wwPDB X-ray Structure Validation Summary Report (i)

Sep 17, 2023 – 10:13 AM EDT

PDB ID	:	4ZNC
Title	:	Fc fragment of human IgG in complex with the C domain of staphylococcal protein A mutant - Q9W
Authors	:	Deis, L.N.; Oas, T.G.
Deposited on	:	2015-05-04
Resolution	:	2.28 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

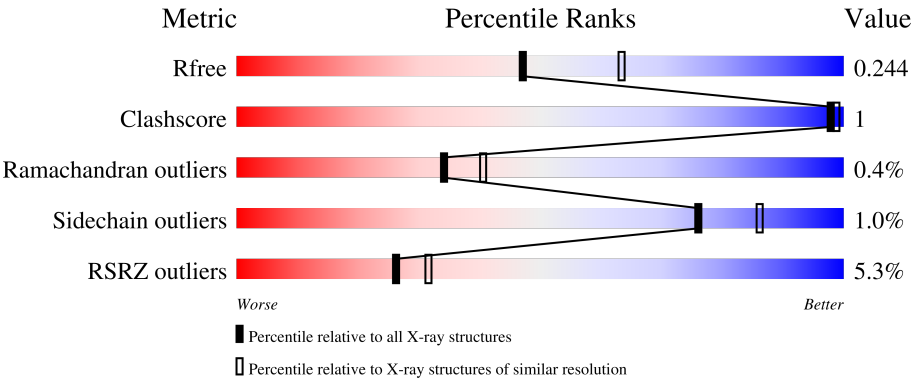
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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}	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	91% 9%
1	B	58	88% • 9%
1	C	58	3% 90% • 9%
2	D	220	3% 93% • 6%
2	E	220	5% 90% 5% 6%

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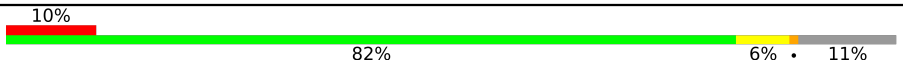
Mol	Chain	Length	Quality of chain
2	F	220	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12392 atoms, of which 6069 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	53	Total	C	H	N	O	0	2	0
			892	286	439	78	89			
1	B	53	Total	C	H	N	O	0	0	0
			852	275	419	73	85			
1	C	53	Total	C	H	N	O	0	0	0
			852	275	419	73	85			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	TRP	GLN	engineered mutation	UNP P38507
B	9	TRP	GLN	engineered mutation	UNP P38507
C	9	TRP	GLN	engineered mutation	UNP P38507

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	207	Total	C	H	N	O	S	0	0	0
			3290	1057	1629	278	318	8			
2	E	207	Total	C	H	N	O	S	0	0	0
			3290	1057	1629	278	318	8			
2	F	195	Total	C	H	N	O	S	0	0	0
			3090	993	1534	258	297	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	24	Total O 24 24	0	0
3	B	19	Total O 19 19	0	0

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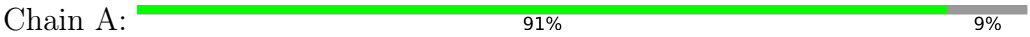
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O 1 1	0	0
3	D	42	Total O 42 42	0	0
3	E	18	Total O 18 18	0	0
3	F	22	Total O 22 22	0	0

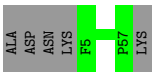
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Immunoglobulin G-binding protein A

Chain A:



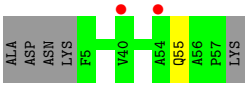


• Molecule 1: Immunoglobulin G-binding protein A

Chain B:

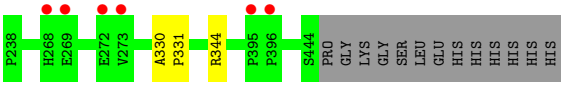
• Molecule 1: Immunoglobulin G-binding protein A

Chain C:



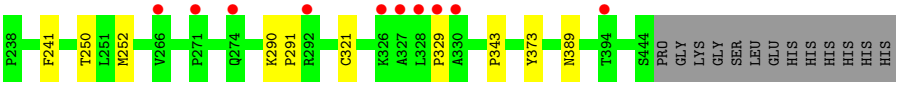
• Molecule 2: Ig gamma-3 chain C region

Chain D:



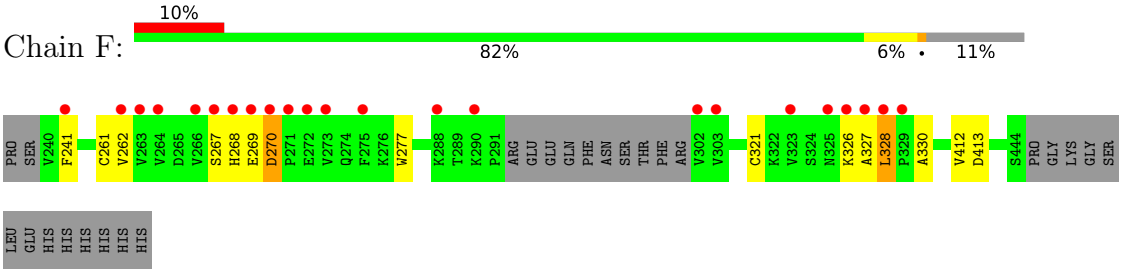
• Molecule 2: Ig gamma-3 chain C region

Chain E:



• Molecule 2: Ig gamma-3 chain C region

Chain F:


10%
82%
6%
11%
PRO SER V240 F241 C261 V262 V263 V264 D265 V266 S267 H268 E269 D270 P271 E272 V273 Q274 F275 K276 W277 K288 T289 K290 P291 ARG GLU GLU GLN PHE ASN SER THR PHE ARG V302 V303 C321 K322 V323 S324 N325 K326 A327 L328 P329 A330 V412 D413 S444 PRO GLY LYS GLY SER
LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	137.95Å 87.21Å 103.25Å 90.00° 91.06° 90.00°	Depositor
Resolution (Å)	34.82 – 2.28 42.48 – 2.27	Depositor EDS
% Data completeness (in resolution range)	94.5 (34.82-2.28) 93.2 (42.48-2.27)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.27Å)	Xtriage
Refinement program	PHENIX dev_1664	Depositor
R, R_{free}	0.196 , 0.242 0.202 , 0.244	Depositor DCC
R_{free} test set	2002 reflections (3.61%)	wwPDB-VP
Wilson B-factor (Å^2)	51.9	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 41.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12392	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.75	0/462	0.76	0/623
1	B	0.79	0/442	0.74	1/597 (0.2%)
1	C	0.75	0/442	0.66	0/597
2	D	0.75	0/1707	0.76	2/2322 (0.1%)
2	E	0.76	0/1707	0.79	2/2322 (0.1%)
2	F	0.74	1/1598 (0.1%)	0.75	1/2175 (0.0%)
All	All	0.75	1/6358 (0.0%)	0.76	6/8636 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	412	VAL	CB-CG2	-5.55	1.41	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	344	ARG	NE-CZ-NH2	-7.15	116.73	120.30
1	B	27	ARG	NE-CZ-NH2	-6.72	116.94	120.30
2	E	252	MET	CG-SD-CE	-6.55	89.72	100.20
2	F	270	ASP	C-N-CD	6.05	141.11	128.40
2	D	344	ARG	NE-CZ-NH1	5.31	122.95	120.30

There are no chirality outliers.

There are no planarity outliers.

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	453	439	436	0	0
1	B	433	419	419	1	0
1	C	433	419	419	0	0
2	D	1661	1629	1629	1	0
2	E	1661	1629	1629	4	0
2	F	1556	1534	1533	4	4
3	A	24	0	0	0	0
3	B	19	0	0	0	0
3	C	1	0	0	0	0
3	D	42	0	0	0	0
3	E	18	0	0	0	0
3	F	22	0	0	0	0
All	All	6323	6069	6065	9	4

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 1.

The worst 5 of 9 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)
1:B:54:ALA:HB2	2:E:389:ASN:HB2	1.89	0.55
2:F:241:PHE:O	2:F:262:VAL:N	2.44	0.47
2:E:343:PRO:HA	2:E:373:TYR:O	2.17	0.45
2:F:327:ALA:O	2:F:328:LEU:HB2	2.16	0.45
2:D:330:ALA:HB1	2:D:331:PRO:HD2	2.00	0.43

All (4) 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)
2:F:326:LYS:O	2:F:326:LYS:HE3[2_659]	0.97	0.63
2:F:326:LYS:HG3	2:F:326:LYS:HE2[2_659]	1.22	0.38
2:F:326:LYS:O	2:F:326:LYS:CE[2_659]	1.83	0.37
2:F:326:LYS:C	2:F:326:LYS:HE3[2_659]	1.59	0.01

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	53/58 (91%)	50 (94%)	3 (6%)	0	100	100
1	B	51/58 (88%)	50 (98%)	1 (2%)	0	100	100
1	C	51/58 (88%)	50 (98%)	1 (2%)	0	100	100
2	D	205/220 (93%)	201 (98%)	4 (2%)	0	100	100
2	E	205/220 (93%)	201 (98%)	3 (2%)	1 (0%)	29	34
2	F	191/220 (87%)	181 (95%)	8 (4%)	2 (1%)	15	16
All	All	756/834 (91%)	733 (97%)	20 (3%)	3 (0%)	34	40

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	269	GLU
2	F	328	LEU
2	E	329	PRO

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	49/51 (96%)	49 (100%)	0	100	100
1	B	47/51 (92%)	47 (100%)	0	100	100
1	C	47/51 (92%)	46 (98%)	1 (2%)	53	68
2	D	195/206 (95%)	195 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	E	195/206 (95%)	194 (100%)	1 (0%)	88 94
2	F	183/206 (89%)	178 (97%)	5 (3%)	44 59
All	All	716/771 (93%)	709 (99%)	7 (1%)	76 86

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	268	HIS
2	F	270	ASP
2	F	413	ASP
2	F	321	CYS
2	F	267	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	392	ASN
2	F	421	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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)

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^{th} 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	53/58 (91%)	0.15	0 100 100	43, 52, 71, 83	0
1	B	53/58 (91%)	0.19	0 100 100	43, 52, 70, 76	0
1	C	53/58 (91%)	0.22	2 (3%) 40 45	50, 69, 81, 91	0
2	D	207/220 (94%)	0.31	6 (2%) 51 57	40, 55, 80, 94	0
2	E	207/220 (94%)	0.41	10 (4%) 30 36	41, 60, 90, 99	0
2	F	195/220 (88%)	0.74	23 (11%) 4 6	41, 64, 96, 104	0
All	All	768/834 (92%)	0.42	41 (5%) 26 31	40, 60, 90, 104	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	268	HIS	7.8
2	F	271	PRO	6.5
2	F	326	LYS	5.8
2	F	267	SER	5.5
2	F	302	VAL	4.2

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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.