Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 10:12 pm BST

PDB ID	:	6GFC
Title	:	Structure of the BTB/POZ domain of human 90K
Authors	:	Ssebyatika, G.; Krey, T.
Deposited on	:	2018-04-29
Resolution	:	3.30 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

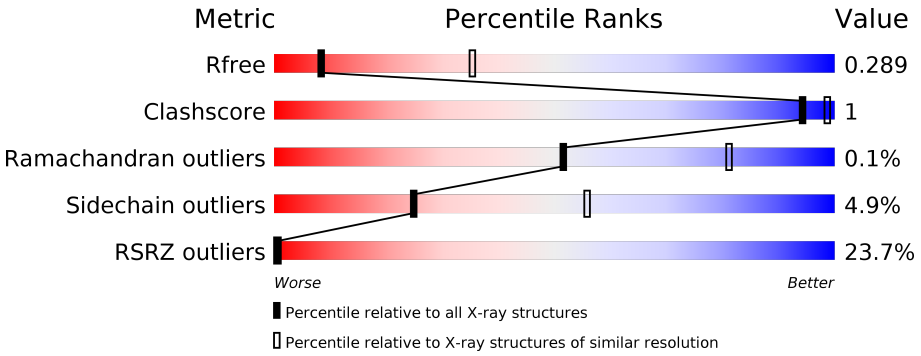
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 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% 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	A	166	13% 67% 5% 28%
1	B	166	18% 70% 7% 23%
1	C	166	14% 67% 5% 28%
1	D	166	15% 69% 5% • 26%
1	F	166	17% 61% 5% 34%
1	G	166	25% 68% 7% 25%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5540 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 Galectin-3-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	119	Total	C	N	O	S	0	0	0
			909	574	151	177	7			
1	B	128	Total	C	N	O	S	0	0	0
			987	619	169	192	7			
1	C	119	Total	C	N	O	S	0	0	0
			909	574	151	177	7			
1	D	123	Total	C	N	O	S	0	0	0
			941	595	158	181	7			
1	F	109	Total	C	N	O	S	0	0	0
			847	537	143	160	7			
1	G	124	Total	C	N	O	S	0	0	0
			947	598	159	183	7			

