WORLD WIDE PDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Oct 5, 2024 – 08:25 AM EDT

PDB ID	:	1BBJ
Title	:	CRYSTAL STRUCTURE OF A CHIMERIC FAB' FRAGMENT OF AN AN-TIBODY BINDING TUMOUR CELLS
Authors	:	Brady, R.L.; Hubbard, R.E.; Todd, R.J.
Deposited on	:	1992-04-30
Resolution	:	3.10 Å(reported)

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

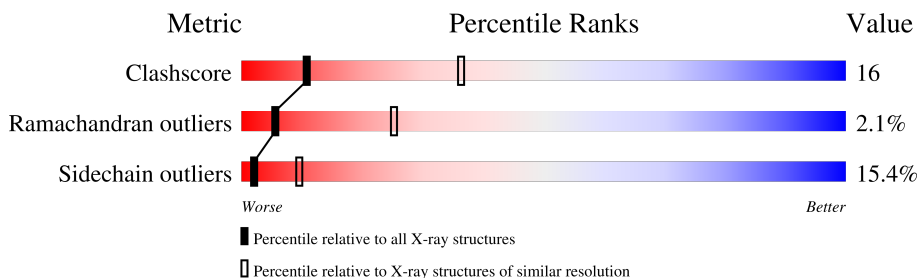|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.10 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	Percentile Ranks	Value
Clashscore		16
Ramachandran outliers		2.1%
Sidechain outliers		15.4%

Worse   *Better*

▊ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	211	50% 39% 9% •
1	L	211	50% 40% 9% •
2	B	212	57% 35% 7% •
2	H	212	57% 35% 7% •

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6466 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 IGG4-KAPPA B72.3 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	211	Total 1630	C 1019	N 274	O 332	S 5	0	0	0
1	A	211	Total 1630	C 1019	N 274	O 332	S 5	0	0	0

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	3	GLN	GLU	conflict	GB 11692743
L	4	MET	LEU	conflict	GB 11692743
L	11	LEU	GLN	conflict	GB 11692743
L	13	VAL	ALA	conflict	GB 11692743
L	15	VAL	LEU	conflict	GB 11692743
L	18	THR	SER	conflict	GB 11692743
L	24	ARG	LEU	conflict	GB 11692743
L	27	GLU	GLN	conflict	GB 11692743
L	28	ASN	THR	conflict	GB 11692743
L	30	TYR	GLY	conflict	GB 11692743
L	31	SER	THR	conflict	GB 11692743
L	32	ASN	TRP	conflict	GB 11692743
L	40	GLN	PRO	conflict	GB 11692743
L	48	VAL	ILE	conflict	GB 11692743
L	53	ASN	SER	conflict	GB 11692743
L	70	GLN	LYS	conflict	GB 11692743
L	71	TYR	PHE	conflict	GB 11692743
L	73	LEU	PHE	conflict	GB 11692743
L	76	ASN	SER	conflict	GB 11692743
L	80	SER	ALA	conflict	GB 11692743
L	84	GLY	VAL	conflict	GB 11692743
L	90	HIS	GLN	conflict	GB 11692743
L	91	PHE	LEU	conflict	GB 11692743
L	92	TRP	TYR	conflict	GB 11692743
L	93	GLY	SER	conflict	GB 11692743

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	103	ARG	LYS	conflict	GB 11692743
L	109	ALA	THR	conflict	GB 11692743
L	110	ASP	VAL	conflict	GB 11692743
L	114	THR	SER	conflict	GB 11692743
A	3	GLN	GLU	conflict	GB 11692743
A	4	MET	LEU	conflict	GB 11692743
A	11	LEU	GLN	conflict	GB 11692743
A	13	VAL	ALA	conflict	GB 11692743
A	15	VAL	LEU	conflict	GB 11692743
A	18	THR	SER	conflict	GB 11692743
A	24	ARG	LEU	conflict	GB 11692743
A	27	GLU	GLN	conflict	GB 11692743
A	28	ASN	THR	conflict	GB 11692743
A	30	TYR	GLY	conflict	GB 11692743
A	31	SER	THR	conflict	GB 11692743
A	32	ASN	TRP	conflict	GB 11692743
A	40	GLN	PRO	conflict	GB 11692743
A	48	VAL	ILE	conflict	GB 11692743
A	53	ASN	SER	conflict	GB 11692743
A	70	GLN	LYS	conflict	GB 11692743
A	71	TYR	PHE	conflict	GB 11692743
A	73	LEU	PHE	conflict	GB 11692743
A	76	ASN	SER	conflict	GB 11692743
A	80	SER	ALA	conflict	GB 11692743
A	84	GLY	VAL	conflict	GB 11692743
A	90	HIS	GLN	conflict	GB 11692743
A	91	PHE	LEU	conflict	GB 11692743
A	92	TRP	TYR	conflict	GB 11692743
A	93	GLY	SER	conflict	GB 11692743
A	103	ARG	LYS	conflict	GB 11692743
A	109	ALA	THR	conflict	GB 11692743
A	110	ASP	VAL	conflict	GB 11692743
A	114	THR	SER	conflict	GB 11692743

