



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 11:08 am BST

PDB ID : 5H7A  
Title : Crystal structure of a repeat protein with four Protein A repeat module  
Authors : Youn, S.J.; Kwon, N.Y.; Lee, J.H.; Kim, J.H.; Lee, H.; Lee, J.O.  
Deposited on : 2016-11-17  
Resolution : 2.70 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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

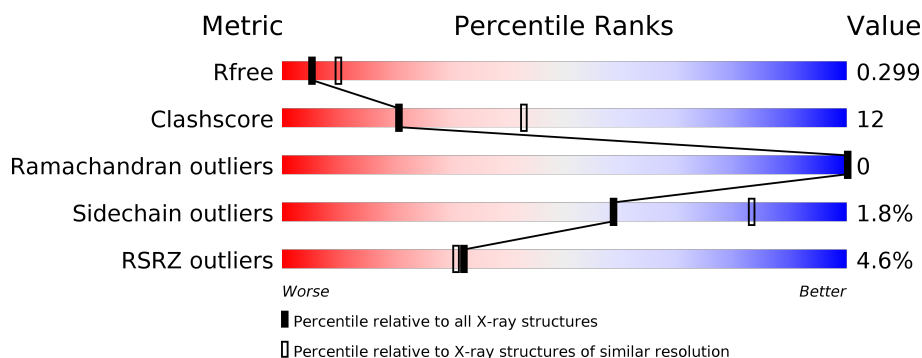
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	A	192	<div> <div>2%</div> <div>75% 23%</div> <div>.</div> </div>
1	B	192	<div> <div>3%</div> <div>72% 26%</div> <div>..</div> </div>
1	C	192	<div> <div>%</div> <div>77% 21%</div> <div>..</div> </div>
1	D	192	<div> <div>7%</div> <div>77% 20%</div> <div>..</div> </div>
1	E	192	<div> <div>%</div> <div>68% 28%</div> <div>..</div> </div>
1	F	192	<div> <div>6%</div> <div>71% 27%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	192	<div><div>8%</div><div><div></div><div>70%</div><div>28%</div></div><div></div></div>
1	H	192	<div><div>12%</div><div><div></div><div>71%</div><div>25%</div></div><div></div></div>
1	I	192	<div><div>4%</div><div><div></div><div>67%</div><div>31%</div></div><div></div></div>
1	J	192	<div><div>7%</div><div><div></div><div>75%</div><div>22%</div></div><div></div></div>
1	K	192	<div><div>4%</div><div><div></div><div>76%</div><div>21%</div></div><div></div></div>
1	L	192	<div><div>%</div><div><div></div><div>61%</div><div>33%</div></div><div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18409 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 Immunoglobulin G-binding protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	189	Total	C	N	O	S	0	0	0
			1519	947	264	307	1			
1	A	188	Total	C	N	O		0	0	0
			1511	942	263	306				
1	D	188	Total	C	N	O		0	0	0
			1511	942	263	306				
1	B	189	Total	C	N	O	S	0	0	0
			1519	947	264	307	1			
1	E	187	Total	C	N	O		0	0	0
			1502	936	261	305				
1	F	188	Total	C	N	O		0	0	0
			1511	942	263	306				
1	G	188	Total	C	N	O		0	0	0
			1511	942	263	306				
1	H	187	Total	C	N	O		0	0	0
			1502	936	261	305				
1	I	188	Total	C	N	O		0	0	0
			1511	942	263	306				
1	J	187	Total	C	N	O		0	0	0
			1502	936	261	305				
1	K	187	Total	C	N	O		0	0	0
			1502	936	261	305				
1	L	186	Total	C	N	O		0	0	0
			1491	927	260	304				

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	30	GLY	-	expression tag	UNP P38507
C	31	SER	-	expression tag	UNP P38507
C	32	HIS	-	expression tag	UNP P38507
C	33	MET	-	expression tag	UNP P38507
C	59	ALA	GLY	engineered mutation	UNP P38507

