



wwPDB EM Validation Summary Report ⓘ

Apr 1, 2025 – 08:56 PM EDT

PDB ID : 6X6J / pdb_00006x6j
EMDB ID : EMD-20021
Title : Cryo-EM Structure of CagX and CagY within the Helicobacter pylori PR
Authors : Sheedlo, M.J.; Chung, J.M.; Sawhney, N.; Durie, C.L.; Cover, T.L.; Ohi, M.D.;
Lacy, D.B.
Deposited on : 2020-05-28
Resolution : 3.50 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev117
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

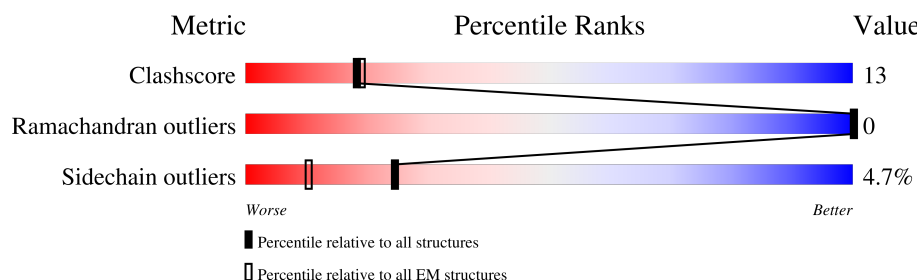
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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.


















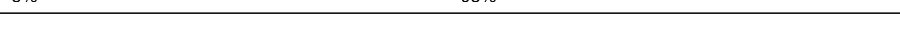
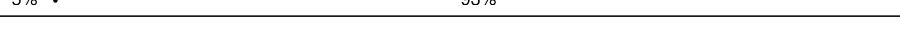
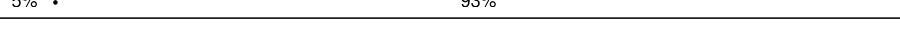
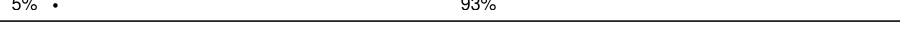
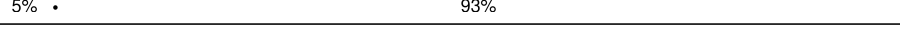
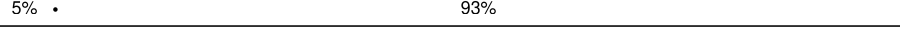
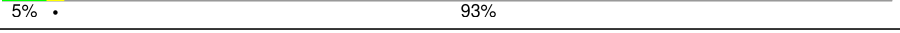


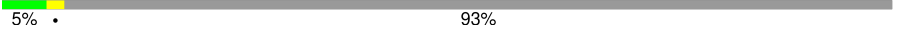
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	AX	521	20% 11% • 69%
1	BX	521	21% 9% • 69%
1	CX	521	19% 12% • 69%
1	DX	521	19% 12% • 69%
1	EX	521	20% 10% • 69%
1	FX	521	21% 10% • 69%
1	GX	521	19% 11% • 69%
1	HX	521	20% 10% • 69%
1	IX	521	21% 9% • 69%

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Mol	Chain	Length	Quality of chain
1	JX	521	 19% 12% • 69%
1	KX	521	 21% 10% • 69%
1	LX	521	 21% 9% • 69%
1	MX	521	 21% 10% • 69%
1	NX	521	 20% 11% • 69%
1	OX	521	 20% 11% • 69%
1	PX	521	 20% 10% • 69%
1	QX	521	 20% 10% • 69%
2	AY	1927	 5% • 93%
2	BY	1927	 • • 93%
2	CY	1927	 5% • 93%
2	DY	1927	 5% • 93%
2	EY	1927	 5% • 93%
2	FY	1927	 5% • 93%
2	GY	1927	 5% • 93%
2	HY	1927	 5% • 93%
2	IY	1927	 5% • 93%
2	JY	1927	 5% • 93%
2	KY	1927	 5% • 93%
2	LY	1927	 5% • 93%
2	MY	1927	 5% • 93%
2	NY	1927	 5% • 93%
2	OY	1927	 5% • 93%
2	PY	1927	 5% • 93%
2	QY	1927	 5% • 93%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 40613 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 Cag pathogenicity island protein (Cag8).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	BX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	CX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	DX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	EX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	FX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	GX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	HX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	IX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	JX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	KX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	LX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	MX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	NX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	OX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	PX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	QX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AX	?	-	GLU	deletion	UNP O25263
AX	516	GLU	LEU	conflict	UNP O25263
BX	?	-	GLU	deletion	UNP O25263
BX	516	GLU	LEU	conflict	UNP O25263
CX	?	-	GLU	deletion	UNP O25263
CX	516	GLU	LEU	conflict	UNP O25263
DX	?	-	GLU	deletion	UNP O25263
DX	516	GLU	LEU	conflict	UNP O25263
EX	?	-	GLU	deletion	UNP O25263
EX	516	GLU	LEU	conflict	UNP O25263
FX	?	-	GLU	deletion	UNP O25263
FX	516	GLU	LEU	conflict	UNP O25263
GX	?	-	GLU	deletion	UNP O25263
GX	516	GLU	LEU	conflict	UNP O25263
HX	?	-	GLU	deletion	UNP O25263
HX	516	GLU	LEU	conflict	UNP O25263
IX	?	-	GLU	deletion	UNP O25263
IX	516	GLU	LEU	conflict	UNP O25263
JX	?	-	GLU	deletion	UNP O25263
JX	516	GLU	LEU	conflict	UNP O25263
KX	?	-	GLU	deletion	UNP O25263
KX	516	GLU	LEU	conflict	UNP O25263
LX	?	-	GLU	deletion	UNP O25263
LX	516	GLU	LEU	conflict	UNP O25263
MX	?	-	GLU	deletion	UNP O25263
MX	516	GLU	LEU	conflict	UNP O25263
NX	?	-	GLU	deletion	UNP O25263
NX	516	GLU	LEU	conflict	UNP O25263
OX	?	-	GLU	deletion	UNP O25263
OX	516	GLU	LEU	conflict	UNP O25263
PX	?	-	GLU	deletion	UNP O25263
PX	516	GLU	LEU	conflict	UNP O25263
QX	?	-	GLU	deletion	UNP O25263
QX	516	GLU	LEU	conflict	UNP O25263

