



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 05:53 PM GMT

PDB ID : 4J4L  
Title : Modular evolution and design of the protein binding interface  
Authors : Cheong, H.K.; Kim, H.J.  
Deposited on : 2013-02-07  
Resolution : 2.30 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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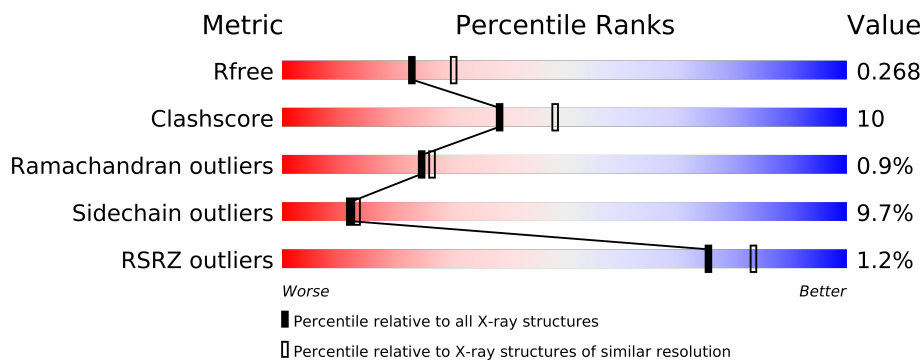
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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. 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	267	
1	B	267	
2	C	168	
2	D	168	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6751 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 Internalin B, Variable lymphocyte receptor B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			2035	1297	345	389	4			
1	B	251	Total	C	N	O	S	0	0	0
			1982	1264	336	378	4			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	ALA	ASP	CONFLICT	UNP D2P9A6
A	302	LEU	-	EXPRESSION TAG	UNP Q4G1L3
A	303	GLU	-	EXPRESSION TAG	UNP Q4G1L3
A	304	HIS	-	EXPRESSION TAG	UNP Q4G1L3
A	305	HIS	-	EXPRESSION TAG	UNP Q4G1L3
A	306	HIS	-	EXPRESSION TAG	UNP Q4G1L3
A	307	HIS	-	EXPRESSION TAG	UNP Q4G1L3
A	308	HIS	-	EXPRESSION TAG	UNP Q4G1L3
A	309	HIS	-	EXPRESSION TAG	UNP Q4G1L3
B	59	ALA	ASP	CONFLICT	UNP D2P9A6
B	302	LEU	-	EXPRESSION TAG	UNP Q4G1L3
B	303	GLU	-	EXPRESSION TAG	UNP Q4G1L3
B	304	HIS	-	EXPRESSION TAG	UNP Q4G1L3
B	305	HIS	-	EXPRESSION TAG	UNP Q4G1L3
B	306	HIS	-	EXPRESSION TAG	UNP Q4G1L3
B	307	HIS	-	EXPRESSION TAG	UNP Q4G1L3
B	308	HIS	-	EXPRESSION TAG	UNP Q4G1L3
B	309	HIS	-	EXPRESSION TAG	UNP Q4G1L3

- Molecule 2 is a protein called Interleukin-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	155	Total	C	N	O	S	0	0	0
			1246	780	216	241	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	166	Total	C	N	O	S	0	0	0
			1330	832	229	260	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	17	GLY	-	EXPRESSION TAG	UNP P05231
C	18	SER	-	EXPRESSION TAG	UNP P05231
D	17	GLY	-	EXPRESSION TAG	UNP P05231
D	18	SER	-	EXPRESSION TAG	UNP P05231

- Molecule 3 is water.

