



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2017 – 06:47 AM EDT

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 : unknown
Resolution : 2.31 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

<http://wwpdb.org/validation/2016/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) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20029824

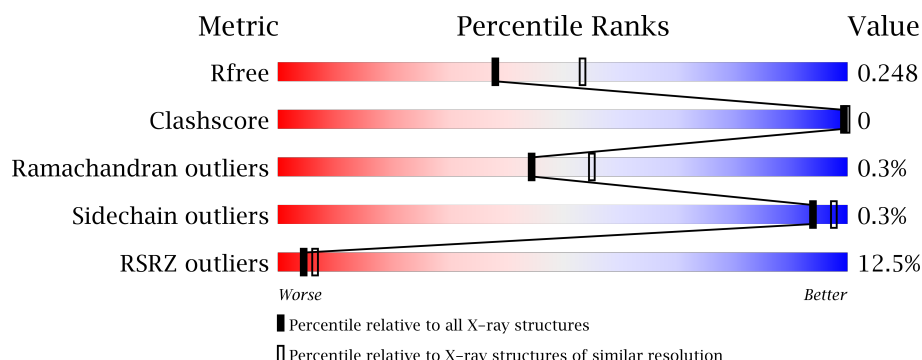
1 Overall quality at a glance

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}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (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 ≥ 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	
1	B	58	
1	C	58	
2	D	220	
2	E	220	

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Mol	Chain	Length	Quality of chain
2	F	220	<div> <div>16%</div> <div> <div></div> <div>93%</div> <div>6%</div> </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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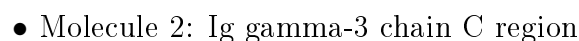
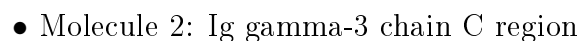
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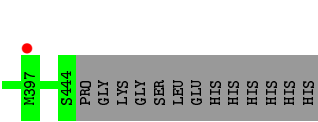
Chain	Residue	Modelled	Actual	Comment	Reference
D	457	HIS	-	expression tag	UNP P01860
E	296	PHE	TYR	conflict	UNP P01860
E	435	HIS	ARG	conflict	UNP P01860
E	436	TYR	PHE	conflict	UNP P01860
E	448	GLY	-	expression tag	UNP P01860
E	449	SER	-	expression tag	UNP P01860
E	450	LEU	-	expression tag	UNP P01860
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.

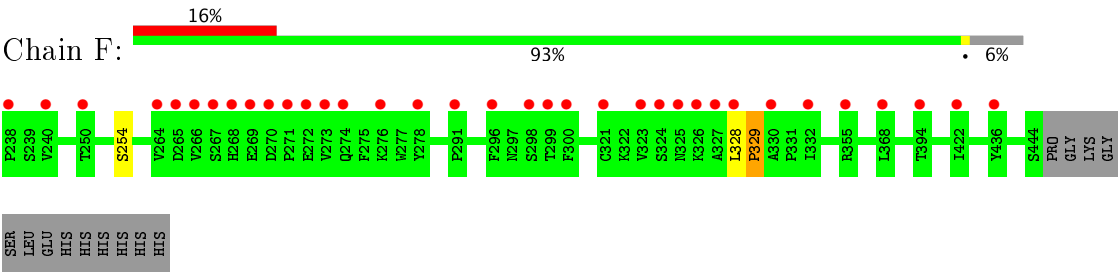
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	23	Total O 23 23	0	0
3	B	18	Total O 18 18	0	0
3	C	23	Total O 23 23	0	0
3	D	38	Total O 38 38	0	0
3	E	29	Total O 29 29	0	0
3	F	34	Total O 34 34	0	0

- Molecule 1: Immunoglobulin G-binding protein A





● 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.210 , 0.251 0.212 , 0.248	Depositor DCC
R_{free} test set	1864 reflections (3.70%)	DCC
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12566	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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](#)

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%)	32	39
2	E	174/220 (79%)	171 (98%)	3 (2%)	0	100	100
2	F	208/220 (94%)	202 (97%)	5 (2%)	1 (0%)	32	39
All	All	755/834 (90%)	740 (98%)	13 (2%)	2 (0%)	44	55

