



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:22 PM GMT

PDB ID : 1FC1  
Title : CRYSTALLOGRAPHIC REFINEMENT AND ATOMIC MODELS OF A HUMAN FC FRAGMENT AND ITS COMPLEX WITH FRAGMENT B OF PROTEIN A FROM STAPHYLOCOCCUS AUREUS AT 2.9-AND 2.8-ANGSTROMS RESOLUTION  
Authors : Deisenhofer, J.  
Deposited on : 1981-05-21  
Resolution : 2.90 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 : 1.7 (RC4), CSD as536be (2015)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

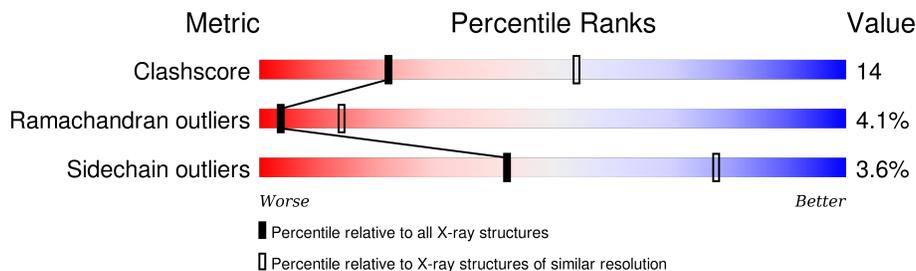
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	224	
1	B	224	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FUC	A	2	X	-	-	-
2	MAN	A	4	X	-	-	-
2	FUC	B	2	X	-	-	-

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
2	MAN	B	4	X	-	-	-

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 3532 atoms, of which 0 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 FC FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	207	Total 1656	C 1054	N 282	O 313	S 7	60	0	1
1	B	207	Total 1656	C 1054	N 282	O 313	S 7	217	0	1

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	272	GLN	GLU	CONFLICT	UNP P01857
A	283	GLN	GLU	CONFLICT	UNP P01857
A	294	GLN	GLU	CONFLICT	UNP P01857
A	312	ASN	ASP	CONFLICT	UNP P01857
A	315	ASP	ASN	CONFLICT	UNP P01857
A	356	GLU	ASP	CONFLICT	UNP P01857
A	358	MET	LEU	CONFLICT	UNP P01857
B	272	GLN	GLU	CONFLICT	UNP P01857
B	283	GLN	GLU	CONFLICT	UNP P01857
B	294	GLN	GLU	CONFLICT	UNP P01857
B	312	ASN	ASP	CONFLICT	UNP P01857
B	315	ASP	ASN	CONFLICT	UNP P01857
B	356	GLU	ASP	CONFLICT	UNP P01857
B	358	MET	LEU	CONFLICT	UNP P01857

- Molecule 2 is a polymer of unknown type called SUGAR (9-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	9	Total 110	C 62	N 4	O 44	18	0
2	B	9	Total 110	C 62	N 4	O 44	55	0



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.40Å 146.40Å 50.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	unknown	Depositor
R, $R_{free}$	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3532	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, GAL, NAG, MAN

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	1.01	4/1702 (0.2%)	1.22	2/2318 (0.1%)
1	B	1.01	4/1702 (0.2%)	1.21	1/2318 (0.0%)
All	All	1.01	8/3404 (0.2%)	1.22	3/4636 (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
1	A	0	17
1	B	0	22
2	A	3	0
2	B	3	0
All	All	6	39

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	381	TRP	NE1-CE2	-7.99	1.27	1.37
1	A	277	TRP	NE1-CE2	-7.94	1.27	1.37
1	B	277	TRP	NE1-CE2	-7.76	1.27	1.37
1	B	313	TRP	NE1-CE2	-7.71	1.27	1.37
1	A	417	TRP	NE1-CE2	-7.63	1.27	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	401	ASP	CB-CA-C	-5.71	98.98	110.40
1	A	297	ASN	N-CA-CB	-5.52	100.66	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	HIS	CA-CB-CG	-5.42	104.39	113.60

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2	FUC	C5,C1
2	A	4	MAN	C1
2	B	2	FUC	C5,C1
2	B	4	MAN	C1

5 of 39 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	259	VAL	Mainchain
1	A	276	ASN	Sidechain
1	A	280	ASP	Mainchain
1	A	287	ALA	Mainchain
1	A	309	LEU	Mainchain

## 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	1656	0	1629	51	4
1	B	1656	0	1629	36	1
2	A	110	0	94	5	0
2	B	110	0	94	1	0
All	All	3532	0	3446	86	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 14.

