



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 12:50 PM UTC

PDB ID : 6X6K / pdb_00006x6k
EMDB ID : EMD-22076
Title : Cryo-EM Structure of the Helicobacter pylori dCag3 OMC
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 : 3.10 Å(reported)

This is a Full wwPDB EM 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/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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

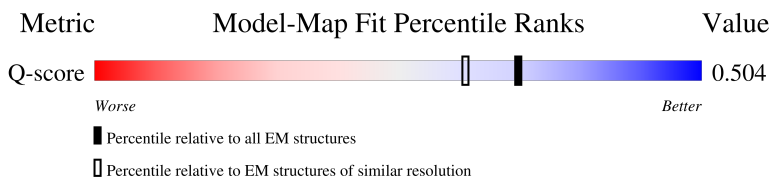
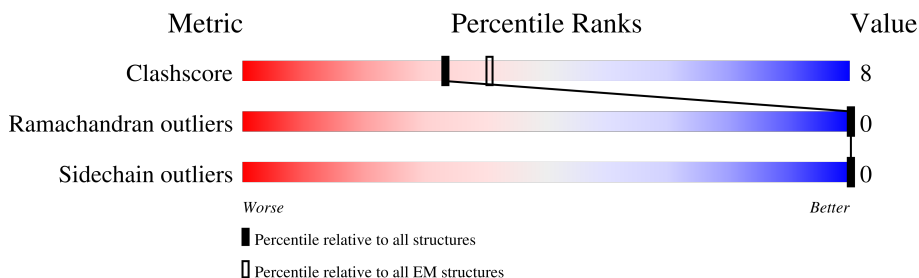
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AT	278	38% 52%12%36%
1	BT	278	36% 52%13%36%
1	CT	278	36% 51%13%36%
1	DT	278	37% 51%13%36%

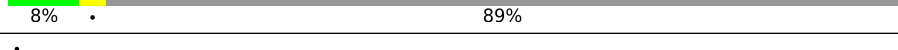
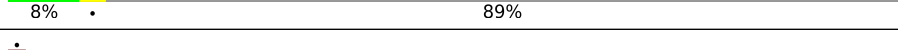
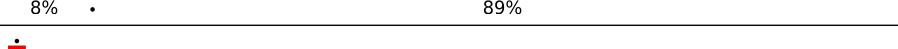
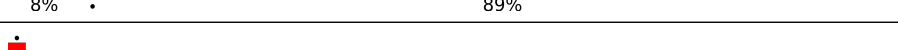
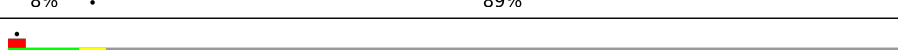
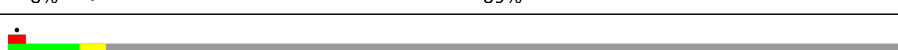
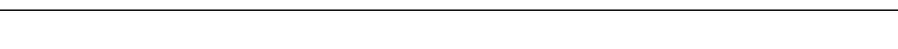
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Mol	Chain	Length	Quality of chain
1	ET	278	
1	FT	278	
1	GT	278	
1	HT	278	
1	IT	278	
1	JT	278	
1	KT	278	
1	LT	278	
1	MT	278	
1	NT	278	
2	AX	522	
2	BX	522	
2	CX	522	
2	DX	522	
2	EX	522	
2	FX	522	
2	GX	522	
2	HX	522	
2	IX	522	
2	JX	522	
2	KX	522	
2	LX	522	
2	MX	522	
2	NX	522	
3	AY	1927	

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Mol	Chain	Length	Quality of chain
3	BY	1927	 8% . 89%
3	CY	1927	 8% . 89%
3	DY	1927	 8% . 89%
3	EY	1927	 8% . 89%
3	FY	1927	 8% . 89%
3	GY	1927	 8% . 89%
3	HY	1927	 8% . 89%
3	IY	1927	 8% . 89%
3	JY	1927	 8% . 89%
3	KY	1927	 8% . 89%
3	LY	1927	 8% . 89%
3	MY	1927	 8% . 89%
3	NY	1927	 8% . 89%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 60970 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AT	179	Total	C	N	O	S	0	0
			1502	957	261	282	2		
1	BT	179	Total	C	N	O	S	0	0
			1502	957	261	282	2		
1	CT	179	Total	C	N	O	S	0	0
			1502	957	261	282	2		
1	DT	179	Total	C	N	O	S	0	0
			1502	957	261	282	2		
1	ET	179	Total	C	N	O	S	0	0
			1502	957	261	282	2		
1	FT	179	Total	C	N	O	S	0	0
			1502	957	261	282	2		
1	GT	179	Total	C	N	O	S	0	0
			1502	957	261	282	2		
1	HT	179	Total	C	N	O	S	0	0
			1502	957	261	282	2		
1	IT	179	Total	C	N	O	S	0	0
			1502	957	261	282	2		
1	JT	179	Total	C	N	O	S	0	0
			1502	957	261	282	2		
1	KT	179	Total	C	N	O	S	0	0
			1502	957	261	282	2		
1	LT	179	Total	C	N	O	S	0	0
			1502	957	261	282	2		
1	MT	179	Total	C	N	O	S	0	0
			1502	957	261	282	2		
1	NT	179	Total	C	N	O	S	0	0
			1502	957	261	282	2		

- Molecule 2 is a protein called Type IV secretion system apparatus protein CagX.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AX	155	Total	C	N	O	S	0	0
			1275	819	222	231	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	BX	155	Total	C	N	O	S	0	0
			1275	819	222	231	3		
2	CX	155	Total	C	N	O	S	0	0
			1275	819	222	231	3		
2	DX	155	Total	C	N	O	S	0	0
			1275	819	222	231	3		
2	EX	155	Total	C	N	O	S	0	0
			1275	819	222	231	3		
2	FX	155	Total	C	N	O	S	0	0
			1275	819	222	231	3		
2	GX	155	Total	C	N	O	S	0	0
			1275	819	222	231	3		
2	HX	155	Total	C	N	O	S	0	0
			1275	819	222	231	3		
2	IX	155	Total	C	N	O	S	0	0
			1275	819	222	231	3		
2	JX	155	Total	C	N	O	S	0	0
			1275	819	222	231	3		
2	KX	155	Total	C	N	O	S	0	0
			1275	819	222	231	3		
2	LX	155	Total	C	N	O	S	0	0
			1275	819	222	231	3		
2	MX	155	Total	C	N	O	S	0	0
			1275	819	222	231	3		
2	NX	155	Total	C	N	O	S	0	0
			1275	819	222	231	3		

- Molecule 3 is a protein called Cag pathogenicity island protein (Cag7).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AY	209	Total	C	N	O	S	0	0
			1578	1014	255	300	9		
3	BY	209	Total	C	N	O	S	0	0
			1578	1014	255	300	9		
3	CY	209	Total	C	N	O	S	0	0
			1578	1014	255	300	9		
3	DY	209	Total	C	N	O	S	0	0
			1578	1014	255	300	9		
3	EY	209	Total	C	N	O	S	0	0
			1578	1014	255	300	9		
3	FY	209	Total	C	N	O	S	0	0
			1578	1014	255	300	9		

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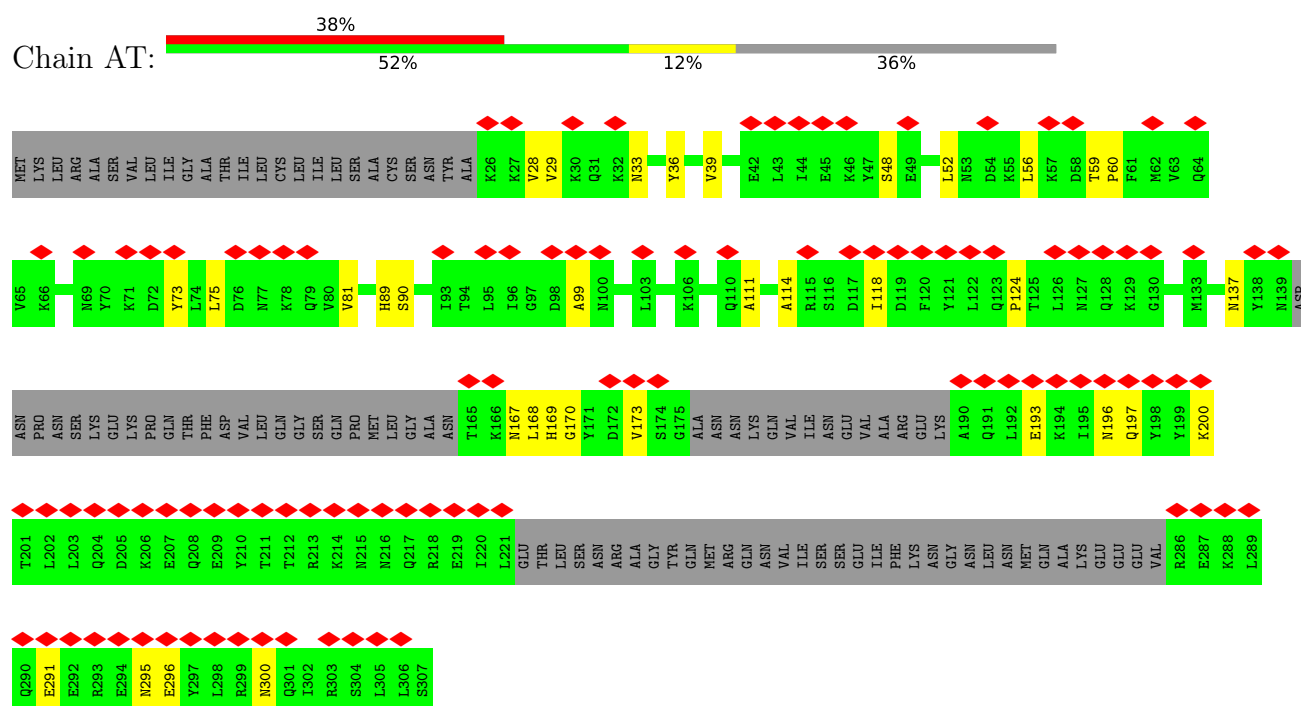
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	GY	209	Total	C	N	O	S	0	0
			1578	1014	255	300	9		
3	HY	209	Total	C	N	O	S	0	0
			1578	1014	255	300	9		
3	IY	209	Total	C	N	O	S	0	0
			1578	1014	255	300	9		
3	JY	209	Total	C	N	O	S	0	0
			1578	1014	255	300	9		
3	KY	209	Total	C	N	O	S	0	0
			1578	1014	255	300	9		
3	LY	209	Total	C	N	O	S	0	0
			1578	1014	255	300	9		
3	MY	209	Total	C	N	O	S	0	0
			1578	1014	255	300	9		
3	NY	209	Total	C	N	O	S	0	0
			1578	1014	255	300	9		

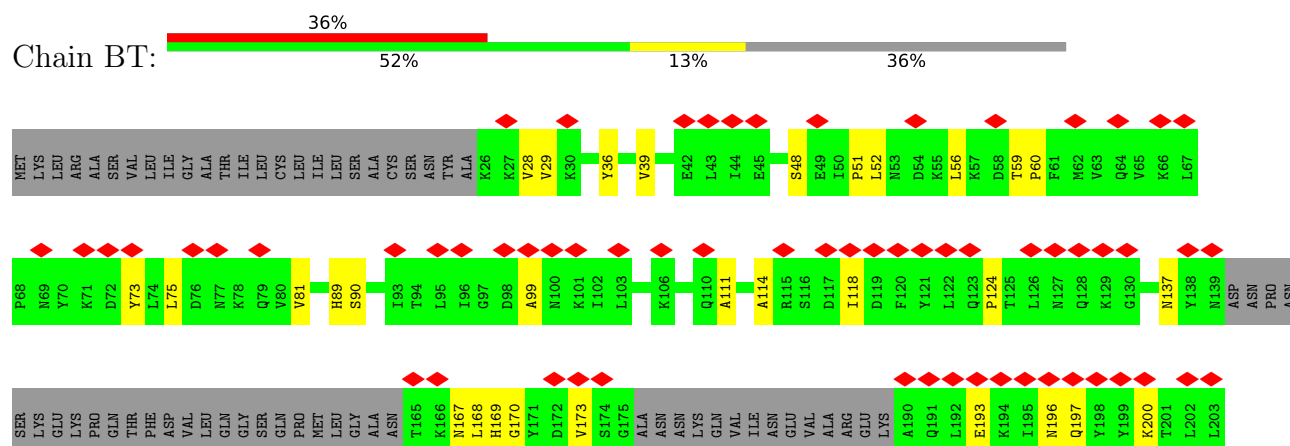
3 Residue-property plots

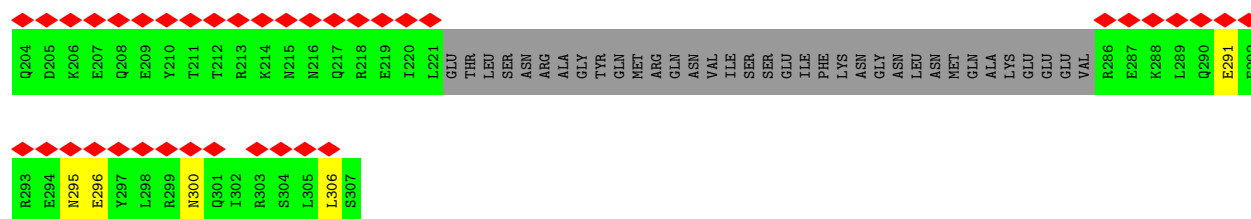
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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

