



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:47 PM GMT

PDB ID : 1F9Q  
Title : CRYSTAL STRUCTURE OF PLATELET FACTOR 4  
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Deposited on : 2000-07-11  
Resolution : 2.00 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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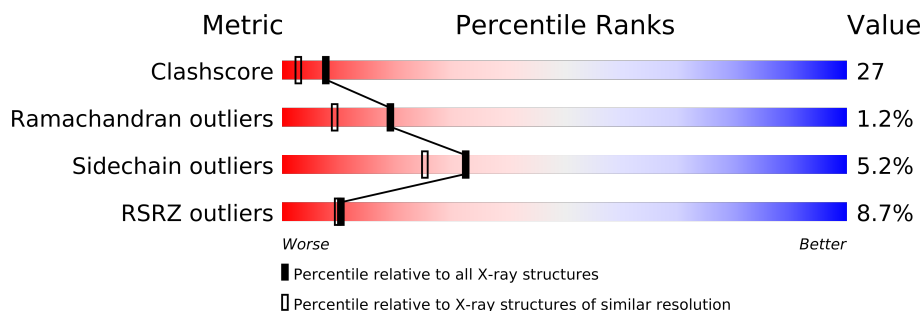
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
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) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.00 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	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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	70	
1	B	70	
1	C	70	
1	D	70	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2198 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 PLATELET FACTOR 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	64	Total	C	N	O	S	0	0	0
			498	317	90	87	4			
1	B	62	Total	C	N	O	S	0	0	0
			482	307	88	83	4			
1	C	62	Total	C	N	O	S	0	0	0
			482	307	88	83	4			
1	D	66	Total	C	N	O	S	0	0	0
			510	323	92	91	4			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	66	Total	O	0	0
			66	66		
2	B	64	Total	O	0	0
			64	64		
2	C	52	Total	O	0	0
			52	52		
2	D	44	Total	O	0	0
			44	44		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.69Å 77.54Å 43.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.00 22.64 – 2.00	Depositor EDS
% Data completeness (in resolution range)	76.5 (15.00-2.00) 76.6 (22.64-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 2.01Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, $R_{free}$	0.227 , 0.275 0.244 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	46.5	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 64.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 14991 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2198	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.59% 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	0.32	0/504	0.60	0/678
1	B	0.33	0/488	0.66	0/656
1	C	0.29	0/488	0.61	0/656
1	D	0.29	0/516	0.68	0/694
All	All	0.31	0/1996	0.64	0/2684

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	498	0	546	27	0
1	B	482	0	531	33	0
1	C	482	0	531	39	0
1	D	510	0	553	41	0
2	A	66	0	0	2	0
2	B	64	0	0	3	0
2	C	52	0	0	3	0
2	D	44	0	0	0	0
All	All	2198	0	2161	113	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 27.

