



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jan 4, 2017 – 03:20 AM EST

PDB ID : 5TCQ
EMDB ID: : EMD-8399
Title : Near-atomic resolution cryo-EM structure of the Salmonella SPI-1 type III secretion injectisome secretin InvG
Authors : Worrall, L.J.; Hong, C.; Vuckovic, M.; Bergeron, J.R.C.; Huang, R.K.; Yu, Z.; Strynadka, N.C.J.
Deposited on : 2016-09-15
Resolution : 3.60 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : unknown
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) : rb-20028442

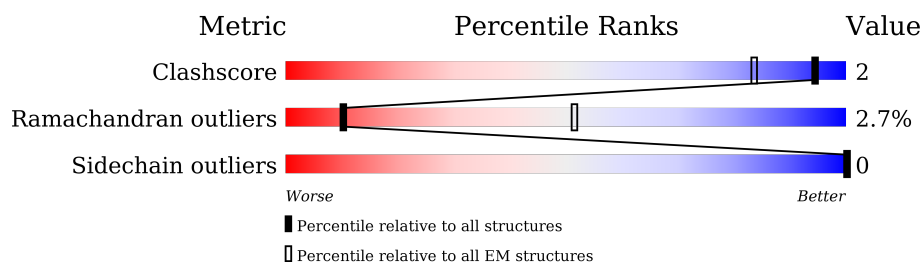
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	562	57% 40%
1	B	562	57% 40%
1	C	562	57% 40%
1	D	562	57% 40%
1	E	562	57% 40%
1	F	562	57% 40%
1	G	562	57% 40%
1	H	562	57% 40%
1	I	562	57% 40%

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Mol	Chain	Length	Quality of chain
1	J	562	 56% . . 40%
1	K	562	 57% . . 40%
1	L	562	 57% . . 40%
1	M	562	 57% . . 40%
1	N	562	 56% . . 40%
1	O	562	 57% . . 40%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 39180 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

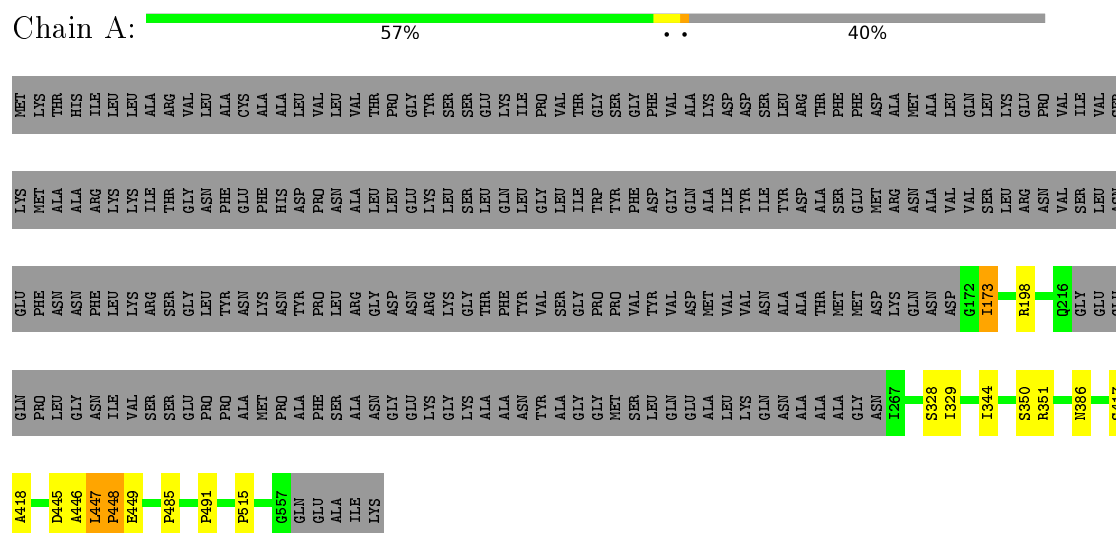
- Molecule 1 is a protein called Protein InvG.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	336	Total	C	N	O	S	0	0
			2612	1648	457	501	6		
1	B	336	Total	C	N	O	S	0	0
			2612	1648	457	501	6		
1	C	336	Total	C	N	O	S	0	0
			2612	1648	457	501	6		
1	D	336	Total	C	N	O	S	0	0
			2612	1648	457	501	6		
1	E	336	Total	C	N	O	S	0	0
			2612	1648	457	501	6		
1	F	336	Total	C	N	O	S	0	0
			2612	1648	457	501	6		
1	G	336	Total	C	N	O	S	0	0
			2612	1648	457	501	6		
1	H	336	Total	C	N	O	S	0	0
			2612	1648	457	501	6		
1	I	336	Total	C	N	O	S	0	0
			2612	1648	457	501	6		
1	J	336	Total	C	N	O	S	0	0
			2612	1648	457	501	6		
1	K	336	Total	C	N	O	S	0	0
			2612	1648	457	501	6		
1	L	336	Total	C	N	O	S	0	0
			2612	1648	457	501	6		
1	M	336	Total	C	N	O	S	0	0
			2612	1648	457	501	6		
1	N	336	Total	C	N	O	S	0	0
			2612	1648	457	501	6		
1	O	336	Total	C	N	O	S	0	0
			2612	1648	457	501	6		

