wwPDB X-ray Structure Validation Summary Report (i)

May 16, 2020 – 07:19 pm BST

PDB ID	:	1DFB
Title	:	STRUCTURE OF A HUMAN MONOCLONAL ANTIBODY FAB FRAGMENT AGAINST GP41 OF HUMAN IMMUNODEFICIENCY VIRUS TYPE I
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Deposited on	:	1992-03-27
Resolution	:	2.70 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 following versions of software and data (see references (i)) were used in the production of this report:

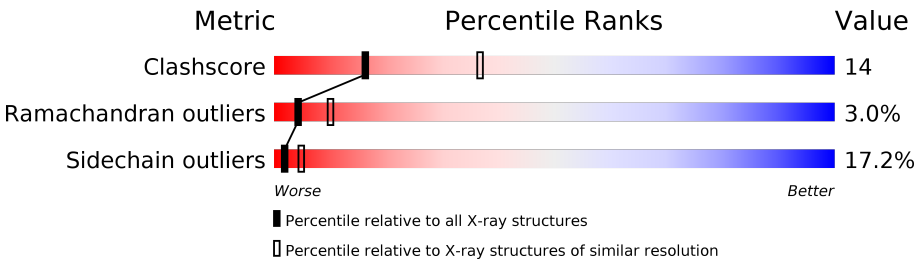
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.70 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	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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 >=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	L	212	54% 32% 11% •
2	H	229	53% 34% 10% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3354 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 IGG1-KAPPA 3D6 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	212	1636	1024	274	332	6	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	31	ARG	PRO	CONFLICT	GB 468243
L	34	ALA	PRO	CONFLICT	GB 468243
L	43	VAL	ALA	CONFLICT	GB 468243
L	76	SER	THR	CONFLICT	GB 468243
L	87	TYR	PHE	CONFLICT	GB 468243
L	90	GLN	HIS	CONFLICT	GB 468243
L	?	-	ARG	DELETION	GB 468243
L	93	SER	PRO	CONFLICT	GB 468243
L	94	TYR	TRP	CONFLICT	GB 468243
L	95	SER	THR	CONFLICT	GB 468243
L	98	PRO	GLN	CONFLICT	GB 468243
L	103	ASP	GLU	CONFLICT	GB 468243

- Molecule 2 is a protein called IGG1-KAPPA 3D6 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	229	1718	1083	288	338	9	0	0	0

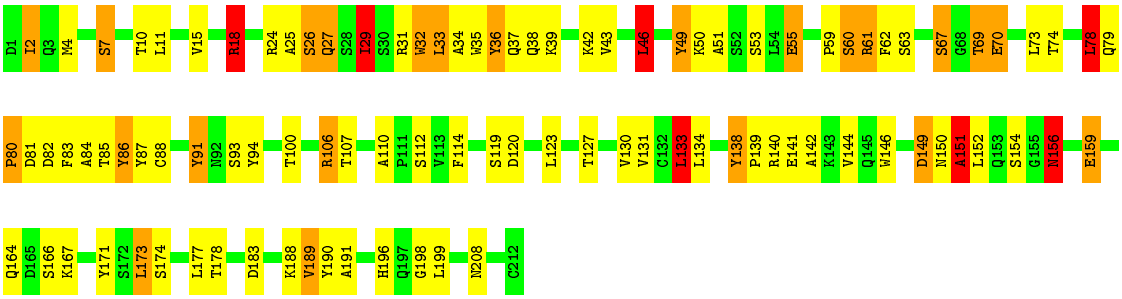
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