- Molecule 2 is a protein called Cag pathogenicity island protein (Cag7).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AY	135	Total	C	N	O	S	0	0
			1050	649	177	220	4		
2	BY	135	Total	C	N	O	S	0	0
			1050	649	177	220	4		

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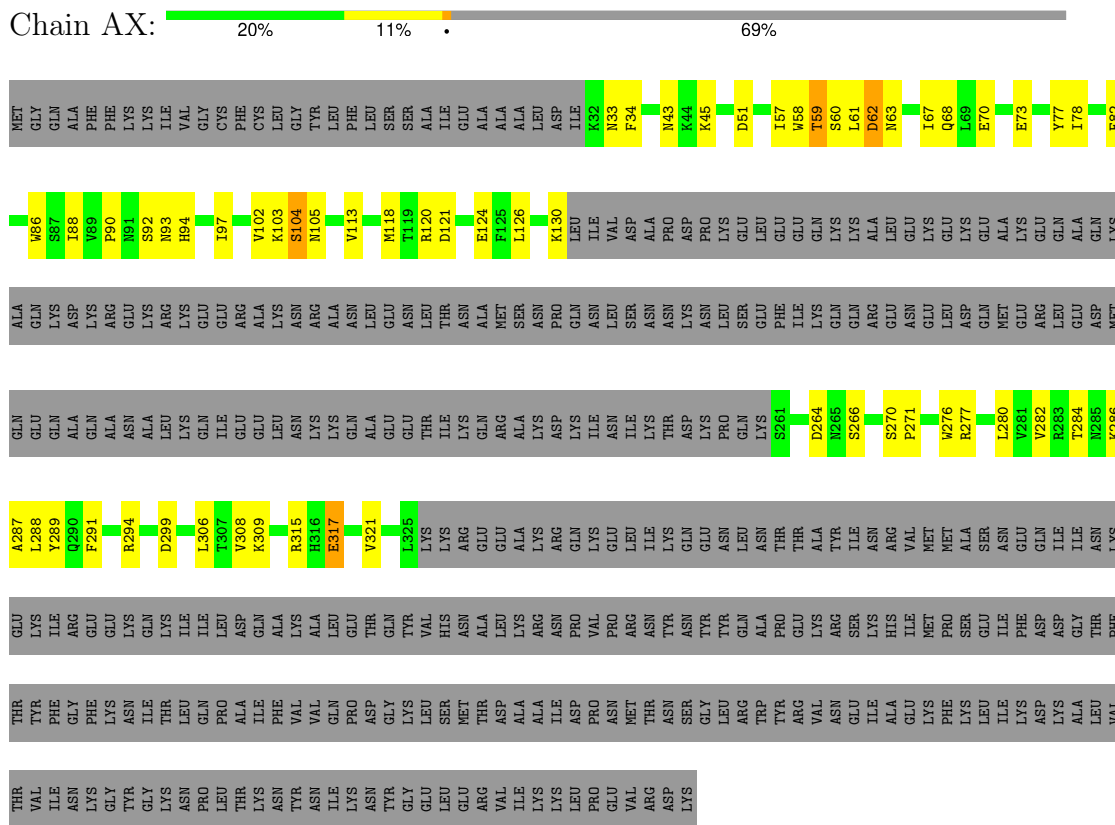
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	CY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	DY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	EY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	FY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	GY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	HY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	IY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	JY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	KY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	LY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	MY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	NY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	OY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	PY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	QY	135	Total 1050	C 649	N 177	O 220	S 4	0	0

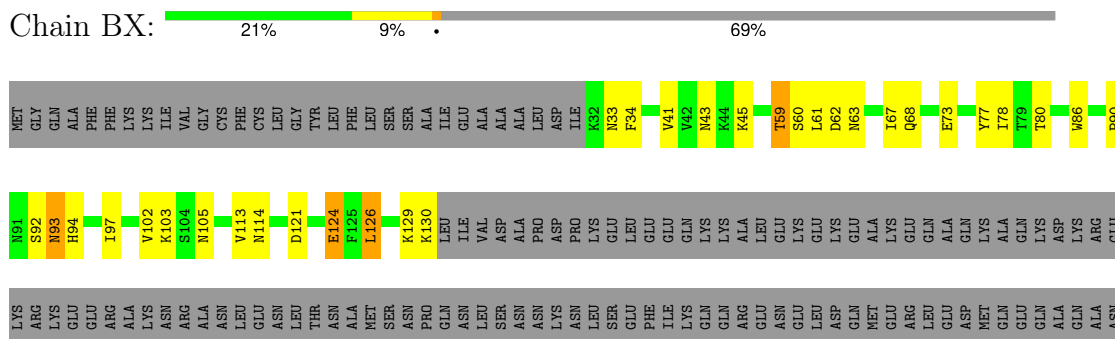
3 Residue-property plots [i](#)

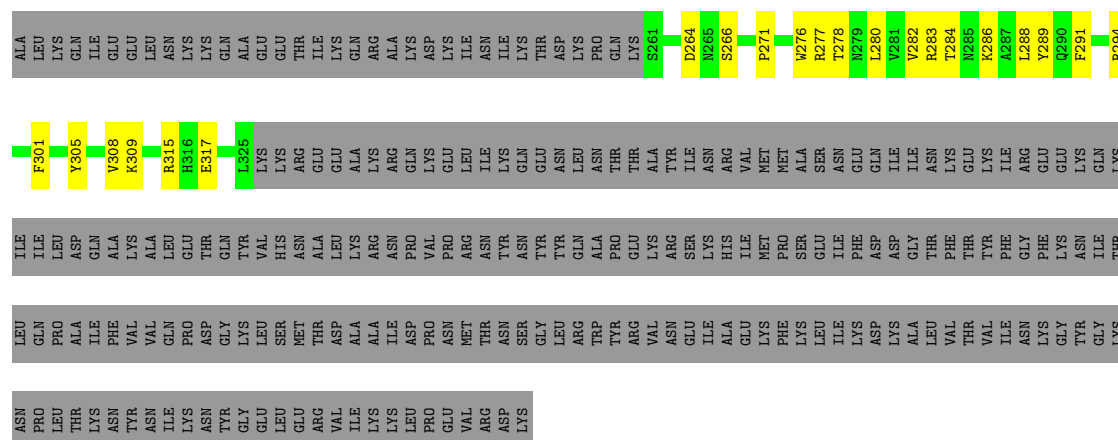
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