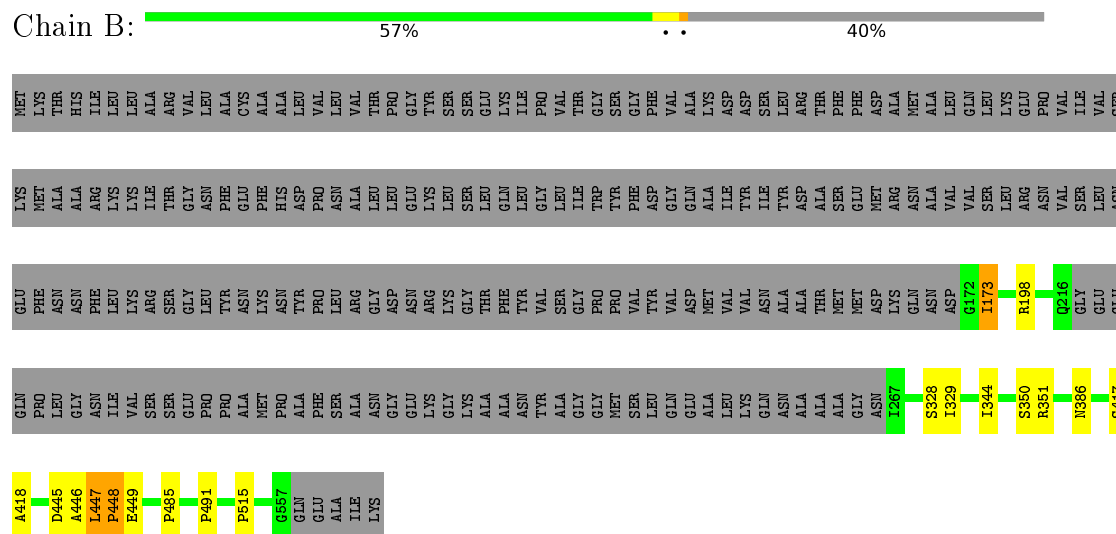
3 Residue-property plots

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. 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.

