wwPDB X-ray Structure Validation Summary Report (i)

Jun 23, 2024 – 10:39 AM EDT

PDB ID	:	5BXF
Title	:	Apo FcRn Structure at pH 4.5
Authors	:	Nam, H.-J.; Taha, M.
Deposited on	:	2015-06-08
Resolution	:	2.85 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:

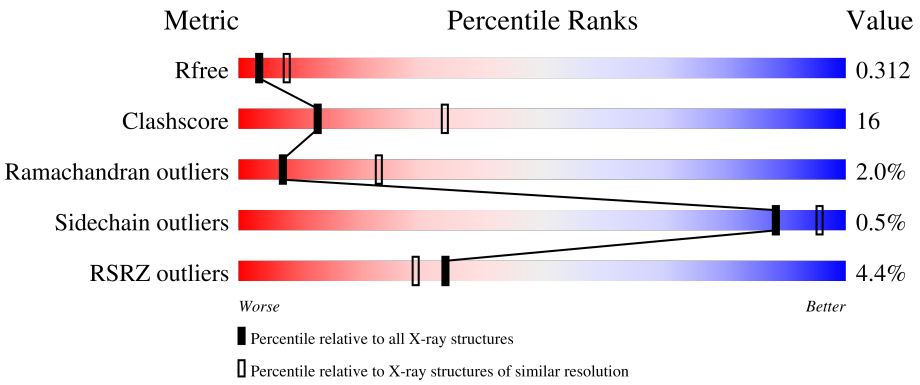
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	300	2%, 67%, 19%, ••, 12%
1	C	300	6%, 61%, 24%, ••, 12%
2	B	119	66%, 17%, 17%
2	D	119	7%, 50%, 32%, •, 17%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5797 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 IgG receptor FcRn large subunit p51.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	263	2069	1324	357	380	8	0	0	0
1	C	263	2069	1324	357	380	8	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	268	VAL	-	expression tag	UNP P55899
A	269	ASP	-	expression tag	UNP P55899
A	270	HIS	-	expression tag	UNP P55899
A	271	HIS	-	expression tag	UNP P55899
A	272	HIS	-	expression tag	UNP P55899
A	273	HIS	-	expression tag	UNP P55899
A	274	HIS	-	expression tag	UNP P55899
A	275	HIS	-	expression tag	UNP P55899
A	276	VAL	-	expression tag	UNP P55899
A	277	ASP	-	expression tag	UNP P55899
C	268	VAL	-	expression tag	UNP P55899
C	269	ASP	-	expression tag	UNP P55899
C	270	HIS	-	expression tag	UNP P55899
C	271	HIS	-	expression tag	UNP P55899
C	272	HIS	-	expression tag	UNP P55899
C	273	HIS	-	expression tag	UNP P55899
C	274	HIS	-	expression tag	UNP P55899
C	275	HIS	-	expression tag	UNP P55899
C	276	VAL	-	expression tag	UNP P55899
C	277	ASP	-	expression tag	UNP P55899

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	99	829	528	140	158	3	0	0	0
2	D	99	829	528	140	158	3	0	0	0

- Molecule 3 is water.

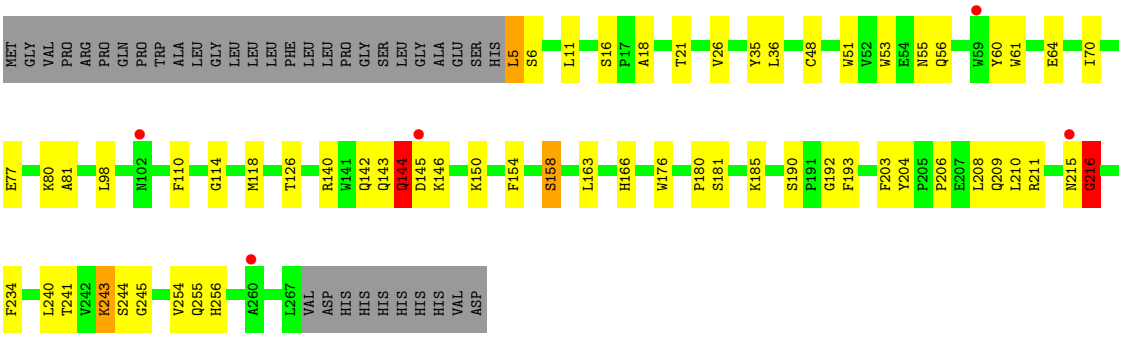
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	C	1	1	1	0	0

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.

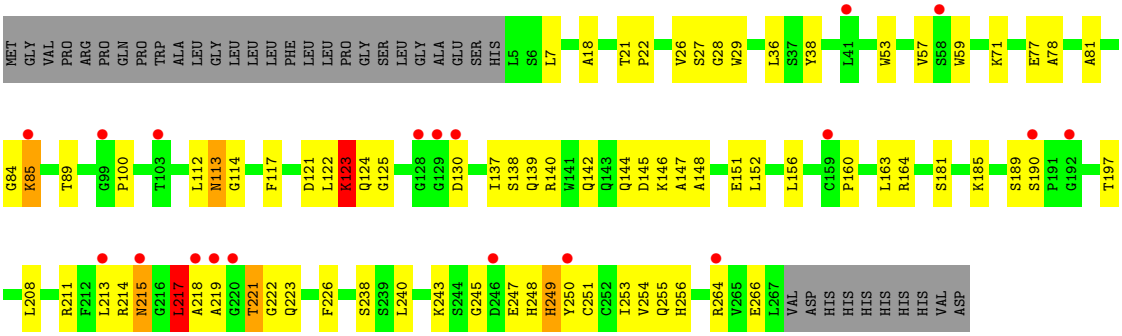
• Molecule 1: IgG receptor FcRn large subunit p51