- Molecule 2 is a protein called IGG4-KAPPA B72.3 FAB (HEAVY CHAIN).

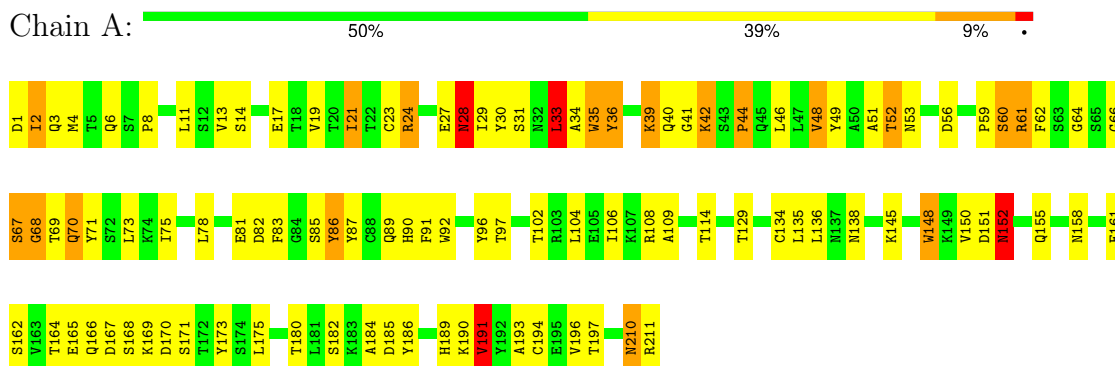| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	212	Total 1603	C 1009	N 266	O 322	S 6	0	0	0
2	B	212	Total 1603	C 1009	N 266	O 322	S 6	0	0	0

3 Residue-property plots ⓘ

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. 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. 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.

Note EDS was not executed.

• Molecule 1: IGG4-KAPPA B72.3 FAB (LIGHT CHAIN)

Chain L:

• Molecule 1: IGG4-KAPPA B72.3 FAB (LIGHT CHAIN)

Chain A:

• Molecule 2: IGG4-KAPPA B72.3 FAB (HEAVY CHAIN)

Chain H:

V182 P186 S187 S188 S189 T192 C197 H201 K202 P203 R211 V212

• Molecule 2: IGG4-KAPPA B72.3 FAB (HEAVY CHAIN)

Chain B:

57%   35%   7%   •

Q1 V2 Q3 L4 Q5 V12 V18 C22 K23 Y27 T28 F29 T30 D31 H32 A33 I34 H35 W36 K40 P41 E42 E46 W47 I48 I51 S52 P53 G54 N55 D56 D57 I58 K59 K65 G66 K67 A68 T69 L70 T71 A72 D73 K74 S77 T78 M81 Q82 S85

L86 Y94 K97 R98 S99 Y100 Y101 G102 H103 W104 T109 L110 S113 S114 T117 F123 P124 L125 C128 S129 R130 S131 T132 S133 E134 S135 C141 L142 V143 P148 E149 P150 V151 T152 V153 S154 W155 N156 L160 T161 S162 P168 S173 S178 L179 S180 S181

V182 P186 S187 S188 S189 T192 C197 H201 K202 P203 R211 V212

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.50Å 93.20Å 208.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.176 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6466	wwPDB-VP
Average B, all atoms (Å²)	35.0	wwPDB-VP

5　Model quality ⓘ

5.1　Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PCA

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	1.13	6/1666 (0.4%)	1.81	44/2261 (1.9%)
1	L	1.13	6/1666 (0.4%)	1.81	44/2261 (1.9%)
2	B	1.12	5/1635 (0.3%)	1.67	29/2225 (1.3%)
2	H	1.12	5/1635 (0.3%)	1.67	29/2225 (1.3%)
All	All	1.13	22/6602 (0.3%)	1.74	146/8972 (1.6%)