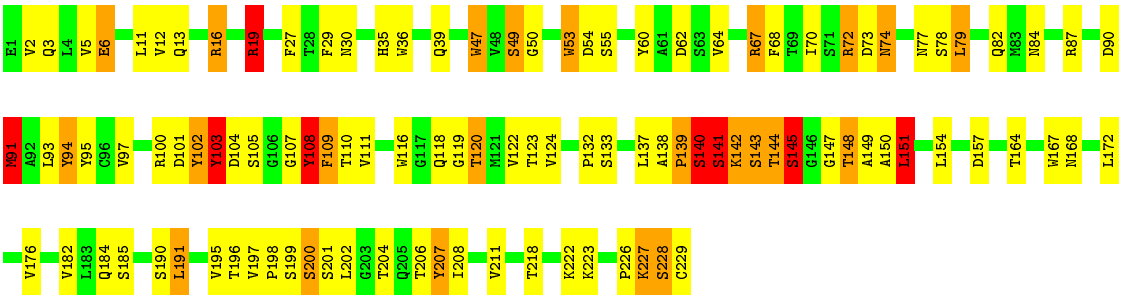
- Molecule 1: IGG1-KAPPA 3D6 FAB (LIGHT CHAIN)

Chain L:



- Molecule 2: IGG1-KAPPA 3D6 FAB (HEAVY CHAIN)

Chain H:



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	66.60Å 74.70Å 105.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.177 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3354	wwPDB-VP
Average B, all atoms ($Å^2$)	12.0	wwPDB-VP

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	L	1.05	2/1672 (0.1%)	1.92	47/2268 (2.1%)
2	H	1.12	3/1760 (0.2%)	2.07	65/2391 (2.7%)
All	All	1.09	5/3432 (0.1%)	2.00	112/4659 (2.4%)

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	L	0	2
2	H	0	2
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	211	VAL	CA-CB	5.86	1.67	1.54
1	L	60	SER	CA-CB	5.82	1.61	1.52
1	L	15	VAL	CA-CB	5.80	1.67	1.54
2	H	167	TRP	CG-CD2	-5.73	1.33	1.43
2	H	116	TRP	CG-CD2	-5.06	1.35	1.43

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	19	ARG	NE-CZ-NH1	11.57	126.09	120.30
2	H	72	ARG	NE-CZ-NH1	10.63	125.61	120.30
2	H	100	ARG	NE-CZ-NH1	10.46	125.53	120.30
2	H	19	ARG	NE-CZ-NH2	-10.22	115.19	120.30
2	H	72	ARG	NE-CZ-NH2	-9.94	115.33	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	102	TYR	Sidechain
2	H	108	TYR	Sidechain
1	L	7	SER	Peptide
1	L	94	TYR	Sidechain

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	L	1636	0	1591	44	0
2	H	1718	0	1668	55	0
All	All	3354	0	3259	95	0

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 95 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)
2:H:101:ASP:HA	2:H:110:THR:HA	1.29	1.10
1:L:2:ILE:HG12	1:L:29:ILE:HD11	1.49	0.93
1:L:159:GLU:HG2	1:L:173:LEU:HD21	1.62	0.80
2:H:139:PRO:HB3	2:H:151:LEU:HB2	1.70	0.73
2:H:35:HIS:HD2	2:H:47:TRP:HE1	1.38	0.71

There are no symmetry-related clashes.

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	L	210/212 (99%)	187 (89%)	16 (8%)	7 (3%)	4 8
2	H	227/229 (99%)	198 (87%)	23 (10%)	6 (3%)	5 13
All	All	437/441 (99%)	385 (88%)	39 (9%)	13 (3%)	4 10

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	156	ASN
2	H	140	SER
2	H	143	SER
1	L	26	SER
1	L	51	ALA

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	L	188/188 (100%)	156 (83%)	32 (17%)	2 5
2	H	191/191 (100%)	158 (83%)	33 (17%)	2 5
All	All	379/379 (100%)	314 (83%)	65 (17%)	2 5

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	178	THR
2	H	19	ARG
2	H	200	SER
1	L	183	ASP
2	H	5	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	153	GLN
2	H	39	GLN
1	L	197	GLN
1	L	92	ASN
1	L	156	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 carbohydrates 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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.