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Chain	Residue	Modelled	Actual	Comment	Reference
C	86	ALA	ASN	engineered mutation	UNP P38507
C	93	SER	HIS	engineered mutation	UNP P38507
C	104	ALA	GLY	engineered mutation	UNP P38507
C	131	ALA	ASN	engineered mutation	UNP P38507
C	149	ALA	GLY	engineered mutation	UNP P38507
C	176	ALA	ASN	engineered mutation	UNP P38507
C	194	ALA	GLY	engineered mutation	UNP P38507
A	30	GLY	-	expression tag	UNP P38507
A	31	SER	-	expression tag	UNP P38507
A	32	HIS	-	expression tag	UNP P38507
A	33	MET	-	expression tag	UNP P38507
A	59	ALA	GLY	engineered mutation	UNP P38507
A	86	ALA	ASN	engineered mutation	UNP P38507
A	93	SER	HIS	engineered mutation	UNP P38507
A	104	ALA	GLY	engineered mutation	UNP P38507
A	131	ALA	ASN	engineered mutation	UNP P38507
A	149	ALA	GLY	engineered mutation	UNP P38507
A	176	ALA	ASN	engineered mutation	UNP P38507
A	194	ALA	GLY	engineered mutation	UNP P38507
D	30	GLY	-	expression tag	UNP P38507
D	31	SER	-	expression tag	UNP P38507
D	32	HIS	-	expression tag	UNP P38507
D	33	MET	-	expression tag	UNP P38507
D	59	ALA	GLY	engineered mutation	UNP P38507
D	86	ALA	ASN	engineered mutation	UNP P38507
D	93	SER	HIS	engineered mutation	UNP P38507
D	104	ALA	GLY	engineered mutation	UNP P38507
D	131	ALA	ASN	engineered mutation	UNP P38507
D	149	ALA	GLY	engineered mutation	UNP P38507
D	176	ALA	ASN	engineered mutation	UNP P38507
D	194	ALA	GLY	engineered mutation	UNP P38507
B	30	GLY	-	expression tag	UNP P38507
B	31	SER	-	expression tag	UNP P38507
B	32	HIS	-	expression tag	UNP P38507
B	33	MET	-	expression tag	UNP P38507
B	59	ALA	GLY	engineered mutation	UNP P38507
B	86	ALA	ASN	engineered mutation	UNP P38507
B	93	SER	HIS	engineered mutation	UNP P38507
B	104	ALA	GLY	engineered mutation	UNP P38507
B	131	ALA	ASN	engineered mutation	UNP P38507
B	149	ALA	GLY	engineered mutation	UNP P38507
B	176	ALA	ASN	engineered mutation	UNP P38507

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Chain	Residue	Modelled	Actual	Comment	Reference
B	194	ALA	GLY	engineered mutation	UNP P38507
E	30	GLY	-	expression tag	UNP P38507
E	31	SER	-	expression tag	UNP P38507
E	32	HIS	-	expression tag	UNP P38507
E	33	MET	-	expression tag	UNP P38507
E	59	ALA	GLY	engineered mutation	UNP P38507
E	86	ALA	ASN	engineered mutation	UNP P38507
E	93	SER	HIS	engineered mutation	UNP P38507
E	104	ALA	GLY	engineered mutation	UNP P38507
E	131	ALA	ASN	engineered mutation	UNP P38507
E	149	ALA	GLY	engineered mutation	UNP P38507
E	176	ALA	ASN	engineered mutation	UNP P38507
E	194	ALA	GLY	engineered mutation	UNP P38507
F	30	GLY	-	expression tag	UNP P38507
F	31	SER	-	expression tag	UNP P38507
F	32	HIS	-	expression tag	UNP P38507
F	33	MET	-	expression tag	UNP P38507
F	59	ALA	GLY	engineered mutation	UNP P38507
F	86	ALA	ASN	engineered mutation	UNP P38507
F	93	SER	HIS	engineered mutation	UNP P38507
F	104	ALA	GLY	engineered mutation	UNP P38507
F	131	ALA	ASN	engineered mutation	UNP P38507
F	149	ALA	GLY	engineered mutation	UNP P38507
F	176	ALA	ASN	engineered mutation	UNP P38507
F	194	ALA	GLY	engineered mutation	UNP P38507
G	30	GLY	-	expression tag	UNP P38507
G	31	SER	-	expression tag	UNP P38507
G	32	HIS	-	expression tag	UNP P38507
G	33	MET	-	expression tag	UNP P38507
G	59	ALA	GLY	engineered mutation	UNP P38507
G	86	ALA	ASN	engineered mutation	UNP P38507
G	93	SER	HIS	engineered mutation	UNP P38507
G	104	ALA	GLY	engineered mutation	UNP P38507
G	131	ALA	ASN	engineered mutation	UNP P38507
G	149	ALA	GLY	engineered mutation	UNP P38507
G	176	ALA	ASN	engineered mutation	UNP P38507
G	194	ALA	GLY	engineered mutation	UNP P38507
H	30	GLY	-	EXPRESSION TAG	UNP P38507
H	31	SER	-	EXPRESSION TAG	UNP P38507
H	32	HIS	-	EXPRESSION TAG	UNP P38507
H	33	MET	-	EXPRESSION TAG	UNP P38507
H	59	ALA	GLY	engineered mutation	UNP P38507

