



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 08:05 PM GMT

PDB ID : 4WWI  
Title : Crystal structure of the C domain of staphylococcal protein A in complex with the Fc fragment of human IgG at 2.3 Angstrom resolution  
Authors : Deis, L.N.; Oas, T.G.  
Deposited on : 2014-11-11  
Resolution : 2.31 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

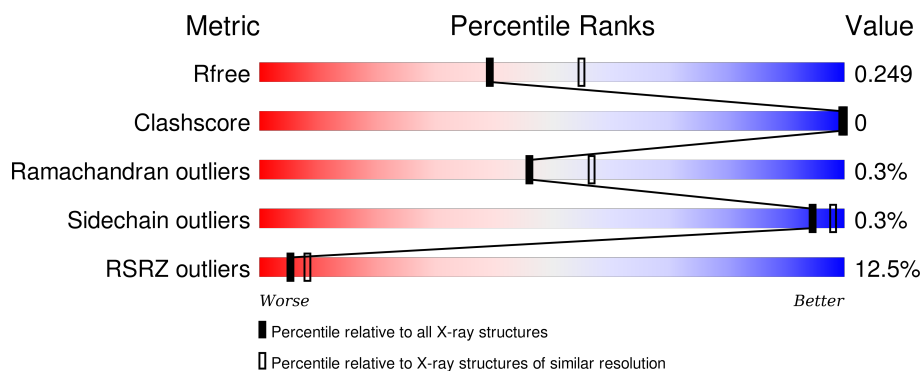
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.31 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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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. 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	58	<div> <div>9%</div> <div>97%</div> <div>..</div> </div>
1	B	58	<div> <div>3%</div> <div>97%</div> <div>.</div> </div>
1	C	58	<div> <div>3%</div> <div>95%</div> <div>5%</div> </div>
2	D	220	<div> <div>11%</div> <div>88%</div> <div>.. 9%</div> </div>
2	E	220	<div> <div>11%</div> <div>80%</div> <div>19%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	220	<div><div></div><div>16%</div><div></div><div>93%</div><div></div><div>6%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12566 atoms, of which 6147 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 Immunoglobulin G-binding protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	57	Total	C	H	N	O	0	4	0
			969	304	478	87	100			
1	B	56	Total	C	H	N	O	0	4	0
			921	290	457	81	93			
1	C	55	Total	C	H	N	O	0	7	0
			978	307	483	87	101			

- Molecule 2 is a protein called Ig gamma-3 chain C region.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	201	Total	C	H	N	O	S	0	6	0
			3258	1047	1615	276	312	8			
2	E	179	Total	C	H	N	O	S	0	9	0
			2929	939	1458	251	273	8			
2	F	207	Total	C	H	N	O	S	0	6	0
			3346	1075	1656	284	323	8			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	296	PHE	TYR	conflict	UNP P01860
D	435	HIS	ARG	conflict	UNP P01860
D	436	TYR	PHE	conflict	UNP P01860
D	448	GLY	-	expression tag	UNP P01860
D	449	SER	-	expression tag	UNP P01860
D	450	LEU	-	expression tag	UNP P01860
D	451	GLU	-	expression tag	UNP P01860
D	452	HIS	-	expression tag	UNP P01860
D	453	HIS	-	expression tag	UNP P01860
D	454	HIS	-	expression tag	UNP P01860
D	455	HIS	-	expression tag	UNP P01860
D	456	HIS	-	expression tag	UNP P01860

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Chain	Residue	Modelled	Actual	Comment	Reference
D	457	HIS	-	expression tag	UNP P01860
E	296	PHE	TYR	conflict	UNP P01860
E	435	HIS	ARG	conflict	UNP P01860
E	436	TYR	PHE	conflict	UNP P01860
E	448	GLY	-	expression tag	UNP P01860
E	449	SER	-	expression tag	UNP P01860
E	450	LEU	-	expression tag	UNP P01860
E	451	GLU	-	expression tag	UNP P01860
E	452	HIS	-	expression tag	UNP P01860
E	453	HIS	-	expression tag	UNP P01860
E	454	HIS	-	expression tag	UNP P01860
E	455	HIS	-	expression tag	UNP P01860
E	456	HIS	-	expression tag	UNP P01860
E	457	HIS	-	expression tag	UNP P01860
F	296	PHE	TYR	conflict	UNP P01860
F	435	HIS	ARG	conflict	UNP P01860
F	436	TYR	PHE	conflict	UNP P01860
F	448	GLY	-	expression tag	UNP P01860
F	449	SER	-	expression tag	UNP P01860
F	450	LEU	-	expression tag	UNP P01860
F	451	GLU	-	expression tag	UNP P01860
F	452	HIS	-	expression tag	UNP P01860
F	453	HIS	-	expression tag	UNP P01860
F	454	HIS	-	expression tag	UNP P01860
F	455	HIS	-	expression tag	UNP P01860
F	456	HIS	-	expression tag	UNP P01860
F	457	HIS	-	expression tag	UNP P01860