Chain A:



• Molecule 1: IgG receptor FcRn large subunit p51

Chain C:



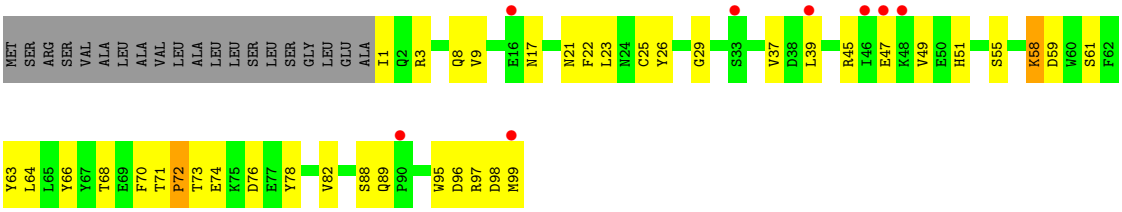
• Molecule 2: Beta-2-microglobulin

Chain B:

• Molecule 2: Beta-2-microglobulin

Chain D:

7%
50%
32%
17%


MET SER ARG SER VAL ALA LEU ALA VAL LEU ALA LEU LEU SER LEU SER GLY LEU GLU ALA I1 Q2 R3 Q8 V9 E16 N17 N21 F22 L23 N24 C25 Y26 G29 S33 V37 D38 L39 R45 I46 E47 K48 V49 E50 H51 S55 K58 D59 W60 S61 F62
Y63 L64 L65 Y66 Y67 T68 E69 F70 T71 P72 T73 E74 K75 D76 E77 Y78 V82 S88 Q89 P90 W95 D96 R97 D98 M99

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	42.18Å 77.58Å 140.55Å 90.00° 93.60° 90.00°	Depositor
Resolution (Å)	46.76 – 2.85 46.76 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.76-2.85) 79.8 (46.76-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.99 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.237 , 0.314 0.241 , 0.312	Depositor DCC
R_{free} test set	1089 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	45.2	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 29.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	5797	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.59% 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 (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	0.52	0/2134	0.72	2/2900 (0.1%)
1	C	0.52	0/2134	0.78	3/2900 (0.1%)
2	B	0.53	0/852	0.67	0/1152
2	D	0.46	0/852	0.65	0/1152
All	All	0.51	0/5972	0.72	5/8104 (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	2
1	C	0	4
All	All	0	6

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	5	LEU	CA-CB-CG	6.76	130.85	115.30
1	C	217	LEU	CA-CB-CG	6.42	130.06	115.30
1	A	216	GLY	N-CA-C	-5.59	99.12	113.10
1	C	215	ASN	N-CA-C	-5.17	97.04	111.00
1	C	85	LYS	CD-CE-NZ	5.10	123.44	111.70

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	GLN	Peptide
1	A	243	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	C	112	LEU	Peptide
1	C	123	LYS	Peptide
1	C	248	HIS	Peptide

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	2069	0	1983	52	0
1	C	2069	0	1983	101	1
2	B	829	0	794	14	0
2	D	829	0	794	34	0
3	C	1	0	0	0	0
All	All	5797	0	5554	186	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 16.

The worst 5 of 186 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:C:217:LEU:HD21	1:C:219:ALA:CB	1.40	1.50
1:C:208:LEU:HD12	1:C:255:GLN:O	1.40	1.15
1:C:249:HIS:NE2	1:C:251:CYS:SG	2.19	1.15
1:C:217:LEU:HG	1:C:219:ALA:N	1.64	1.12
1:C:217:LEU:CD2	1:C:219:ALA:CB	2.29	1.10

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:C:130:ASP:OD2	1:C:189:SER:OG[2_655]	2.06	0.14

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	261/300 (87%)	240 (92%)	17 (6%)	4 (2%)	10 30
1	C	261/300 (87%)	233 (89%)	21 (8%)	7 (3%)	5 16
2	B	97/119 (82%)	91 (94%)	5 (5%)	1 (1%)	15 40
2	D	97/119 (82%)	86 (89%)	9 (9%)	2 (2%)	7 22
All	All	716/838 (85%)	650 (91%)	52 (7%)	14 (2%)	7 23

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	100	PRO
1	C	113	ASN
1	C	123	LYS
1	C	147	ALA
2	B	97	ARG

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	217/248 (88%)	216 (100%)	1 (0%)	88 96
1	C	217/248 (88%)	216 (100%)	1 (0%)	88 96
2	B	94/109 (86%)	94 (100%)	0	100 100
2	D	94/109 (86%)	93 (99%)	1 (1%)	73 90
All	All	622/714 (87%)	619 (100%)	3 (0%)	88 96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ILE
1	C	243	LYS
2	D	58	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	A	255	GLN
1	C	223	GLN
1	C	249	HIS
2	D	17	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	263/300 (87%)	0.15	5 (1%)	66	64	19, 36, 66, 75	0
1	C	263/300 (87%)	0.40	19 (7%)	15	11	29, 47, 81, 90	0
2	B	99/119 (83%)	-0.07	0	100	100	21, 31, 48, 63	0
2	D	99/119 (83%)	0.33	8 (8%)	12	8	29, 46, 70, 75	0
All	All	724/838 (86%)	0.23	32 (4%)	34	29	19, 41, 71, 90	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	99	MET	3.7
1	C	219	ALA	3.6
2	D	46	ILE	3.4
1	C	58	SER	3.4
1	A	145	ASP	3.3

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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.