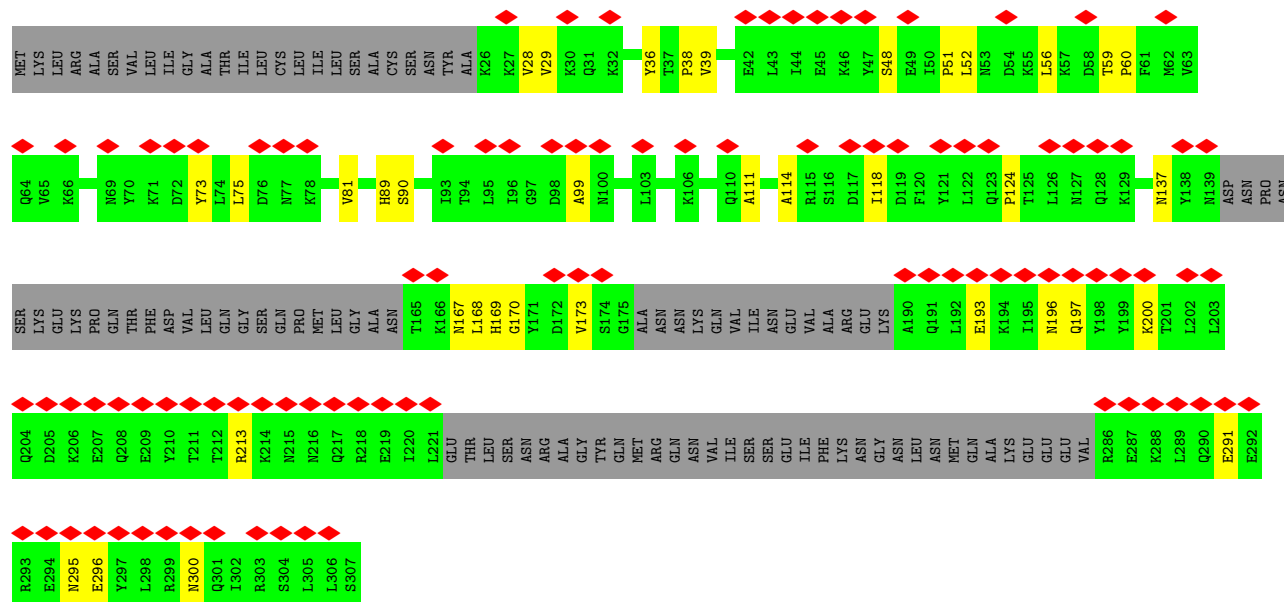


• Molecule 1: Cag pathogenicity island protein

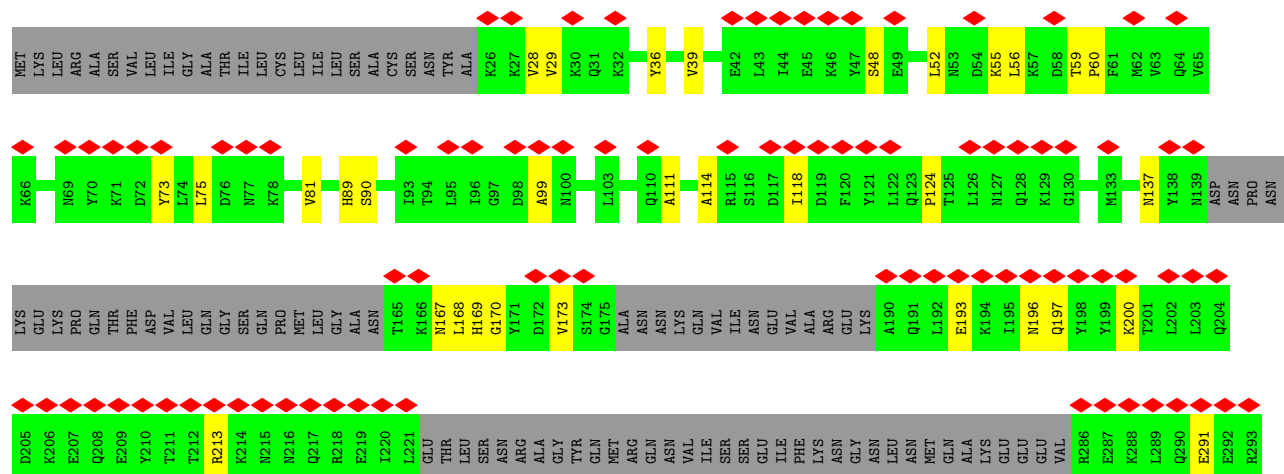
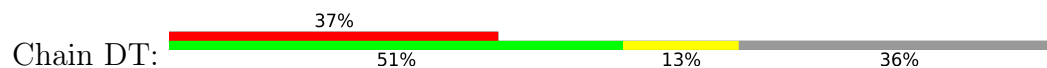


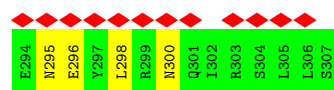


• Molecule 1: Cag pathogenicity island protein

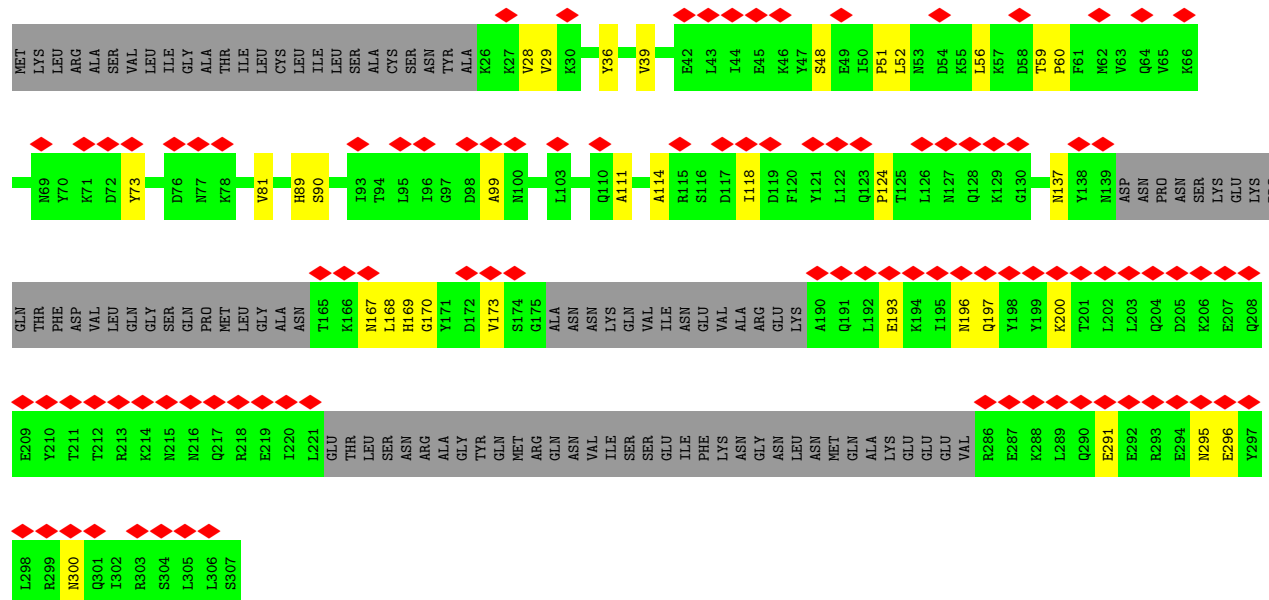


• Molecule 1: Cag pathogenicity island protein

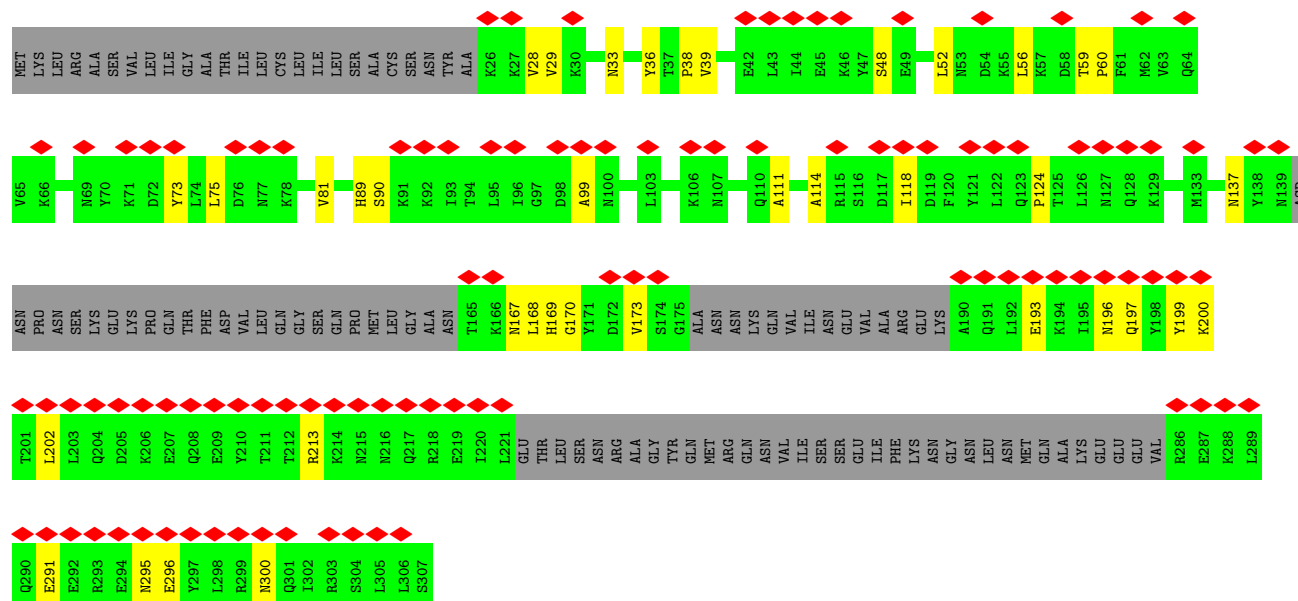
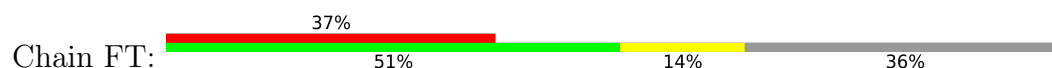