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Chain	Residue	Modelled	Actual	Comment	Reference
H	86	ALA	ASN	engineered mutation	UNP P38507
H	93	SER	HIS	engineered mutation	UNP P38507
H	104	ALA	GLY	engineered mutation	UNP P38507
H	131	ALA	ASN	engineered mutation	UNP P38507
H	149	ALA	GLY	engineered mutation	UNP P38507
H	176	ALA	ASN	engineered mutation	UNP P38507
H	194	ALA	GLY	engineered mutation	UNP P38507
I	30	GLY	-	expression tag	UNP P38507
I	31	SER	-	expression tag	UNP P38507
I	32	HIS	-	expression tag	UNP P38507
I	33	MET	-	expression tag	UNP P38507
I	59	ALA	GLY	engineered mutation	UNP P38507
I	86	ALA	ASN	engineered mutation	UNP P38507
I	93	SER	HIS	engineered mutation	UNP P38507
I	104	ALA	GLY	engineered mutation	UNP P38507
I	131	ALA	ASN	engineered mutation	UNP P38507
I	149	ALA	GLY	engineered mutation	UNP P38507
I	176	ALA	ASN	engineered mutation	UNP P38507
I	194	ALA	GLY	engineered mutation	UNP P38507
J	30	GLY	-	expression tag	UNP P38507
J	31	SER	-	expression tag	UNP P38507
J	32	HIS	-	expression tag	UNP P38507
J	33	MET	-	expression tag	UNP P38507
J	59	ALA	GLY	engineered mutation	UNP P38507
J	86	ALA	ASN	engineered mutation	UNP P38507
J	93	SER	HIS	engineered mutation	UNP P38507
J	104	ALA	GLY	engineered mutation	UNP P38507
J	131	ALA	ASN	engineered mutation	UNP P38507
J	149	ALA	GLY	engineered mutation	UNP P38507
J	176	ALA	ASN	engineered mutation	UNP P38507
J	194	ALA	GLY	engineered mutation	UNP P38507
K	30	GLY	-	expression tag	UNP P38507
K	31	SER	-	expression tag	UNP P38507
K	32	HIS	-	expression tag	UNP P38507
K	33	MET	-	expression tag	UNP P38507
K	59	ALA	GLY	engineered mutation	UNP P38507
K	86	ALA	ASN	engineered mutation	UNP P38507
K	93	SER	HIS	engineered mutation	UNP P38507
K	104	ALA	GLY	engineered mutation	UNP P38507
K	131	ALA	ASN	engineered mutation	UNP P38507
K	149	ALA	GLY	engineered mutation	UNP P38507
K	176	ALA	ASN	engineered mutation	UNP P38507

