wwPDB X-ray Structure Validation Summary Report (i)

Jan 8, 2017 – 10:24 PM EST

PDB ID	:	5JQ6
Title	:	Crystal structure of ClfA in complex with the Fab fragment of Tefibazumab
Authors	:	Ganesh, V.K.
Deposited on	:	2016-05-04
Resolution	:	2.40 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

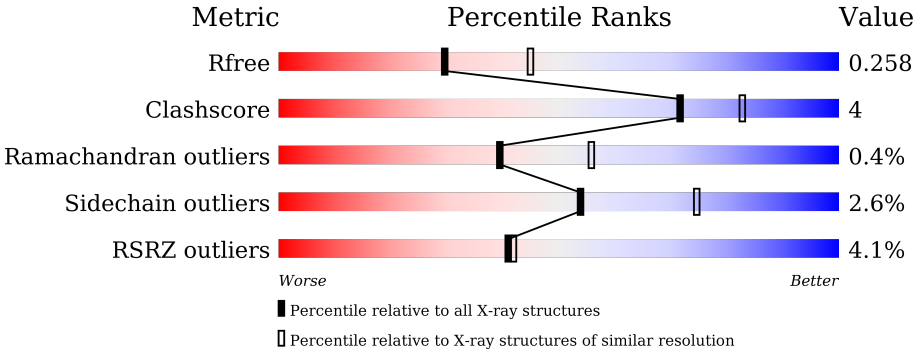
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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. 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	329	2%, 87%, 10%, •
2	H	222	5%, 82%, 8%, •, 8%
3	L	216	6%, 85%, 12%, • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5551 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 Clumping factor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	320	2393	1499	399	490	5	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	217	MET	-	initiating methionine	UNP G0XY13
A	218	ARG	-	expression tag	UNP G0XY13
A	219	GLY	-	expression tag	UNP G0XY13
A	220	SER	-	expression tag	UNP G0XY13
A	221	HIS	-	expression tag	UNP G0XY13
A	222	HIS	-	expression tag	UNP G0XY13
A	223	HIS	-	expression tag	UNP G0XY13
A	224	HIS	-	expression tag	UNP G0XY13
A	225	HIS	-	expression tag	UNP G0XY13
A	226	HIS	-	expression tag	UNP G0XY13
A	227	GLY	-	expression tag	UNP G0XY13
A	228	SER	-	expression tag	UNP G0XY13
A	327	CYS	ASP	engineered mutation	UNP G0XY13
A	541	CYS	LYS	engineered mutation	UNP G0XY13

- Molecule 2 is a protein called Tefibazumab FAB FRAGMENT HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	204	1464	931	246	281	6	0	0	0

- Molecule 3 is a protein called Tefibazumab FAB FRAGMENT LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	212	1489	934	249	300	6	0	0	0

- Molecule 4 is water.

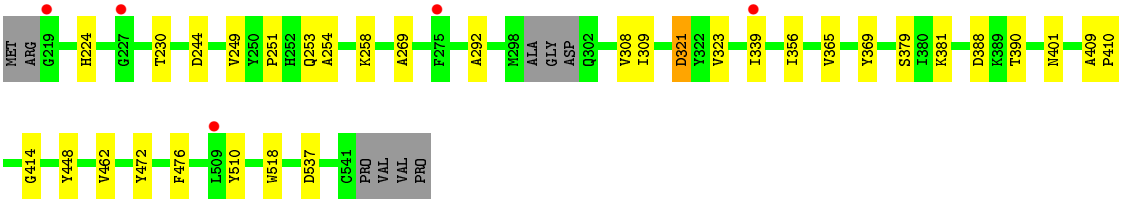
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	106	106	106	0	0
			Total	O		
4	H	60	60	60	0	0
			Total	O		
4	L	39	39	39	0	0

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 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.