- Molecule 1: Cag pathogenicity island protein (Cag8)



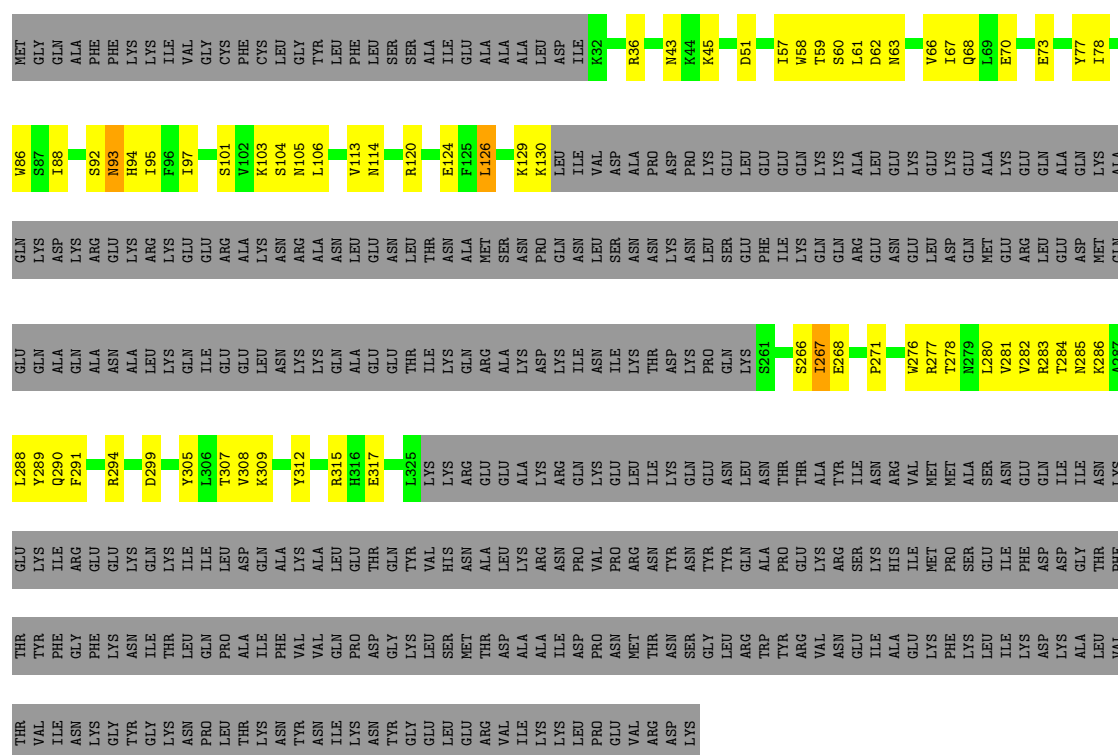
- Molecule 1: Cag pathogenicity island protein (Cag8)





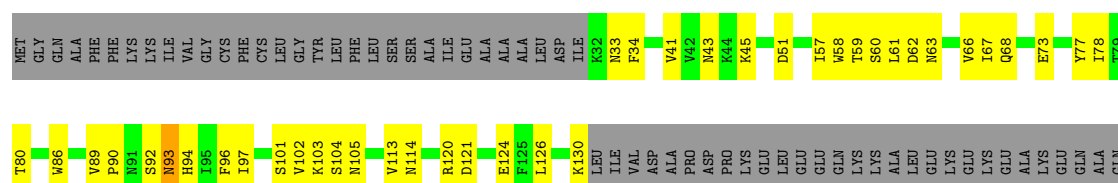
• Molecule 1: Cag pathogenicity island protein (Cag8)

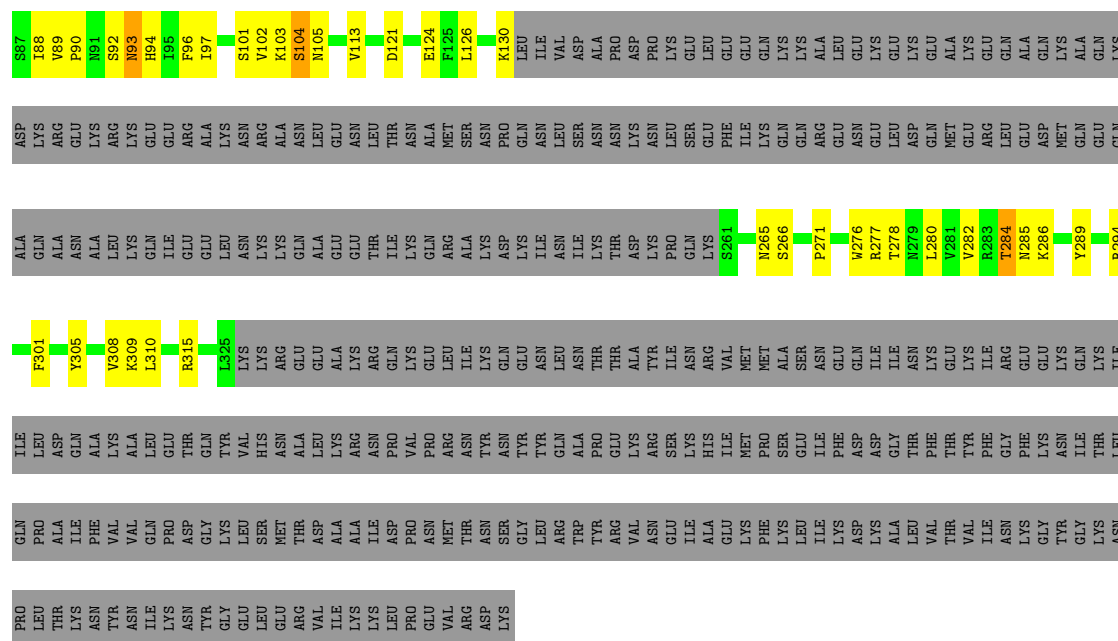
Chain CX: 19% 12% 69%



• Molecule 1: Cag pathogenicity island protein (Cag8)