• Molecule 1: Protein InvG

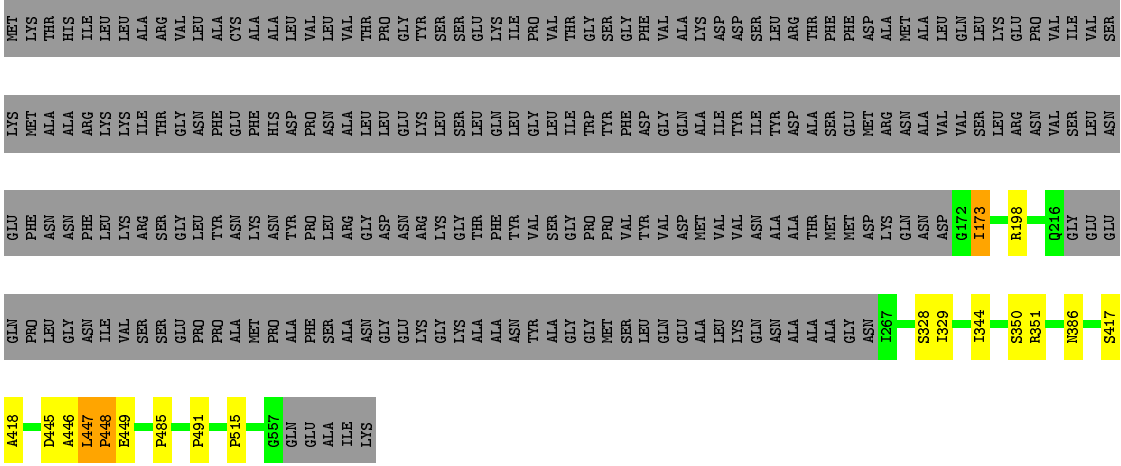


• Molecule 1: Protein InvG



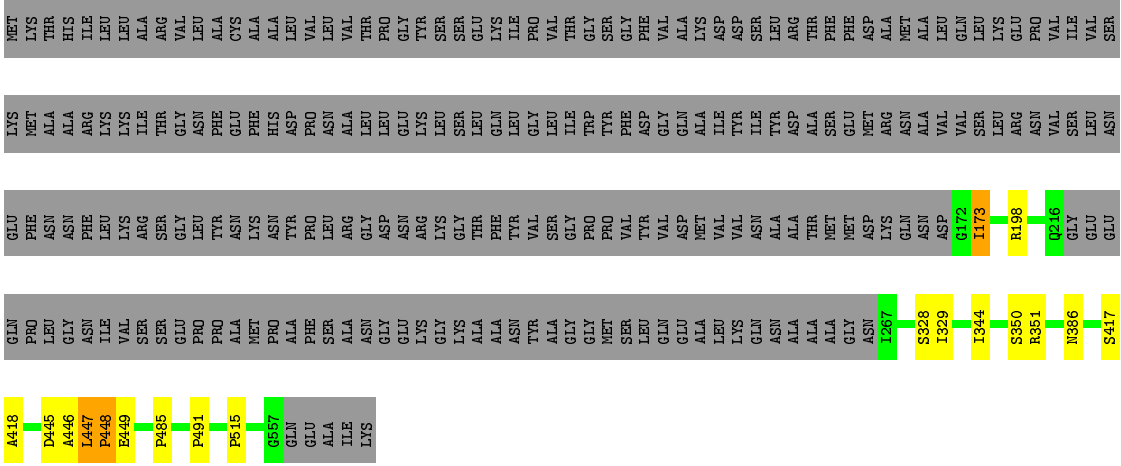
• Molecule 1: Protein InvG





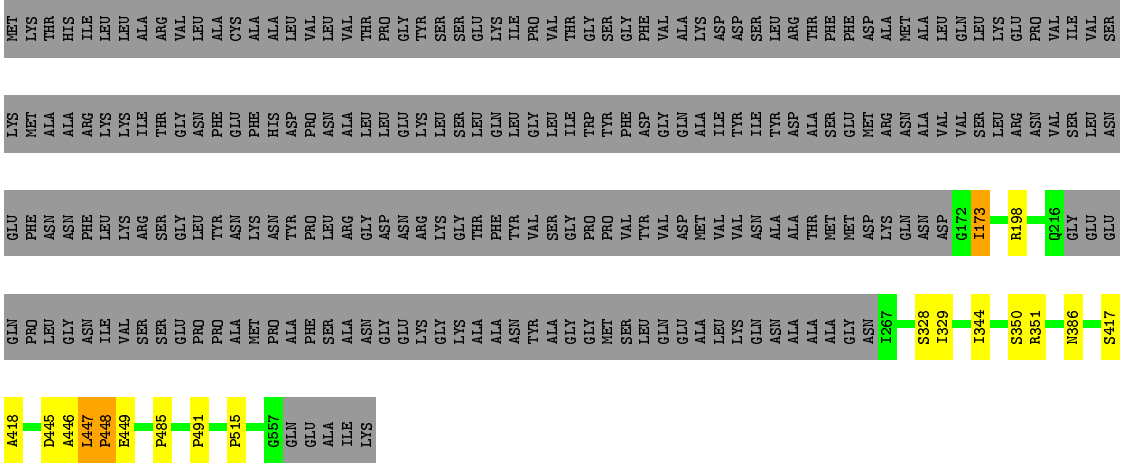
• Molecule 1: Protein InvG

