



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 17, 2014 – 01:41 AM EDT

PDB ID : 4NQS  
Title : Knob-into-hole IgG Fc  
Authors : Eigenbrot, C.; Ultsch, M.  
Deposited on : 2013-11-25  
Resolution : 2.64 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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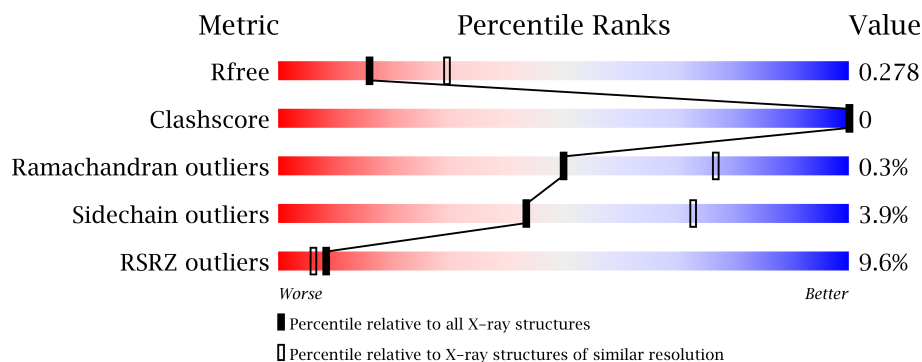
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable22978  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22978

# 1 Overall quality at a glance









The reported resolution of this entry is 2.64 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))
$R_{free}$	66092	2393 (2.68-2.60)
Clashscore	79885	2915 (2.68-2.60)
Ramachandran outliers	78287	2865 (2.68-2.60)
Sidechain outliers	78261	2865 (2.68-2.60)
RSRZ outliers	66119	2393 (2.68-2.60)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	213	
1	G	213	
2	B	213	
2	H	213	
3	D	34	
3	E	34	
3	I	34	
3	J	34	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7832 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	0
			1668	1059	282	320	7			
1	G	208	Total	C	N	O	S	0	0	0
			1656	1051	280	318	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	356	GLU	ASP	SEE REMARK 999	UNP P01857
A	358	MET	LEU	SEE REMARK 999	UNP P01857
A	366	SER	THR	ENGINEERED MUTATION	UNP P01857
A	368	ALA	LEU	ENGINEERED MUTATION	UNP P01857
A	407	VAL	TYR	ENGINEERED MUTATION	UNP P01857
G	356	GLU	ASP	SEE REMARK 999	UNP P01857
G	358	MET	LEU	SEE REMARK 999	UNP P01857
G	366	SER	THR	ENGINEERED MUTATION	UNP P01857
G	368	ALA	LEU	ENGINEERED MUTATION	UNP P01857
G	407	VAL	TYR	ENGINEERED MUTATION	UNP P01857

- Molecule 2 is a protein called Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	207	Total	C	N	O	S	0	0	0
			1666	1063	280	316	7			
2	H	207	Total	C	N	O	S	0	0	0
			1666	1063	280	316	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	356	GLU	ASP	SEE REMARK 999	UNP P01857
B	358	MET	LEU	SEE REMARK 999	UNP P01857

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Chain	Residue	Modelled	Actual	Comment	Reference
B	366	TRP	THR	ENGINEERED MUTATION	UNP P01857
H	356	GLU	ASP	SEE REMARK 999	UNP P01857
H	358	MET	LEU	SEE REMARK 999	UNP P01857
H	366	TRP	THR	ENGINEERED MUTATION	UNP P01857

- Molecule 3 is a protein called miniZ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	34	Total 291	C 176	N 57	O 55	S 3	0	0	0
3	E	34	Total 291	C 176	N 57	O 55	S 3	0	0	0
3	I	34	Total 291	C 176	N 57	O 55	S 3	0	0	0
3	J	34	Total 291	C 176	N 57	O 55	S 3	0	0	0

- Molecule 4 is water.

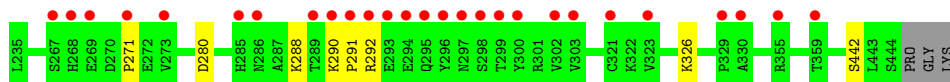
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	O 2	0	0
4	B	3	Total 3	O 3	0	0
4	D	1	Total 1	O 1	0	0
4	G	1	Total 1	O 1	0	0
4	H	4	Total 4	O 4	0	0
4	I	1	Total 1	O 1	0	0