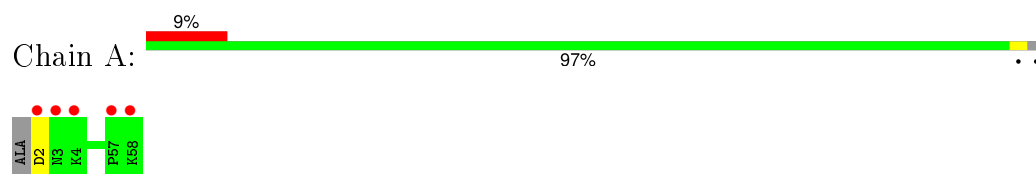
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	23	Total O 23 23	0	0
3	B	18	Total O 18 18	0	0
3	C	23	Total O 23 23	0	0
3	D	38	Total O 38 38	0	0
3	E	29	Total O 29 29	0	0
3	F	34	Total O 34 34	0	0

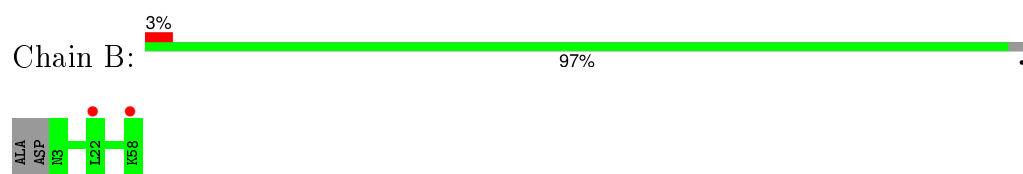
### 3 Residue-property plots [i](#)

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

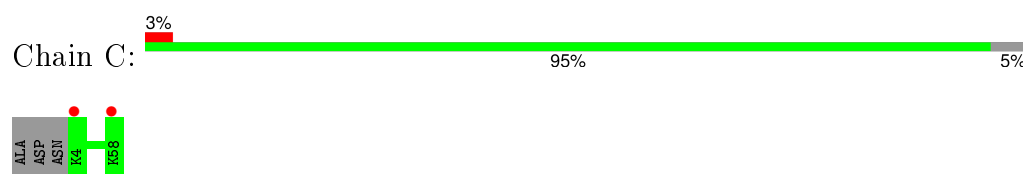
- Molecule 1: Immunoglobulin G-binding protein A



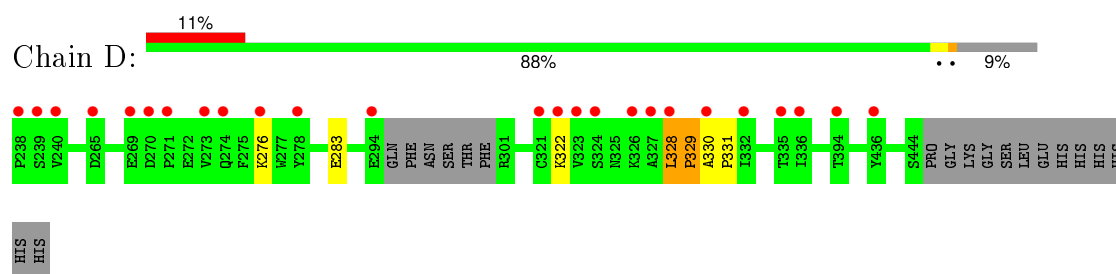
- Molecule 1: Immunoglobulin G-binding protein A



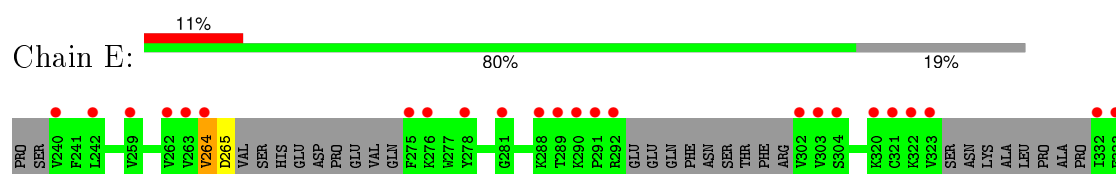
- Molecule 1: Immunoglobulin G-binding protein A