Chain D: 57% 40%



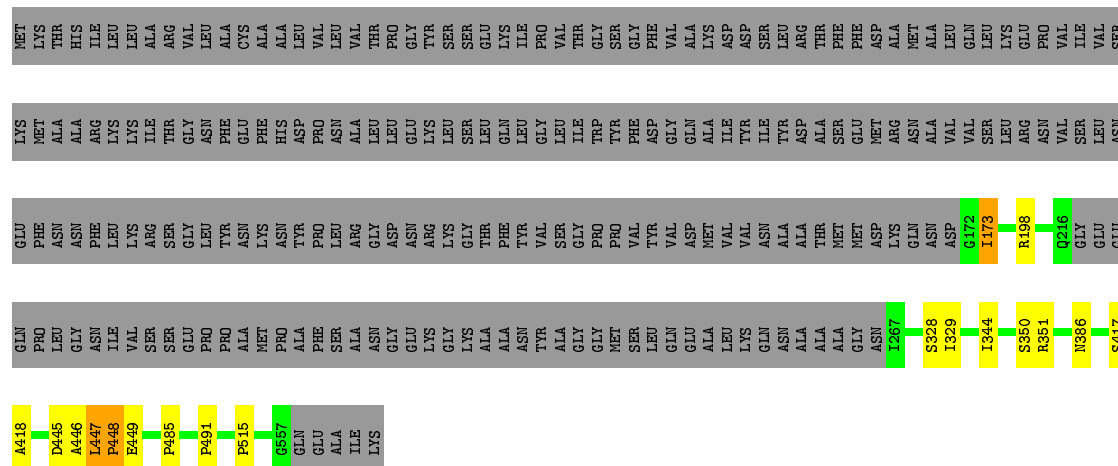
• Molecule 1: Protein InvG

Chain E: 57% 40%



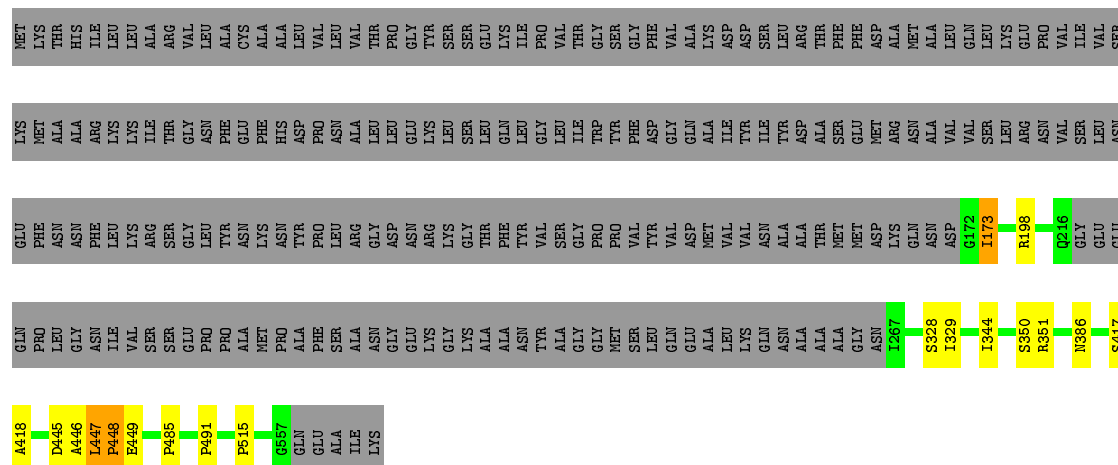
- Molecule 1: Protein InvG

Chain F:  57% .. 40%



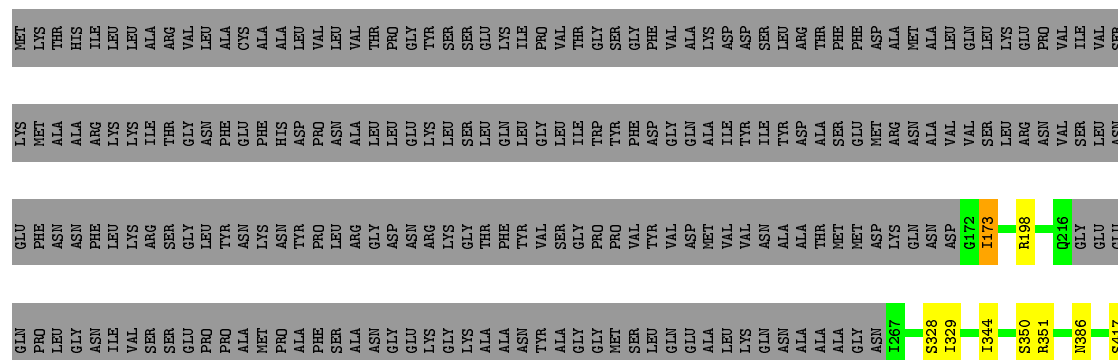