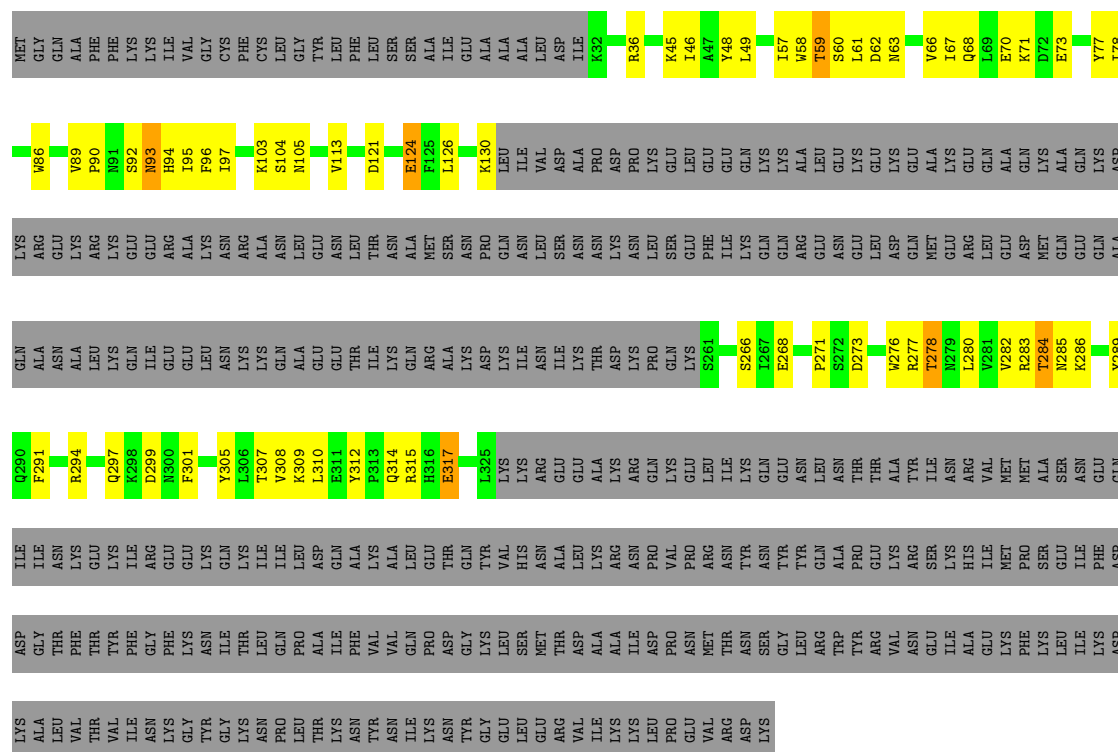
Chain DX: 19% 12% 69%





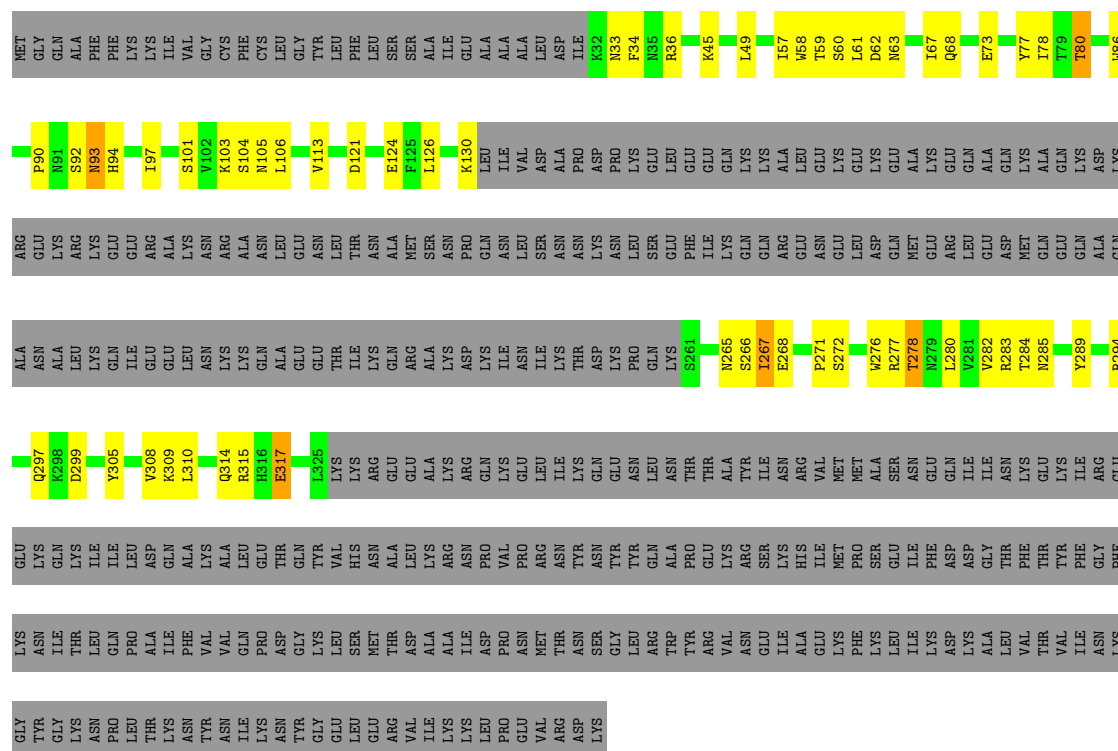
• Molecule 1: Cag pathogenicity island protein (Cag8)