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Chain	Residue	Modelled	Actual	Comment	Reference
K	194	ALA	GLY	engineered mutation	UNP P38507
L	30	GLY	-	expression tag	UNP P38507
L	31	SER	-	expression tag	UNP P38507
L	32	HIS	-	expression tag	UNP P38507
L	33	MET	-	expression tag	UNP P38507
L	59	ALA	GLY	engineered mutation	UNP P38507
L	86	ALA	ASN	engineered mutation	UNP P38507
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L	104	ALA	GLY	engineered mutation	UNP P38507
L	131	ALA	ASN	engineered mutation	UNP P38507
L	149	ALA	GLY	engineered mutation	UNP P38507
L	176	ALA	ASN	engineered mutation	UNP P38507
L	194	ALA	GLY	engineered mutation	UNP P38507

- Molecule 2 is water.

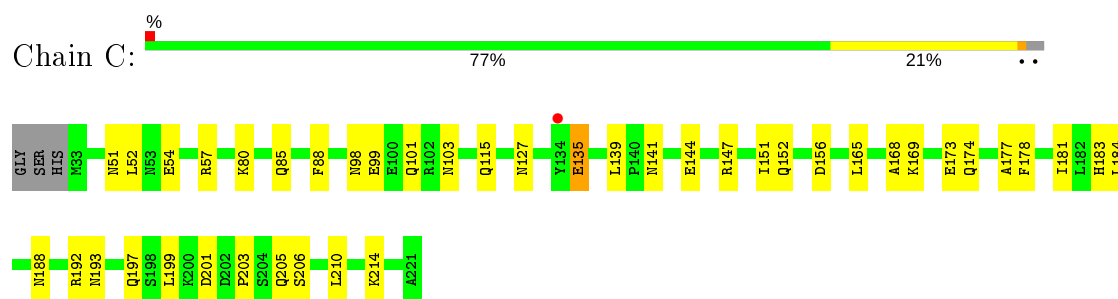
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	25	Total O 25 25	0	0
2	A	28	Total O 28 28	0	0
2	D	28	Total O 28 28	0	0
2	B	22	Total O 22 22	0	0
2	E	29	Total O 29 29	0	0
2	F	24	Total O 24 24	0	0
2	G	27	Total O 27 27	0	0
2	H	20	Total O 20 20	0	0
2	I	39	Total O 39 39	0	0
2	J	26	Total O 26 26	0	0
2	K	19	Total O 19 19	0	0
2	L	30	Total O 30 30	0	0



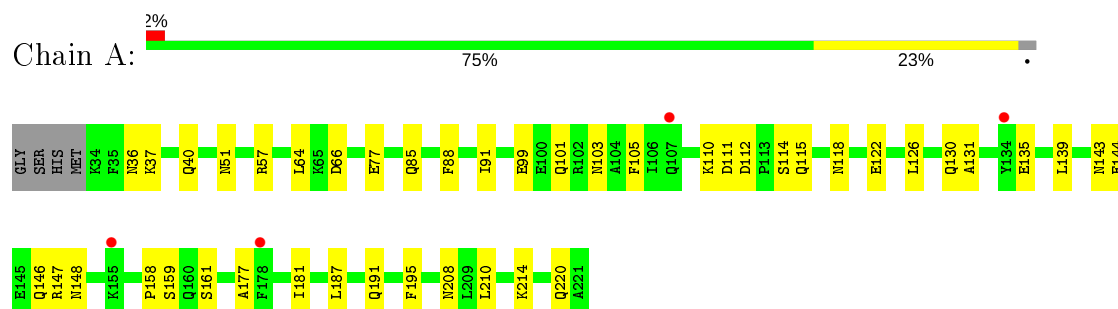
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