- Molecule 1: Protein InvG

Chain G: 57% .. 40%



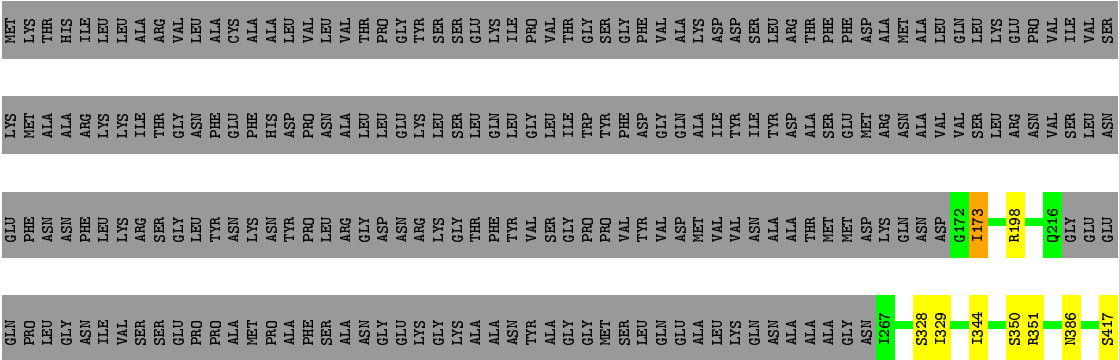
- Molecule 1: Protein InvG

Chain H:  57% .. 40%

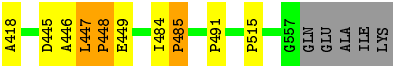
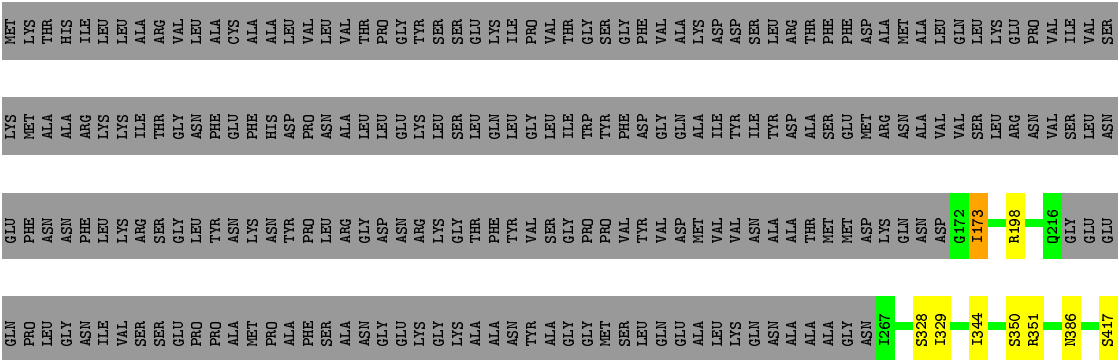