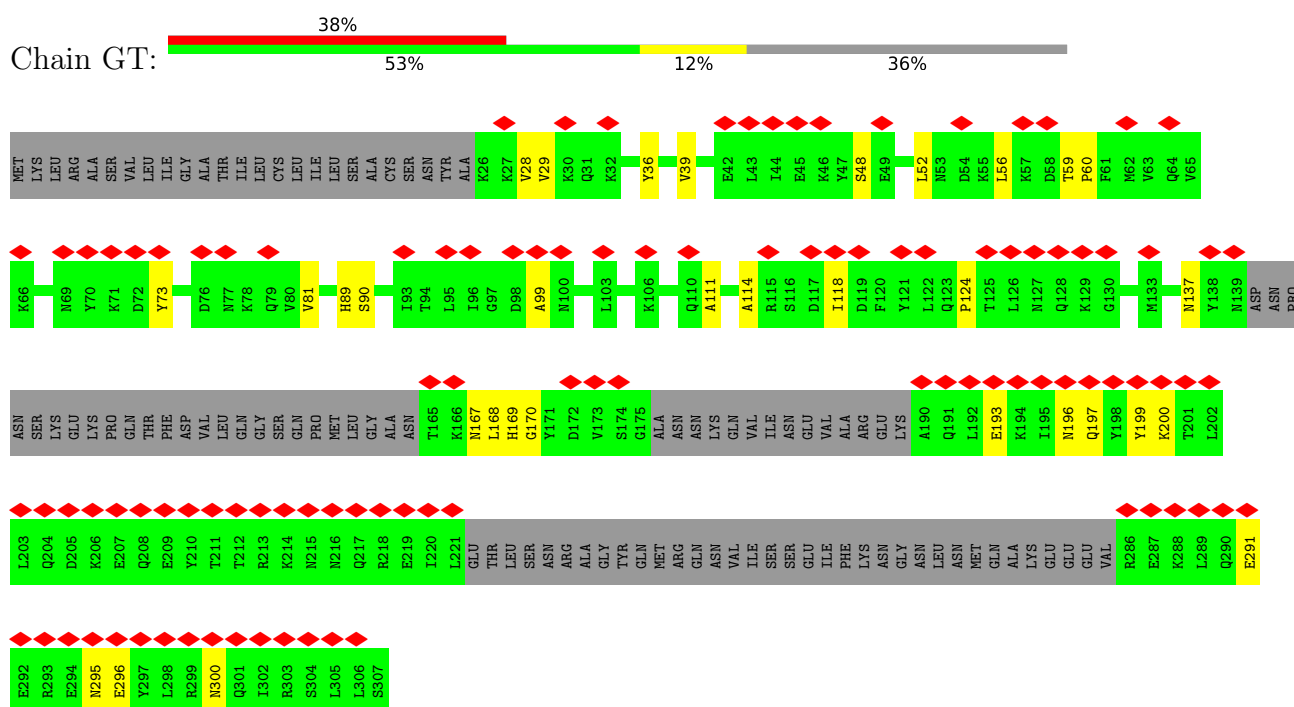
• Molecule 1: Cag pathogenicity island protein



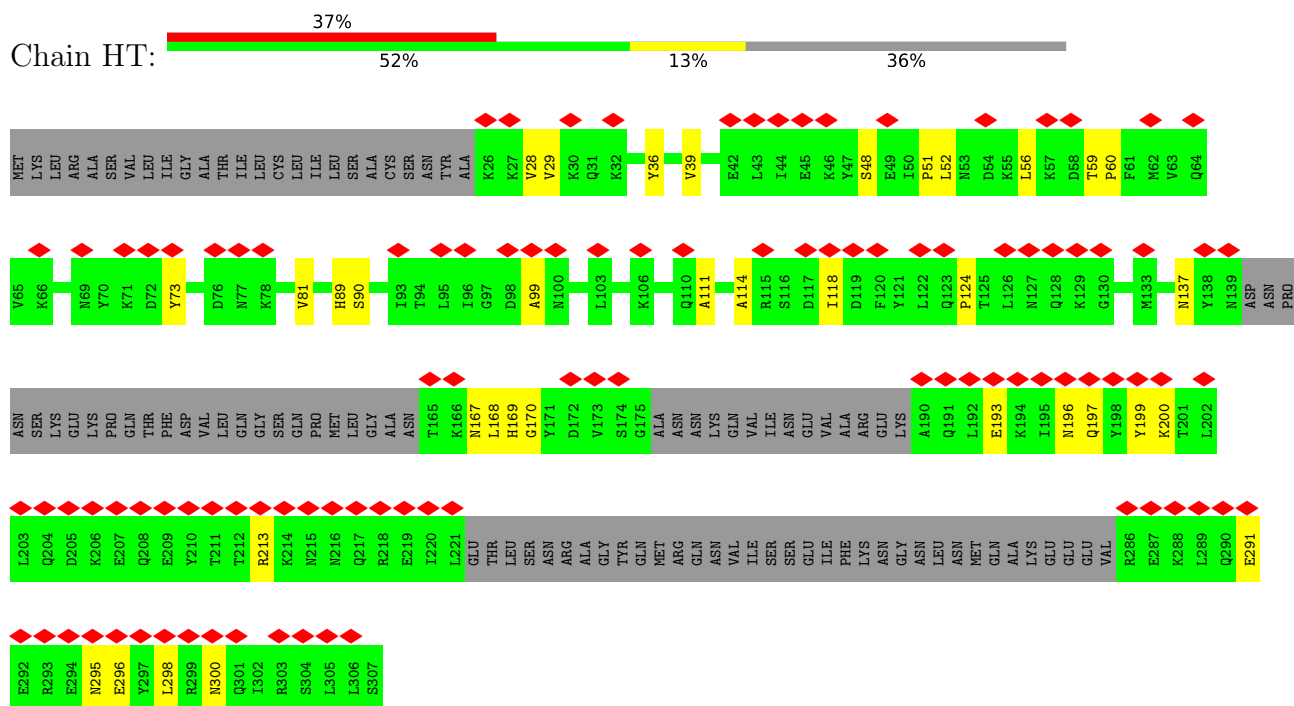
• Molecule 1: Cag pathogenicity island protein



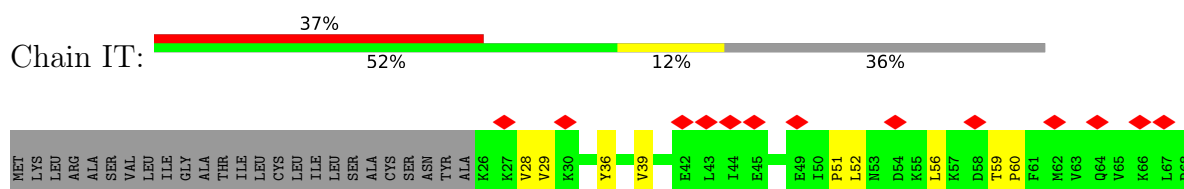
• Molecule 1: Cag pathogenicity island protein

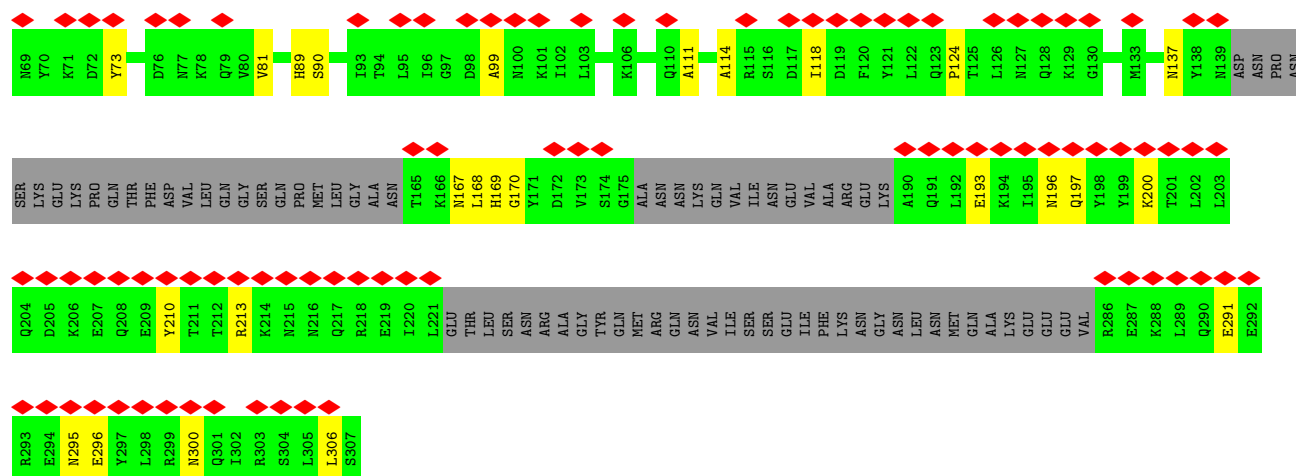


• Molecule 1: Cag pathogenicity island protein

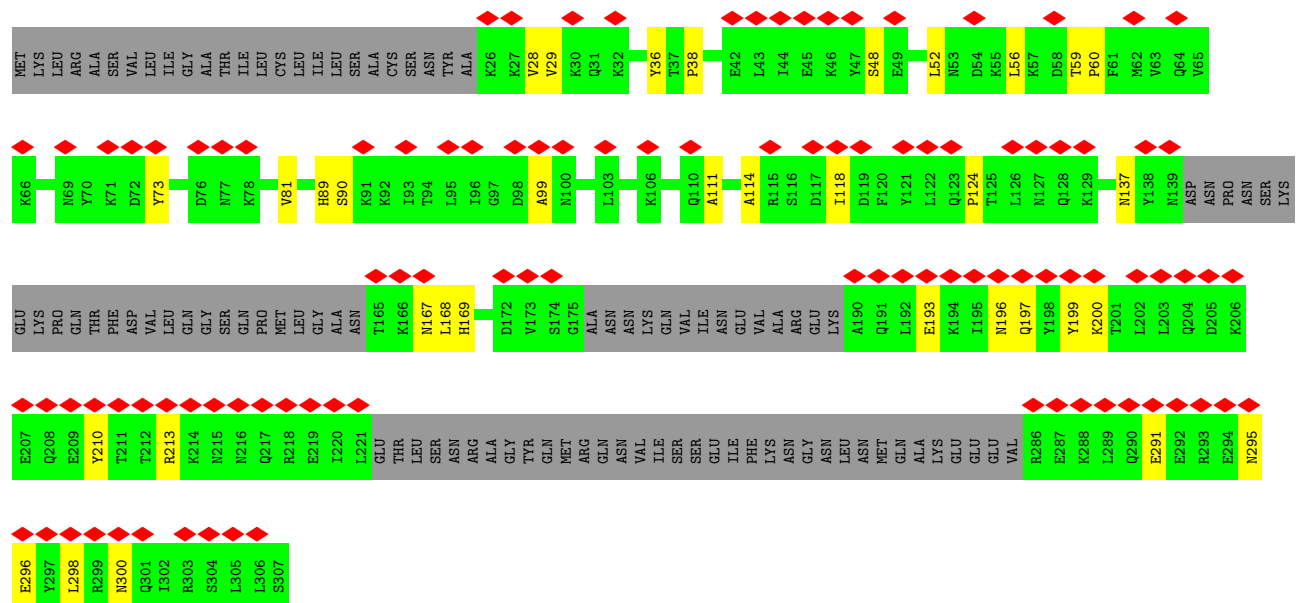
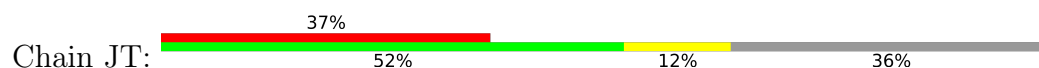


• Molecule 1: Cag pathogenicity island protein

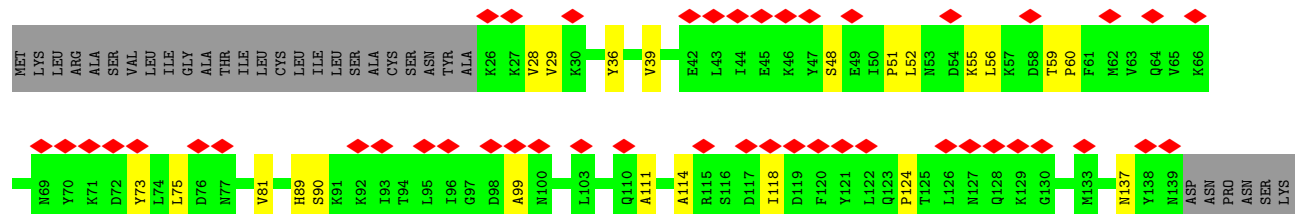
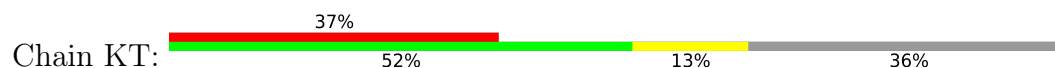