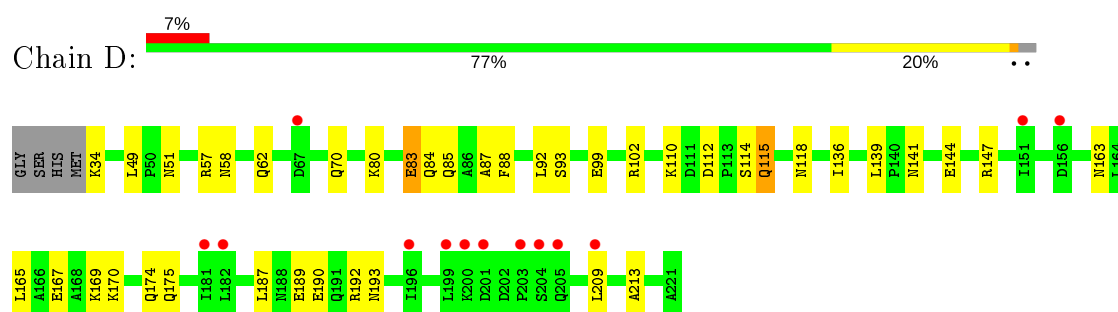
- Molecule 1: Immunoglobulin G-binding protein A



- Molecule 1: Immunoglobulin G-binding protein A

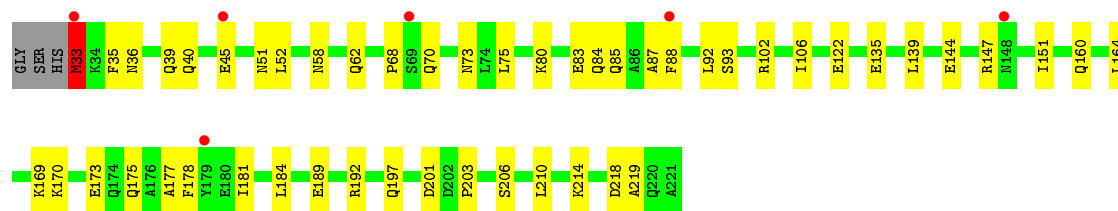


- Molecule 1: Immunoglobulin G-binding protein A

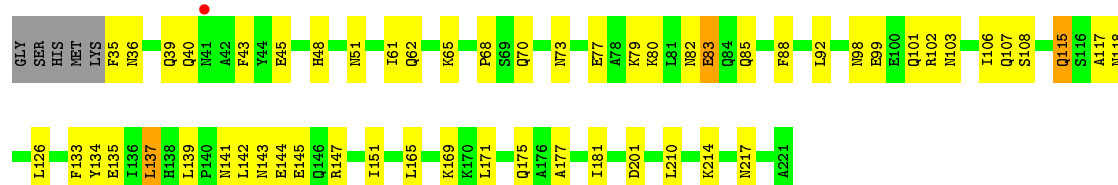


- Molecule 1: Immunoglobulin G-binding protein A

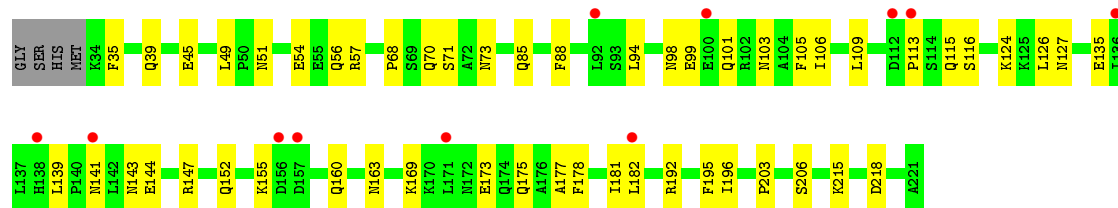




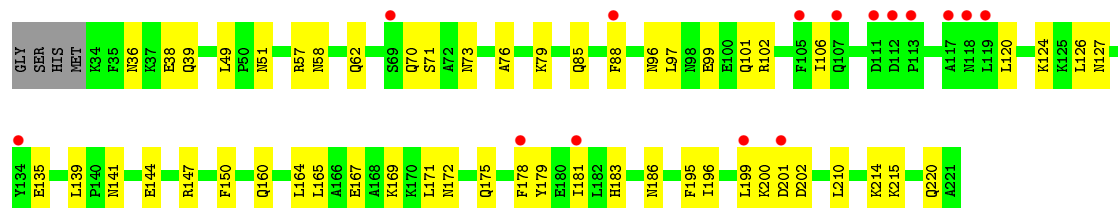
• Molecule 1: Immunoglobulin G-binding protein A