There are 234 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	122	ARG	-	expression tag	UNP H9FUB4
A	123	SER	-	expression tag	UNP H9FUB4
A	251	SER	-	expression tag	UNP H9FUB4
A	252	ARG	-	expression tag	UNP H9FUB4
A	253	ASP	-	expression tag	UNP H9FUB4
A	254	ASP	-	expression tag	UNP H9FUB4
A	255	ASP	-	expression tag	UNP H9FUB4
A	256	ASP	-	expression tag	UNP H9FUB4
A	257	LYS	-	expression tag	UNP H9FUB4
A	258	ALA	-	expression tag	UNP H9FUB4
A	259	GLY	-	expression tag	UNP H9FUB4
A	260	TRP	-	expression tag	UNP H9FUB4
A	261	SER	-	expression tag	UNP H9FUB4
A	262	HIS	-	expression tag	UNP H9FUB4
A	263	PRO	-	expression tag	UNP H9FUB4
A	264	GLN	-	expression tag	UNP H9FUB4
A	265	PHE	-	expression tag	UNP H9FUB4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	266	GLU	-	expression tag	UNP H9FUB4
A	267	LYS	-	expression tag	UNP H9FUB4
A	268	GLY	-	expression tag	UNP H9FUB4
A	269	GLY	-	expression tag	UNP H9FUB4
A	270	GLY	-	expression tag	UNP H9FUB4
A	271	SER	-	expression tag	UNP H9FUB4
A	272	GLY	-	expression tag	UNP H9FUB4
A	273	GLY	-	expression tag	UNP H9FUB4
A	274	GLY	-	expression tag	UNP H9FUB4
A	275	SER	-	expression tag	UNP H9FUB4
A	276	GLY	-	expression tag	UNP H9FUB4
A	277	GLY	-	expression tag	UNP H9FUB4
A	278	GLY	-	expression tag	UNP H9FUB4
A	279	SER	-	expression tag	UNP H9FUB4
A	280	TRP	-	expression tag	UNP H9FUB4
A	281	SER	-	expression tag	UNP H9FUB4
A	282	HIS	-	expression tag	UNP H9FUB4
A	283	PRO	-	expression tag	UNP H9FUB4
A	284	GLN	-	expression tag	UNP H9FUB4
A	285	PHE	-	expression tag	UNP H9FUB4
A	286	GLU	-	expression tag	UNP H9FUB4
A	287	LYS	-	expression tag	UNP H9FUB4
B	122	ARG	-	expression tag	UNP H9FUB4
B	123	SER	-	expression tag	UNP H9FUB4
B	251	SER	-	expression tag	UNP H9FUB4
B	252	ARG	-	expression tag	UNP H9FUB4
B	253	ASP	-	expression tag	UNP H9FUB4
B	254	ASP	-	expression tag	UNP H9FUB4
B	255	ASP	-	expression tag	UNP H9FUB4
B	256	ASP	-	expression tag	UNP H9FUB4
B	257	LYS	-	expression tag	UNP H9FUB4
B	258	ALA	-	expression tag	UNP H9FUB4
B	259	GLY	-	expression tag	UNP H9FUB4
B	260	TRP	-	expression tag	UNP H9FUB4
B	261	SER	-	expression tag	UNP H9FUB4
B	262	HIS	-	expression tag	UNP H9FUB4
B	263	PRO	-	expression tag	UNP H9FUB4
B	264	GLN	-	expression tag	UNP H9FUB4
B	265	PHE	-	expression tag	UNP H9FUB4
B	266	GLU	-	expression tag	UNP H9FUB4
B	267	LYS	-	expression tag	UNP H9FUB4
B	268	GLY	-	expression tag	UNP H9FUB4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	269	GLY	-	expression tag	UNP H9FUB4
B	270	GLY	-	expression tag	UNP H9FUB4
B	271	SER	-	expression tag	UNP H9FUB4
B	272	GLY	-	expression tag	UNP H9FUB4
B	273	GLY	-	expression tag	UNP H9FUB4
B	274	GLY	-	expression tag	UNP H9FUB4
B	275	SER	-	expression tag	UNP H9FUB4
B	276	GLY	-	expression tag	UNP H9FUB4
B	277	GLY	-	expression tag	UNP H9FUB4
B	278	GLY	-	expression tag	UNP H9FUB4
B	279	SER	-	expression tag	UNP H9FUB4
B	280	TRP	-	expression tag	UNP H9FUB4
B	281	SER	-	expression tag	UNP H9FUB4
B	282	HIS	-	expression tag	UNP H9FUB4
B	283	PRO	-	expression tag	UNP H9FUB4
B	284	GLN	-	expression tag	UNP H9FUB4
B	285	PHE	-	expression tag	UNP H9FUB4
B	286	GLU	-	expression tag	UNP H9FUB4
B	287	LYS	-	expression tag	UNP H9FUB4
C	122	ARG	-	expression tag	UNP H9FUB4
C	123	SER	-	expression tag	UNP H9FUB4
C	251	SER	-	expression tag	UNP H9FUB4
C	252	ARG	-	expression tag	UNP H9FUB4
C	253	ASP	-	expression tag	UNP H9FUB4
C	254	ASP	-	expression tag	UNP H9FUB4
C	255	ASP	-	expression tag	UNP H9FUB4
C	256	ASP	-	expression tag	UNP H9FUB4
C	257	LYS	-	expression tag	UNP H9FUB4
C	258	ALA	-	expression tag	UNP H9FUB4
C	259	GLY	-	expression tag	UNP H9FUB4
C	260	TRP	-	expression tag	UNP H9FUB4
C	261	SER	-	expression tag	UNP H9FUB4
C	262	HIS	-	expression tag	UNP H9FUB4
C	263	PRO	-	expression tag	UNP H9FUB4
C	264	GLN	-	expression tag	UNP H9FUB4
C	265	PHE	-	expression tag	UNP H9FUB4
C	266	GLU	-	expression tag	UNP H9FUB4
C	267	LYS	-	expression tag	UNP H9FUB4
C	268	GLY	-	expression tag	UNP H9FUB4
C	269	GLY	-	expression tag	UNP H9FUB4
C	270	GLY	-	expression tag	UNP H9FUB4
C	271	SER	-	expression tag	UNP H9FUB4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	272	GLY	-	expression tag	UNP H9FUB4
C	273	GLY	-	expression tag	UNP H9FUB4
C	274	GLY	-	expression tag	UNP H9FUB4
C	275	SER	-	expression tag	UNP H9FUB4
C	276	GLY	-	expression tag	UNP H9FUB4
C	277	GLY	-	expression tag	UNP H9FUB4
C	278	GLY	-	expression tag	UNP H9FUB4
C	279	SER	-	expression tag	UNP H9FUB4
C	280	TRP	-	expression tag	UNP H9FUB4
C	281	SER	-	expression tag	UNP H9FUB4
C	282	HIS	-	expression tag	UNP H9FUB4