All (113) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:354:ASP:HB3	1:D:356:GLN:OE1	1.76	0.86
1:A:16:THR:HG23	1:D:307:ASP:OD1	1.78	0.84
1:A:23:HIS:HA	1:A:46:LYS:HD2	1.60	0.82
1:C:247:ASN:N	1:C:247:ASN:HD22	1.77	0.82
1:B:156:GLN:HE21	1:B:158:PRO:HB2	1.47	0.79
1:C:247:ASN:H	1:C:247:ASN:ND2	1.80	0.78
1:A:11:LEU:HG	1:D:311:LEU:HD13	1.66	0.76
1:D:364:ILE:O	1:D:368:LEU:HB2	1.87	0.74
1:C:247:ASN:N	1:C:247:ASN:ND2	2.36	0.74
1:D:357:ALA:HA	1:D:360:TYR:CE1	2.24	0.73
1:C:260:TYR:O	1:C:264:ILE:HG22	1.91	0.71
1:A:11:LEU:HD21	1:D:311:LEU:HB2	1.73	0.71
1:B:161:LYS:O	1:B:165:LYS:HD2	1.91	0.70
1:C:231:LYS:HB2	1:D:367:LEU:HD22	1.74	0.69
1:D:319:VAL:HG11	1:D:351:ILE:CD1	2.23	0.69
1:D:320:ARG:HB3	1:D:322:ARG:HH12	1.59	0.67
1:A:20:ARG:HB2	1:A:23:HIS:ND1	2.10	0.66
1:D:322:ARG:HH11	1:D:322:ARG:HB2	1.60	0.65
1:B:156:GLN:NE2	1:B:158:PRO:HB2	2.10	0.65
1:D:320:ARG:HB3	1:D:322:ARG:NH1	2.12	0.64
1:D:311:LEU:HD23	1:D:342:ILE:CD1	2.28	0.62
1:D:322:ARG:NH1	1:D:322:ARG:H	1.98	0.62
1:D:364:ILE:HG22	1:D:368:LEU:HD22	1.81	0.62
1:A:23:HIS:O	1:A:46:LYS:HG3	2.00	0.62
1:A:68:LEU:HD21	1:B:141:LEU:HD11	1.82	0.62
1:B:150:LYS:HE2	1:C:228:GLU:OE2	2.00	0.61
1:C:223:HIS:O	1:C:245:LEU:HA	2.01	0.61
1:B:157:ALA:HB3	1:B:158:PRO:HD3	1.84	0.60
1:B:156:GLN:HG2	1:B:158:PRO:HD2	1.85	0.59
1:B:165:LYS:N	1:B:165:LYS:HE3	2.16	0.59
1:C:241:LEU:HD11	1:D:368:LEU:HD11	1.84	0.59
1:B:157:ALA:HA	1:B:160:TYR:CE1	2.38	0.59
1:B:109:GLN:HE22	1:C:216:THR:CG2	2.16	0.58
1:D:319:VAL:HG11	1:D:351:ILE:HD11	1.84	0.58
1:D:311:LEU:HD23	1:D:342:ILE:HD13	1.87	0.57
1:B:111:LEU:CD1	1:C:252:CYS:SG	2.93	0.56
1:C:265:LYS:HA	1:C:268:LEU:HD12	1.88	0.56
1:D:359:LEU:O	1:D:363:ILE:HG13	2.06	0.56
1:A:24:ILE:CD1	1:A:63:ILE:HD13	2.36	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:341:LEU:HD13	1:D:355:LEU:CD2	2.37	0.55
1:A:68:LEU:HD13	1:B:160:TYR:CZ	2.42	0.55
1:A:7:ASP:N	2:A:509:HOH:O	2.39	0.55
1:C:211:LEU:HD23	1:C:211:LEU:O	2.08	0.54
1:B:146:LYS:HG2	1:D:348:GLY:HA3	1.89	0.54
1:C:237:PRO:HD3	2:C:539:HOH:O	2.08	0.53
1:C:209:GLN:N	2:C:539:HOH:O	2.41	0.53
1:C:247:ASN:H	1:C:247:ASN:HD22	1.42	0.53
1:A:67:LEU:HD11	1:B:131:LYS:HB2	1.91	0.53
1:C:213:VAL:HG23	1:C:214:LYS:N	2.24	0.52
1:D:318:GLN:O	1:D:319:VAL:HG13	2.10	0.52
1:D:319:VAL:HG11	1:D:351:ILE:HD13	1.91	0.52
1:C:213:VAL:HG23	1:C:214:LYS:H	1.74	0.52
1:C:260:TYR:CE2	1:D:368:LEU:HD21	2.45	0.51
1:C:266:LYS:HE3	1:D:331:LYS:NZ	2.24	0.51
1:A:61:LYS:HB3	2:A:462:HOH:O	2.11	0.51
1:C:264:ILE:O	1:C:268:LEU:HG	2.11	0.51
1:A:31:LYS:HE3	1:B:170:SER:HA	1.93	0.50
1:A:35:HIS:CD2	1:A:35:HIS:H	2.28	0.50
1:A:64:ILE:HD13	1:B:164:ILE:HD13	1.92	0.50
1:A:16:THR:CG2	1:D:307:ASP:OD1	2.57	0.49
1:C:244:THR:OG1	1:C:250:LYS:HE2	2.12	0.49
1:B:128:GLU:OE1	1:C:250:LYS:HE3	2.13	0.49
1:B:145:LEU:HD22	1:B:145:LEU:N	2.27	0.49
1:D:324:ILE:CD1	1:D:363:ILE:HD13	2.43	0.48
1:B:164:ILE:O	1:B:168:LEU:HB2	2.14	0.48
1:B:124:ILE:HG22	1:B:167:LEU:HD21	1.95	0.48
1:A:67:LEU:CD1	1:B:131:LYS:HB2	2.44	0.47
1:D:341:LEU:HD13	1:D:355:LEU:HD22	1.96	0.47
1:C:224:ILE:HD12	1:C:263:ILE:CG2	2.44	0.47
1:D:356:GLN:HB2	1:D:358:PRO:HD2	1.94	0.47
1:D:364:ILE:CG2	1:D:368:LEU:HD22	2.44	0.47
1:A:62:LYS:O	1:A:65:LYS:HG2	2.15	0.47
1:B:109:GLN:NE2	1:C:216:THR:CG2	2.78	0.47
1:A:31:LYS:CE	1:B:170:SER:HA	2.45	0.46
1:D:320:ARG:HB2	1:D:323:HIS:HD2	1.80	0.46
1:A:7:ASP:OD2	1:D:316:THR:HG23	2.16	0.45
1:B:138:THR:HG21	2:B:498:HOH:O	2.17	0.45
1:C:256:GLN:HB2	1:C:256:GLN:HE21	1.52	0.45
1:B:160:TYR:C	1:B:160:TYR:CD2	2.90	0.45
1:C:224:ILE:HD12	1:C:263:ILE:HG23	1.98	0.45
1:C:246:LYS:HG3	1:C:247:ASN:HD22	1.81	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:360:TYR:O	1:D:364:ILE:HG13	2.16	0.45
1:C:260:TYR:HA	1:C:263:ILE:HD12	2.00	0.44
1:D:360:TYR:C	1:D:362:LYS:H	2.21	0.44
1:B:141:LEU:HD22	1:B:155:LEU:HD23	1.99	0.44
1:A:23:HIS:HA	1:A:46:LYS:CD	2.40	0.43
1:D:336:CYS:HA	1:D:337:PRO:HD3	1.88	0.43
1:A:57:ALA:HA	1:A:58:PRO:HD3	1.87	0.43
1:B:111:LEU:HD23	1:B:142:ILE:HD11	2.01	0.43
1:C:245:LEU:HD12	1:C:249:ARG:HB3	1.99	0.43
1:A:69:GLU:O	1:A:70:SER:HB3	2.18	0.43
1:B:109:GLN:N	1:B:135:HIS:O	2.51	0.43
1:B:109:GLN:NE2	1:C:216:THR:HG21	2.32	0.43
1:D:357:ALA:N	1:D:358:PRO:CD	2.81	0.43
1:A:39:ALA:HB2	2:B:536:HOH:O	2.19	0.43
1:A:11:LEU:CG	1:D:311:LEU:HD13	2.41	0.43
1:D:360:TYR:C	1:D:362:LYS:N	2.71	0.43
1:C:253:LEU:HD22	2:C:609:HOH:O	2.18	0.42
1:A:9:GLN:O	1:D:311:LEU:HD12	2.19	0.42
1:B:111:LEU:HG	1:C:211:LEU:HD21	2.01	0.42
1:A:54:ASP:OD1	1:A:56:GLN:HG2	2.19	0.42
1:D:351:ILE:HD12	1:D:353:LEU:HD21	2.01	0.41
1:C:260:TYR:HA	1:C:263:ILE:HB	2.02	0.41
1:D:322:ARG:CB	1:D:322:ARG:HH11	2.28	0.41
1:B:168:LEU:HD12	1:B:168:LEU:HA	1.86	0.41
1:C:222:ARG:HE	1:C:222:ARG:HB2	1.71	0.41
1:B:111:LEU:HD11	1:C:252:CYS:SG	2.61	0.41
1:C:236:CYS:HA	1:C:237:PRO:HD3	1.80	0.41
1:C:245:LEU:HD12	1:C:249:ARG:HD3	2.02	0.41
1:C:259:LEU:HD22	1:C:263:ILE:HD11	2.02	0.40
1:D:318:GLN:HG3	1:D:318:GLN:O	2.18	0.40
1:C:211:LEU:HD23	1:C:211:LEU:C	2.42	0.40
1:B:159:LEU:HB3	2:B:458:HOH:O	2.20	0.40