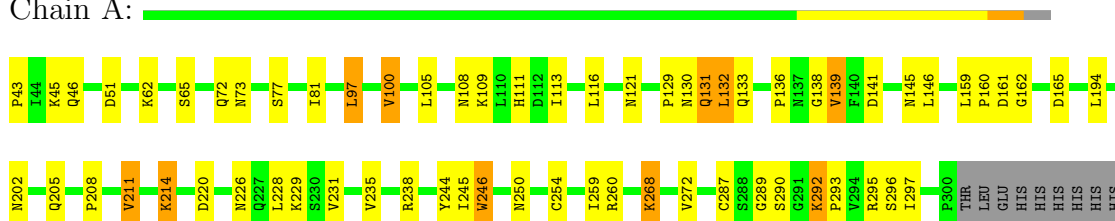
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	61	Total	O	0	0
			61	61		
3	B	28	Total	O	0	0
			28	28		
3	C	37	Total	O	0	0
			37	37		
3	D	32	Total	O	0	0
			32	32		

### 3 Residue-property plots

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.

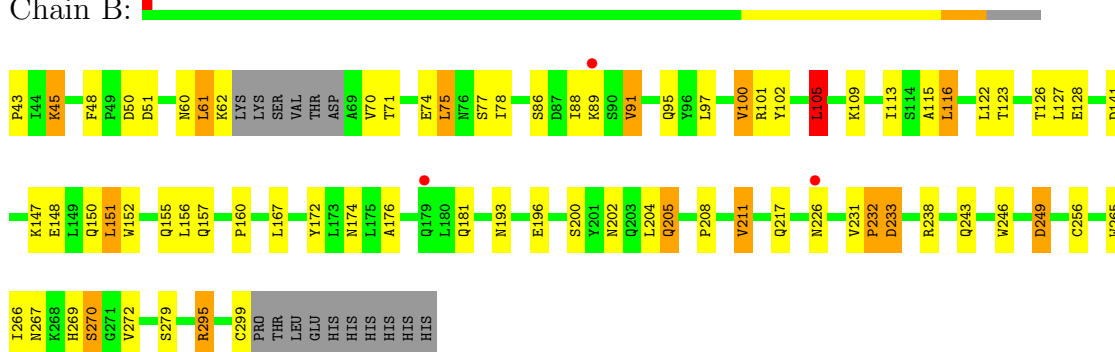
- Molecule 1: Internalin B, Variable lymphocyte receptor B

Chain A:



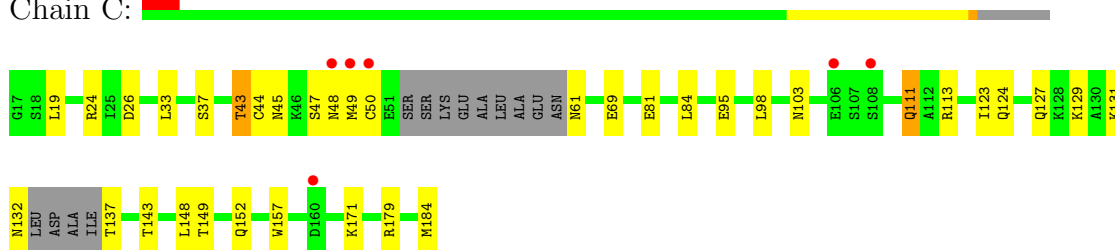
- Molecule 1: Internalin B, Variable lymphocyte receptor B

Chain B:



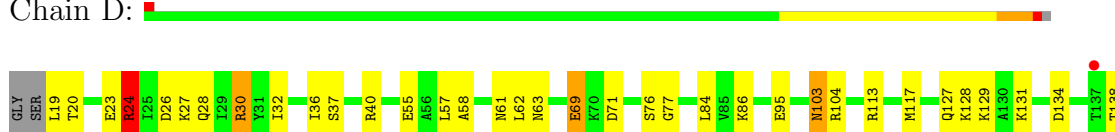
- Molecule 2: Interleukin-6

Chain C:



- Molecule 2: Interleukin-6

Chain D:



T142	Q154	N155	Q156	M161	L165	R168	S169	F170	K171	E172	L181	R182	Q183	M184
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.32Å 134.00Å 148.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.09 – 2.30 61.09 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.2 (61.09-2.30) 95.2 (61.09-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.88 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.205 , 0.268 0.204 , 0.268	Depositor DCC
$R_{free}$ test set	2017 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 20.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 40123 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6751	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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	0.81	1/2075 (0.0%)	0.90	2/2821 (0.1%)
1	B	0.69	1/2020 (0.0%)	0.84	3/2745 (0.1%)
2	C	0.81	1/1259 (0.1%)	0.89	0/1687
2	D	0.76	0/1345	0.92	6/1807 (0.3%)
All	All	0.77	3/6699 (0.0%)	0.88	11/9060 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	246	TRP	CD2-CE2	6.02	1.48	1.41
2	C	157	TRP	CD2-CE2	5.96	1.48	1.41
1	B	246	TRP	CD2-CE2	5.13	1.47	1.41

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	30	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	B	151	LEU	CA-CB-CG	6.76	130.84	115.30
2	D	24	ARG	NE-CZ-NH1	6.13	123.36	120.30
2	D	84	LEU	CB-CG-CD1	-6.08	100.66	111.00
2	D	30	ARG	NE-CZ-NH2	-5.94	117.33	120.30

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	2035	0	2058	46	0
1	B	1982	0	2001	45	0
2	C	1246	0	1261	18	0
2	D	1330	0	1348	27	0
3	A	61	0	0	7	0
3	B	28	0	0	3	0
3	C	37	0	0	2	0
3	D	32	0	0	5	0
All	All	6751	0	6668	130	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 10.

The worst 5 of 130 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:154:GLN:NE2	3:D:231:HOH:O	1.99	0.89
1:A:208:PRO:HB2	1:A:211:VAL:HG13	1.54	0.87
1:A:226:ASN:HB2	1:A:250:ASN:HD21	1.47	0.78
2:C:111:GLN:HE21	2:C:111:GLN:H	1.31	0.78
2:C:111:GLN:HE21	2:C:111:GLN:N	1.82	0.77

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	256/267 (96%)	241 (94%)	14 (6%)	1 (0%)	43	52
1	B	247/267 (92%)	224 (91%)	18 (7%)	5 (2%)	11	8
2	C	149/168 (89%)	146 (98%)	3 (2%)	0	100	100
2	D	164/168 (98%)	156 (95%)	7 (4%)	1 (1%)	33	39
All	All	816/870 (94%)	767 (94%)	42 (5%)	7 (1%)	25	26

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	GLY
1	B	160	PRO
1	B	233	ASP
1	B	270	SER
2	D	131	LYS

### 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	233/242 (96%)	212 (91%)	21 (9%)	14	15
1	B	226/242 (93%)	205 (91%)	21 (9%)	13	14
2	C	142/152 (93%)	127 (89%)	15 (11%)	10	10
2	D	151/152 (99%)	135 (89%)	16 (11%)	10	10
All	All	752/788 (95%)	679 (90%)	73 (10%)	12	13

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	155	GLN
1	B	279	SER
2	D	134	ASP
1	B	211	VAL
2	C	37	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	150	GLN
1	B	217	GLN
2	D	127	GLN
1	B	169	ASN
1	B	193	ASN

### 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	258/267 (96%)	-0.18	0 100 100	11, 27, 45, 65	0
1	B	251/267 (94%)	0.02	3 (1%) 75 83	17, 40, 64, 82	0
2	C	155/168 (92%)	0.06	6 (3%) 37 48	11, 29, 58, 83	1 (0%)
2	D	166/168 (98%)	-0.15	1 (0%) 86 92	14, 29, 57, 76	1 (0%)
All	All	830/870 (95%)	-0.07	10 (1%) 75 83	11, 31, 58, 83	2 (0%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	50	CYS	5.0
2	C	48	ASN	3.2
2	C	106	GLU	3.0
2	C	49	MET	2.7
1	B	179	GLN	2.5

### 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.