Chain GX: 19% 11% 69%

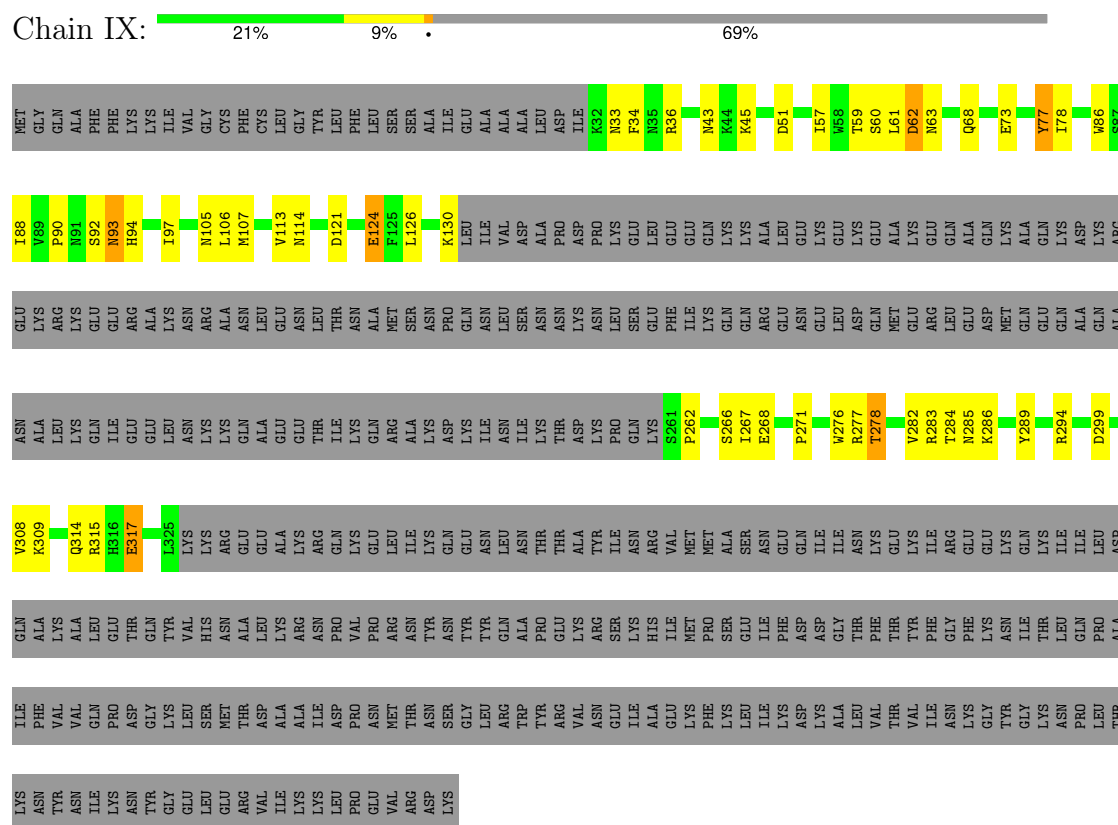


• Molecule 1: Cag pathogenicity island protein (Cag8)

Chain HX: 20% 10% 69%



• Molecule 1: Cag pathogenicity island protein (Cag8)



• Molecule 1: Cag pathogenicity island protein (Cag8)

Response	Percentage
Yes	19%
No	12%
Don't know	69%



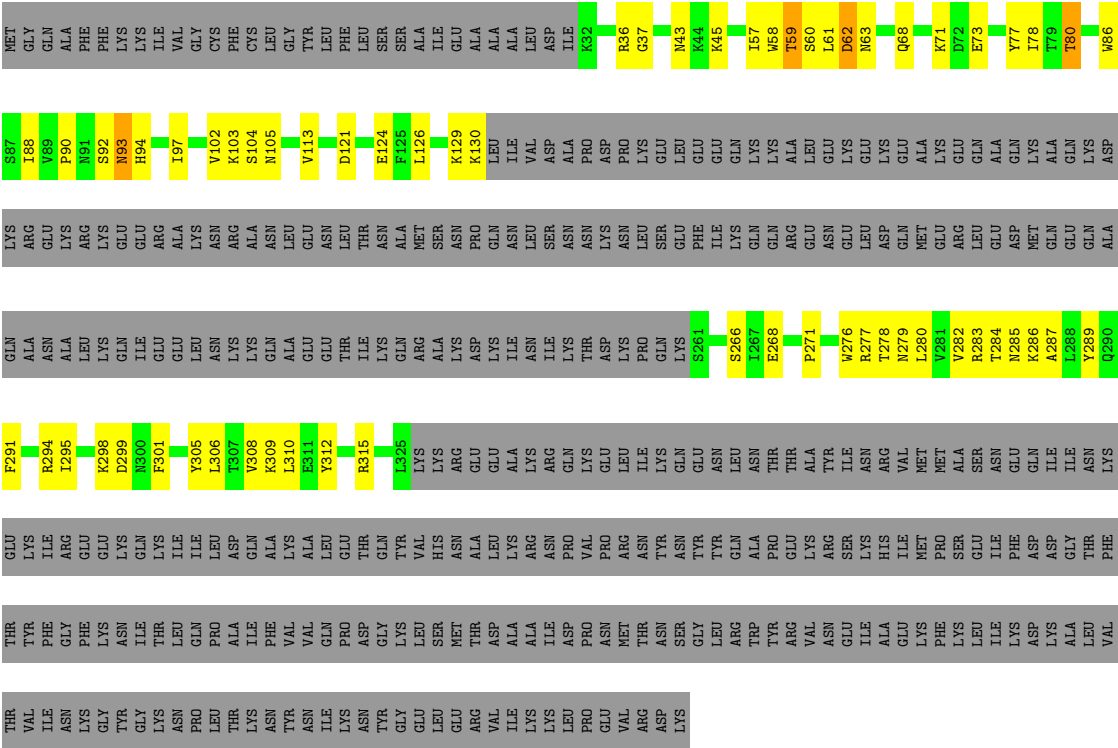
21% 10% • 69%



LYS ASN
GLN PRO
LEU THR
PHE LYS
ASN TYR
ILE LYS
VAL ASN
GLY TYR
GLU GLY
LEU LEU
GLU ARG
VAL VAL
ILE LYS
PHE LYS
SER LYS
SER LYS
ALA LYS
ILE PRO
GLU PRO
VAL VAL
ASP ASP
LYS LYS

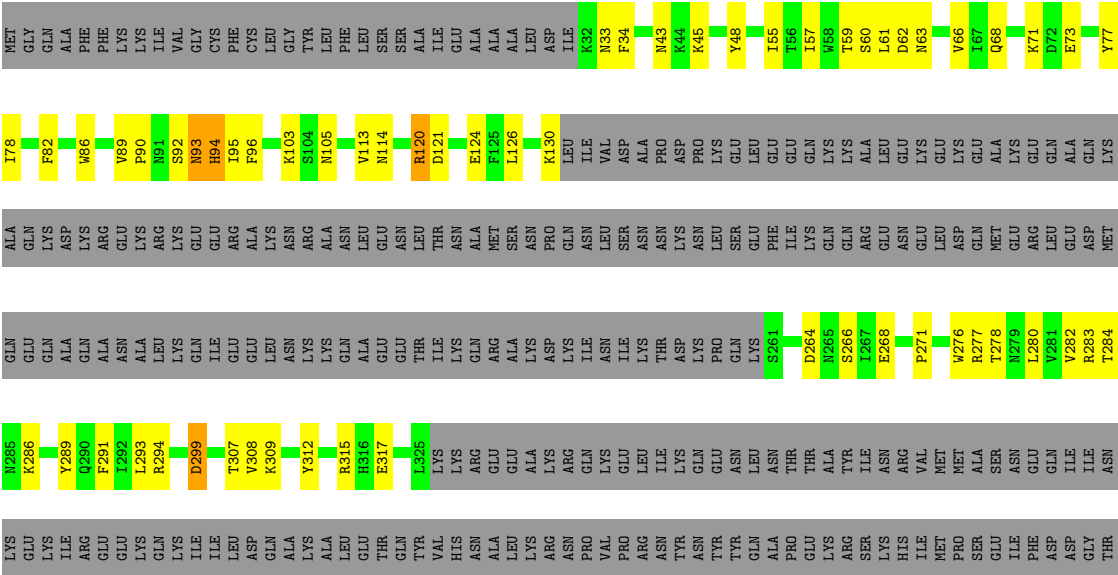
● Molecule 1: Cag pathogenicity island protein (Cag8)