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	62/70 (89%)	59 (95%)	3 (5%)	0	100	100
1	B	60/70 (86%)	53 (88%)	6 (10%)	1 (2%)	14	5
1	C	60/70 (86%)	57 (95%)	2 (3%)	1 (2%)	14	5
1	D	64/70 (91%)	57 (89%)	6 (9%)	1 (2%)	14	5
All	All	246/280 (88%)	226 (92%)	17 (7%)	3 (1%)	19	9

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	358	PRO
1	C	269	GLU
1	B	134	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	58/62 (94%)	57 (98%)	1 (2%)	73	75
1	B	56/62 (90%)	52 (93%)	4 (7%)	21	14
1	C	56/62 (90%)	51 (91%)	5 (9%)	14	8
1	D	59/62 (95%)	57 (97%)	2 (3%)	49	45
All	All	229/248 (92%)	217 (95%)	12 (5%)	32	25

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	B	141	LEU
1	B	153	LEU
1	B	165	LYS
1	B	168	LEU
1	C	247	ASN

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Mol	Chain	Res	Type
1	C	255	LEU
1	C	256	GLN
1	C	259	LEU
1	C	264	ILE
1	D	318	GLN
1	D	322	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	B	109	GLN
1	B	118	GLN
1	B	123	HIS
1	B	156	GLN
1	C	209	GLN
1	C	247	ASN
1	C	256	GLN
1	D	309	GLN
1	D	323	HIS

### 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	64/70 (91%)	0.32	3 (4%) 30 29	37, 52, 83, 89	0
1	B	62/70 (88%)	0.20	3 (4%) 29 28	32, 48, 70, 81	0
1	C	62/70 (88%)	0.92	7 (11%) 6 5	42, 69, 88, 97	0
1	D	66/70 (94%)	0.64	9 (13%) 4 3	35, 58, 95, 99	0
All	All	254/280 (90%)	0.52	22 (8%) 10 10	32, 58, 89, 99	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	270	SER	6.4
1	D	319	VAL	4.9
1	C	256	GLN	4.4
1	B	170	SER	4.0
1	D	320	ARG	4.0
1	C	257	ALA	3.6
1	D	357	ALA	3.0
1	A	58	PRO	2.8
1	C	263	ILE	2.8
1	C	269	GLU	2.7
1	A	18	GLN	2.6
1	D	358	PRO	2.5
1	D	327	LEU	2.4
1	D	356	GLN	2.4
1	D	318	GLN	2.3
1	C	237	PRO	2.2
1	B	113	VAL	2.2
1	D	367	LEU	2.2
1	A	23	HIS	2.1
1	B	109	GLN	2.1
1	C	260	TYR	2.1
1	D	326	SER	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.