wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 10:00 PM GMT

PDB ID	:	1RMF
Title	:	STRUCTURES OF A MONOCLONAL ANTI-ICAM-1 ANTIBODY R6.5 FRAGMENT AT 2.8 ANGSTROMS RESOLUTION
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Deposited on	:	1994-12-16
Resolution	:	2.80 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:

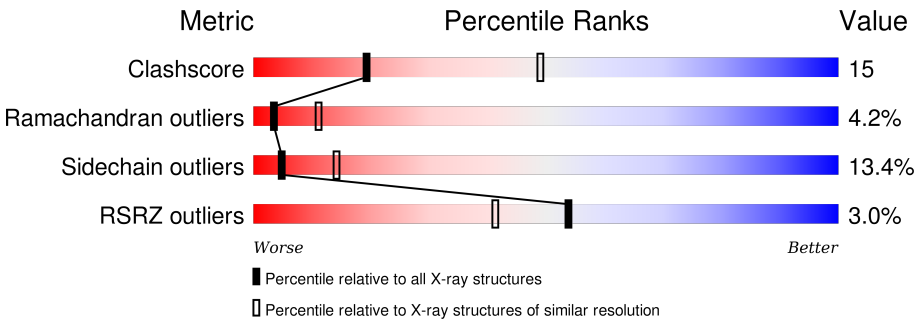
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.80 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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	L	219	72% 24% • •
2	H	216	6% 52% 33% 13% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4208 atoms, of which 850 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 IGG2A-KAPPA R6.5 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	L	219	2095	1052	404	290	342	7	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	7	SER	THR	CONFLICT	PIR S16112
L	36	ASN	THR	CONFLICT	PIR S16112
L	39	HIS	TYR	CONFLICT	PIR S16112
L	45	SER	PRO	CONFLICT	PIR S16112
L	48	ALA	SER	CONFLICT	PIR S16112
L	51	LEU	PRO	CONFLICT	PIR S16112
L	55	LYS	ARG	CONFLICT	PIR S16112
L	94	SER	PHE	CONFLICT	PIR S16112
L	96	SER	GLY	CONFLICT	PIR S16112
L	101	LEU	TYR	CONFLICT	PIR S16112
L	108	LYS	ARG	CONFLICT	PIR S16112

- Molecule 2 is a protein called IGG2A-KAPPA R6.5 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	H	216	1996	1034	368	265	324	5	0	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	6	GLN	GLU	CONFLICT	GB 2852989
H	30	ILE	THR	CONFLICT	GB 2852989
H	33	ALA	PRO	CONFLICT	GB 2852989
H	34	ILE	MET	CONFLICT	GB 2852989
H	39	GLU	GLN	CONFLICT	GB 2852989

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Chain	Residue	Modelled	Actual	Comment	Reference
H	53	ALA	THR	CONFLICT	GB 2852989
H	55	SER	TYR	CONFLICT	GB 2852989
H	57	ASP	ASN	CONFLICT	GB 2852989
H	62	GLN	ARG	CONFLICT	GB 2852989
H	63	LYS	ASN	CONFLICT	GB 2852989
H	77	ASN	SER	CONFLICT	GB 2852989
H	81	LEU	MET	CONFLICT	GB 2852989
H	99	GLY	-	INSERTION	GB 2852989
H	100	GLY	-	INSERTION	GB 2852989
H	101	TRP	-	INSERTION	GB 2852989
H	103	LEU	ASN	CONFLICT	GB 2852989
H	?	-	ASP	DELETION	GB 2852989
H	?	-	GLY	DELETION	GB 2852989
H	?	-	TYR	DELETION	GB 2852989
H	?	-	TYR	DELETION	GB 2852989
H	105	SER	GLY	CONFLICT	GB 2852989
H	107	ASP	ALA	CONFLICT	GB 2852989
H	114	THR	LEU	CONFLICT	GB 2852989
H	115	LEU	VAL	CONFLICT	GB 2852989
H	119	SER	ALA	CONFLICT	GB 2852989
H	128	THR	TYR	CONFLICT	GB 2852989
H	146	VAL	CYS	CONFLICT	GB 2852989

- Molecule 3 is water.

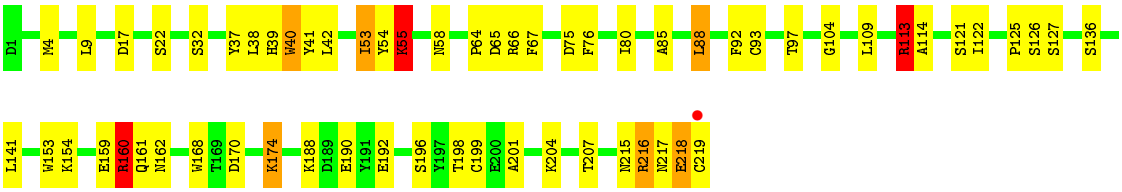
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	H	O		
3	H	18	54	36	18	0	0
			Total	H	O		
3	L	21	63	42	21	0	0

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.