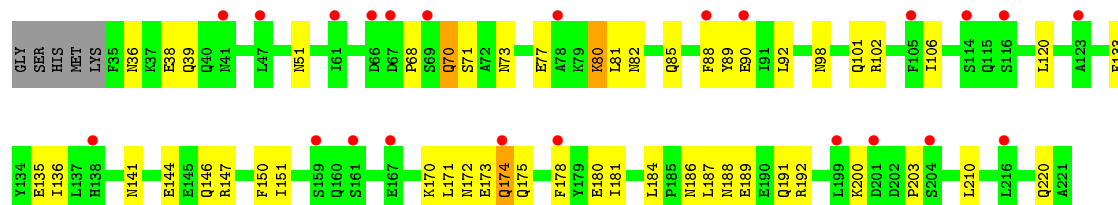
• Molecule 1: Immunoglobulin G-binding protein A



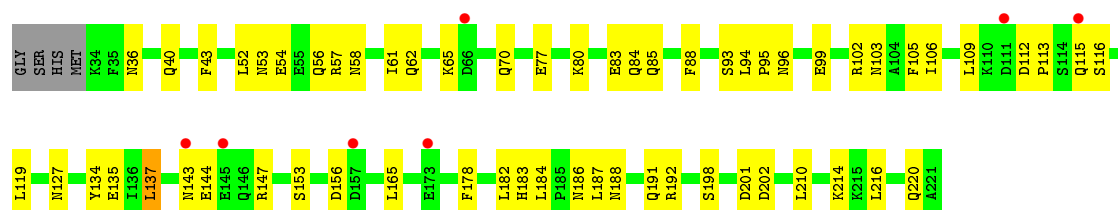
• Molecule 1: Immunoglobulin G-binding protein A



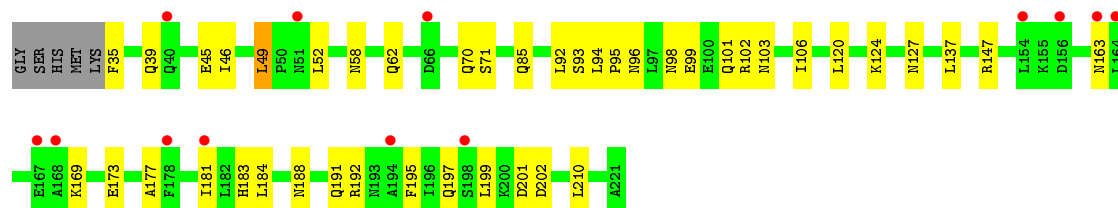
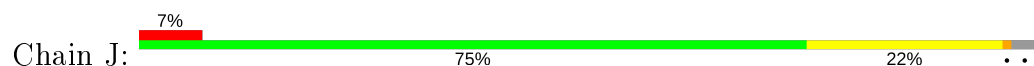
• Molecule 1: Immunoglobulin G-binding protein A



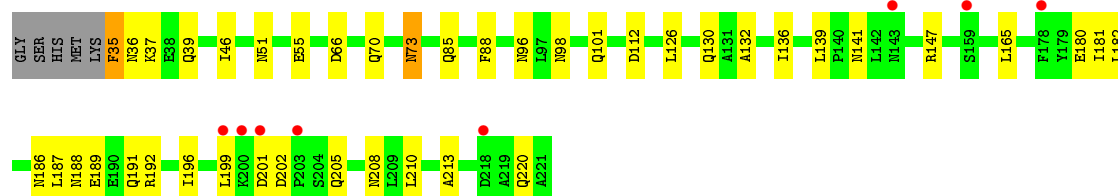
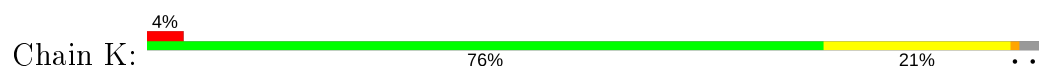
- Molecule 1: Immunoglobulin G-binding protein A