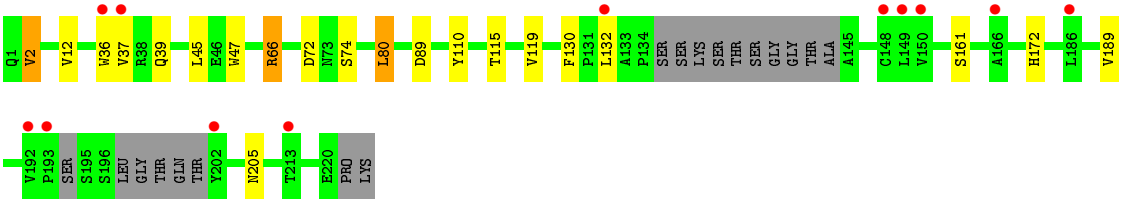
- Molecule 1: Clumping factor A

Chain A:



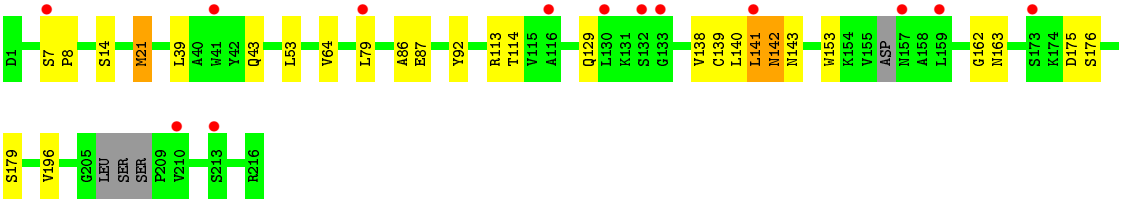
- Molecule 2: Tefibazumab FAB FRAGMENT HEAVY CHAIN

Chain H:



- Molecule 3: Tefibazumab FAB FRAGMENT LIGHT CHAIN

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	234.29Å 84.09Å 48.63Å 90.00° 98.90° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 19.89 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-2.40) 99.5 (19.89-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.208 , 0.259 0.209 , 0.258	Depositor DCC
R_{free} test set	1812 reflections (5.24%)	DCC
Wilson B-factor (Å^2)	58.0	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 54.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5551	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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	0.51	0/2443	0.64	0/3346
2	H	0.47	0/1502	0.64	1/2050 (0.0%)
3	L	0.50	0/1520	0.61	0/2078
All	All	0.50	0/5465	0.63	1/7474 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	66	ARG	NE-CZ-NH1	5.22	122.91	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2393	0	2222	17	0
2	H	1464	0	1310	14	0
3	L	1489	0	1271	17	0
4	A	106	0	0	1	0
4	H	60	0	0	0	0
4	L	39	0	0	1	0
All	All	5551	0	4803	44	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 4.

The worst 5 of 44 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)
3:L:113:ARG:NH1	3:L:114:THR:O	2.07	0.86
3:L:162:GLY:O	3:L:163:ASN:CG	2.25	0.74
3:L:21:MET:HE1	3:L:92:TYR:CB	2.31	0.61
3:L:141:LEU:HD23	3:L:141:LEU:N	2.18	0.57
1:A:249:VAL:HG23	1:A:365:VAL:HG11	1.87	0.56

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	A	316/329 (96%)	304 (96%)	12 (4%)	0	100	100
2	H	196/222 (88%)	190 (97%)	6 (3%)	0	100	100
3	L	206/216 (95%)	193 (94%)	10 (5%)	3 (2%)	13	17
All	All	718/767 (94%)	687 (96%)	28 (4%)	3 (0%)	39	56

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	175	ASP
3	L	143	ASN
3	L	196	VAL

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	258/288 (90%)	253 (98%)	5 (2%)	65	83
2	H	141/188 (75%)	139 (99%)	2 (1%)	74	88
3	L	136/191 (71%)	129 (95%)	7 (5%)	29	46
All	All	535/667 (80%)	521 (97%)	14 (3%)	54	74

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	80	LEU
3	L	14	SER
3	L	141	LEU
2	H	2	VAL
3	L	87	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	172	HIS

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)

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	320/329 (97%)	-0.17	5 (1%)	74	74	41, 61, 93, 176	0
2	H	204/222 (91%)	-0.01	12 (5%)	26	26	47, 66, 123, 145	0
3	L	212/216 (98%)	0.13	13 (6%)	25	25	45, 82, 103, 117	0
All	All	736/767 (95%)	-0.04	30 (4%)	41	42	41, 67, 110, 176	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	219	GLY	4.7
2	H	148	CYS	3.9
1	A	275	PHE	3.8
2	H	192	VAL	3.6
3	L	132	SER	3.5

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 carbohydrates 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.