



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5I1I
Title : CRYSTAL STRUCTURE OF HUMAN GERMLINE ANTIBODY IGHV3-53/IGKV4-1
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Deposited on : 2016-02-05
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
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-20027939

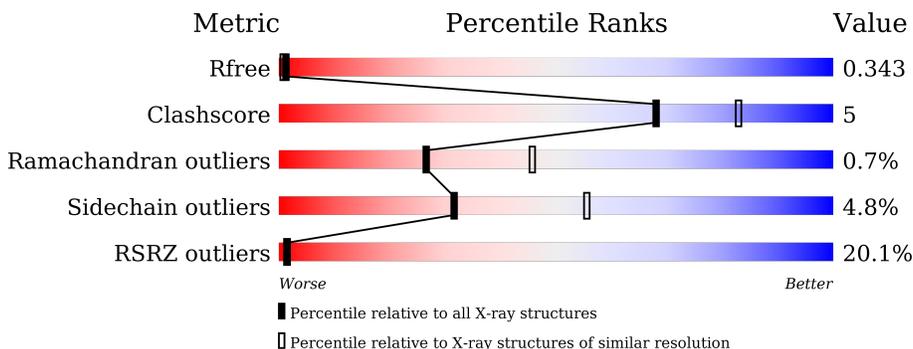
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 $\leq 5\%$. 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	220	
2	H	227	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3239 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 FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	219	1693	1062	282	344	5	0	0	0

- Molecule 2 is a protein called FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	209	1525	965	256	298	6	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	10	Total	O	0	0
			10	10		
3	H	11	Total	O	0	0
			11	11		

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	68.05Å 68.05Å 95.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.50 28.16 – 2.51	Depositor EDS
% Data completeness (in resolution range)	98.3 (15.00-2.50) 98.7 (28.16-2.51)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.18 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.250 , 0.337 0.255 , 0.343	Depositor DCC
R_{free} test set	844 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 67.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l 0.049 for h,-h-k,-l 0.033 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3239	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	L	0.34	0/1730	0.55	0/2352
2	H	0.34	0/1560	0.58	0/2129
All	All	0.34	0/3290	0.56	0/4481

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 [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	1693	0	1641	18	0
2	H	1525	0	1471	14	0
3	H	11	0	0	0	0
3	L	10	0	0	0	0
All	All	3239	0	3112	30	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 5.

All (30) 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:12:ILE:HD12	2:H:85:LEU:HD13	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:204:HIS:CD2	1:L:206:GLY:H	2.14	0.66
1:L:34:ASN:HD22	1:L:36:LYS:H	1.49	0.61
1:L:55:TYR:HB2	2:H:105:LEU:HD22	1.86	0.58
2:H:53:SER:HA	2:H:71:ARG:HH12	1.68	0.58
1:L:151:LYS:HB3	1:L:203:THR:HB	1.85	0.57
2:H:7:THR:HG23	2:H:21:SER:HB2	1.85	0.57
1:L:168:SER:HB2	2:H:172:PRO:HG2	1.89	0.55
1:L:126:PRO:HG3	1:L:136:ALA:HB1	1.89	0.54
1:L:39:LEU:HD13	1:L:77:PHE:CD1	2.43	0.53
1:L:11:LEU:HD21	1:L:19:ALA:HB1	1.93	0.49
2:H:12:ILE:HD11	2:H:114:VAL:HG13	1.94	0.49
1:L:12:ALA:O	1:L:113:LYS:HD3	2.11	0.49
2:H:200:ILE:HA	2:H:214:LYS:O	2.14	0.48
2:H:4:LEU:O	2:H:109:GLY:HA3	2.15	0.47
2:H:108:TRP:N	2:H:108:TRP:CD1	2.83	0.46
1:L:39:LEU:HD13	1:L:77:PHE:CE1	2.50	0.46
2:H:33:TYR:HB2	2:H:98:TYR:HB2	1.96	0.46
1:L:113:LYS:HE2	1:L:113:LYS:HB3	1.81	0.46
1:L:67:ARG:HB2	1:L:82:SER:O	2.15	0.45
2:H:59:TYR:OH	2:H:68:THR:HA	2.17	0.45
1:L:204:HIS:HD2	1:L:206:GLY:H	1.64	0.45
1:L:37:ASN:O	1:L:56:TRP:HA	2.17	0.44
1:L:67:ARG:CZ	1:L:85:GLN:HG3	2.47	0.44
1:L:57:ALA:HB1	1:L:77:PHE:HE2	1.83	0.44
2:H:38:ARG:HG2	2:H:48:VAL:CG2	2.49	0.43
2:H:33:TYR:CD2	2:H:52:TYR:HD1	2.39	0.41
1:L:21:ILE:HD12	1:L:79:LEU:HD23	2.01	0.41
1:L:37:ASN:HB2	1:L:57:ALA:HB2	2.03	0.41
2:H:155:VAL:HG23	2:H:183:LEU:HD21	2.03	0.40

