



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:44 AM GMT

PDB ID : 2IG2
Title : DIR PRIMAERSTRUKTUR DES KRISTALLISIERBAREN MONOKLONALEN IMMUNOGLOBULINS IGG1 KOL. II. AMINOSAEURESEQUENZ DER L-KETTE, LAMBDA-TYP, SUBGRUPPE I (GERMAN)
Authors : Marquart, M.; Huber, R.
Deposited on : 1989-04-18
Resolution : 3.00 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

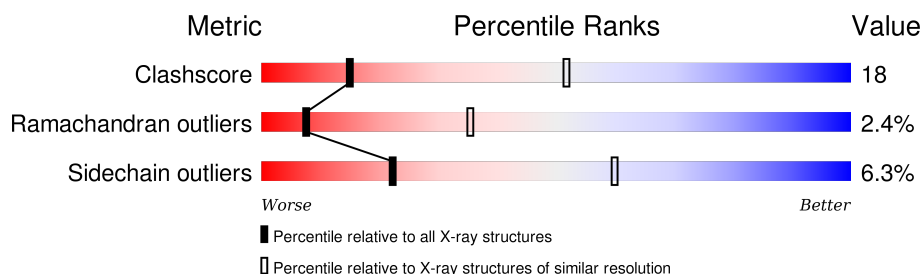
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	216	
2	H	455	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3379 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-LAMBDA KOL FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	216	Total	C	N	O	S	54	0	0
			1602	999	269	327	7			

- Molecule 2 is a protein called IGG1-LAMBDA KOL FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	239	Total	C	N	O	S	53	0	1
			1777	1113	305	348	11			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	6	GLN	GLU	CONFLICT	UNP P01772
H	23	SER	ALA	CONFLICT	UNP P01772
H	24	SER	ALA	CONFLICT	UNP P01772
H	28	ILE	THR	CONFLICT	UNP P01772
H	31	SER	ASN	CONFLICT	UNP P01772
H	33	ALA	GLY	CONFLICT	UNP P01772
H	35	TYR	HIS	CONFLICT	UNP P01772
H	50	ILE	ALA	CONFLICT	UNP P01772
H	53	ASP	TYR	CONFLICT	UNP P01772
H	57	ASP	ASN	CONFLICT	UNP P01772
H	58	GLN	LYS	CONFLICT	UNP P01772
H	59	HIS	TYR	CONFLICT	UNP P01772
H	73	ASN	ASP	CONFLICT	UNP P01772
H	74	ASP	ASN	CONFLICT	UNP P01772
H	80	PHE	TYR	CONFLICT	UNP P01772
H	81	LEU	MET	CONFLICT	UNP P01772
H	84	ASP	ASN	CONFLICT	UNP P01772
H	88	PRO	ALA	CONFLICT	UNP P01772
H	92	GLY	ALA	CONFLICT	UNP P01772
H	95	PHE	TYR	CONFLICT	UNP P01772

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Chain	Residue	Modelled	Actual	Comment	Reference
H	99	ASP	GLU	CONFLICT	UNP P01772
H	101	GLY	ARG	CONFLICT	UNP P01772
H	101A	HIS	TRP	CONFLICT	UNP P01772
H	101B	GLY	VAL	CONFLICT	UNP P01772
H	101C	PHE	ARG	CONFLICT	UNP P01772
H	101D	CYS	TYR	CONFLICT	UNP P01772
H	102	SER	THR	CONFLICT	UNP P01772
H	103	SER	THR	CONFLICT	UNP P01772
H	104	ALA	VAL	CONFLICT	UNP P01772
H	104A	SER	THR	CONFLICT	UNP P01772
H	104B	CYS	THR	CONFLICT	UNP P01772
H	104C	PHE	ILE	CONFLICT	UNP P01772
H	?	-	TYR	DELETION	UNP P01772
H	?	-	TYR	DELETION	UNP P01772
H	105	PRO	PHE	CONFLICT	UNP P01772
H	113	PRO	LEU	CONFLICT	UNP P01772
H	153	GLN	GLU	CONFLICT	UNP P01772
H	273	GLN	GLU	CONFLICT	UNP P01772
H	284	GLN	GLU	CONFLICT	UNP P01772
H	295	GLN	GLU	CONFLICT	UNP P01772
H	313	ASN	ASP	CONFLICT	UNP P01772
H	316	ASP	ASN	CONFLICT	UNP P01772