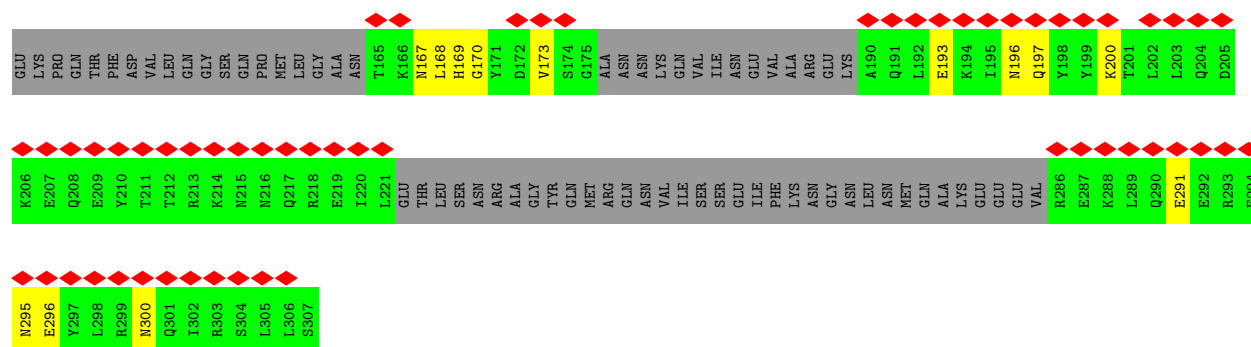


• Molecule 1: Cag pathogenicity island protein

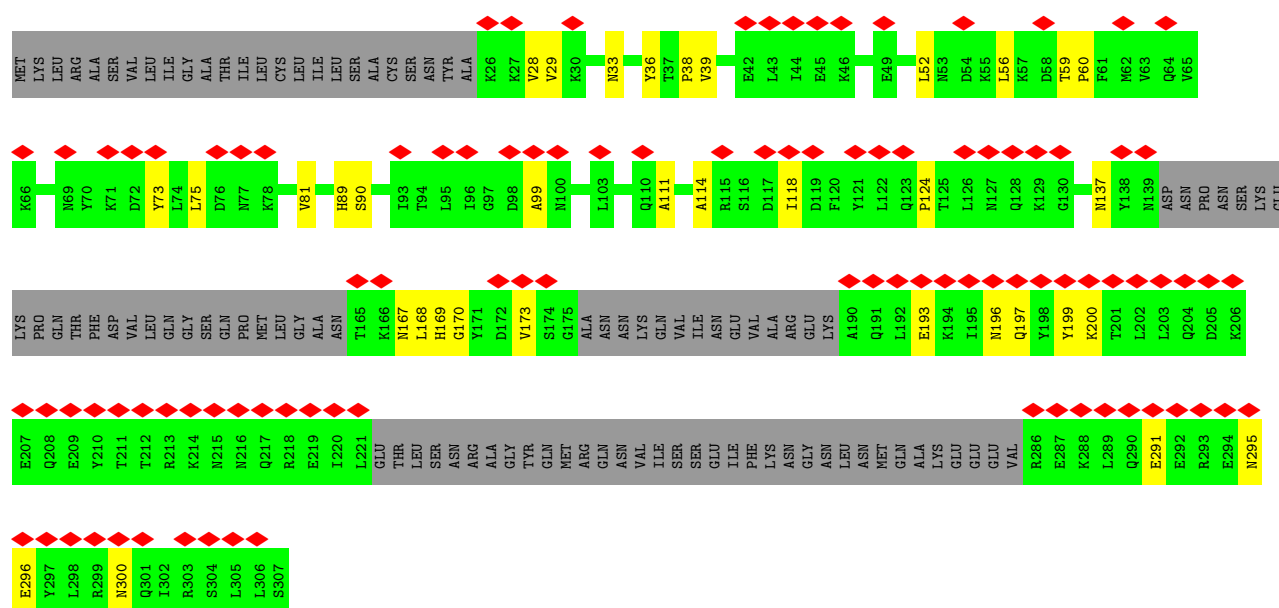


• Molecule 1: Cag pathogenicity island protein

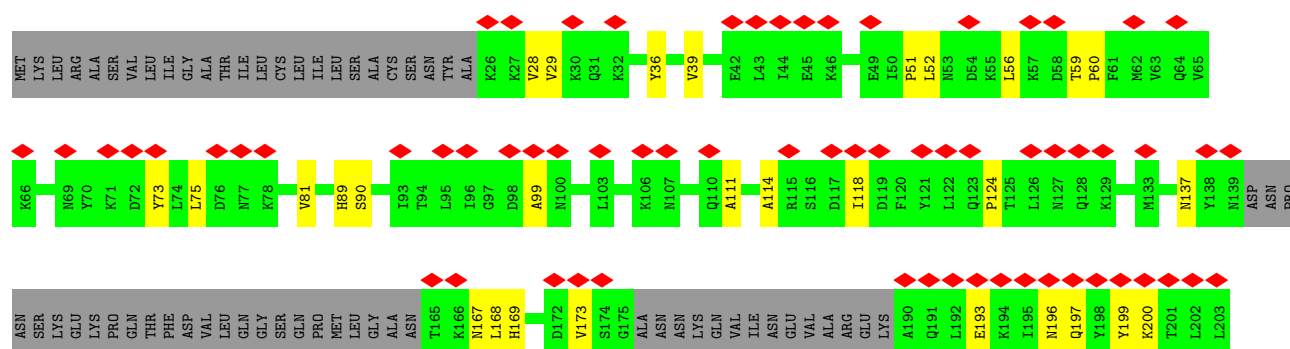
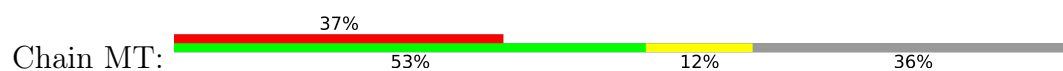


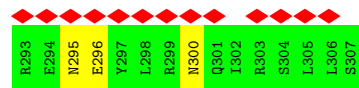


• Molecule 1: Cag pathogenicity island protein

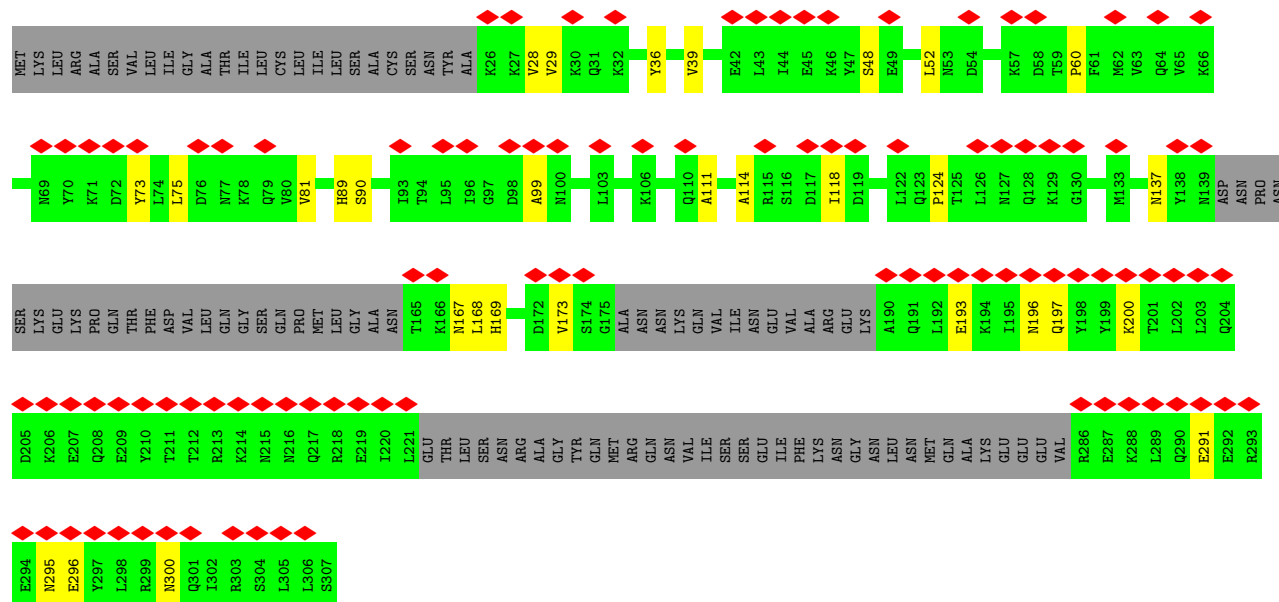


• Molecule 1: Cag pathogenicity island protein

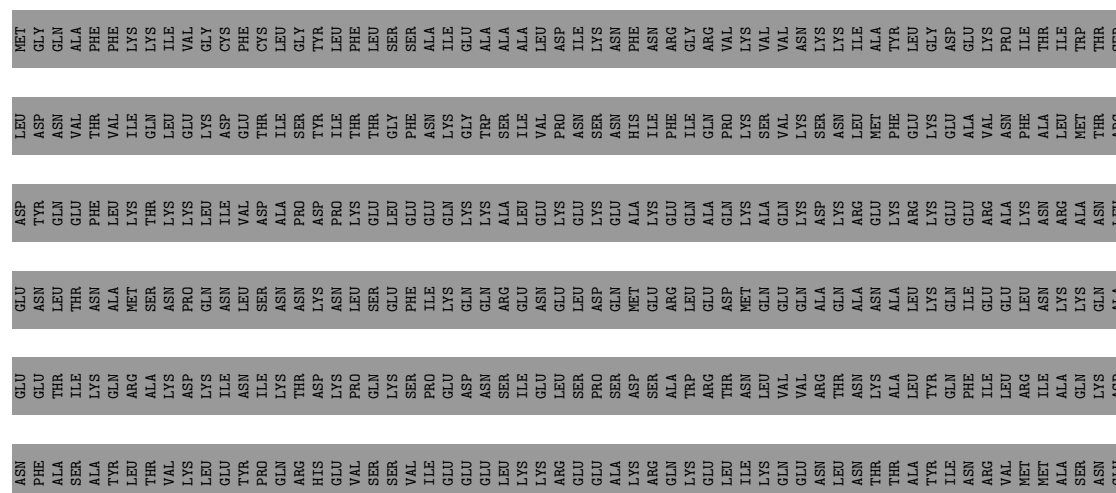


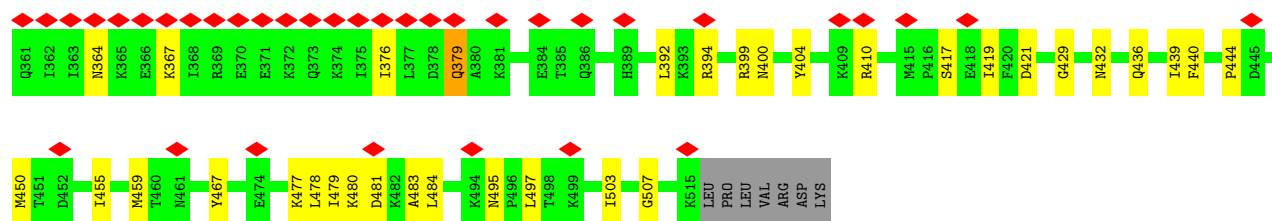


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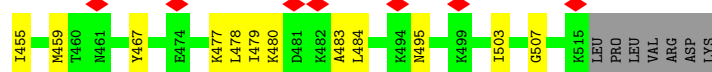
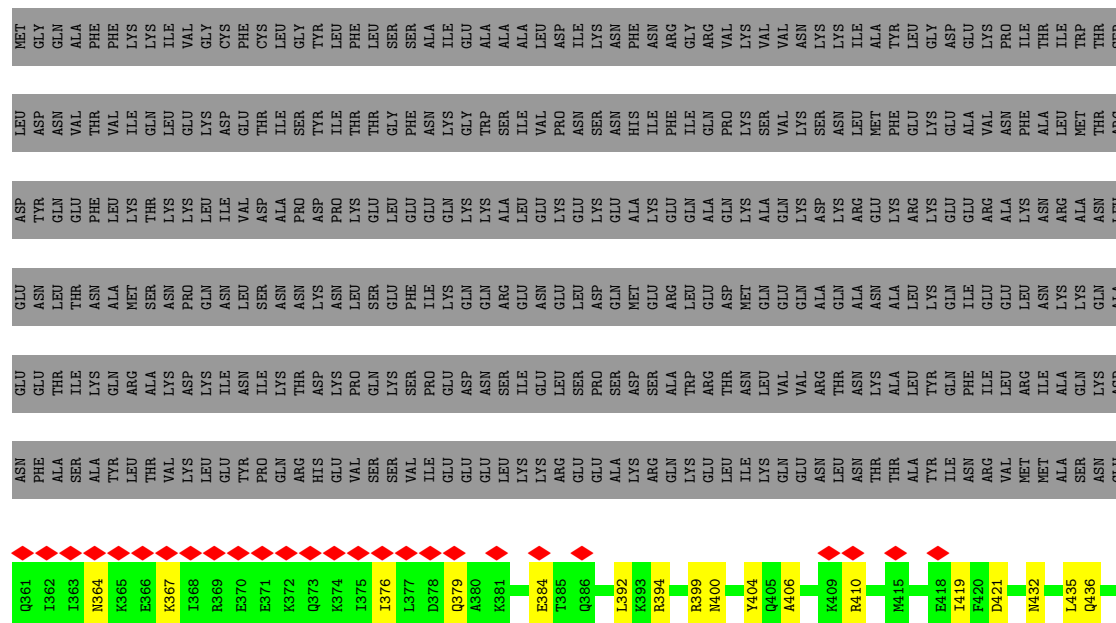