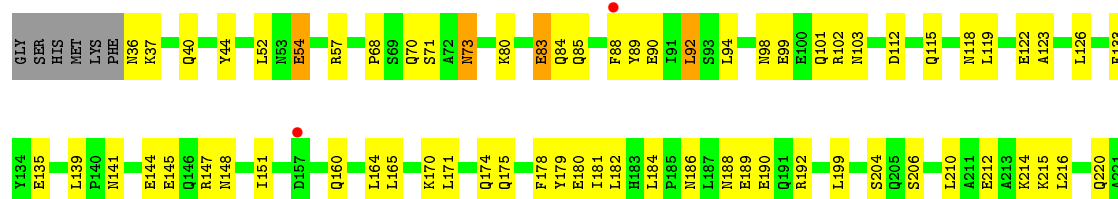
- Molecule 1: Immunoglobulin G-binding protein A



- Molecule 1: Immunoglobulin G-binding protein A



- Molecule 1: Immunoglobulin G-binding protein A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.41Å 80.80Å 130.33Å 89.83° 89.62° 90.12°	Depositor
Resolution (Å)	34.30 – 2.70 32.68 – 2.63	Depositor EDS
% Data completeness (in resolution range)	94.6 (34.30-2.70) 93.4 (32.68-2.63)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.246 , 0.285 0.255 , 0.299	Depositor DCC
$R_{free}$ test set	2018 reflections (3.20%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.7	Xtriage
Anisotropy	0.580	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 17.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.059 for h,-k,-l 0.368 for -h,k,-l 0.046 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	18409	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.68 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9691e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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

### 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	0.31	0/1534	0.48	0/2072
1	B	0.30	0/1542	0.55	1/2082 (0.0%)
1	C	0.30	0/1542	0.48	0/2082
1	D	0.29	0/1534	0.46	0/2072
1	E	0.31	0/1525	0.53	1/2061 (0.0%)
1	F	0.29	0/1534	0.46	0/2072
1	G	0.30	0/1534	0.49	0/2072
1	H	0.29	0/1525	0.48	0/2061
1	I	0.28	0/1534	0.50	1/2072 (0.0%)
1	J	0.28	0/1525	0.48	1/2061 (0.0%)
1	K	0.28	0/1525	0.50	0/2061
1	L	0.27	0/1513	0.48	1/2045 (0.0%)
All	All	0.29	0/18367	0.49	5/24813 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	33	MET	CB-CA-C	7.46	125.32	110.40
1	E	137	LEU	CA-CB-CG	7.18	131.81	115.30
1	I	137	LEU	CA-CB-CG	6.60	130.48	115.30
1	J	199	LEU	CA-CB-CG	6.06	129.24	115.30
1	L	92	LEU	CA-CB-CG	5.70	128.40	115.30

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	1511	0	1469	37	0
1	B	1519	0	1478	32	0
1	C	1519	0	1478	31	0
1	D	1511	0	1469	36	0
1	E	1502	0	1456	42	0
1	F	1511	0	1469	34	0
1	G	1511	0	1469	43	0
1	H	1502	0	1456	37	0
1	I	1511	0	1469	49	0
1	J	1502	0	1456	33	0
1	K	1502	0	1456	34	0
1	L	1491	0	1447	55	0
2	A	28	0	0	9	0
2	B	22	0	0	6	0
2	C	25	0	0	8	0
2	D	28	0	0	14	0
2	E	29	0	0	16	0
2	F	24	0	0	2	0
2	G	27	0	0	9	0
2	H	20	0	0	8	0
2	I	39	0	0	8	0
2	J	26	0	0	7	0
2	K	19	0	0	9	0
2	L	30	0	0	11	0
All	All	18409	0	17572	440	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 12.