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	4
1	L	0	4
2	B	0	4
2	H	0	4
All	All	0	16

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	142	LEU	C-N	-12.31	1.05	1.34
2	H	142	LEU	C-N	-12.29	1.05	1.34
2	B	54	GLY	C-N	11.50	1.60	1.34
2	H	54	GLY	C-N	11.48	1.60	1.34
1	A	148	TRP	C-N	-9.16	1.12	1.34

The worst 5 of 146 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	28	ASN	O-C-N	-14.55	99.42	122.70
1	L	28	ASN	O-C-N	-14.52	99.47	122.70
1	A	168	SER	C-N-CA	-10.79	94.74	121.70
1	L	168	SER	C-N-CA	-10.77	94.77	121.70
1	A	148	TRP	CD1-CG-CD2	10.26	114.51	106.30

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	42	GLU	Mainchain
1	L	152	ASN	Mainchain
1	L	28	ASN	Peptide
1	L	33	LEU	Mainchain
1	L	70	GLN	Mainchain

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	1630	0	1561	65	0
1	L	1630	0	1561	65	1
2	B	1603	0	1561	42	0
2	H	1603	0	1561	42	1
All	All	6466	0	6244	208	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 208 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:L:106:ILE:HD11	1:L:171:SER:OG	1.55	1.07
1:A:106:ILE:HD11	1:A:171:SER:OG	1.55	1.07
2:H:98:ARG:O	2:H:98:ARG:HG2	1.50	1.06
2:B:2:VAL:HG11	2:B:98:ARG:HH21	0.94	1.06
2:B:98:ARG:O	2:B:98:ARG:HG2	1.50	1.06

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:L:13:VAL:CG1	2:H:192:THR:CG2[4_466]	1.87	0.33

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	209/211 (99%)	187 (90%)	17 (8%)	5 (2%)	5	22
1	L	209/211 (99%)	187 (90%)	17 (8%)	5 (2%)	5	22
2	B	210/212 (99%)	186 (89%)	20 (10%)	4 (2%)	6	27
2	H	210/212 (99%)	186 (89%)	20 (10%)	4 (2%)	6	27
All	All	838/846 (99%)	746 (89%)	74 (9%)	18 (2%)	5	25

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	52	THR
2	H	56	ASP
1	A	52	THR
2	B	56	ASP
1	L	60	SER

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	183/183 (100%)	158 (86%)	25 (14%)	3	13
1	L	183/183 (100%)	158 (86%)	25 (14%)	3	13
2	B	181/181 (100%)	150 (83%)	31 (17%)	1	7
2	H	181/181 (100%)	150 (83%)	31 (17%)	1	7
All	All	728/728 (100%)	616 (85%)	112 (15%)	2	9

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
2	B	188	SER
1	A	129	THR
2	B	182	VAL
2	B	133	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	89	GLN
2	B	156	ASN
1	L	89	GLN
1	L	32	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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).

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PCA	H	1	2	7,8,9	1.84	1 (14%)	9,10,12	1.94	3 (33%)
2	PCA	B	1	2	7,8,9	1.85	1 (14%)	9,10,12	1.94	3 (33%)

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	PCA	H	1	2	-	0/0/11/13	0/1/1/1
2	PCA	B	1	2	-	0/0/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	PCA	CD-N	4.47	1.45	1.34
2	H	1	PCA	CD-N	4.42	1.45	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1	PCA	OE-CD-CG	-3.10	121.20	126.72
2	B	1	PCA	OE-CD-CG	-3.09	121.20	126.72
2	H	1	PCA	OE-CD-N	-2.89	118.70	124.96
2	B	1	PCA	OE-CD-N	-2.89	118.71	124.96
2	H	1	PCA	O-C-CA	-2.47	118.42	124.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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 ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	L	4
1	A	4
2	H	3
2	B	3

The worst 5 of 14 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	54:GLY	C	55:ASN	N	1.60
1	B	54:GLY	C	55:ASN	N	1.60
1	L	135:LEU	C	136:LEU	N	1.18
1	H	28:THR	C	29:PHE	N	1.18
1	A	135:LEU	C	136:LEU	N	1.18

6　Fit of model and data ⓘ

6.1　Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3　Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4　Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5　Other polymers ⓘ

EDS was not executed - this section is therefore empty.