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	135.60 Å 135.60 Å 82.10 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	EREF	Depositor
R, R_{free}	0.207 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3379	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

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	L	1.09	4/1640 (0.2%)	1.38	9/2238 (0.4%)
2	H	1.08	5/1825 (0.3%)	1.31	5/2486 (0.2%)
All	All	1.09	9/3465 (0.3%)	1.35	14/4724 (0.3%)

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	24
2	H	0	22
All	All	0	46

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	108	TRP	NE1-CE2	-8.23	1.26	1.37
2	H	52	TRP	NE1-CE2	-8.15	1.26	1.37
2	H	47	TRP	NE1-CE2	-8.09	1.27	1.37
1	L	90	TRP	NE1-CE2	-7.91	1.27	1.37
1	L	150	TRP	NE1-CE2	-7.74	1.27	1.37

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	60	ARG	NE-CZ-NH1	8.84	124.72	120.30
2	H	72	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	L	170	SER	O-C-N	6.67	133.37	122.70
2	H	207	PRO	N-CA-CB	6.07	110.58	103.30
1	L	170	SER	N-CA-CB	5.71	119.07	110.50

There are no chirality outliers.

5 of 46 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	1	GLN	Mainchain
1	L	37	GLN	Sidechain
1	L	38	LEU	Mainchain
1	L	53	ARG	Mainchain
1	L	6	GLN	Sidechain

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	L	1602	0	1559	53	266
2	H	1777	0	1706	64	194
All	All	3379	0	3265	112	273

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 18.

The worst 5 of 112 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:9:GLY:HA3	2:H:18:LEU:HD22	1.51	0.90
2:H:164:LEU:HD21	2:H:187:VAL:HG21	1.61	0.83
2:H:122:LYS:HD2	2:H:180:LEU:HD21	1.60	0.82
1:L:196:GLN:HB3	1:L:205:GLU:HG2	1.66	0.78
1:L:183:THR:HG22	1:L:185:GLU:HG3	1.66	0.77

The worst 5 of 273 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)
1:L:200:GLU:C	2:H:188:THR:C[6_556]	0.33	1.87
1:L:108:LEU:CG	2:H:162:GLY:O[6_556]	0.43	1.77
1:L:111:PRO:CA	2:H:186:VAL:CA[6_556]	0.51	1.69
1:L:111:PRO:CD	2:H:186:VAL:N[6_556]	0.62	1.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:169:GLN:CD	1:L:171:ASN:O[6_556]	0.63	1.57

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	214/216 (99%)	176 (82%)	32 (15%)	6 (3%)	6	30
2	H	237/455 (52%)	203 (86%)	29 (12%)	5 (2%)	9	40
All	All	451/671 (67%)	379 (84%)	61 (14%)	11 (2%)	7	35

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	77	LEU
1	L	213	CYS
2	H	137	SER
2	H	166	SER
1	L	49	ARG

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	180/180 (100%)	170 (94%)	10 (6%)	26	65
2	H	202/402 (50%)	188 (93%)	14 (7%)	19	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	382/582 (66%)	358 (94%)	24 (6%)	22	60

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	3	GLN
2	H	52	TRP
2	H	214	LYS
2	H	13	GLN
2	H	22	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	77	ASN
2	H	82	GLN
2	H	202	ASN
2	H	73	ASN
2	H	153	GLN

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 [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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.