Chain AX:



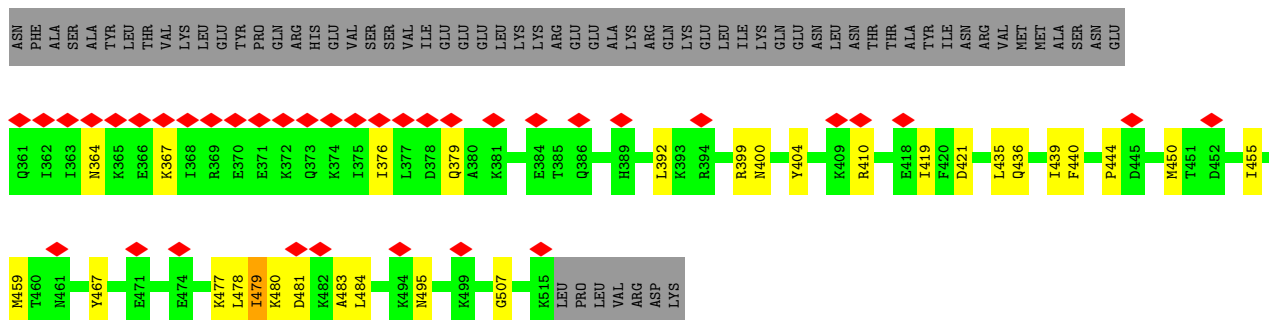


• Molecule 2: Type IV secretion system apparatus protein CagX

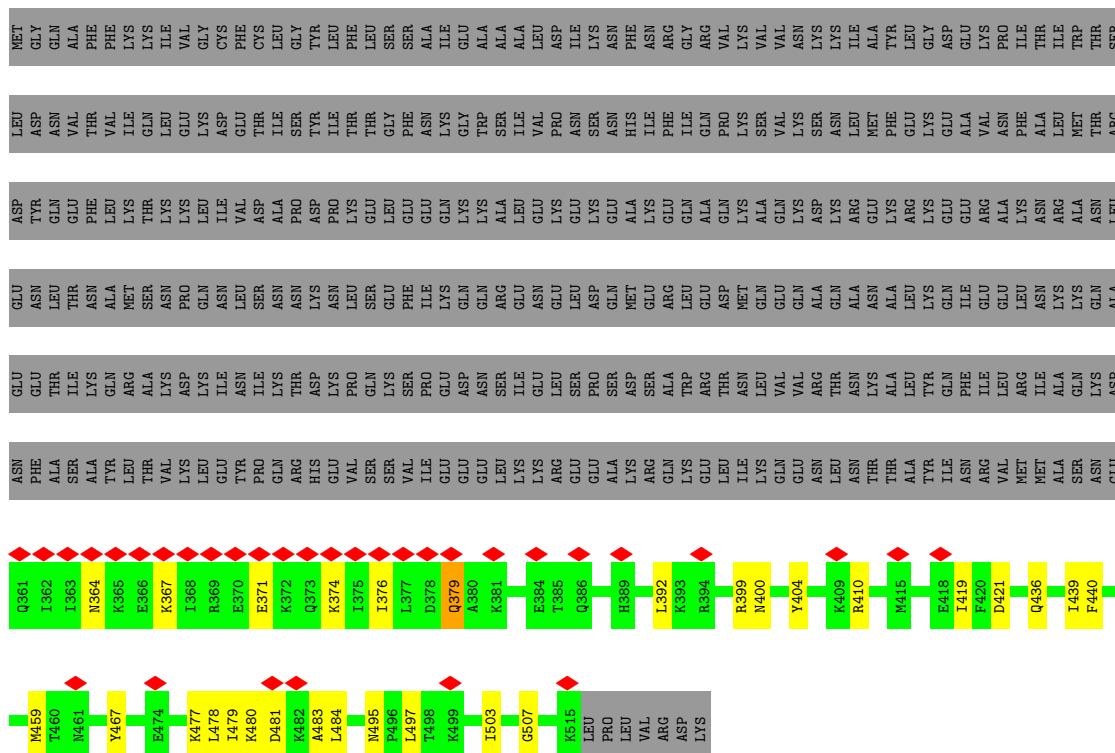


• Molecule 2: Type IV secretion system apparatus protein CagX

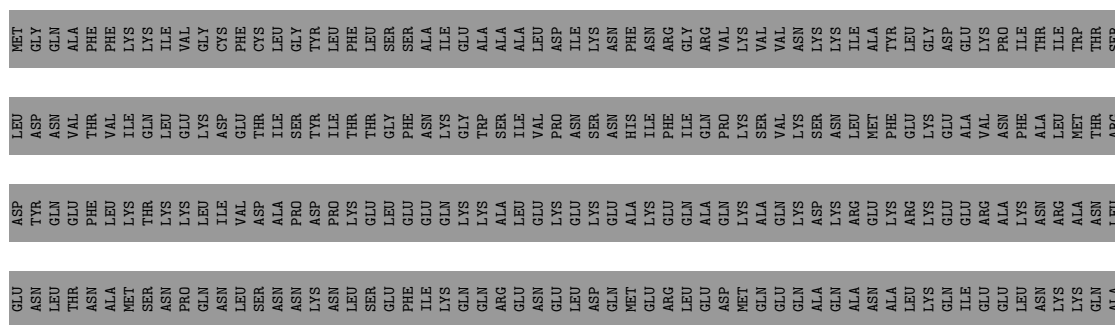


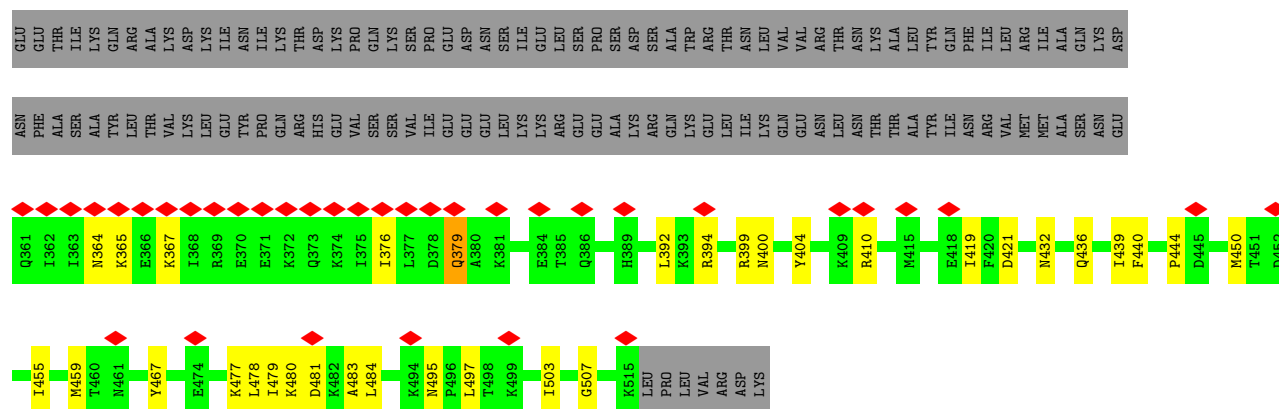


- Molecule 2: Type IV secretion system apparatus protein CagX

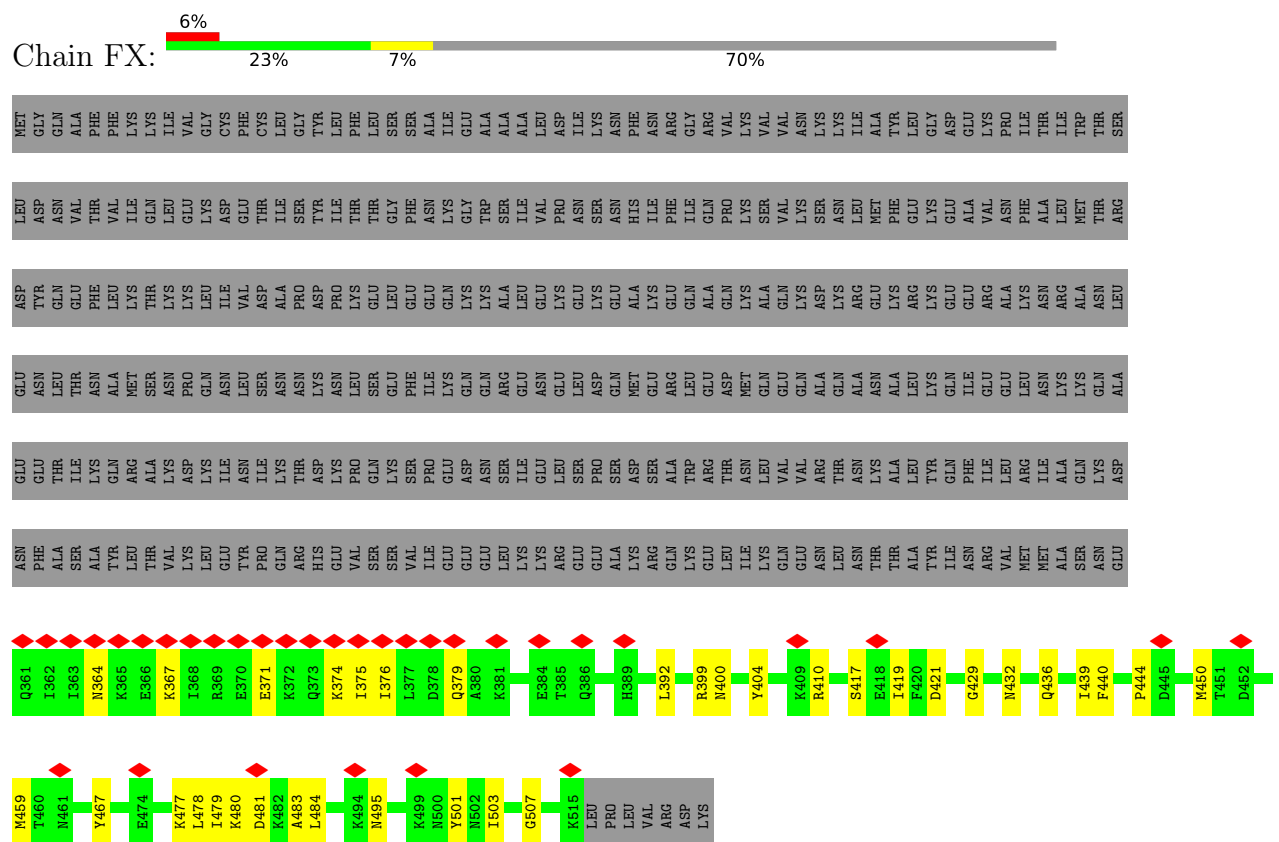


- Molecule 2: Type IV secretion system apparatus protein CagX

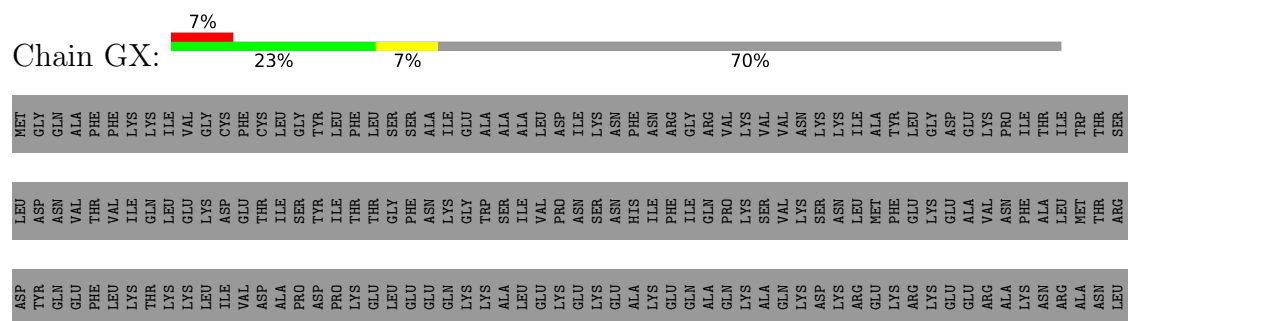


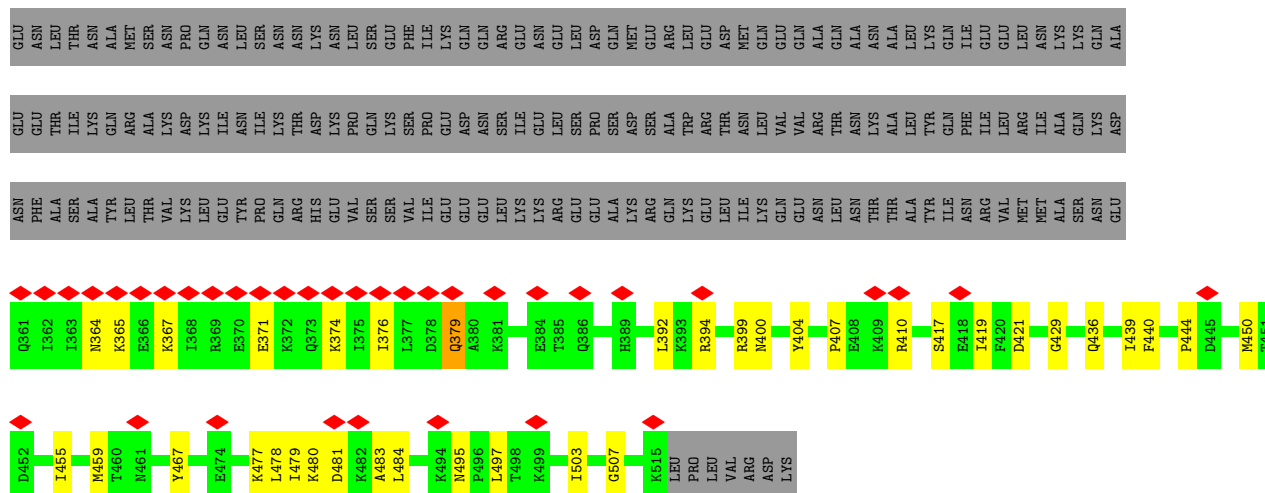


• Molecule 2: Type IV secretion system apparatus protein CagX

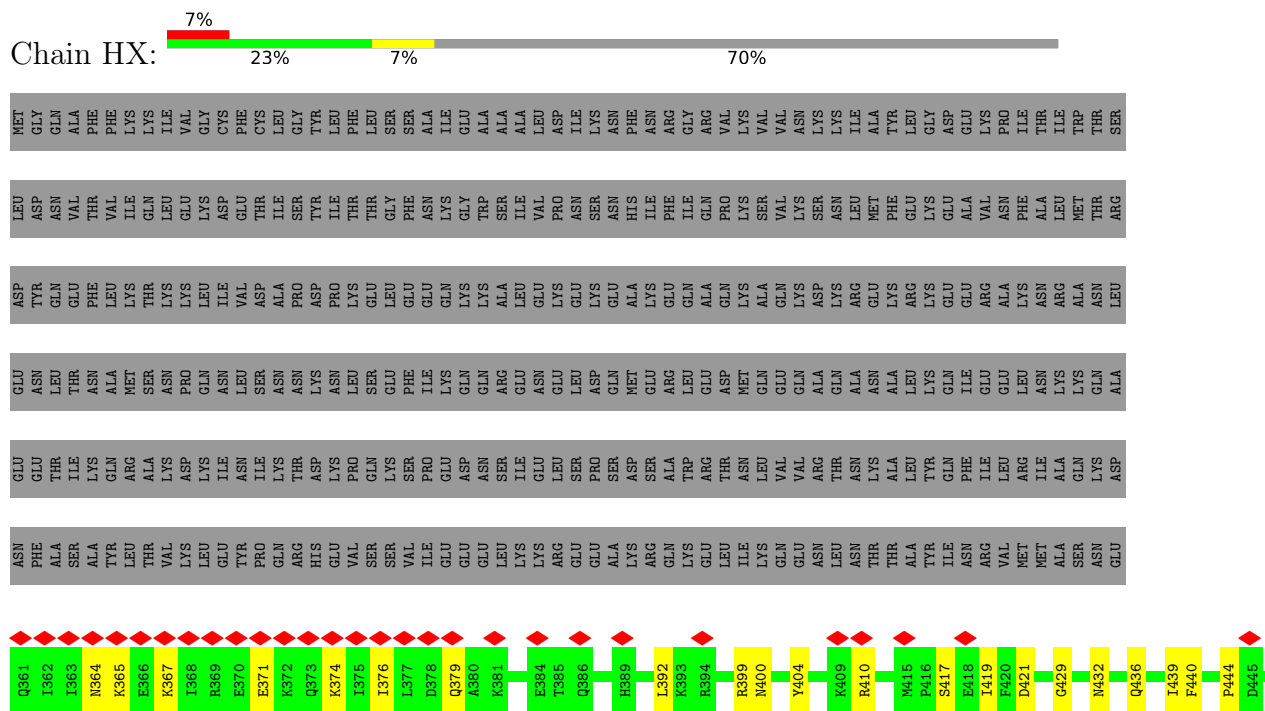


• Molecule 2: Type IV secretion system apparatus protein CagX

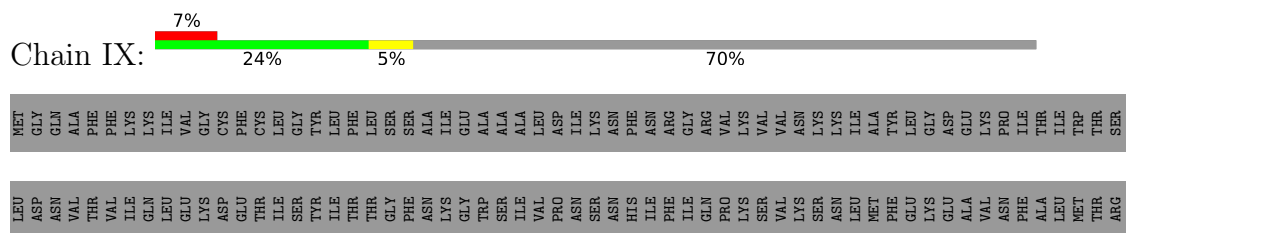


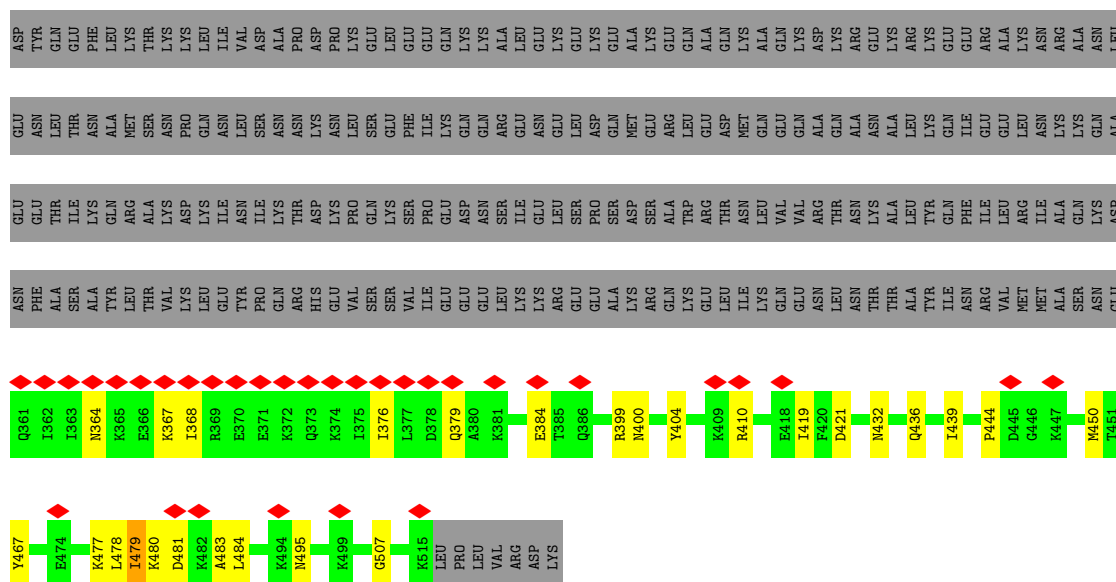


• Molecule 2: Type IV secretion system apparatus protein CagX

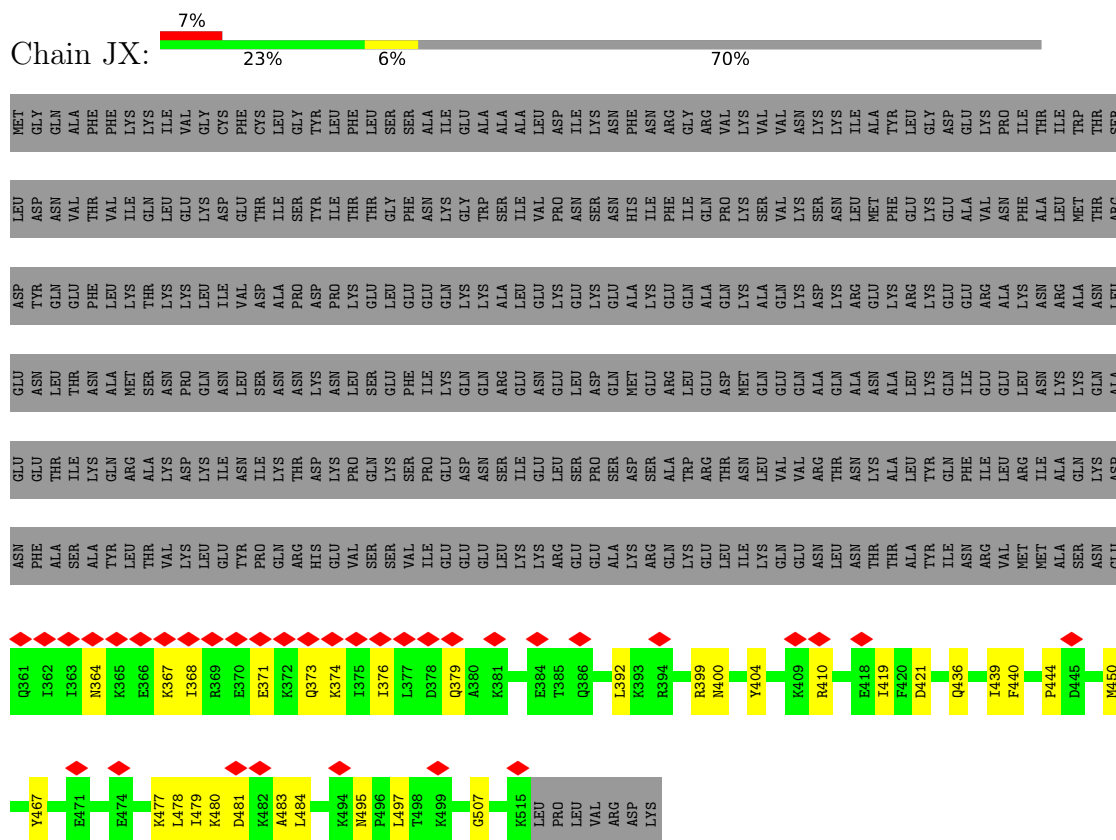


• Molecule 2: Type IV secretion system apparatus protein CagX

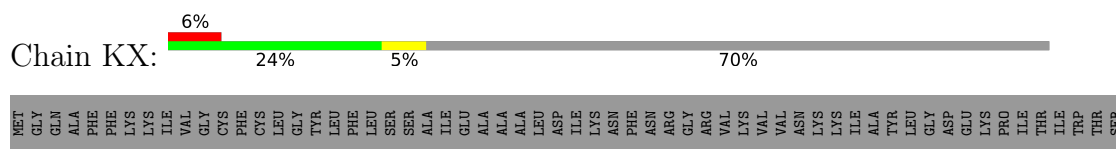


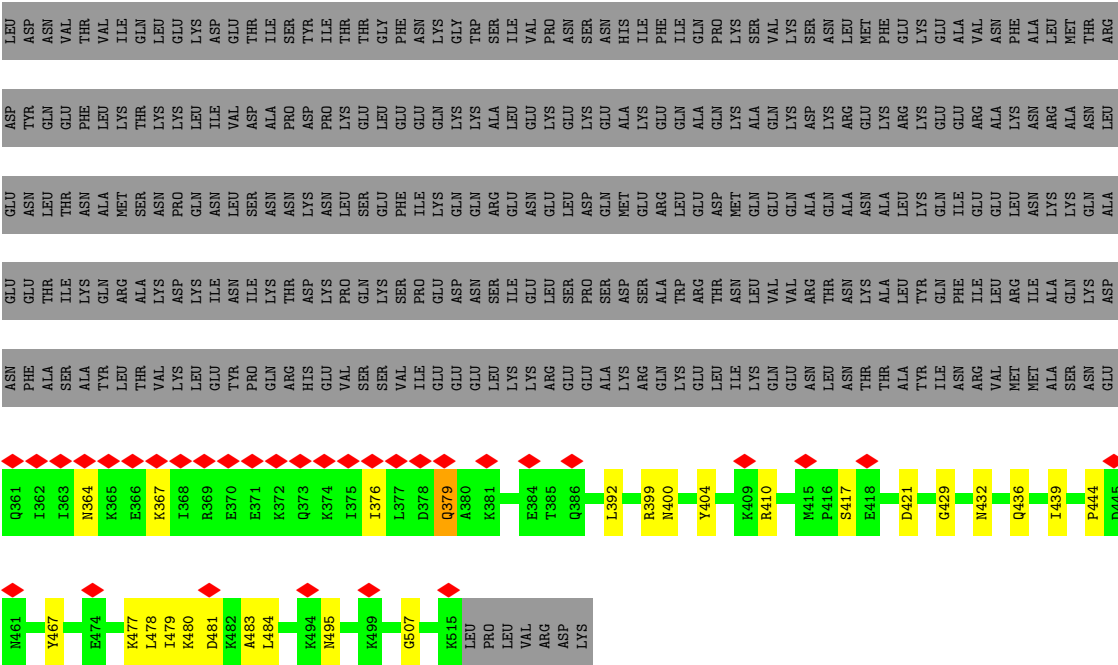


• Molecule 2: Type IV secretion system apparatus protein CagX

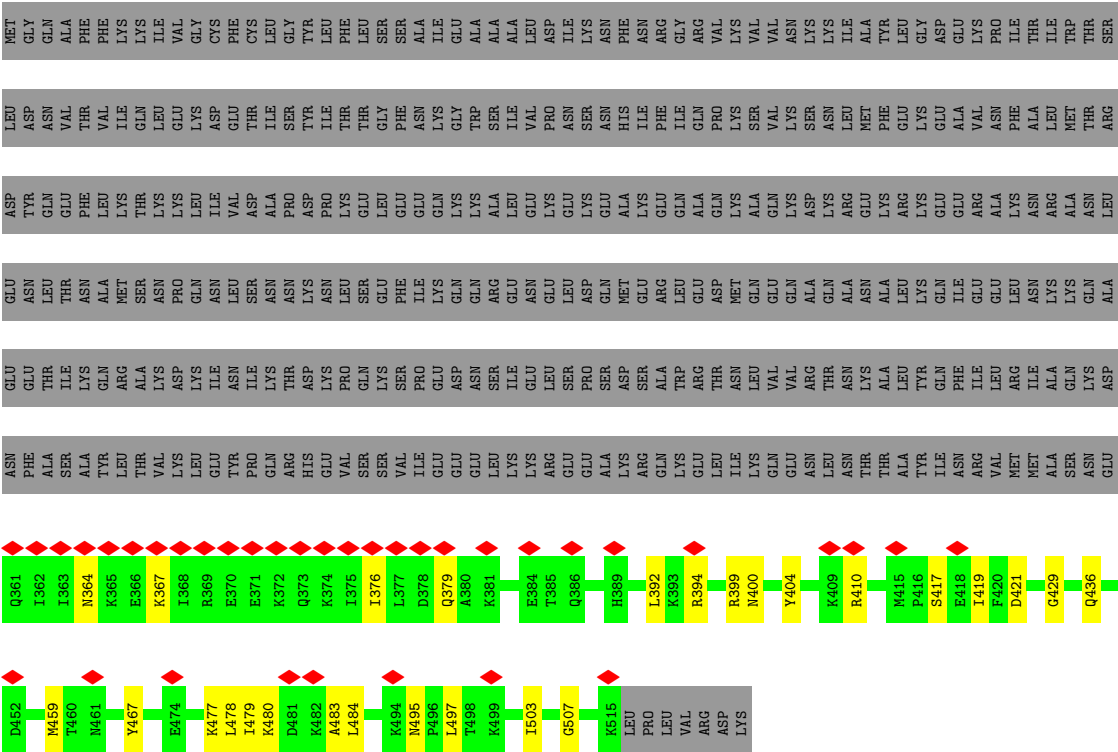


• Molecule 2: Type IV secretion system apparatus protein CagX





• Molecule 2: Type IV secretion system apparatus protein CagX