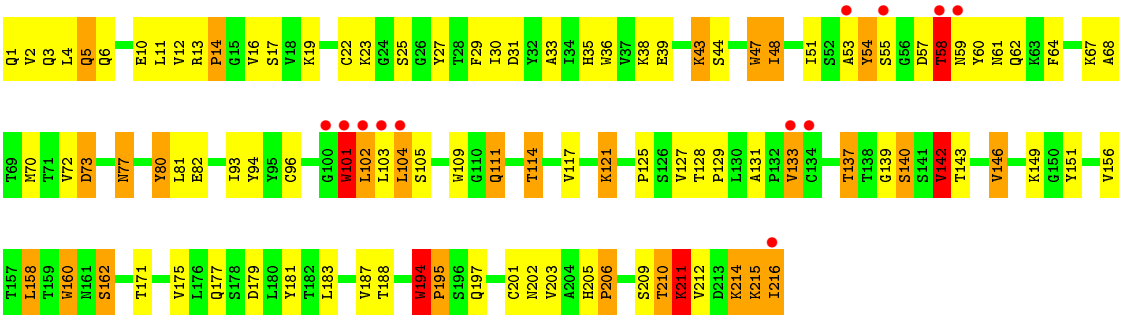
- Molecule 1: IGG2A-KAPPA R6.5 FAB (LIGHT CHAIN)

Chain L:



- Molecule 2: IGG2A-KAPPA R6.5 FAB (HEAVY CHAIN)

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	40.36Å 137.76Å 91.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.50 – 2.80 41.03 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.50-2.80) 82.9 (41.03-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.17 (at 2.69Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.188 , (Not available) 0.207 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	37.4	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 79.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 12179 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	4208	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	L	0.93	0/1728	1.47	20/2342 (0.9%)
2	H	1.03	1/1668 (0.1%)	1.63	27/2278 (1.2%)
All	All	0.98	1/3396 (0.0%)	1.55	47/4620 (1.0%)

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
2	H	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	44	SER	CA-CB	5.22	1.60	1.52

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	101	TRP	CD1-CG-CD2	10.57	114.76	106.30
2	H	211	LYS	N-CA-C	10.12	138.33	111.00
1	L	168	TRP	CD1-CG-CD2	9.37	113.79	106.30
2	H	36	TRP	CD1-CG-CD2	9.20	113.66	106.30
2	H	109	TRP	CD1-CG-CD2	9.09	113.57	106.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	131	ALA	Peptide
2	H	181	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	H	194	TRP	Peptide
2	H	215	LYS	Mainchain

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	1691	404	1636	28	0
2	H	1628	368	1607	79	0
3	H	18	36	0	0	0
3	L	21	42	0	0	0
All	All	3358	850	3243	97	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 15.

The worst 5 of 97 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:146:VAL:HG11	2:H:201:CYS:SG	1.97	1.04
2:H:202:ASN:HA	2:H:211:LYS:HB3	1.49	0.95
2:H:146:VAL:HG21	2:H:201:CYS:SG	2.20	0.81
2:H:13:ARG:HG2	2:H:14:PRO:HD2	1.61	0.81
2:H:4:LEU:HD22	2:H:22:CYS:SG	2.22	0.79

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	217/219 (99%)	193 (89%)	18 (8%)	6 (3%)	6 21
2	H	214/216 (99%)	175 (82%)	27 (13%)	12 (6%)	2 6
All	All	431/435 (99%)	368 (85%)	45 (10%)	18 (4%)	3 11

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	216	ARG
1	L	217	ASN
2	H	43	LYS
2	H	62	GLN
2	H	133	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	L	196/196 (100%)	175 (89%)	21 (11%)	8 24
2	H	185/185 (100%)	155 (84%)	30 (16%)	3 8
All	All	381/381 (100%)	330 (87%)	51 (13%)	5 14

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	10	GLU
2	H	31	ASP
2	H	211	LYS
2	H	14	PRO
2	H	48	ILE

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

Mol	Chain	Res	Type
2	H	35	HIS
2	H	202	ASN
2	H	59	ASN
1	L	215	ASN
2	H	177	GLN

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	L	219/219 (100%)	-0.59	1 (0%)	91	88	2, 12, 23, 36	0
2	H	216/216 (100%)	-0.24	12 (5%)	28	18	2, 15, 27, 32	0
All	All	435/435 (100%)	-0.42	13 (2%)	54	41	2, 13, 25, 36	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	219	CYS	6.3
2	H	53	ALA	5.2
2	H	104	LEU	4.5
2	H	58	THR	4.2
2	H	103	LEU	4.2

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.