wwPDB X-ray Structure Validation Summary Report (i)

Jan 10, 2017 – 09:45 AM EST

PDB ID	:	5T6P
Title	:	Crystal structure of therapeutic mAB AR20.5 in complex with MUC1 peptide
Authors	:	Brooks, C.L.; Movahedin, M.
Deposited on	:	2016-09-01
Resolution	:	1.97 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:

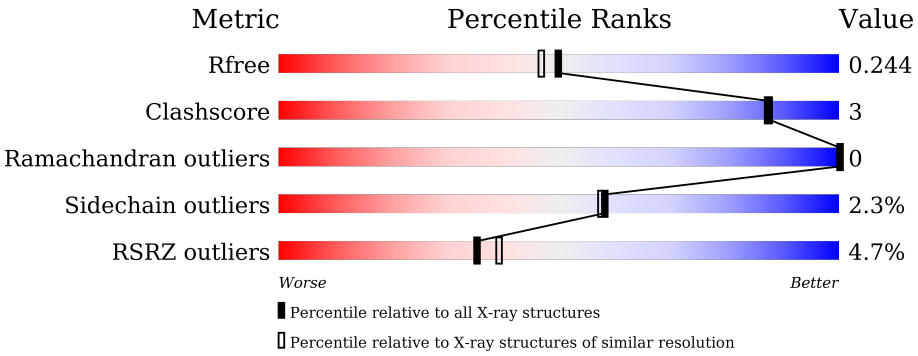
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 1.97 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	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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	216	91% 8%
1	C	216	94% 6%
2	B	215	7% 90% 5%
2	D	215	9% 87% 8%
3	E	8	63% 13% 25%
3	F	8	50% 13% 13% 25%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13470 atoms, of which 6436 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 Fab fragment AR20.5 - Light Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	216	Total	C	H	N	O	S	0	0	0
			3322	1059	1638	286	333	6			
1	C	216	Total	C	H	N	O	S	0	0	0
			3324	1059	1640	286	333	6			

- Molecule 2 is a protein called Fab Fragment - Heavy Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	206	Total	C	H	N	O	S	0	0	0
			3106	1006	1537	253	303	7			
2	D	206	Total	C	H	N	O	S	0	0	0
			3106	1006	1537	253	303	7			

- Molecule 3 is a protein called MUC1 Peptide Fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	6	Total	C	H	N	O	0	0	0
			87	27	42	9	9			
3	F	6	Total	C	H	N	O	0	0	0
			87	27	42	9	9			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	125	Total	O	0	0
			125	125		
4	B	91	Total	O	0	0
			91	91		
4	C	130	Total	O	0	0
			130	130		
4	D	82	Total	O	0	0
			82	82		

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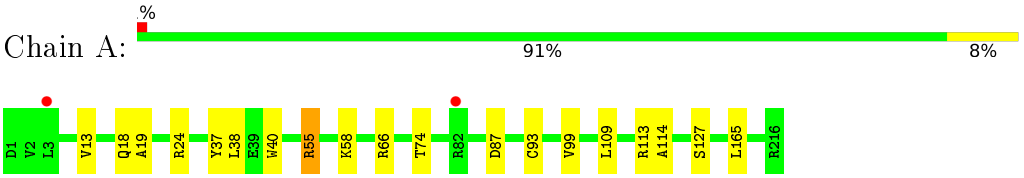
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	5	Total O 5 5	0	0
4	F	5	Total O 5 5	0	0

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.

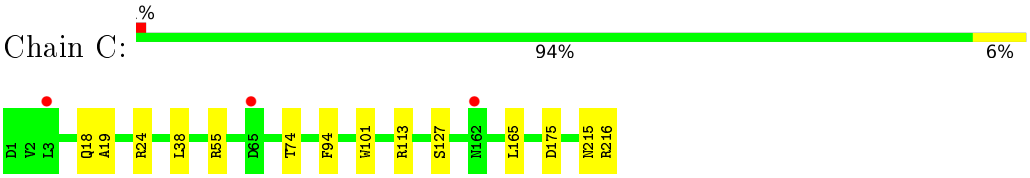
- Molecule 1: Fab fragment AR20.5 - Light Chain

Chain A:



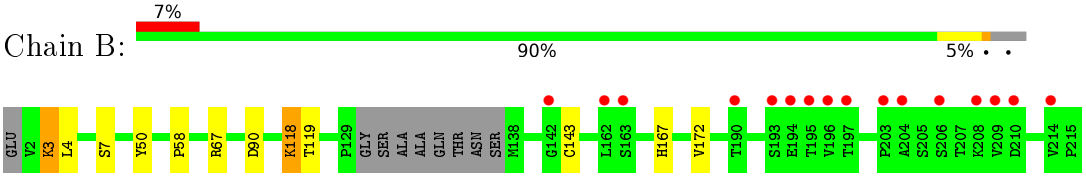
- Molecule 1: Fab fragment AR20.5 - Light Chain

Chain C:



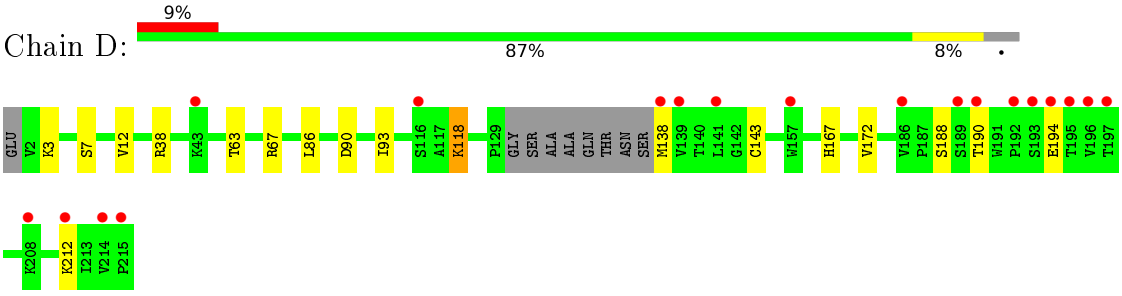
- Molecule 2: Fab Fragment - Heavy Chain

Chain B:



- Molecule 2: Fab Fragment - Heavy Chain

Chain D:



- Molecule 3: MUC1 Peptide Fragment

Chain E:

• Molecule 3: MUC1 Peptide Fragment

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	69.70Å 69.70Å 363.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.44 – 1.97 46.44 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.44-1.97) 99.8 (46.44-1.97)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.11 (at 1.97Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.221 , 0.232 0.230 , 0.244	Depositor DCC
R_{free} test set	3606 reflections (4.87%)	DCC
Wilson B-factor (Å^2)	32.3	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 35.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.066 for -h,-k,l	Xtriage
Reported twinning fraction	0.100 for -h,-k,l	Depositor
Outliers	0 of 74059 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13470	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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

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	0.31	0/1724	0.52	0/2338
1	C	0.29	0/1724	0.51	0/2338
2	B	0.31	0/1614	0.53	0/2208
2	D	0.32	0/1614	0.51	0/2208
3	E	0.33	0/46	0.54	0/63
3	F	0.24	0/46	0.52	0/63
All	All	0.31	0/6768	0.52	0/9218

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1684	1638	1640	11	0
1	C	1684	1640	1640	8	0
2	B	1569	1537	1537	6	0
2	D	1569	1537	1537	9	0
3	E	45	42	42	3	0
3	F	45	42	42	4	0
4	A	125	0	0	0	1
4	B	91	0	0	1	0
4	C	130	0	0	0	2
4	D	82	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	5	0	0	0	0
4	F	5	0	0	0	0
All	All	7034	6436	6438	34	3

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 3.

The worst 5 of 34 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:A:58:LYS:NZ	3:F:3:ASP:OD2	2.00	0.94
2:D:118:LYS:NZ	4:D:302:HOH:O	2.18	0.65
1:A:99:VAL:HG11	3:F:8:PRO:HB3	1.83	0.61
3:F:3:ASP:OD1	3:F:3:ASP:N	2.35	0.56
2:B:67:ARG:NH2	2:B:90:ASP:OD2	2.39	0.55

All (3) 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)
4:C:378:HOH:O	4:C:393:HOH:O[4_545]	1.96	0.24
4:A:376:HOH:O	4:A:385:HOH:O[6_865]	2.00	0.20
4:C:356:HOH:O	4:C:390:HOH:O[4_655]	2.08	0.12

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	214/216 (99%)	209 (98%)	5 (2%)	0	100	100
1	C	214/216 (99%)	211 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	202/215 (94%)	200 (99%)	2 (1%)	0	100	100
2	D	202/215 (94%)	200 (99%)	2 (1%)	0	100	100
3	E	4/8 (50%)	4 (100%)	0	0	100	100
3	F	4/8 (50%)	4 (100%)	0	0	100	100
All	All	840/878 (96%)	828 (99%)	12 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	193/193 (100%)	190 (98%)	3 (2%)	70	71
1	C	193/193 (100%)	191 (99%)	2 (1%)	82	84
2	B	178/184 (97%)	173 (97%)	5 (3%)	51	48
2	D	178/184 (97%)	173 (97%)	5 (3%)	51	48
3	E	5/6 (83%)	4 (80%)	1 (20%)	1	0
3	F	5/6 (83%)	4 (80%)	1 (20%)	1	0
All	All	752/766 (98%)	735 (98%)	17 (2%)	58	57

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	167	HIS
1	C	38	LEU
2	D	143	CYS
2	B	143	CYS
2	D	167	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules 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^{th} 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	216/216 (100%)	0.41	2 (0%) 85 87	21, 36, 59, 87	0
1	C	216/216 (100%)	0.34	3 (1%) 78 80	19, 36, 67, 93	0
2	B	206/215 (95%)	0.60	16 (7%) 16 19	24, 44, 85, 119	0
2	D	206/215 (95%)	0.61	19 (9%) 11 13	21, 45, 89, 127	0
3	E	6/8 (75%)	0.07	0 100 100	31, 37, 39, 49	0
3	F	6/8 (75%)	0.36	0 100 100	28, 34, 38, 47	0
All	All	856/878 (97%)	0.49	40 (4%) 35 39	19, 40, 79, 127	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	195	THR	7.5
2	D	196	VAL	4.6
2	B	203	PRO	4.6
2	B	195	THR	4.2
2	B	204	ALA	3.8

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 (i)

There are no such residues in this entry.