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	217/220 (99%)	204 (94%)	12 (6%)	1 (0%)	34	55
2	H	205/227 (90%)	183 (89%)	20 (10%)	2 (1%)	19	34
All	All	422/447 (94%)	387 (92%)	32 (8%)	3 (1%)	26	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	73	ASN
1	L	57	ALA
2	H	76	ASN

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	193/195 (99%)	183 (95%)	10 (5%)	29	51
2	H	164/191 (86%)	157 (96%)	7 (4%)	35	61
All	All	357/386 (92%)	340 (95%)	17 (5%)	31	55

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	14	SER
1	L	18	ARG
1	L	34	ASN
1	L	39	LEU
1	L	71	SER
1	L	113	LYS
1	L	153	GLN
1	L	160	LEU
1	L	182	SER
1	L	205	GLN
2	H	34	MET
2	H	38	ARG
2	H	77	THR

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Mol	Chain	Res	Type
2	H	105	LEU
2	H	108	TRP
2	H	113	LEU
2	H	121	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	27	GLN
1	L	34	ASN
1	L	153	GLN
1	L	204	HIS
2	H	76	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

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, 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	219/220 (99%)	1.06	38 (17%) 2 2	59, 85, 110, 125	0
2	H	209/227 (92%)	1.36	48 (22%) 1 1	58, 88, 133, 166	0
All	All	428/447 (95%)	1.21	86 (20%) 1 1	58, 87, 122, 166	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	30	SER	10.7
2	H	77	THR	5.9
2	H	102	TYR	5.9
2	H	65	GLY	5.5
2	H	72	ASP	5.4
2	H	105	LEU	5.4
2	H	79	TYR	5.1
2	H	70	SER	5.0
2	H	23	ALA	4.6
2	H	74	SER	4.6
2	H	78	LEU	4.5
1	L	174	SER	4.5
2	H	73	ASN	4.5
2	H	56	SER	4.4
2	H	33	TYR	4.2
2	H	4	LEU	4.1
2	H	75	LYS	4.0
2	H	64	LYS	4.0
1	L	175	LYS	3.9
2	H	198	THR	3.9
1	L	2	ILE	3.9
2	H	26	GLY	3.9
2	H	55	GLY	3.8
2	H	52	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
2	H	58	TYR	3.8
2	H	50	VAL	3.6
2	H	27	PHE	3.3
2	H	28	THR	3.3
1	L	72	GLY	3.3
1	L	139	VAL	3.3
1	L	76	ASP	3.2
2	H	103	GLY	3.2
2	H	192	SER	3.2
1	L	86	ALA	3.1
2	H	71	ARG	3.1
2	H	31	SER	3.1
1	L	56	TRP	3.0
2	H	51	ILE	3.0
1	L	33	SER	2.9
2	H	100	GLY	2.9
1	L	39	LEU	2.9
2	H	196	THR	2.8
1	L	141	LEU	2.8
2	H	5	VAL	2.8
1	L	85	GLN	2.8
2	H	61	ASP	2.8
1	L	1	ASP	2.8
1	L	97	TYR	2.7
1	L	184	THR	2.7
1	L	16	GLY	2.7
2	H	76	ASN	2.6
1	L	15	LEU	2.6
2	H	101	ILE	2.6
1	L	158	ASN	2.6
1	L	35	ASN	2.5
2	H	104	GLU	2.5
1	L	196	LYS	2.5
2	H	45	LEU	2.5
2	H	147	VAL	2.5
2	H	193	SER	2.4
1	L	24	LYS	2.4
1	L	14	SER	2.4
2	H	195	GLY	2.4
1	L	55	TYR	2.4
1	L	193	GLU	2.4
1	L	183	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	82	SER	2.3
1	L	87	GLU	2.3
2	H	17	SER	2.3
2	H	161	SER	2.2
1	L	22	ASN	2.2
1	L	41	TRP	2.2
2	H	12	ILE	2.2
2	H	189	VAL	2.1
1	L	73	SER	2.1
1	L	62	SER	2.1
1	L	65	PRO	2.1
1	L	52	LEU	2.1
2	H	54	GLY	2.1
1	L	40	ALA	2.1
2	H	194	LEU	2.1
2	H	146	LEU	2.0
1	L	34	ASN	2.0
1	L	54	ILE	2.0
1	L	197	VAL	2.0
1	L	104	PHE	2.0

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.