wwPDB X-ray Structure Validation Summary Report (i)

May 29, 2024 – 05:23 PM EDT

PDB ID	:	2FB4
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	:	1.90 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

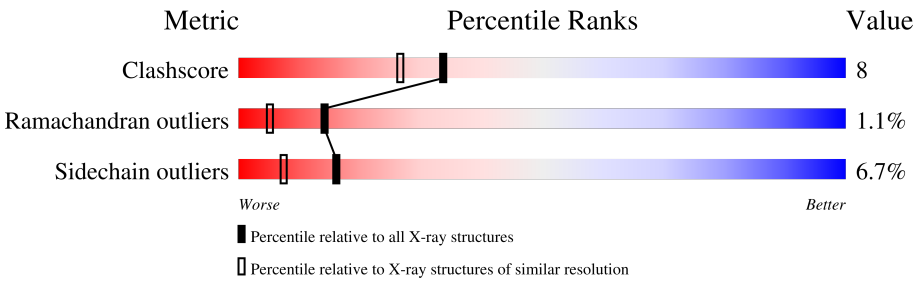
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.90 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	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	216	68% 26% 5%
2	H	229	73% 23% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3417 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
			Total	C	N	O	S			
1	L	216	1602	999	269	327	7	93	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	229	1710	1073	292	336	9	77	0	0

There are 37 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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	L	37	37	37	0	0
			Total	O		
3	H	68	68	68	0	0

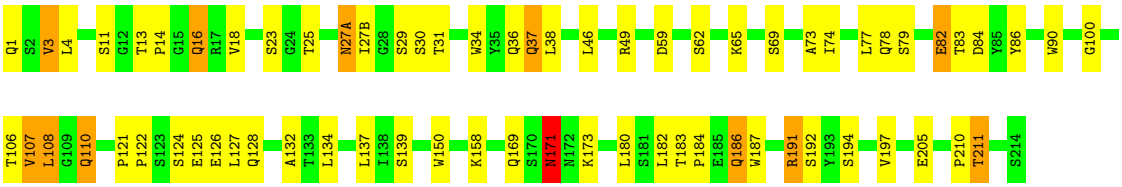
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

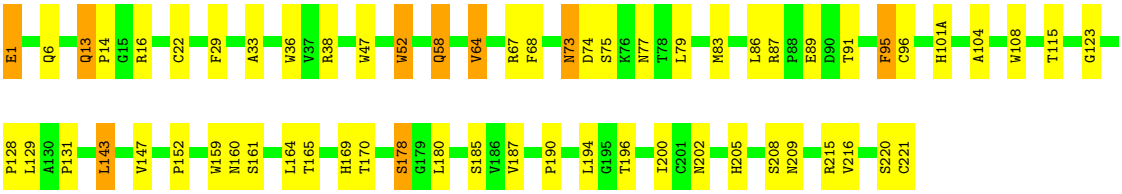
• Molecule 1: IGG1-LAMBDA KOL FAB (LIGHT CHAIN)

Chain L: 68% 26% 5%



• Molecule 2: IGG1-LAMBDA KOL FAB (HEAVY CHAIN)

Chain H: 73% 23% •



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.30Å 138.90Å 40.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	EREF	Depositor
R, R_{free}	0.189 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3417	wwPDB-VP
Average B, all atoms ($Å^2$)	17.0	wwPDB-VP

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	1.06	4/1640 (0.2%)	1.22	4/2238 (0.2%)
2	H	1.08	5/1755 (0.3%)	1.16	3/2387 (0.1%)
All	All	1.07	9/3395 (0.3%)	1.18	7/4625 (0.2%)

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	16
2	H	0	14
All	All	0	30

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	187	TRP	NE1-CE2	-7.92	1.27	1.37
1	L	90	TRP	NE1-CE2	-7.89	1.27	1.37
1	L	150	TRP	NE1-CE2	-7.80	1.27	1.37
2	H	36	TRP	NE1-CE2	-7.72	1.27	1.37
2	H	52	TRP	NE1-CE2	-7.69	1.27	1.37

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	87	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	L	191	ARG	N-CA-CB	7.09	123.37	110.60
1	L	197	VAL	CA-CB-CG2	5.84	119.66	110.90
1	L	171	ASN	N-CA-CB	-5.81	100.15	110.60
2	H	38	ARG	NE-CZ-NH2	-5.80	117.40	120.30

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	1	GLN	Mainchain
1	L	16	GLN	Sidechain
1	L	29	SER	Mainchain
1	L	37	GLN	Sidechain
1	L	74	ILE	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	1602	0	1559	29	3
2	H	1710	0	1644	23	3
3	H	68	0	0	1	0
3	L	37	0	0	0	0
All	All	3417	0	3203	52	4

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 8.

The worst 5 of 52 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:L:82:GLU:HG3	1:L:107:VAL:HG23	1.44	0.99
1:L:77:LEU:HD21	1:L:107:VAL:HG22	1.43	0.97
1:L:27(A):ASN:HD22	1:L:27(B):ILE:H	1.19	0.90
1:L:25:THR:H	1:L:27(A):ASN:HD21	1.26	0.79
2:H:6:GLN:HE21	2:H:96:CYS:H	1.30	0.78

All (4) 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:211:THR:CG2	2:H:101(A):HIS:CG[3_656]	1.83	0.37
1:L:65:LYS:O	1:L:110:GLN:NE2[2_665]	1.99	0.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:211:THR:CG2	2:H:101(A):HIS:CB[3_656]	2.15	0.05
2:H:104:ALA:N	2:H:221:CYS:O[3_646]	2.19	0.01

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%)	201 (94%)	9 (4%)	4 (2%)	8 1
2	H	227/229 (99%)	220 (97%)	6 (3%)	1 (0%)	34 24
All	All	441/445 (99%)	421 (96%)	15 (3%)	5 (1%)	14 5

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	3	VAL
1	L	211	THR
1	L	158	LYS
2	H	220	SER
1	L	110	GLN

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%)	166 (92%)	14 (8%)	12 5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	H	193/193 (100%)	182 (94%)	11 (6%)	20 11
All	All	373/373 (100%)	348 (93%)	25 (7%)	16 7

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	1	GLU
2	H	58	GLN
2	H	209	ASN
2	H	52	TRP
2	H	64	VAL

Sometimes 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	202	ASN
2	H	205	HIS
2	H	209	ASN
1	L	171	ASN
2	H	39	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 monosaccharides 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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.