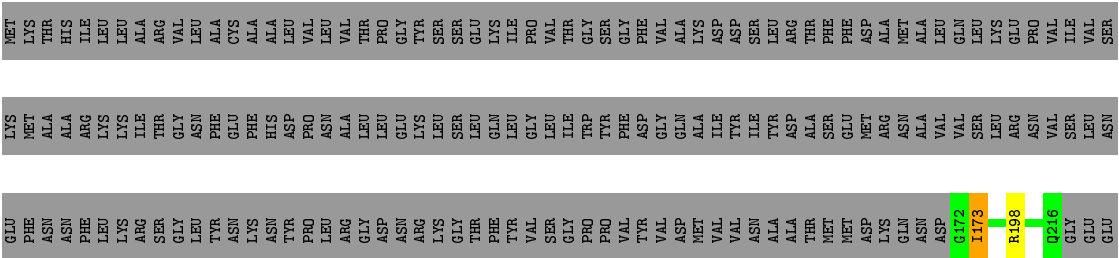
• Molecule 1: Protein InvG

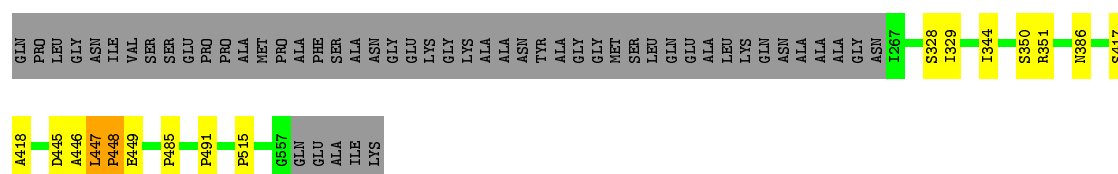


• Molecule 1: Protein InvG

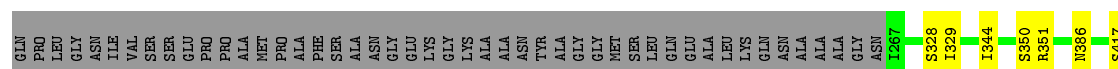
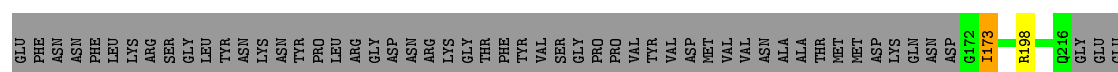


• Molecule 1: Protein InvG

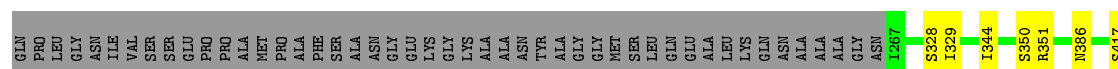
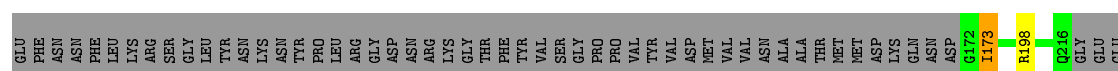
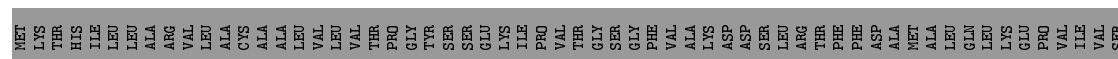