Chain NX: 20% 11% 69%

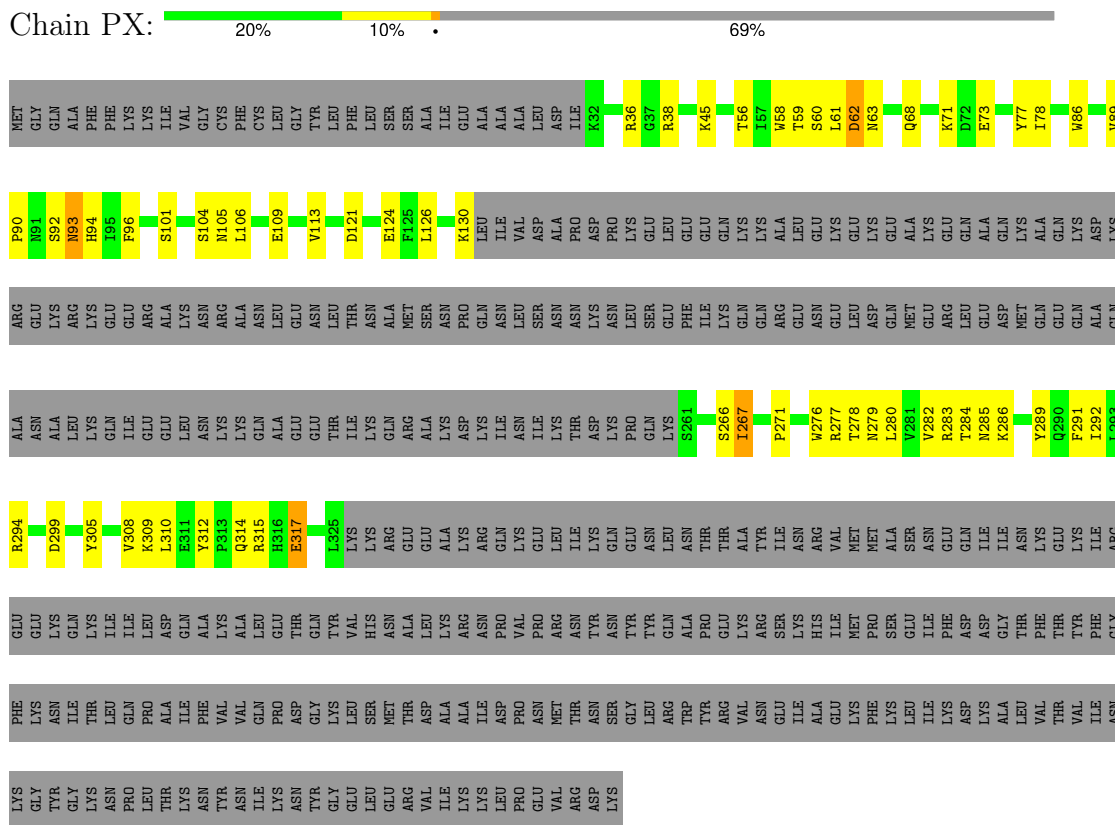


● Molecule 1: Cag pathogenicity island protein (Cag8)

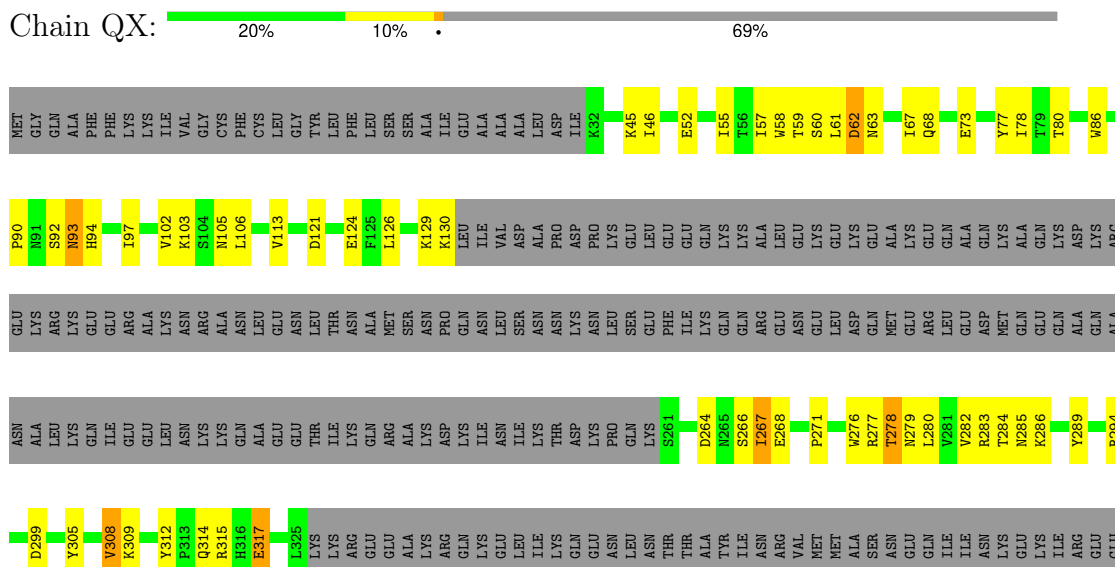
Chain OX: 20% 11% 69%



- Molecule 1: Cag pathogenicity island protein (Cag8)



- Molecule 1: Cag pathogenicity island protein (Cag8)