The worst 5 of 440 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:D:85:GLN:O	1:D:88:PHE:HB2	1.51	1.09
1:L:85:GLN:O	1:L:88:PHE:HB2	1.68	0.93
1:G:51:ASN:O	1:G:85:GLN:NE2	2.03	0.91
1:H:77:GLU:O	2:H:301:HOH:O	1.88	0.90
1:D:99:GLU:OE2	2:D:301:HOH:O	1.88	0.89

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	186/192 (97%)	179 (96%)	7 (4%)	0	100	100
1	B	187/192 (97%)	181 (97%)	6 (3%)	0	100	100
1	C	187/192 (97%)	183 (98%)	4 (2%)	0	100	100
1	D	186/192 (97%)	178 (96%)	8 (4%)	0	100	100
1	E	185/192 (96%)	181 (98%)	4 (2%)	0	100	100
1	F	186/192 (97%)	181 (97%)	5 (3%)	0	100	100
1	G	186/192 (97%)	182 (98%)	4 (2%)	0	100	100
1	H	185/192 (96%)	179 (97%)	6 (3%)	0	100	100
1	I	186/192 (97%)	180 (97%)	6 (3%)	0	100	100
1	J	185/192 (96%)	178 (96%)	7 (4%)	0	100	100
1	K	185/192 (96%)	173 (94%)	12 (6%)	0	100	100
1	L	184/192 (96%)	176 (96%)	8 (4%)	0	100	100
All	All	2228/2304 (97%)	2151 (96%)	77 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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	163/166 (98%)	162 (99%)	1 (1%)	86	95
1	B	164/166 (99%)	160 (98%)	4 (2%)	49	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	164/166 (99%)	161 (98%)	3 (2%)	59	83
1	D	163/166 (98%)	160 (98%)	3 (2%)	59	83
1	E	162/166 (98%)	159 (98%)	3 (2%)	57	82
1	F	163/166 (98%)	161 (99%)	2 (1%)	71	88
1	G	163/166 (98%)	162 (99%)	1 (1%)	86	95
1	H	162/166 (98%)	157 (97%)	5 (3%)	40	69
1	I	163/166 (98%)	160 (98%)	3 (2%)	59	83
1	J	162/166 (98%)	159 (98%)	3 (2%)	57	82
1	K	162/166 (98%)	159 (98%)	3 (2%)	57	82
1	L	161/166 (97%)	156 (97%)	5 (3%)	40	69
All	All	1952/1992 (98%)	1916 (98%)	36 (2%)	59	83

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	167	GLU
1	H	174	GLN
1	L	54	GLU
1	H	80	LYS
1	H	181	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	175	GLN
1	H	205	GLN
1	J	191	GLN
1	F	73	ASN
1	H	73	ASN

### 5.3.3 RNA ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	188/192 (97%)	0.51	4 (2%) 63 65	22, 36, 52, 67	0
1	B	189/192 (98%)	0.52	6 (3%) 47 48	22, 33, 53, 63	0
1	C	189/192 (98%)	0.27	1 (0%) 91 92	15, 29, 40, 48	0
1	D	188/192 (97%)	0.59	13 (6%) 16 15	21, 35, 60, 85	0
1	E	187/192 (97%)	0.28	1 (0%) 91 92	18, 28, 43, 56	0
1	F	188/192 (97%)	0.62	11 (5%) 22 21	19, 35, 49, 67	0
1	G	188/192 (97%)	0.61	15 (7%) 12 10	23, 34, 55, 69	0
1	H	187/192 (97%)	0.80	23 (12%) 4 3	24, 36, 51, 56	0
1	I	188/192 (97%)	0.44	7 (3%) 41 41	19, 31, 46, 70	0
1	J	187/192 (97%)	0.62	13 (6%) 16 14	22, 36, 51, 73	0
1	K	187/192 (97%)	0.51	8 (4%) 35 33	18, 34, 57, 77	0
1	L	186/192 (96%)	0.45	2 (1%) 80 82	18, 36, 48, 58	0
All	All	2252/2304 (97%)	0.52	104 (4%) 32 31	15, 34, 52, 85	0

The worst 5 of 104 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	178	PHE	6.3
1	G	178	PHE	5.2
1	H	69	SER	4.5
1	D	201	ASP	4.5
1	H	174	GLN	3.8

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

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.