• Molecule 2: Type IV secretion system apparatus protein CagX



Amino Acid Category	Number of Amino Acids
D452	1
M459	2
T460	2
N461	2
Y467	2
E474	1
K477	3
L478	3
I479	3
K480	3
D481	3
K482	3
A483	3
L484	3
K494	3
N495	3
P496	3
L497	3
T498	3
K499	3
I503	1
G507	1
K515	1
LEU	2
PRO	2
LEU	2
VAL	2
ARG	2
ASP	2
LYS	2
Q361	1
T362	1
I363	1
N364	1
K365	1
E366	1
K367	1
T368	1
R369	1
E370	1
E371	1
K372	1
Q373	1
K374	1
L375	1
L376	1
L377	1
D378	1
Q379	1
A380	1
K381	1
E384	1
T385	1
Q386	1
H389	1
L392	1
R399	1
N400	1
Y404	1
P407	1
E408	1
K409	1
R410	1
S417	1
F418	1
T419	1
F420	1
D421	1
G429	1
N432	1
Q436	1
L439	1
F440	1
P444	1
D445	1
K450	1
T451	1

Chain NX:

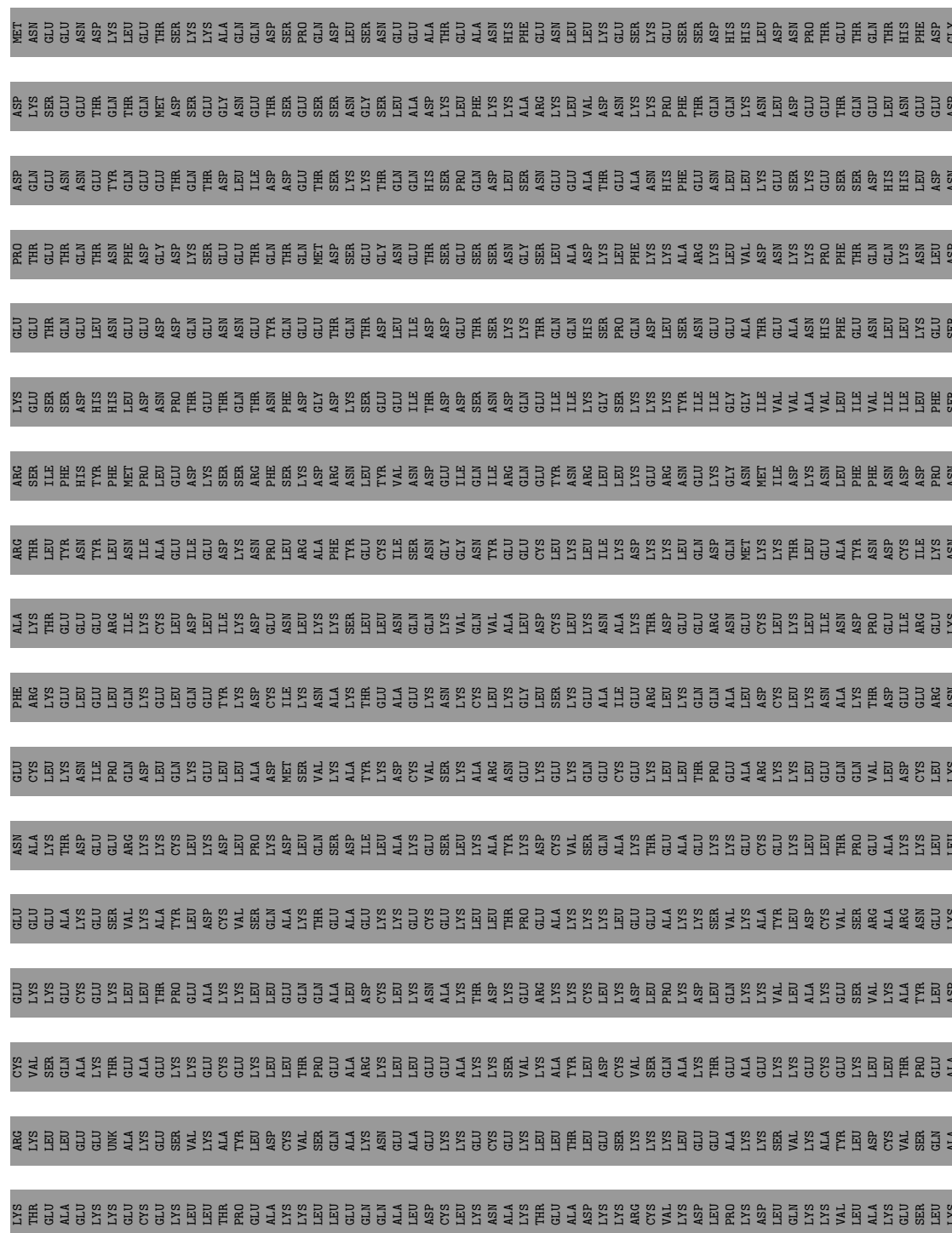
D452	Q361	GLU	ASN	GLU	GLU	ASN	ASP	LEU	MET
D459	Q362	THR	PHE	THR	GLU	ASN	TYR	ASP	GLY
T460	Q363	ILE	ALA	ILE	THR	THR	GLN	ASN	GLN
N461	Q364	LYS	ALA	LYS	ASN	ASN	PHE	THR	PHE
Y467	K365	ARG	LEU	ARG	GLN	MET	LEU	VAL	LYS
E474	K366	THR	THR	ALA	SER	ASN	THR	GLN	LYS
K477	K367	LYS	LYS	ASP	VAL	ASN	LYS	GLU	ILE
L478	K368	LYS	LEU	LYS	GLN	GLN	LEU	LYS	GLY
I479	E370	GLU	GLU	ILE	ASN	ASN	ILE	ASP	VAL
K480	E371	ASN	TYR	ASN	TYR	LEU	VAL	GLU	CYS
D481	K372	GLN	PRO	ILE	SER	ASN	ASP	THR	PHE
K482	K373	THR	ARG	LYS	GLN	ASN	ALA	ILE	LEU
A483	K374	ASP	HIS	THR	THR	ASN	PRO	SER	LEU