- Molecule 1: Protein InvG

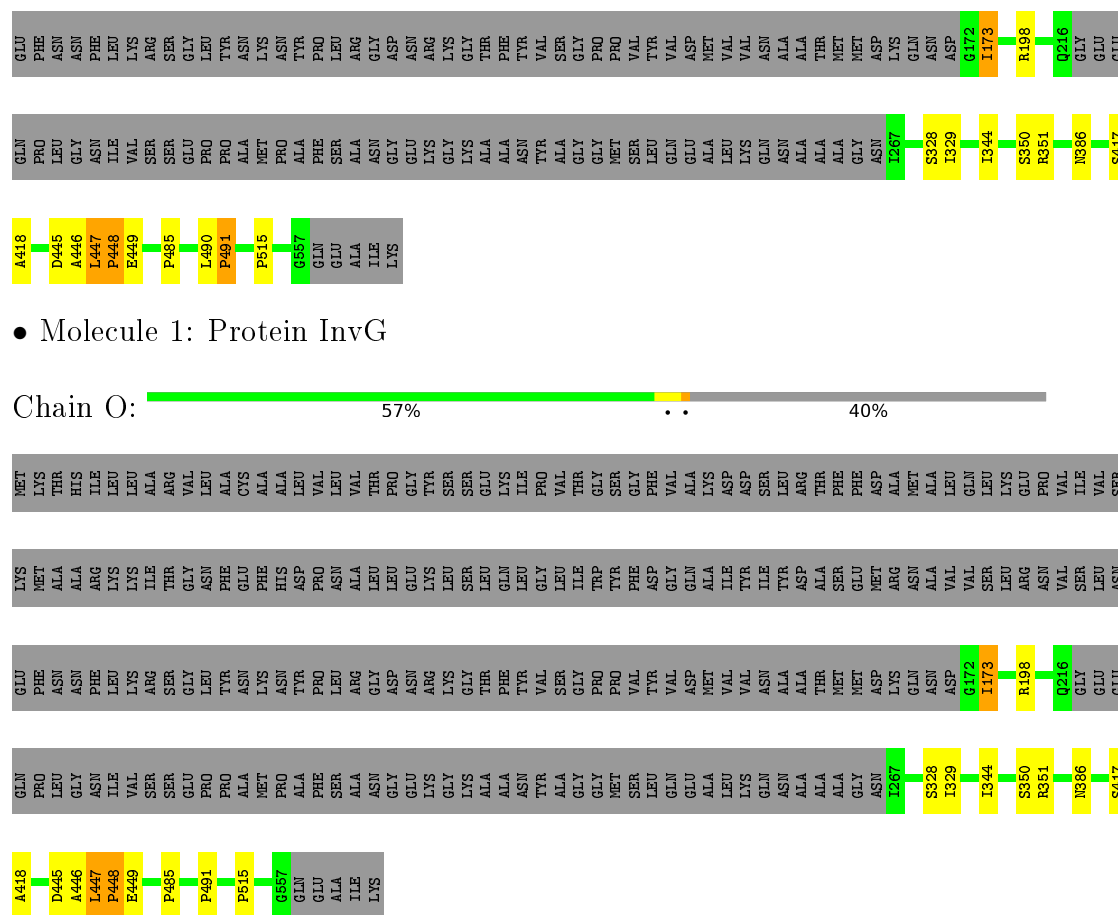


- Molecule 1: Protein InvG



- Molecule 1: Protein InvG





4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	83900	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	29240	Depositor
Image detector	Not provided	Depositor

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 >2	RMSZ	# Z >2
1	A	0.74	0/2651	0.69	0/3592
1	B	0.74	0/2651	0.70	0/3592
1	C	0.74	0/2651	0.69	0/3592
1	D	0.74	0/2651	0.69	0/3592
1	E	0.74	0/2651	0.69	0/3592
1	F	0.74	0/2651	0.69	0/3592
1	G	0.74	0/2651	0.70	0/3592
1	H	0.74	0/2651	0.69	0/3592
1	I	0.74	0/2651	0.69	0/3592
1	J	0.74	0/2651	0.70	0/3592
1	K	0.74	0/2651	0.70	0/3592
1	L	0.74	0/2651	0.70	0/3592
1	M	0.74	0/2651	0.70	0/3592
1	N	0.74	0/2651	0.69	0/3592
1	O	0.74	0/2651	0.70	0/3592
All	All	0.74	0/39765	0.69	0/53880