C	283	PRO	-	expression tag	UNP H9FUB4
C	284	GLN	-	expression tag	UNP H9FUB4
C	285	PHE	-	expression tag	UNP H9FUB4
C	286	GLU	-	expression tag	UNP H9FUB4
C	287	LYS	-	expression tag	UNP H9FUB4
D	122	ARG	-	expression tag	UNP H9FUB4
D	123	SER	-	expression tag	UNP H9FUB4
D	251	SER	-	expression tag	UNP H9FUB4
D	252	ARG	-	expression tag	UNP H9FUB4
D	253	ASP	-	expression tag	UNP H9FUB4
D	254	ASP	-	expression tag	UNP H9FUB4
D	255	ASP	-	expression tag	UNP H9FUB4
D	256	ASP	-	expression tag	UNP H9FUB4
D	257	LYS	-	expression tag	UNP H9FUB4
D	258	ALA	-	expression tag	UNP H9FUB4
D	259	GLY	-	expression tag	UNP H9FUB4
D	260	TRP	-	expression tag	UNP H9FUB4
D	261	SER	-	expression tag	UNP H9FUB4
D	262	HIS	-	expression tag	UNP H9FUB4
D	263	PRO	-	expression tag	UNP H9FUB4
D	264	GLN	-	expression tag	UNP H9FUB4
D	265	PHE	-	expression tag	UNP H9FUB4
D	266	GLU	-	expression tag	UNP H9FUB4
D	267	LYS	-	expression tag	UNP H9FUB4
D	268	GLY	-	expression tag	UNP H9FUB4
D	269	GLY	-	expression tag	UNP H9FUB4
D	270	GLY	-	expression tag	UNP H9FUB4
D	271	SER	-	expression tag	UNP H9FUB4
D	272	GLY	-	expression tag	UNP H9FUB4
D	273	GLY	-	expression tag	UNP H9FUB4
D	274	GLY	-	expression tag	UNP H9FUB4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	275	SER	-	expression tag	UNP H9FUB4
D	276	GLY	-	expression tag	UNP H9FUB4
D	277	GLY	-	expression tag	UNP H9FUB4
D	278	GLY	-	expression tag	UNP H9FUB4
D	279	SER	-	expression tag	UNP H9FUB4
D	280	TRP	-	expression tag	UNP H9FUB4
D	281	SER	-	expression tag	UNP H9FUB4
D	282	HIS	-	expression tag	UNP H9FUB4
D	283	PRO	-	expression tag	UNP H9FUB4
D	284	GLN	-	expression tag	UNP H9FUB4
D	285	PHE	-	expression tag	UNP H9FUB4
D	286	GLU	-	expression tag	UNP H9FUB4
D	287	LYS	-	expression tag	UNP H9FUB4
F	122	ARG	-	expression tag	UNP H9FUB4
F	123	SER	-	expression tag	UNP H9FUB4
F	251	SER	-	expression tag	UNP H9FUB4
F	252	ARG	-	expression tag	UNP H9FUB4
F	253	ASP	-	expression tag	UNP H9FUB4
F	254	ASP	-	expression tag	UNP H9FUB4
F	255	ASP	-	expression tag	UNP H9FUB4
F	256	ASP	-	expression tag	UNP H9FUB4
F	257	LYS	-	expression tag	UNP H9FUB4
F	258	ALA	-	expression tag	UNP H9FUB4
F	259	GLY	-	expression tag	UNP H9FUB4
F	260	TRP	-	expression tag	UNP H9FUB4
F	261	SER	-	expression tag	UNP H9FUB4
F	262	HIS	-	expression tag	UNP H9FUB4
F	263	PRO	-	expression tag	UNP H9FUB4
F	264	GLN	-	expression tag	UNP H9FUB4
F	265	PHE	-	expression tag	UNP H9FUB4
F	266	GLU	-	expression tag	UNP H9FUB4
F	267	LYS	-	expression tag	UNP H9FUB4
F	268	GLY	-	expression tag	UNP H9FUB4
F	269	GLY	-	expression tag	UNP H9FUB4
F	270	GLY	-	expression tag	UNP H9FUB4
F	271	SER	-	expression tag	UNP H9FUB4
F	272	GLY	-	expression tag	UNP H9FUB4
F	273	GLY	-	expression tag	UNP H9FUB4
F	274	GLY	-	expression tag	UNP H9FUB4
F	275	SER	-	expression tag	UNP H9FUB4
F	276	GLY	-	expression tag	UNP H9FUB4
F	277	GLY	-	expression tag	UNP H9FUB4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	278	GLY	-	expression tag	UNP H9FUB4
F	279	SER	-	expression tag	UNP H9FUB4
F	280	TRP	-	expression tag	UNP H9FUB4
F	281	SER	-	expression tag	UNP H9FUB4
F	282	HIS	-	expression tag	UNP H9FUB4
F	283	PRO	-	expression tag	UNP H9FUB4
F	284	GLN	-	expression tag	UNP H9FUB4
F	285	PHE	-	expression tag	UNP H9FUB4
F	286	GLU	-	expression tag	UNP H9FUB4
F	287	LYS	-	expression tag	UNP H9FUB4
G	122	ARG	-	expression tag	UNP H9FUB4
G	123	SER	-	expression tag	UNP H9FUB4
G	251	SER	-	expression tag	UNP H9FUB4
G	252	ARG	-	expression tag	UNP H9FUB4
G	253	ASP	-	expression tag	UNP H9FUB4
G	254	ASP	-	expression tag	UNP H9FUB4
G	255	ASP	-	expression tag	UNP H9FUB4
G	256	ASP	-	expression tag	UNP H9FUB4
G	257	LYS	-	expression tag	UNP H9FUB4
G	258	ALA	-	expression tag	UNP H9FUB4
G	259	GLY	-	expression tag	UNP H9FUB4
G	260	TRP	-	expression tag	UNP H9FUB4
G	261	SER	-	expression tag	UNP H9FUB4
G	262	HIS	-	expression tag	UNP H9FUB4
G	263	PRO	-	expression tag	UNP H9FUB4
G	264	GLN	-	expression tag	UNP H9FUB4
G	265	PHE	-	expression tag	UNP H9FUB4
G	266	GLU	-	expression tag	UNP H9FUB4
G	267	LYS	-	expression tag	UNP H9FUB4
G	268	GLY	-	expression tag	UNP H9FUB4
G	269	GLY	-	expression tag	UNP H9FUB4
G	270	GLY	-	expression tag	UNP H9FUB4
G	271	SER	-	expression tag	UNP H9FUB4
G	272	GLY	-	expression tag	UNP H9FUB4
G	273	GLY	-	expression tag	UNP H9FUB4
G	274	GLY	-	expression tag	UNP H9FUB4
G	275	SER	-	expression tag	UNP H9FUB4
G	276	GLY	-	expression tag	UNP H9FUB4
G	277	GLY	-	expression tag	UNP H9FUB4
G	278	GLY	-	expression tag	UNP H9FUB4
G	279	SER	-	expression tag	UNP H9FUB4
G	280	TRP	-	expression tag	UNP H9FUB4