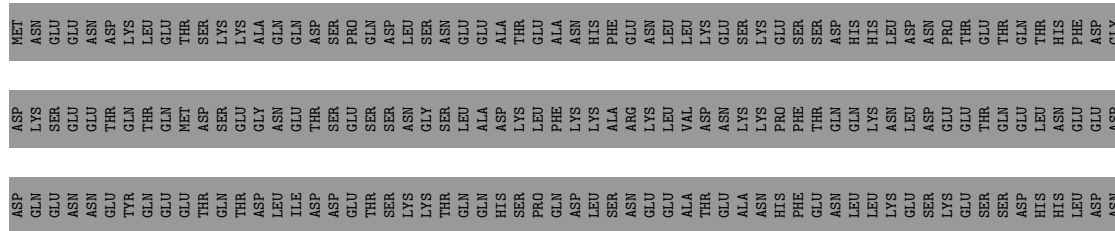


[illegible]

- Molecule 2: Cag pathogenicity island protein (Cag7)

Chain AY: 5% • 93%

[illegible]





- Molecule 2: Cag pathogenicity island protein (Cag7)

Chain CY: 5% . 93%

[illegible]



GLY	ASN
-----	-----

- Molecule 2: Cag pathogenicity island protein (Cag7)

Chain DY: 5% . 93%

[illegible]



[illegible]









[illegible]

- Molecule 2: Cag pathogenicity island protein (Cag7)

Chain LY:  5% 93%

[illegible]

- Molecule 2: Cag pathogenicity island protein (Cag7)

Chain MY: 5% . 93%

MET	ASN	GLU	GLU	ASN	ASP	LYS	LEU	THR	SER	LYS	LYS	ALA	GLN	GLN	ASP	SER	PRO	GLN	ASP	LEU	SER	ASN	GLU	GLU	ALA	ALA	PHE	GLU	ASN	LEU	LEU	LYS	GLU	SER	LYS	GLU	SER	ASP	HIS	HIS	LEU	ASP	ASN	PRO	THR	GLU	THR	GLN	THR	HIS	PHE	ASP	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



● Molecule 2: Cag pathogenicity island protein (Cag7)

Chain NY: 93%



[illegible]

- Molecule 2: Cag pathogenicity island protein (Cag7)

Chain OY: 5% . 93%

[illegible]



[illegible]



TYR
LYS
ASN
GLU
GLY
ASP
SER
ILE
LYS
ILE
LEU
THR
MET
ASP
ASP
ILE
ASP
PHE
SER
GLY
VAL
TYR
ASP
VAL
LYS
ILE
THR
ASN
LYS
SER
VAL
VAL
ASP
GLU
ILE
ILE
LYS
GLN
SER
THR
LYS
THR
LEU
SER
ARG
GLU
HIS
GLU
ILE
THR
THR
SER
PRO
LYS
GLY
ASN

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20929	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	59.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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	AX	0.39	0/1365	0.46	0/1845
1	BX	0.39	0/1365	0.46	0/1845
1	CX	0.39	0/1365	0.46	0/1845
1	DX	0.40	0/1365	0.46	0/1845
1	EX	0.39	0/1365	0.46	0/1845
1	FX	0.39	0/1365	0.46	0/1845
1	GX	0.39	0/1365	0.46	0/1845
1	HX	0.40	0/1365	0.46	0/1845
1	IX	0.39	0/1365	0.46	0/1845
1	JX	0.40	0/1365	0.46	0/1845
1	KX	0.39	0/1365	0.46	0/1845
1	LX	0.39	0/1365	0.46	0/1845
1	MX	0.39	0/1365	0.46	0/1845
1	NX	0.39	0/1365	0.46	0/1845
1	OX	0.39	0/1365	0.46	0/1845
1	PX	0.39	0/1365	0.46	0/1845
1	QX	0.40	0/1365	0.46	0/1845
2	AY	0.30	0/1061	0.41	0/1432
2	BY	0.30	0/1061	0.42	0/1432
2	CY	0.31	0/1061	0.43	0/1432
2	DY	0.31	0/1061	0.42	0/1432
2	EY	0.30	0/1061	0.42	0/1432
2	FY	0.30	0/1061	0.41	0/1432
2	GY	0.30	0/1061	0.42	0/1432
2	HY	0.33	0/1061	0.45	0/1432
2	IY	0.30	0/1061	0.41	0/1432
2	JY	0.31	0/1061	0.43	0/1432
2	KY	0.30	0/1061	0.42	0/1432
2	LY	0.30	0/1061	0.42	0/1432
2	MY	0.30	0/1061	0.42	0/1432
2	NY	0.30	0/1061	0.42	0/1432
2	OY	0.31	0/1061	0.42	0/1432
2	PY	0.30	0/1061	0.41	0/1432
2	QY	0.30	0/1061	0.41	0/1432

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.36	0/41242	0.44	0/55709

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	AX	1339	0	1355	47	0
1	BX	1339	0	1355	37	0
1	CX	1339	0	1355	54	0
1	DX	1339	0	1355	53	0
1	EX	1339	0	1355	43	0
1	FX	1339	0	1355	43	0
1	GX	1339	0	1355	48	0
1	HX	1339	0	1355	43	0
1	IX	1339	0	1355	41	0
1	JX	1339	0	1355	54	0
1	KX	1339	0	1355	40	0
1	LX	1339	0	1355	39	0
1	MX	1339	0	1355	43	0
1	NX	1339	0	1355	50	0
1	OX	1339	0	1355	42	0
1	PX	1339	0	1355	41	0
1	QX	1339	0	1355	44	0
2	AY	1050	0	1038	32	0
2	BY	1050	0	1038	36	0
2	CY	1050	0	1038	28	0
2	DY	1050	0	1038	29	0
2	EY	1050	0	1038	32	0
2	FY	1050	0	1038	28	0
2	GY	1050	0	1038	28	0
2	HY	1050	0	1038	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	IY	1050	0	1038	32	0
2	JY	1050	0	1038	32	0
2	KY	1050	0	1038	28	0
2	LY	1050	0	1038	24	0
2	MY	1050	0	1038	32	0
2	NY	1050	0	1038	29	0
2	OY	1050	0	1038	23	0
2	PY	1050	0	1038	24	0
2	QY	1050	0	1038	31	0
All	All	40613	0	40681	1048	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 13.