### 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.

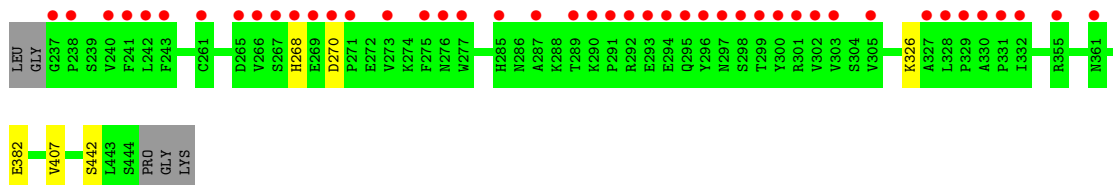
- Molecule 1: Ig gamma-1 chain C region

Chain A: 



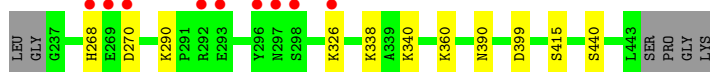
- Molecule 1: Ig gamma-1 chain C region

Chain G: 



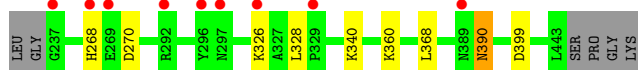
- Molecule 2: Ig gamma-1 chain C region

Chain B: 



- Molecule 2: Ig gamma-1 chain C region

Chain H: 



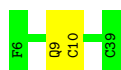
- Molecule 3: miniZ

Chain D: 

There are no outlier residues recorded for this chain.

- Molecule 3: miniZ

Chain E: 



- Molecule 3: miniZ

Chain I: 



- Molecule 3: miniZ

Chain J: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.24Å 66.08Å 102.90Å 90.00° 95.18° 90.00°	Depositor
Resolution (Å)	46.50 – 2.64 44.86 – 2.64	Depositor EDS
% Data completeness (in resolution range)	97.0 (46.50-2.64) 97.1 (44.86-2.64)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, $R_{free}$	0.229 , 0.266 0.239 , 0.278	Depositor DCC
$R_{free}$ test set	961 reflections (3.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.0	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 11.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 30472 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7832	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.19% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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  >5	RMSZ	# Z  >5
1	A	0.40	0/1713	0.62	0/2332
1	G	0.39	0/1701	0.58	0/2316
2	B	0.39	0/1714	0.60	0/2335
2	H	0.37	0/1714	0.62	0/2335
3	D	0.38	0/295	0.59	0/393
3	E	0.38	0/295	0.61	0/393
3	I	0.37	0/295	0.55	0/393
3	J	0.39	0/295	0.58	0/393
All	All	0.39	0/8022	0.60	0/10890

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1668	0	0	0	0
1	G	1656	0	0	0	0
2	B	1666	0	0	0	0
2	H	1666	0	0	0	0
3	D	291	0	0	0	0
3	E	291	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	291	0	0	0	0
3	J	291	0	0	0	0
4	A	2	0	0	0	0
4	B	3	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
4	H	4	0	0	0	0
4	I	1	0	0	0	0
All	All	7832	0	0	0	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 0.

There are no clashes within the asymmetric unit.

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	A	208/213 (98%)	196 (94%)	10 (5%)	2 (1%)	22	43
1	G	206/213 (97%)	199 (97%)	7 (3%)	0	100	100
2	B	205/213 (96%)	198 (97%)	7 (3%)	0	100	100
2	H	205/213 (96%)	198 (97%)	6 (3%)	1 (0%)	38	66
3	D	32/34 (94%)	32 (100%)	0	0	100	100
3	E	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
3	I	32/34 (94%)	32 (100%)	0	0	100	100
3	J	32/34 (94%)	32 (100%)	0	0	100	100
All	All	952/988 (96%)	918 (96%)	31 (3%)	3 (0%)	50	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	PRO
2	H	390	ASN
1	A	271	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	194/196 (99%)	188 (97%)	6 (3%)	52	80
1	G	193/196 (98%)	187 (97%)	6 (3%)	52	80
2	B	193/197 (98%)	182 (94%)	11 (6%)	29	53
2	H	193/197 (98%)	184 (95%)	9 (5%)	36	64
3	D	32/32 (100%)	32 (100%)	0	100	100
3	E	32/32 (100%)	30 (94%)	2 (6%)	25	47
3	I	32/32 (100%)	32 (100%)	0	100	100
3	J	32/32 (100%)	31 (97%)	1 (3%)	52	80
All	All	901/914 (99%)	866 (96%)	35 (4%)	43	73

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	280	ASP
1	A	288	LYS
1	A	290	LYS
1	A	292	ARG
1	A	326	LYS
1	A	442	SER
2	B	268	HIS
2	B	270	ASP
2	B	290	LYS
2	B	326	LYS
2	B	338	LYS
2	B	340	LYS
2	B	360	LYS
2	B	390	ASN
2	B	399	ASP