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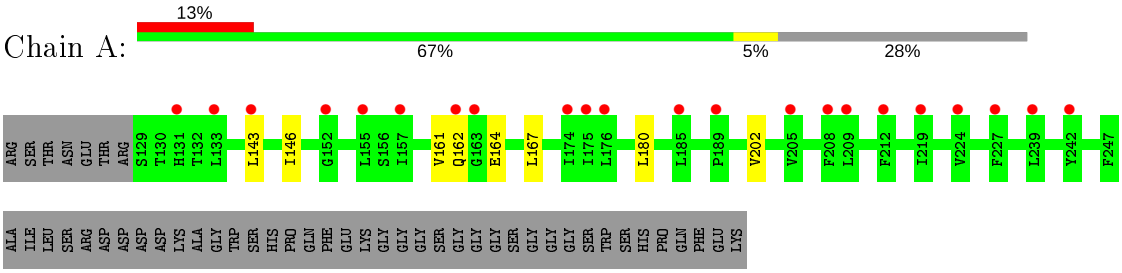
Chain	Residue	Modelled	Actual	Comment	Reference
G	281	SER	-	expression tag	UNP H9FUB4
G	282	HIS	-	expression tag	UNP H9FUB4
G	283	PRO	-	expression tag	UNP H9FUB4
G	284	GLN	-	expression tag	UNP H9FUB4
G	285	PHE	-	expression tag	UNP H9FUB4
G	286	GLU	-	expression tag	UNP H9FUB4
G	287	LYS	-	expression tag	UNP H9FUB4