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%)	91	96
2	E	171/206 (83%)	170 (99%)	1 (1%)	89	95
2	F	198/206 (96%)	198 (100%)	0	100	100
All	All	721/771 (94%)	719 (100%)	2 (0%)	94	97

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

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	A	57/58 (98%)	0.69	5 (8%)	11 15	43, 53, 91, 102	0
1	B	56/58 (96%)	0.53	2 (3%)	43 50	45, 60, 87, 99	0
1	C	55/58 (94%)	0.50	2 (3%)	43 50	40, 51, 79, 97	0
2	D	201/220 (91%)	0.90	25 (12%)	4 7	38, 60, 98, 107	1 (0%)
2	E	179/220 (81%)	1.04	25 (13%)	3 5	38, 61, 94, 101	0
2	F	207/220 (94%)	1.15	35 (16%)	2 2	38, 59, 95, 102	1 (0%)
All	All	755/834 (90%)	0.93	94 (12%)	4 6	38, 58, 96, 107	2 (0%)

All (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
2	D	322	LYS	6.3
2	F	326	LYS	6.2
1	A	58	LYS	6.0
2	E	292	ARG	6.0
2	D	326	LYS	5.7
2	E	321	CYS	5.6
1	A	2	ASP	5.5
2	D	324	SER	5.2
2	E	264	VAL	5.1
2	D	270	ASP	5.1
2	E	289	THR	5.0
2	E	323	VAL	5.0
2	E	263	VAL	4.9
2	D	239	SER	4.8

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Mol	Chain	Res	Type	RSRZ
2	E	262	VAL	4.7
2	F	299	THR	4.7
2	D	273	VAL	4.6
2	F	270	ASP	4.5
1	B	58	LYS	4.5
2	F	267	SER	4.4
2	E	275	PHE	4.2
2	F	269	GLU	4.2
2	E	278	TYR	4.2
2	F	273[A]	VAL	4.2
1	A	4	LYS	4.0
2	F	268	HIS	3.9
2	D	238	PRO	3.9
2	F	325	ASN	3.9
2	F	323	VAL	3.9
2	F	296	PHE	3.8
2	D	327	ALA	3.8
2	F	271	PRO	3.8
2	E	240	VAL	3.8
2	E	322	LYS	3.8
2	E	291	PRO	3.8
2	E	290	LYS	3.6
2	F	274	GLN	3.6
2	F	266	VAL	3.5
2	F	300	PHE	3.5
2	D	274	GLN	3.4
2	D	323	VAL	3.3
2	D	332	ILE	3.3
2	F	265	ASP	3.2
2	F	278	TYR	3.2
2	F	240	VAL	3.1
2	F	330	ALA	3.1
2	D	240	VAL	3.1
1	C	58	LYS	3.1
1	A	3	ASN	3.1
2	D	271	PRO	3.1
2	D	336	ILE	3.0
2	F	332[A]	ILE	2.9
2	D	265	ASP	2.9
2	D	335	THR	2.9
2	E	333	GLU	2.9
2	F	324	SER	2.8

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Mol	Chain	Res	Type	RSRZ
2	F	291	PRO	2.8
2	E	276	LYS	2.8
2	E	288	LYS	2.8
2	F	250	THR	2.7
2	F	327	ALA	2.7
2	D	330	ALA	2.7
2	F	321	CYS	2.6
2	E	320	LYS	2.6
2	D	321	CYS	2.6
2	E	397	MET	2.6
2	D	269	GLU	2.6
2	F	298	SER	2.5
2	E	304	SER	2.5
2	D	436[A]	TYR	2.5
2	F	276	LYS	2.5
1	C	4	LYS	2.4
2	F	394	THR	2.4
2	F	272	GLU	2.4
1	A	57	PRO	2.4
2	F	436[A]	TYR	2.3
2	F	355	ARG	2.3
2	E	242	LEU	2.2
2	D	394	THR	2.2
2	F	422	ILE	2.2
2	D	278	TYR	2.2
2	E	259	VAL	2.1
2	D	276	LYS	2.1
2	D	328	LEU	2.1
2	F	368	LEU	2.1
1	B	22	LEU	2.1
2	D	294	GLU	2.0
2	F	238	PRO	2.0
2	E	281	GLY	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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.