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Mol	Chain	Res	Type
2	B	415	SER
2	B	440	SER
3	E	9	GLN
3	E	10	CYS
1	G	268	HIS
1	G	270	ASP
1	G	326	LYS
1	G	382	GLU
1	G	407	VAL
1	G	442	SER
2	H	268	HIS
2	H	270	ASP
2	H	326	LYS
2	H	328	LEU
2	H	340	LYS
2	H	360	LYS
2	H	368	LEU
2	H	390	ASN
2	H	399	ASP
3	J	38	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	210/213 (98%)	0.74	27 (12%) 4 3	20, 50, 126, 172	0
1	G	208/213 (97%)	0.94	44 (21%) 1 1	20, 59, 133, 149	0
2	B	207/213 (97%)	-0.02	9 (4%) 34 30	19, 34, 85, 117	0
2	H	207/213 (97%)	-0.01	9 (4%) 34 30	19, 35, 82, 107	0
3	D	34/34 (100%)	-0.04	0 100 100	26, 34, 57, 61	0
3	E	34/34 (100%)	-0.07	0 100 100	19, 41, 58, 64	0
3	I	34/34 (100%)	-0.09	1 (2%) 49 47	25, 35, 60, 69	0
3	J	34/34 (100%)	0.17	3 (8%) 10 7	22, 42, 64, 68	0
All	All	968/988 (97%)	0.35	93 (9%) 8 6	19, 41, 112, 172	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	296	TYR	12.9
1	A	295	GLN	11.8
1	A	291	PRO	11.1
1	A	292	ARG	10.3
1	G	297	ASN	9.0
1	A	290	LYS	8.5
1	A	294	GLU	8.1
1	G	296	TYR	7.9
1	A	297	ASN	7.8
1	A	300	TYR	7.4
1	A	298	SER	7.3
1	A	289	THR	7.1
1	G	269	GLU	7.0
1	G	267	SER	6.3
1	G	292	ARG	6.2
1	G	299	THR	6.1

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Mol	Chain	Res	Type	RSRZ
1	G	275	PHE	5.9
1	G	268	HIS	5.8
1	A	299	THR	5.7
1	G	298	SER	5.3
2	H	297	ASN	5.2
1	G	273	VAL	5.1
1	G	291	PRO	5.1
2	B	298	SER	5.1
1	G	329	PRO	5.0
1	G	300	TYR	4.9
1	A	268	HIS	4.7
1	G	277	TRP	4.3
1	G	294	GLU	4.3
2	B	297	ASN	4.2
1	G	271	PRO	4.1
1	A	330	ALA	4.0
3	J	38	ASP	4.0
1	A	302	VAL	3.9
3	J	39	CYS	3.9
1	G	243	PHE	3.8
2	B	292	ARG	3.7
1	G	285	HIS	3.6
1	G	266	VAL	3.5
1	G	330	ALA	3.5
1	G	241	PHE	3.4
1	G	305	VAL	3.4
1	A	293	GLU	3.4
2	H	296	TYR	3.3
1	A	269	GLU	3.3
1	G	293	GLU	3.3
1	G	261	CYS	3.3
1	G	295	GLN	3.3
1	G	287	ALA	3.2
1	A	267	SER	3.2
1	G	270	ASP	3.1
1	A	303	VAL	3.0
1	G	355	ARG	3.0
1	A	285	HIS	3.0
2	B	269	GLU	2.9
1	A	273	VAL	2.9
1	G	238	PRO	2.9
1	G	276	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	327	ALA	2.8
1	G	242	LEU	2.8
2	H	389	ASN	2.8
1	G	328	LEU	2.7
1	A	359	THR	2.7
1	A	355	ARG	2.7
1	A	321	CYS	2.6
1	G	237	GLY	2.6
1	G	332	ILE	2.6
2	H	237	GLY	2.6
2	H	269	GLU	2.5
1	G	303	VAL	2.5
1	G	240	VAL	2.5
2	H	326	LYS	2.5
1	G	331	PRO	2.4
1	G	302	VAL	2.4
1	G	290	LYS	2.4
2	B	296	TYR	2.4
2	H	329	PRO	2.4
1	G	265	ASP	2.4
1	A	329	PRO	2.3
1	G	289	THR	2.3
2	H	292	ARG	2.3
1	G	361	ASN	2.3
2	B	270	ASP	2.2
2	H	268	HIS	2.2
2	B	293	GLU	2.2
1	A	271	PRO	2.2
1	A	323	VAL	2.2
3	I	39	CYS	2.2
3	J	6	PHE	2.1
1	A	286	ASN	2.1
2	B	326	LYS	2.0
1	G	301	ARG	2.0
2	B	268	HIS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

### 6.5 Other polymers ⓘ

There are no such residues in this entry.