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 the various outlier classes 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.

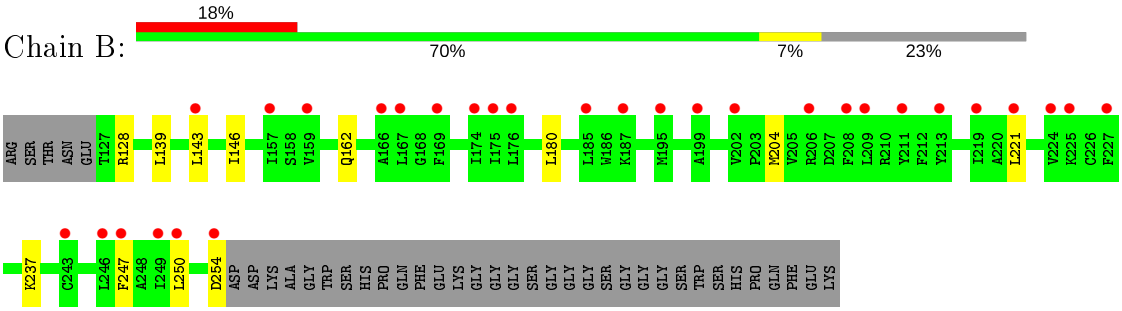
- Molecule 1: Galectin-3-binding protein

Chain A:



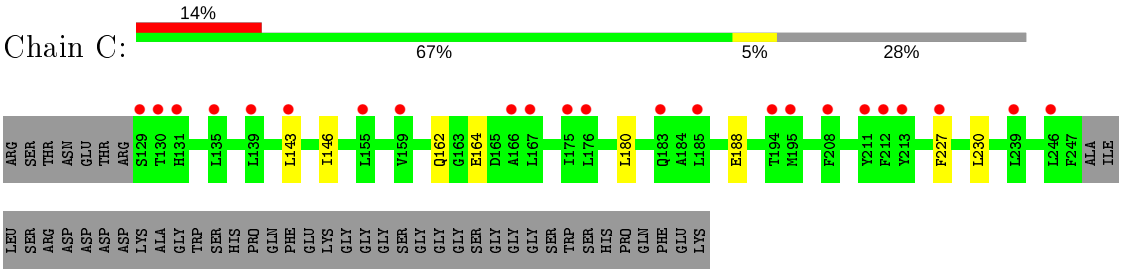
- Molecule 1: Galectin-3-binding protein

Chain B:



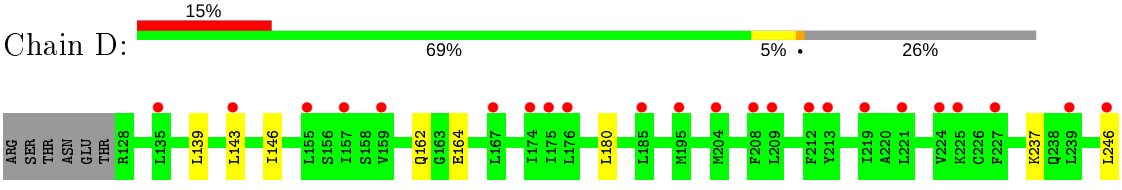
- Molecule 1: Galectin-3-binding protein

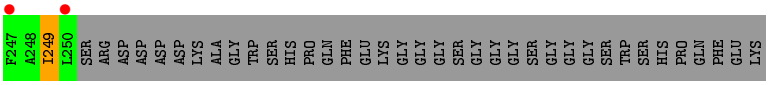
Chain C:



- Molecule 1: Galectin-3-binding protein

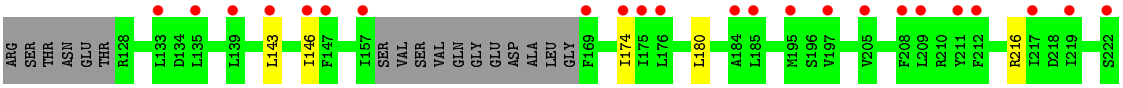
Chain D:

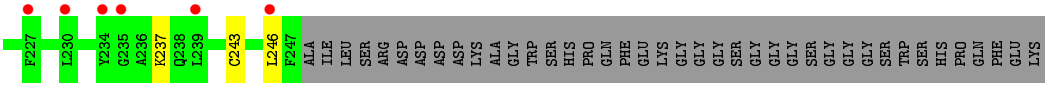




- Molecule 1: Galectin-3-binding protein

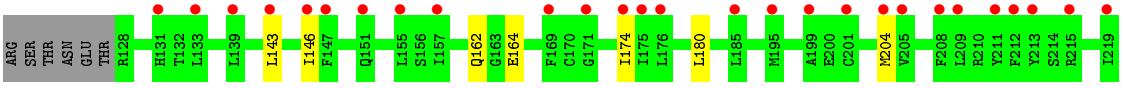
Chain F:

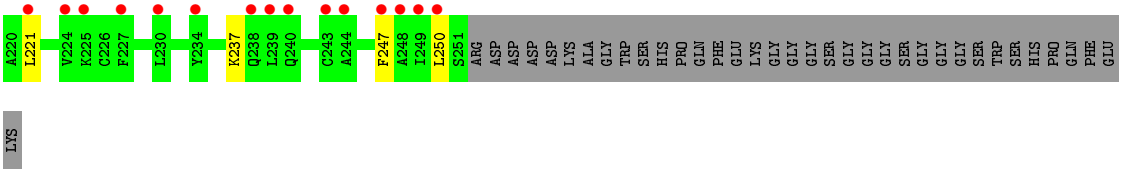




- Molecule 1: Galectin-3-binding protein

Chain G:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	181.74Å 181.74Å 173.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 128.51 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-3.30) 100.0 (128.51-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 3.33Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.267 , 0.287 0.281 , 0.289	Depositor DCC
R_{free} test set	1106 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	177.9	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 89.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.010 for l,-k,h 0.035 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5540	wwPDB-VP
Average B, all atoms (Å^2)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	A	0.37	0/925	0.56	0/1251
1	B	0.37	0/1003	0.58	0/1355
1	C	0.37	0/925	0.57	0/1251
1	D	0.36	0/957	0.57	0/1294
1	F	0.37	0/862	0.55	0/1163
1	G	0.36	0/963	0.56	0/1302
All	All	0.37	0/5635	0.56	0/7616

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

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	909	0	882	3	0
1	B	987	0	966	3	0
1	C	909	0	882	3	0
1	D	941	0	922	2	0
1	F	847	0	826	3	0
1	G	947	0	927	3	0
All	All	5540	0	5405	14	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 1.

All (14) 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:F:174:ILE:HD12	1:G:174:ILE:HD12	1.85	0.58
1:B:143:LEU:HA	1:B:146:ILE:HD12	1.90	0.54
1:F:143:LEU:HA	1:F:146:ILE:HD12	1.89	0.54
1:A:143:LEU:HA	1:A:146:ILE:HD12	1.90	0.54
1:D:143:LEU:HA	1:D:146:ILE:HD12	1.90	0.53
1:C:143:LEU:HA	1:C:146:ILE:HD12	1.89	0.53
1:G:143:LEU:HA	1:G:146:ILE:HD12	1.89	0.53
1:F:243:CYS:HA	1:F:246:LEU:HD12	1.91	0.52
1:G:221:LEU:HD12	1:G:250:LEU:HD22	1.94	0.48
1:A:161:VAL:HG21	1:A:202:VAL:HG22	1.96	0.47
1:B:221:LEU:HD12	1:B:250:LEU:HD22	1.97	0.47
1:C:227:PHE:HA	1:C:230:LEU:HD12	2.00	0.44
1:C:143:LEU:HD22	1:D:139:LEU:HD22	2.00	0.43
1:A:143:LEU:HD22	1:B:139:LEU:HD22	2.02	0.41