The worst 5 of 86 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:274:LYS:HB3	1:B:324:SER:HB2	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ASN:HB3	1:A:299:THR:HG22	1.61	0.81
1:A:328:LEU:HD21	1:A:332:ILE:HG13	1.64	0.77
1:A:250:THR:HG22	1:A:257:PRO:HB3	1.68	0.76
1:A:296:TYR:HD2	2:A:1:NAG:H62	1.52	0.75

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)
1:A:389:ASN:OD1	1:B:389:ASN:ND2[4_566]	1.69	0.51
1:A:268:HIS:CG	1:A:285:HIS:NE2[2_674]	1.81	0.39
1:A:268:HIS:ND1	1:A:285:HIS:NE2[2_674]	2.01	0.19
1:A:268:HIS:CB	1:A:285:HIS:NE2[2_674]	2.16	0.04

## 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	205/224 (92%)	179 (87%)	18 (9%)	8 (4%)	4	15
1	B	205/224 (92%)	179 (87%)	17 (8%)	9 (4%)	3	12
All	All	410/448 (92%)	358 (87%)	35 (8%)	17 (4%)	3	14

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	297	ASN
1	B	268	HIS
1	B	292	ARG
1	B	297	ASN
1	A	285	HIS

### 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	193/207 (93%)	186 (96%)	7 (4%)	42	78
1	B	193/207 (93%)	186 (96%)	7 (4%)	42	78
All	All	386/414 (93%)	372 (96%)	14 (4%)	42	78

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	434	ASN
1	B	284	VAL
1	B	390	ASN
1	A	425	CYS
1	B	376	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	438	GLN
1	B	283	GLN
1	B	418	GLN
1	A	421	ASN
1	B	419	GLN

### 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

18 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	A	1	1,2	14,14,15	0.70	0	15,19,21	1.73	2 (13%)
2	FUC	A	2	2	10,10,11	0.80	0	14,14,16	1.73	2 (14%)
2	NAG	A	3	2	14,14,15	0.97	0	15,19,21	1.59	2 (13%)
2	MAN	A	4	2	11,11,12	0.54	0	14,15,17	1.55	2 (14%)
2	MAN	A	5	2	11,11,12	0.55	0	14,15,17	1.37	2 (14%)
2	NAG	A	6	2	14,14,15	0.92	0	15,19,21	1.80	1 (6%)
2	GAL	A	7	2	11,11,12	0.53	0	14,15,17	1.67	3 (21%)
2	MAN	A	8	2	11,11,12	0.76	0	14,15,17	1.62	1 (7%)
2	NAG	A	9	2	14,14,15	0.78	0	15,19,21	2.02	1 (6%)
2	NAG	B	1	1,2	14,14,15	0.75	0	15,19,21	1.57	1 (6%)
2	FUC	B	2	2	10,10,11	0.76	0	14,14,16	1.68	1 (7%)
2	NAG	B	3	2	14,14,15	0.91	1 (7%)	15,19,21	1.40	1 (6%)
2	MAN	B	4	2	11,11,12	0.62	0	14,15,17	1.94	2 (14%)
2	MAN	B	5	2	11,11,12	0.62	0	14,15,17	1.64	1 (7%)
2	NAG	B	6	2	14,14,15	0.81	0	15,19,21	1.80	1 (6%)
2	GAL	B	7	2	11,11,12	0.59	0	14,15,17	1.35	1 (7%)
2	MAN	B	8	2	11,11,12	0.86	1 (9%)	14,15,17	1.69	1 (7%)
2	NAG	B	9	2	14,14,15	0.93	1 (7%)	15,19,21	1.75	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1	1,2	-	0/6/23/26	0/1/1/1
2	FUC	A	2	2	2/2/4/5	0/0/17/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	3	2	-	0/6/23/26	0/1/1/1
2	MAN	A	4	2	1/1/4/5	0/2/19/22	0/1/1/1
2	MAN	A	5	2	-	0/2/19/22	0/1/1/1
2	NAG	A	6	2	-	0/6/23/26	0/1/1/1
2	GAL	A	7	2	-	0/2/19/22	0/1/1/1
2	MAN	A	8	2	-	0/2/19/22	0/1/1/1
2	NAG	A	9	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	FUC	B	2	2	2/2/4/5	0/0/17/20	0/1/1/1
2	NAG	B	3	2	-	0/6/23/26	0/1/1/1
2	MAN	B	4	2	1/1/4/5	0/2/19/22	0/1/1/1
2	MAN	B	5	2	-	0/2/19/22	0/1/1/1
2	NAG	B	6	2	-	0/6/23/26	0/1/1/1
2	GAL	B	7	2	-	0/2/19/22	0/1/1/1
2	MAN	B	8	2	-	0/2/19/22	0/1/1/1
2	NAG	B	9	2	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	NAG	C1-C2	2.00	1.55	1.52
2	B	8	MAN	C2-C3	2.40	1.55	1.52
2	B	9	NAG	C1-C2	2.47	1.55	1.52

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	7	GAL	O5-C1-C2	-2.67	106.53	110.86
2	A	4	MAN	O3-C3-C4	-2.37	105.00	110.34
2	B	4	MAN	O3-C3-C4	-2.34	105.08	110.34
2	A	1	NAG	C4-C3-C2	-2.06	108.02	111.23
2	A	2	FUC	O5-C5-C6	2.02	109.46	106.13

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	4	MAN	C1
2	A	4	MAN	C1
2	B	2	FUC	C5
2	B	2	FUC	C1
2	A	2	FUC	C5

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	NAG	2	0
2	A	7	GAL	3	0
2	B	7	GAL	1	0

## 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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers

EDS was not executed - this section will therefore be empty.