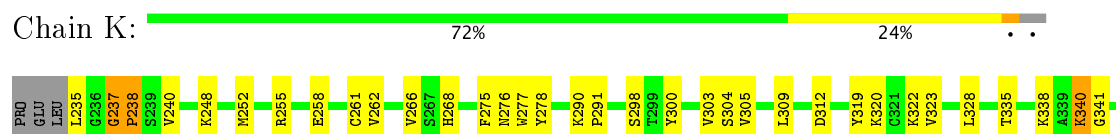
- Molecule 3: Complement C1q subcomponent subunit C



- Molecule 4: Immunoglobulin gamma-1 heavy chain



- Molecule 4: Immunoglobulin gamma-1 heavy chain



R344	E345	P346	C367	F372	T373	P374	I377	H381	N390	T393	L406	Y407	S408	K414	Q418	H429	E430	A431	L432	H433	I434	L443	S444	PRO	GLY	LYS
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## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	79120	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.49	0/1080	0.76	0/1463
2	B	0.44	0/1074	0.71	0/1448
3	C	0.51	0/1037	0.77	0/1412
4	H	0.49	1/1769 (0.1%)	0.91	4/2408 (0.2%)
4	K	0.64	2/1722 (0.1%)	1.31	7/2346 (0.3%)
All	All	0.53	3/6682 (0.0%)	0.97	11/9077 (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
4	H	0	1
4	K	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	237	GLY	C-N	17.76	1.68	1.34
4	H	342	GLN	C-N	13.03	1.59	1.34
4	K	340	LYS	C-N	7.13	1.45	1.33

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	340	LYS	O-C-N	-39.97	55.25	123.20
4	K	237	GLY	C-N-CD	-23.35	69.22	120.60
4	H	342	GLN	CA-C-N	-20.25	60.41	117.10
4	K	237	GLY	O-C-N	-18.03	86.83	121.10
4	H	342	GLN	O-C-N	17.93	155.18	121.10



There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	H	342	GLN	Mainchain
4	K	340	LYS	Mainchain

## 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	1052	0	1015	17	0
2	B	1053	0	1033	41	0
3	C	1010	0	979	30	0
4	H	1721	0	1693	105	0
4	K	1676	0	1645	52	0
5	A	75	0	0	0	0
5	B	43	0	0	3	0
5	C	76	0	0	4	0
5	H	2	0	0	5	0
5	K	2	0	0	0	0
All	All	6710	0	6365	215	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 17.

The worst 5 of 215 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)
4:K:237:GLY:C	4:K:238:PRO:CD	1.80	1.50
4:K:237:GLY:C	4:K:238:PRO:N	1.68	1.47
3:C:195:ASP:OD2	4:H:331:PRO:CB	1.81	1.28
4:H:234:LEU:HA	5:H:502:HOH:O	1.11	1.25
3:C:195:ASP:OD1	4:H:322:LYS:NZ	1.74	1.18

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 PDB entries followed by that with respect to all EM entries.

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	131/133 (98%)	124 (95%)	7 (5%)	0	100	100
2	B	130/132 (98%)	121 (93%)	7 (5%)	2 (2%)	12	53
3	C	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
4	H	214/216 (99%)	193 (90%)	16 (8%)	5 (2%)	7	43
4	K	208/216 (96%)	198 (95%)	8 (4%)	2 (1%)	18	61
All	All	810/826 (98%)	760 (94%)	41 (5%)	9 (1%)	21	60

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	342	GLN
4	H	445	PRO
4	K	238	PRO
4	K	341	GLY
4	H	446	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 PDB entries followed by that with respect to all EM entries.

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	117/117 (100%)	116 (99%)	1 (1%)	82	91
2	B	115/115 (100%)	110 (96%)	5 (4%)	33	64
3	C	113/113 (100%)	112 (99%)	1 (1%)	82	91
4	H	200/200 (100%)	186 (93%)	14 (7%)	18	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	K	195/200 (98%)	191 (98%)	4 (2%)	59	80
All	All	740/745 (99%)	715 (97%)	25 (3%)	46	69

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	H	296	TYR
4	H	325	ASN
4	K	377	ILE
4	H	311	GLN
4	H	328	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
4	H	390	ASN
4	H	421	ASN
4	K	421	ASN
4	H	347	GLN
4	H	361	ASN

### 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 ⓘ

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	237:GLY	C	238:PRO	N	1.68