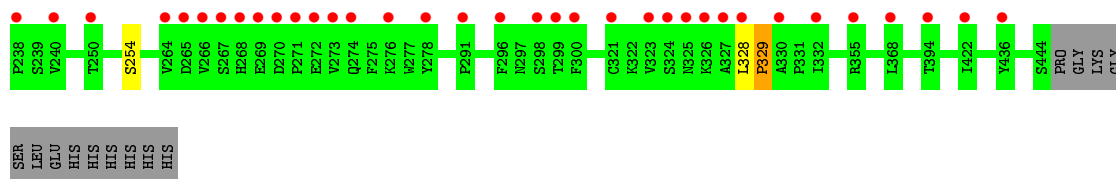


- Molecule 2: Ig gamma-3 chain C region



- Molecule 2: Ig gamma-3 chain C region





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.92Å 88.12Å 101.04Å 90.00° 90.95° 90.00°	Depositor
Resolution (Å)	41.18 – 2.31 44.06 – 2.31	Depositor EDS
% Data completeness (in resolution range)	94.0 (41.18-2.31) 93.7 (44.06-2.31)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 2.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.210 , 0.251 0.212 , 0.249	Depositor DCC
$R_{free}$ test set	1870 reflections (3.70%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.2	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 41.9	EDS
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 53496 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12566	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.24	0/498	0.41	0/667
1	B	0.23	0/471	0.36	0/631
1	C	0.22	0/508	0.35	0/682
2	D	0.32	2/1688 (0.1%)	0.47	2/2295 (0.1%)
2	E	0.22	0/1508	0.40	0/2044
2	F	0.29	1/1737 (0.1%)	0.43	1/2362 (0.0%)
All	All	0.27	3/6410 (0.0%)	0.42	3/8681 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	329	PRO	N-CD	5.19	1.55	1.47
2	D	331	PRO	N-CD	5.15	1.55	1.47
2	D	329	PRO	N-CD	5.13	1.55	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	330	ALA	C-N-CD	5.80	140.57	128.40
2	D	328	LEU	C-N-CD	5.65	140.27	128.40
2	F	328	LEU	C-N-CD	5.54	140.04	128.40

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	A	491	478	471	0	1
1	B	464	457	441	0	0
1	C	495	483	475	0	0
2	D	1643	1615	1603	2	0
2	E	1471	1458	1436	1	0
2	F	1690	1656	1647	0	1
3	A	23	0	0	0	0
3	B	18	0	0	0	0
3	C	23	0	0	0	0
3	D	38	0	0	0	0
3	E	29	0	0	0	0
3	F	34	0	0	0	0
All	All	6419	6147	6073	3	1

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 0.

All (3) 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:D:276:LYS:HB2	2:D:322:LYS:HB3	2.00	0.42
2:D:276:LYS:HE3	2:D:283:GLU:OE2	2.20	0.42
2:E:264:VAL:HA	2:E:265:ASP:HA	1.82	0.42

All (1) 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)
1:A:2:ASP:O	2:F:254:SER:O[4_558]	1.75	0.45

## 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	58/58 (100%)	58 (100%)	0	0	100	100
1	B	55/58 (95%)	54 (98%)	1 (2%)	0	100	100
1	C	60/58 (103%)	59 (98%)	1 (2%)	0	100	100
2	D	200/220 (91%)	196 (98%)	3 (2%)	1 (0%)	34	41
2	E	174/220 (79%)	171 (98%)	3 (2%)	0	100	100
2	F	208/220 (94%)	202 (97%)	5 (2%)	1 (0%)	34	41
All	All	755/834 (90%)	740 (98%)	13 (2%)	2 (0%)	46	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	329	PRO
2	F	329	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	54/51 (106%)	54 (100%)	0	100	100
1	B	51/51 (100%)	51 (100%)	0	100	100
1	C	55/51 (108%)	55 (100%)	0	100	100
2	D	192/206 (93%)	191 (100%)	1 (0%)	92	97
2	E	171/206 (83%)	170 (99%)	1 (1%)	90	96
2	F	198/206 (96%)	198 (100%)	0	100	100
All	All	721/771 (94%)	719 (100%)	2 (0%)	94	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	328	LEU
2	E	264	VAL

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 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 ⓘ

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, 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	57/58 (98%)	0.69	5 (8%) 12 18	43, 53, 91, 102	0
1	B	56/58 (96%)	0.53	2 (3%) 46 55	45, 60, 87, 99	0
1	C	55/58 (94%)	0.50	2 (3%) 46 55	40, 51, 79, 97	0
2	D	201/220 (91%)	0.90	25 (12%) 5 8	38, 60, 98, 107	1 (0%)
2	E	179/220 (81%)	1.04	25 (13%) 4 6	38, 61, 94, 101	0
2	F	207/220 (94%)	1.15	35 (16%) 2 3	38, 59, 95, 102	1 (0%)
All	All	755/834 (90%)	0.93	94 (12%) 5 8	38, 58, 96, 107	2 (0%)

The worst 5 of 94 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	328	LEU	8.8
2	E	302	VAL	7.9
2	E	332	ILE	7.6
2	E	303	VAL	6.6
2	F	264	VAL	6.4

### 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 [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.