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	117/166 (70%)	112 (96%)	5 (4%)	0	100 100
1	B	126/166 (76%)	121 (96%)	5 (4%)	0	100 100
1	C	117/166 (70%)	113 (97%)	4 (3%)	0	100 100
1	D	121/166 (73%)	116 (96%)	4 (3%)	1 (1%)	19 51
1	F	105/166 (63%)	102 (97%)	3 (3%)	0	100 100
1	G	122/166 (74%)	118 (97%)	4 (3%)	0	100 100
All	All	708/996 (71%)	682 (96%)	25 (4%)	1 (0%)	51 81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	249	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	100/136 (74%)	96 (96%)	4 (4%)	31	61
1	B	109/136 (80%)	102 (94%)	7 (6%)	17	46
1	C	100/136 (74%)	96 (96%)	4 (4%)	31	61
1	D	103/136 (76%)	97 (94%)	6 (6%)	20	50
1	F	93/136 (68%)	90 (97%)	3 (3%)	39	67
1	G	104/136 (76%)	98 (94%)	6 (6%)	20	50
All	All	609/816 (75%)	579 (95%)	30 (5%)	25	56

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	GLN
1	A	164	GLU
1	A	167	LEU
1	A	180	LEU
1	B	128	ARG
1	B	162	GLN
1	B	180	LEU
1	B	204	MET
1	B	237	LYS
1	B	247	PHE
1	B	254	ASP
1	C	162	GLN
1	C	164	GLU
1	C	180	LEU
1	C	188	GLU
1	D	162	GLN

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Mol	Chain	Res	Type
1	D	164	GLU
1	D	180	LEU
1	D	237	LYS
1	D	246	LEU
1	D	249	ILE
1	F	180	LEU
1	F	216	ARG
1	F	237	LYS
1	G	162	GLN
1	G	164	GLU
1	G	180	LEU
1	G	204	MET
1	G	237	LYS
1	G	247	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