L484	K375	GLU	GLU	LYS	LYS	ASN	PRO	ILE	TYR
K494	L376	VAL	VAL	PRO	SER	PHE	GLU	THR	GLY
N495	D378	ILE	ILE	GLU	GLU	ILE	GLU	THR	LEU
P496	K379	GLU	GLU	ASP	GLU	LYS	GLN	LYS	ALA
L497	K380	GLU	GLU	ASN	ASN	GLN	LYS	TRP	ALA
T498	K381	LEU	LEU	SER	SER	ARG	ALA	SER	ALA
K499	K381	LYS	LYS	ILE	ILE	GLU	LYS	ILE	ALA
I503	E384	LYS	LYS	GLU	GLU	ASN	GLU	VAL	LEU
G507	T385	ARG	ARG	LEU	LEU	GLU	LYS	PRO	ASP
K515	Q386	GLU	GLU	SER	SER	LEU	GLU	ASN	ILE
LEU	H389	ALA	LYS	SER	SER	GLU	LYS	SER	LYS
PRO	L392	GLN	ARG	ALA	ALA	GLU	GLU	GLU	ASN
VAL	K393	LYS	GLN	TRP	TRP	LEU	GLN	ILE	PHE
LEU	R394	GLU	GLU	ARG	GLU	GLU	ALA	GLN	GLY
ASP	R399	ILE	LEU	THR	THR	ASP	GLN	PRO	ARG
ARG	N400	LYS	LYS	ASN	ASN	MET	LYS	LYS	VAL
LYS	Y404	GLN	GLN	VAL	VAL	GLU	ALA	SER	VAL
	Y404	GLU	GLU	VAL	VAL	GLN	GLN	VAL	VAL
	K409	ASN	ASN	ARG	ARG	ALA	LYS	LYS	ASN
	R410	LEU	ASN	THR	THR	GLN	LYS	ASN	LYS
	S417	THR	THR	LYS	LYS	ALA	GLU	MET	ALA
	E418	ALA	ALA	ALA	LEU	LEU	ARG	PHE	PHE
	L419	TYR	TYR	TYR	TYR	TYR	ARG	GLU	GLU
	F420	ILE	ILE	GLN	GLN	GLN	LYS	LYS	GLY
	D421	ASN	ASN	PHE	PHE	ILE	GLU	ALA	ASP
	G429	ARG	ARG	ILE	ILE	GLU	ARG	VAL	LYS
	N432	VAL	VAL	LEU	LEU	GLU	ALA	ASN	PRO
	Q436	MET	MET	ARG	ARG	GLU	LYS	ASN	ILE
		MET	MET	ILE	ILE	LEU	LYS	PHE	THR
		ALA	ALA	ALA	ALA	ASN	ARG	ALA	ILE
		SER	SER	GLN	GLN	LYS	ALA	MET	TRP
		ASN	ASN	LYS	LYS	GLN	LEU	THR	THR
		GLU	GLU	ASP	ASP	ALA	ASN	LEU	SER