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	2612	0	2678	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2612	0	2678	8	0
1	C	2612	0	2678	8	0
1	D	2612	0	2678	8	0
1	E	2612	0	2678	8	0
1	F	2612	0	2678	8	0
1	G	2612	0	2678	8	0
1	H	2612	0	2678	8	0
1	I	2612	0	2678	8	0
1	J	2612	0	2678	9	0
1	K	2612	0	2678	8	0
1	L	2612	0	2678	8	0
1	M	2612	0	2678	8	0
1	N	2612	0	2678	9	0
1	O	2612	0	2678	8	0
All	All	39180	0	40170	122	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 2.

The worst 5 of 122 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:E:173:ILE:O	1:E:173:ILE:HG22	1.92	0.70
1:H:173:ILE:HG22	1:H:173:ILE:O	1.92	0.70
1:I:173:ILE:O	1:I:173:ILE:HG22	1.92	0.70
1:D:173:ILE:HG22	1:D:173:ILE:O	1.92	0.70
1:F:173:ILE:O	1:F:173:ILE:HG22	1.92	0.69

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 PDB entries followed by that with respect to all EM entries.

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	332/562 (59%)	312 (94%)	11 (3%)	9 (3%)	6	46
1	B	332/562 (59%)	312 (94%)	11 (3%)	9 (3%)	6	46
1	C	332/562 (59%)	312 (94%)	11 (3%)	9 (3%)	6	46
1	D	332/562 (59%)	312 (94%)	11 (3%)	9 (3%)	6	46
1	E	332/562 (59%)	312 (94%)	11 (3%)	9 (3%)	6	46
1	F	332/562 (59%)	312 (94%)	11 (3%)	9 (3%)	6	46
1	G	332/562 (59%)	312 (94%)	11 (3%)	9 (3%)	6	46
1	H	332/562 (59%)	312 (94%)	11 (3%)	9 (3%)	6	46
1	I	332/562 (59%)	312 (94%)	11 (3%)	9 (3%)	6	46
1	J	332/562 (59%)	312 (94%)	11 (3%)	9 (3%)	6	46
1	K	332/562 (59%)	312 (94%)	11 (3%)	9 (3%)	6	46
1	L	332/562 (59%)	312 (94%)	11 (3%)	9 (3%)	6	46
1	M	332/562 (59%)	312 (94%)	11 (3%)	9 (3%)	6	46
1	N	332/562 (59%)	312 (94%)	11 (3%)	9 (3%)	6	46
1	O	332/562 (59%)	312 (94%)	11 (3%)	9 (3%)	6	46
All	All	4980/8430 (59%)	4680 (94%)	165 (3%)	135 (3%)	10	46

5 of 135 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	446	ALA
1	B	446	ALA
1	B	515	PRO
1	C	446	ALA
1	C	515	PRO

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 PDB entries followed by that with respect to all EM entries.

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	294/477 (62%)	294 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	294/477 (62%)	294 (100%)	0	100	100
1	C	294/477 (62%)	294 (100%)	0	100	100
1	D	294/477 (62%)	294 (100%)	0	100	100
1	E	294/477 (62%)	294 (100%)	0	100	100
1	F	294/477 (62%)	294 (100%)	0	100	100
1	G	294/477 (62%)	294 (100%)	0	100	100
1	H	294/477 (62%)	294 (100%)	0	100	100
1	I	294/477 (62%)	294 (100%)	0	100	100
1	J	294/477 (62%)	294 (100%)	0	100	100
1	K	294/477 (62%)	294 (100%)	0	100	100
1	L	294/477 (62%)	294 (100%)	0	100	100
1	M	294/477 (62%)	294 (100%)	0	100	100
1	N	294/477 (62%)	294 (100%)	0	100	100
1	O	294/477 (62%)	294 (100%)	0	100	100
All	All	4410/7155 (62%)	4410 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

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.