The worst 5 of 1048 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:LX:126:LEU:O	1:LX:130:LYS:HB2	1.65	0.96
1:MX:126:LEU:O	1:MX:130:LYS:HB2	1.68	0.93
1:QX:126:LEU:O	1:QX:130:LYS:HB2	1.68	0.93
1:NX:126:LEU:O	1:NX:130:LYS:HB2	1.71	0.91
1:JX:126:LEU:O	1:JX:130:LYS:HB2	1.71	0.91

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	AX	160/521 (31%)	154 (96%)	6 (4%)	0	100	100
1	BX	160/521 (31%)	151 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CX	160/521 (31%)	154 (96%)	6 (4%)	0	100	100
1	DX	160/521 (31%)	156 (98%)	4 (2%)	0	100	100
1	EX	160/521 (31%)	153 (96%)	7 (4%)	0	100	100
1	FX	160/521 (31%)	152 (95%)	8 (5%)	0	100	100
1	GX	160/521 (31%)	153 (96%)	7 (4%)	0	100	100
1	HX	160/521 (31%)	155 (97%)	5 (3%)	0	100	100
1	IX	160/521 (31%)	154 (96%)	6 (4%)	0	100	100
1	JX	160/521 (31%)	151 (94%)	9 (6%)	0	100	100
1	KX	160/521 (31%)	157 (98%)	3 (2%)	0	100	100
1	LX	160/521 (31%)	154 (96%)	6 (4%)	0	100	100
1	MX	160/521 (31%)	155 (97%)	5 (3%)	0	100	100
1	NX	160/521 (31%)	156 (98%)	4 (2%)	0	100	100
1	OX	160/521 (31%)	152 (95%)	8 (5%)	0	100	100
1	PX	160/521 (31%)	154 (96%)	6 (4%)	0	100	100
1	QX	160/521 (31%)	154 (96%)	6 (4%)	0	100	100
2	AY	133/1927 (7%)	127 (96%)	6 (4%)	0	100	100
2	BY	133/1927 (7%)	128 (96%)	5 (4%)	0	100	100
2	CY	133/1927 (7%)	129 (97%)	4 (3%)	0	100	100
2	DY	133/1927 (7%)	126 (95%)	7 (5%)	0	100	100
2	EY	133/1927 (7%)	127 (96%)	6 (4%)	0	100	100
2	FY	133/1927 (7%)	123 (92%)	10 (8%)	0	100	100
2	GY	133/1927 (7%)	129 (97%)	4 (3%)	0	100	100
2	HY	133/1927 (7%)	126 (95%)	7 (5%)	0	100	100
2	IY	133/1927 (7%)	128 (96%)	5 (4%)	0	100	100
2	JY	133/1927 (7%)	127 (96%)	6 (4%)	0	100	100
2	KY	133/1927 (7%)	126 (95%)	7 (5%)	0	100	100
2	LY	133/1927 (7%)	127 (96%)	6 (4%)	0	100	100
2	MY	133/1927 (7%)	126 (95%)	7 (5%)	0	100	100
2	NY	133/1927 (7%)	127 (96%)	6 (4%)	0	100	100
2	OY	133/1927 (7%)	129 (97%)	4 (3%)	0	100	100
2	PY	133/1927 (7%)	127 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QY	133/1927 (7%)	128 (96%)	5 (4%)	0	100	100
All	All	4981/41616 (12%)	4775 (96%)	206 (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 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	AX	152/469 (32%)	143 (94%)	9 (6%)	16	44
1	BX	152/469 (32%)	142 (93%)	10 (7%)	14	41
1	CX	152/469 (32%)	143 (94%)	9 (6%)	16	44
1	DX	152/469 (32%)	145 (95%)	7 (5%)	23	52
1	EX	152/469 (32%)	140 (92%)	12 (8%)	10	34
1	FX	152/469 (32%)	146 (96%)	6 (4%)	27	56
1	GX	152/469 (32%)	142 (93%)	10 (7%)	14	41
1	HX	152/469 (32%)	143 (94%)	9 (6%)	16	44
1	IX	152/469 (32%)	142 (93%)	10 (7%)	14	41
1	JX	152/469 (32%)	143 (94%)	9 (6%)	16	44
1	KX	152/469 (32%)	142 (93%)	10 (7%)	14	41
1	LX	152/469 (32%)	140 (92%)	12 (8%)	10	34
1	MX	152/469 (32%)	143 (94%)	9 (6%)	16	44
1	NX	152/469 (32%)	147 (97%)	5 (3%)	33	61
1	OX	152/469 (32%)	141 (93%)	11 (7%)	12	37
1	PX	152/469 (32%)	146 (96%)	6 (4%)	27	56
1	QX	152/469 (32%)	142 (93%)	10 (7%)	14	41
2	AY	115/1724 (7%)	112 (97%)	3 (3%)	41	66
2	BY	115/1724 (7%)	111 (96%)	4 (4%)	31	59
2	CY	115/1724 (7%)	111 (96%)	4 (4%)	31	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	DY	115/1724 (7%)	110 (96%)	5 (4%)	25	54
2	EY	115/1724 (7%)	114 (99%)	1 (1%)	75	86
2	FY	115/1724 (7%)	112 (97%)	3 (3%)	41	66
2	GY	115/1724 (7%)	112 (97%)	3 (3%)	41	66
2	HY	115/1724 (7%)	111 (96%)	4 (4%)	31	59
2	IY	115/1724 (7%)	111 (96%)	4 (4%)	31	59
2	JY	115/1724 (7%)	113 (98%)	2 (2%)	56	75
2	KY	115/1724 (7%)	112 (97%)	3 (3%)	41	66
2	LY	115/1724 (7%)	111 (96%)	4 (4%)	31	59
2	MY	115/1724 (7%)	111 (96%)	4 (4%)	31	59
2	NY	115/1724 (7%)	111 (96%)	4 (4%)	31	59
2	OY	115/1724 (7%)	112 (97%)	3 (3%)	41	66
2	PY	115/1724 (7%)	111 (96%)	4 (4%)	31	59
2	QY	115/1724 (7%)	110 (96%)	5 (4%)	25	54
All	All	4539/37281 (12%)	4325 (95%)	214 (5%)	24	51

5 of 214 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	MX	78	ILE
1	PX	317	GLU
2	NY	1499	GLU
1	MX	270	SER
1	OX	93	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 116 such sidechains are listed below:

Mol	Chain	Res	Type
2	DY	1549	ASN
2	QY	1476	HIS
2	GY	1583	GLN
2	PY	1594	ASN
2	NY	1549	ASN

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 oligosaccharides 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 Map visualisation

This section contains visualisations of the EMDB entry EMD-20021. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.