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, 95^{th} 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	A	119/166 (71%)	1.13	22 (18%)	1	1	71, 96, 129, 149	0
1	B	128/166 (77%)	1.25	30 (23%)	0	1	82, 108, 137, 151	0
1	C	119/166 (71%)	1.12	23 (19%)	1	1	94, 128, 178, 192	0
1	D	123/166 (74%)	1.08	25 (20%)	1	1	87, 109, 141, 203	0
1	F	109/166 (65%)	1.22	29 (26%)	0	0	141, 165, 202, 219	0
1	G	124/166 (74%)	1.35	42 (33%)	0	0	132, 147, 182, 217	0
All	All	722/996 (72%)	1.19	171 (23%)	0	1	71, 123, 182, 219	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	129	SER	8.6
1	F	205	VAL	6.5
1	C	185	LEU	6.1
1	C	166	ALA	5.8
1	F	185	LEU	5.8
1	B	249	ILE	5.7
1	B	254	ASP	5.7
1	G	249	ILE	5.2
1	F	227	PHE	4.8
1	F	234	TYR	4.8
1	F	212	PHE	4.8
1	A	185	LEU	4.8
1	F	217	ILE	4.7
1	G	221	LEU	4.7
1	C	159	VAL	4.6
1	C	208	PHE	4.6
1	G	185	LEU	4.5
1	G	213	TYR	4.5
1	F	209	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	195	MET	4.4
1	F	195	MET	4.3
1	D	250	LEU	4.3
1	G	227	PHE	4.3
1	B	219	ILE	4.3
1	D	225	LYS	4.2
1	G	247	PHE	4.2
1	F	139	LEU	4.1
1	F	208	PHE	4.1
1	A	227	PHE	3.9
1	A	162	GLN	3.9
1	G	212	PHE	3.9
1	G	175	ILE	3.9
1	G	209	LEU	3.9
1	G	139	LEU	3.9
1	D	185	LEU	3.8
1	F	169	PHE	3.8
1	G	243	CYS	3.7
1	D	224	VAL	3.7
1	B	227	PHE	3.7
1	B	206	ARG	3.7
1	C	239	LEU	3.6
1	D	175	ILE	3.6
1	F	157	ILE	3.6
1	G	234	TYR	3.5
1	A	155	LEU	3.5
1	B	185	LEU	3.5
1	F	147	PHE	3.5
1	B	243	CYS	3.4
1	C	227	PHE	3.4
1	G	248	ALA	3.4
1	G	155	LEU	3.4
1	B	166	ALA	3.4
1	D	221	LEU	3.4
1	G	239	LEU	3.4
1	D	208	PHE	3.4
1	G	199	ALA	3.3
1	C	195	MET	3.3
1	C	131	HIS	3.3
1	B	157	ILE	3.3
1	C	246	LEU	3.2
1	F	176	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	195	MET	3.2
1	G	174	ILE	3.2
1	G	250	LEU	3.2
1	B	199	ALA	3.2
1	F	246	LEU	3.1
1	F	133	LEU	3.1
1	A	219	ILE	3.1
1	C	211	TYR	3.1
1	C	167	LEU	3.1
1	D	157	ILE	3.1
1	C	212	PHE	3.1
1	F	219	ILE	3.1
1	G	208	PHE	3.0
1	G	215	ARG	3.0
1	C	143	LEU	3.0
1	B	225	LYS	3.0
1	G	204	MET	3.0
1	G	133	LEU	2.9
1	B	221	LEU	2.9
1	D	167	LEU	2.9
1	G	176	LEU	2.9
1	C	175	ILE	2.9
1	D	246	LEU	2.9
1	D	212	PHE	2.9
1	D	247	PHE	2.8
1	G	146	ILE	2.8
1	B	213	TYR	2.8
1	G	230	LEU	2.8
1	B	250	LEU	2.8
1	G	171	GLY	2.8
1	F	230	LEU	2.8
1	C	139	LEU	2.8
1	G	201	CYS	2.7
1	G	143	LEU	2.7
1	A	242	TYR	2.7
1	A	205	VAL	2.7
1	F	239	LEU	2.7
1	B	246	LEU	2.7
1	A	224	VAL	2.7
1	B	167	LEU	2.6
1	A	163	GLY	2.6
1	G	240	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	175	ILE	2.6
1	B	174	ILE	2.6
1	B	175	ILE	2.6
1	C	155	LEU	2.6
1	D	204	MET	2.6
1	B	247	PHE	2.6
1	G	225	LYS	2.6
1	B	143	LEU	2.6
1	D	176	LEU	2.6
1	G	205	VAL	2.6
1	G	238	GLN	2.6
1	D	227	PHE	2.5
1	C	176	LEU	2.5
1	F	222	SER	2.5
1	G	219	ILE	2.5
1	G	131	HIS	2.5
1	G	157	ILE	2.5
1	A	189	PRO	2.5
1	A	174	ILE	2.5
1	D	159	VAL	2.4
1	F	211	TYR	2.4
1	B	169	PHE	2.4
1	B	208	PHE	2.4
1	D	219	ILE	2.4
1	D	143	LEU	2.4
1	B	159	VAL	2.4
1	B	209	LEU	2.4
1	D	155	LEU	2.4
1	F	143	LEU	2.4
1	F	174	ILE	2.4
1	G	147	PHE	2.4
1	F	146	ILE	2.4
1	C	130	THR	2.3
1	D	195	MET	2.3
1	B	176	LEU	2.3
1	A	143	LEU	2.3
1	A	157	ILE	2.3
1	C	183	GLN	2.3
1	F	135	LEU	2.3
1	A	209	LEU	2.3
1	F	184	ALA	2.3
1	D	174	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	176	LEU	2.2
1	A	212	PHE	2.2
1	C	213	TYR	2.2
1	A	131	HIS	2.2
1	D	213	TYR	2.2
1	G	244	ALA	2.2
1	B	224	VAL	2.2
1	C	135	LEU	2.1
1	A	133	LEU	2.1
1	A	239	LEU	2.1
1	B	211	TYR	2.1
1	G	224	VAL	2.1
1	B	187	LYS	2.1
1	G	211	TYR	2.1
1	F	197	VAL	2.1
1	G	151	GLN	2.1
1	B	202	VAL	2.1
1	D	209	LEU	2.1
1	F	235	GLY	2.1
1	A	208	PHE	2.0
1	D	239	LEU	2.0
1	D	135	LEU	2.0
1	G	169	PHE	2.0
1	C	194	THR	2.0
1	A	152	GLY	2.0
1	F	175	ILE	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.