wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 08:40 PM GMT

PDB ID	:	1LGB
Title	:	INTERACTION OF A LEGUME LECTIN WITH THE N2 FRAGMENT OF HUMAN LACTOTRANSFERRIN OR WITH THE ISOLATED BIANTENNARY GLYCOPEPTIDE: ROLE OF THE FUCOSE MOIETY
Authors	:	Bourne, Y.; Cambillau, C.
Deposited on	:	1994-01-07
Resolution	:	3.30 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 (i)) were used in the production of this report:

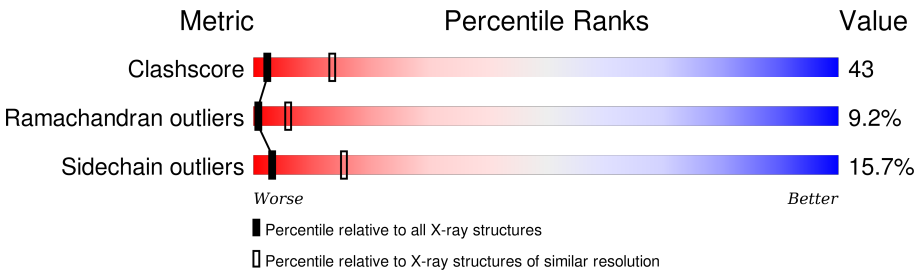
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	181	28% 52% 18% •
2	B	53	42% 42% • • 11%
3	C	159	36% 48% 14% •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3119 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 LEGUME ISOLECTIN II (ALPHA CHAIN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	181	1403	893	231	279	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	PRO	GLN	CONFLICT	UNP P04122
A	153	ALA	LYS	CONFLICT	UNP P04122
A	168	GLY	ALA	CONFLICT	UNP P04122

- Molecule 2 is a protein called LEGUME ISOLECTIN II (BETA CHAIN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	47	371	244	57	70	0	0	1

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	47	ALA	SER	CONFLICT	UNP P12307

- Molecule 3 is a protein called LACTOTRANSFERRIN (N2 FRAGMENT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	159	1233	779	214	232	8	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	200	LYS	ARG	CONFLICT	UNP P02788

- Molecule 4 is a polymer of unknown type called SUGAR (9-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	C	9	110	62	4	44	0	0

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
5	A	1	1	1	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
6	A	1	1	1	0	0

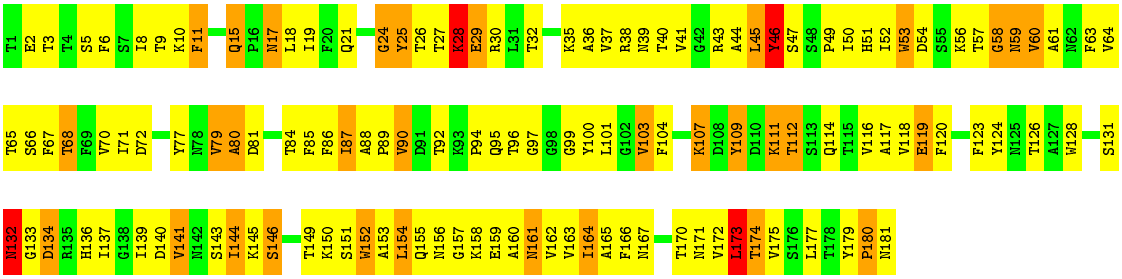
3 Residue-property plots (i)

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.

Note EDS was not executed.

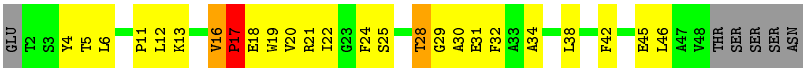
- Molecule 1: LEGUME ISOLECTIN II (ALPHA CHAIN)

Chain A:



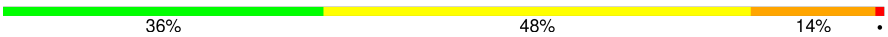
- Molecule 2: LEGUME ISOLECTIN II (BETA CHAIN)

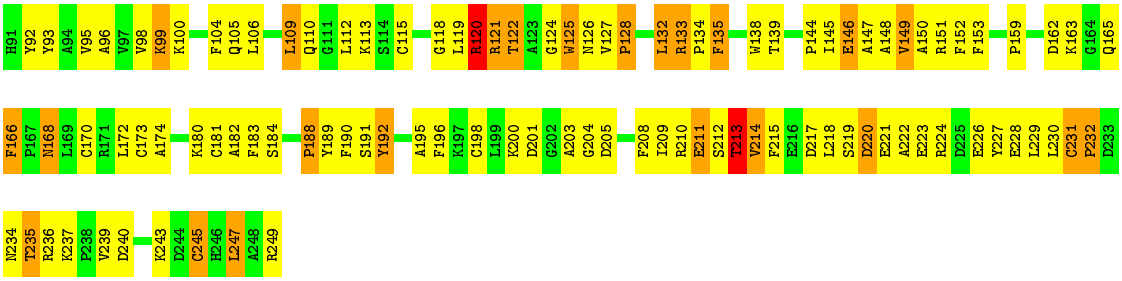
Chain B:



- Molecule 3: LACTOTRANSFERRIN (N2 FRAGMENT)

Chain C:





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	63.50Å 63.50Å 251.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-3.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.210 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3119	wwPDB-VP
Average B, all atoms ($Å^2$)	42.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, CA, MN, GAL, FUC, MAN

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	0.49	0/1438	0.82	2/1963 (0.1%)
2	B	0.53	0/383	0.77	0/525
3	C	0.57	1/1265 (0.1%)	0.82	3/1710 (0.2%)
All	All	0.53	1/3086 (0.0%)	0.81	5/4198 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	121	ARG	C-N	-6.13	1.20	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	121	ARG	O-C-N	-10.44	106.00	122.70
3	C	121	ARG	CA-C-O	6.47	133.68	120.10
3	C	201	ASP	C-N-CA	5.39	133.62	122.30
1	A	145	LYS	N-CA-C	-5.36	96.54	111.00
1	A	173	LEU	CA-CB-CG	5.09	127.01	115.30

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	A	1403	0	1349	154	0
2	B	371	0	347	45	0
3	C	1233	0	1173	100	0
4	C	110	0	94	3	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
All	All	3119	0	2963	262	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 43.

The worst 5 of 262 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)
3:C:229:LEU:HD22	3:C:245:CYS:SG	2.14	0.87
1:A:43:ARG:HB3	2:B:25:SER:HB2	1.58	0.83
3:C:122:THR:HA	3:C:126:ASN:HB2	1.65	0.79
1:A:6:PHE:CE1	2:B:42:PHE:HB3	2.20	0.77
3:C:221:GLU:HA	3:C:224:ARG:HE	1.49	0.76

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	A	179/181 (99%)	137 (76%)	26 (14%)	16 (9%)	1 6
2	B	45/53 (85%)	38 (84%)	6 (13%)	1 (2%)	8 41
3	C	157/159 (99%)	119 (76%)	20 (13%)	18 (12%)	0 3
All	All	381/393 (97%)	294 (77%)	52 (14%)	35 (9%)	1 6

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	GLY
1	A	28	LYS
1	A	36	ALA
1	A	132	ASN
1	A	144	ILE

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	155/155 (100%)	126 (81%)	29 (19%)	2 9
2	B	39/46 (85%)	35 (90%)	4 (10%)	9 34
3	C	130/130 (100%)	112 (86%)	18 (14%)	4 20
All	All	324/331 (98%)	273 (84%)	51 (16%)	3 15

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

Mol	Chain	Res	Type
1	A	161	ASN
1	A	181	ASN
3	C	231	CYS
1	A	173	LEU
2	B	12	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
3	C	110	GLN
1	A	132	ASN
1	A	21	GLN
2	B	35	HIS

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)

9 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	MAN	C	501	4	11,11,12	0.51	0	14,15,17	0.99	1 (7%)
4	BMA	C	502	4	11,11,12	0.53	0	14,15,17	0.75	0
4	MAN	C	503	4	11,11,12	0.54	0	14,15,17	0.84	1 (7%)
4	NAG	C	504	4	14,14,15	0.50	0	15,19,21	0.53	0
4	NAG	C	505	4	14,14,15	0.54	0	15,19,21	0.86	0
4	GAL	C	507	4	11,11,12	0.45	0	14,15,17	0.55	0
4	NAG	C	508	4	14,14,15	0.54	0	15,19,21	0.93	1 (6%)
4	NAG	C	509	3,4	14,14,15	0.69	0	15,19,21	1.11	1 (6%)
4	FUC	C	510	4	10,10,11	0.75	0	14,14,16	1.23	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	C	501	4	-	0/2/19/22	0/1/1/1
4	BMA	C	502	4	-	0/2/19/22	0/1/1/1
4	MAN	C	503	4	-	0/2/19/22	0/1/1/1
4	NAG	C	504	4	-	0/6/23/26	0/1/1/1
4	NAG	C	505	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GAL	C	507	4	-	0/2/19/22	0/1/1/1
4	NAG	C	508	4	-	0/6/23/26	0/1/1/1
4	NAG	C	509	3,4	-	0/6/23/26	0/1/1/1
4	FUC	C	510	4	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	509	NAG	C4-C3-C2	-3.51	105.77	111.23
4	C	508	NAG	C2-N2-C7	-3.09	119.06	123.04
4	C	503	MAN	C1-O5-C5	2.22	115.07	112.25
4	C	501	MAN	C3-C4-C5	2.41	114.40	110.20
4	C	510	FUC	C1-C2-C3	2.74	112.78	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	501	MAN	2	0
4	C	504	NAG	1	0

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 will therefore be empty.

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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