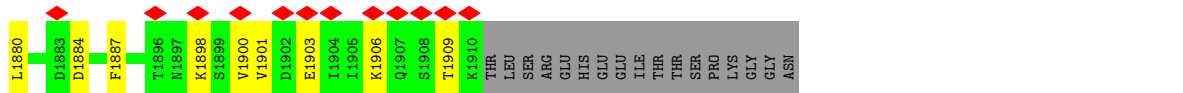
[illegible]











Chain EY:





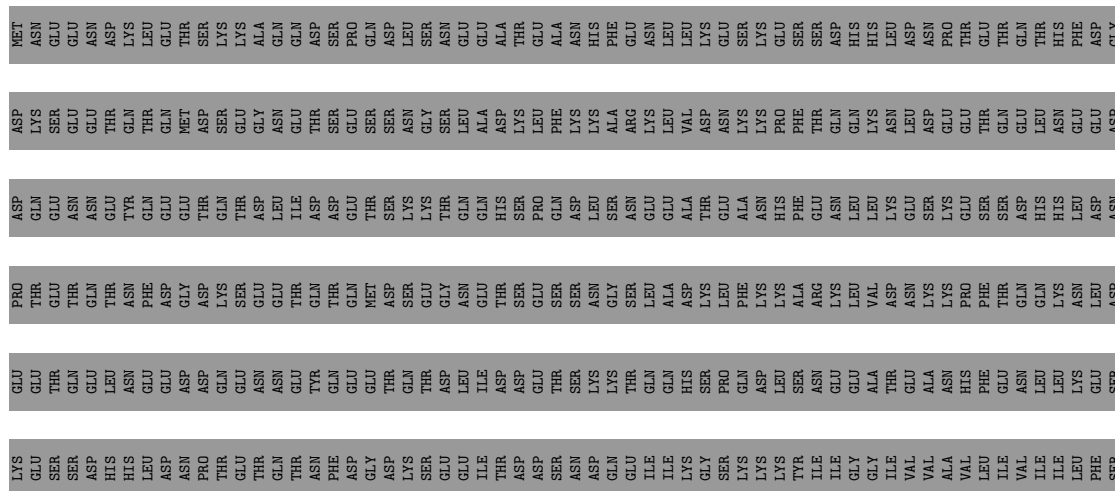




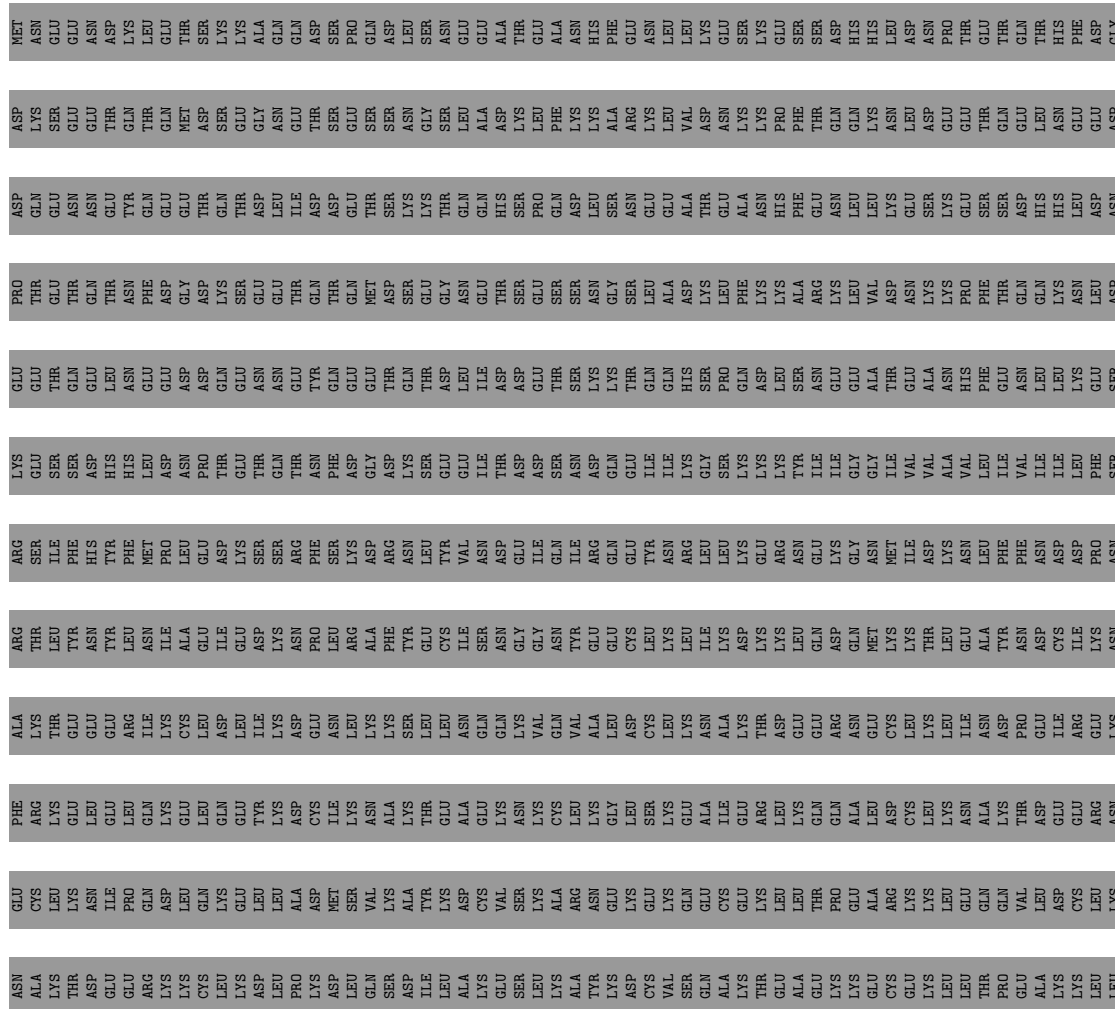






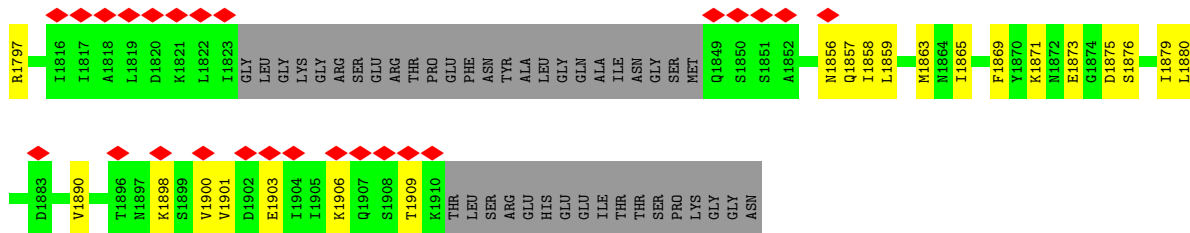












Chain LY: 8% 89%











4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C14	Depositor
Number of particles used	7337	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 ($e^-/\text{\AA}^2$)	59.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.049	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.015	Depositor
Map size ($\text{\AA}$)	510.0, 510.0, 510.0	wwPDB
Map dimensions	510, 510, 510	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0, 1.0, 1.0	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 >5	RMSZ	# Z >5
1	AT	0.33	0/1525	0.69	3/2049 (0.1%)
1	BT	0.33	0/1525	0.69	3/2049 (0.1%)
1	CT	0.33	0/1525	0.69	3/2049 (0.1%)
1	DT	0.33	0/1525	0.69	3/2049 (0.1%)
1	ET	0.33	0/1525	0.69	3/2049 (0.1%)
1	FT	0.33	0/1525	0.69	3/2049 (0.1%)
1	GT	0.33	0/1525	0.69	3/2049 (0.1%)
1	HT	0.33	0/1525	0.69	3/2049 (0.1%)
1	IT	0.33	0/1525	0.69	3/2049 (0.1%)
1	JT	0.33	0/1525	0.69	3/2049 (0.1%)
1	KT	0.33	0/1525	0.69	3/2049 (0.1%)
1	LT	0.33	0/1525	0.69	3/2049 (0.1%)
1	MT	0.33	0/1525	0.69	3/2049 (0.1%)
1	NT	0.33	0/1525	0.69	3/2049 (0.1%)
2	AX	0.50	0/1301	0.69	1/1752 (0.1%)
2	BX	0.50	0/1301	0.69	0/1752
2	CX	0.50	0/1301	0.69	0/1752
2	DX	0.50	0/1301	0.69	1/1752 (0.1%)
2	EX	0.50	0/1301	0.69	1/1752 (0.1%)
2	FX	0.50	0/1301	0.69	0/1752
2	GX	0.50	0/1301	0.69	1/1752 (0.1%)
2	HX	0.50	0/1301	0.69	0/1752
2	IX	0.50	0/1301	0.69	0/1752
2	JX	0.50	0/1301	0.69	0/1752
2	KX	0.50	0/1301	0.69	1/1752 (0.1%)
2	LX	0.50	0/1301	0.69	0/1752
2	MX	0.50	0/1301	0.69	1/1752 (0.1%)
2	NX	0.50	0/1301	0.69	0/1752
3	AY	0.52	0/1602	0.70	0/2170
3	BY	0.53	0/1602	0.70	0/2170
3	CY	0.53	0/1602	0.70	0/2170
3	DY	0.53	0/1602	0.70	0/2170
3	EY	0.52	0/1602	0.70	0/2170
3	FY	0.53	0/1602	0.70	0/2170

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	GY	0.53	0/1602	0.70	0/2170
3	HY	0.53	0/1602	0.70	0/2170
3	IY	0.53	0/1602	0.70	0/2170
3	JY	0.53	0/1602	0.70	0/2170
3	KY	0.53	0/1602	0.70	0/2170
3	LY	0.52	0/1602	0.70	0/2170
3	MY	0.53	0/1602	0.70	0/2170
3	NY	0.53	0/1602	0.70	0/2170
All	All	0.46	0/61992	0.69	48/83594 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AX	0	1
2	BX	0	1
2	CX	0	1
2	DX	0	1
2	EX	0	1
2	FX	0	1
2	GX	0	1
2	HX	0	1
2	IX	0	1
2	JX	0	1
2	KX	0	1
2	LX	0	1
2	MX	0	1
2	NX	0	1
All	All	0	14

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DT	197	GLN	N-CA-CB	5.64	119.59	110.40
1	GT	197	GLN	N-CA-CB	5.63	119.58	110.40
1	NT	197	GLN	N-CA-CB	5.63	119.58	110.40
1	FT	197	GLN	N-CA-CB	5.62	119.56	110.40
1	LT	197	GLN	N-CA-CB	5.61	119.55	110.40
1	KT	197	GLN	N-CA-CB	5.61	119.54	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CT	197	GLN	N-CA-CB	5.60	119.53	110.40
1	BT	197	GLN	N-CA-CB	5.60	119.52	110.40
1	JT	197	GLN	N-CA-CB	5.59	119.52	110.40
1	HT	197	GLN	N-CA-CB	5.59	119.52	110.40
1	IT	197	GLN	N-CA-CB	5.59	119.52	110.40
1	MT	197	GLN	N-CA-CB	5.58	119.49	110.40
1	ET	197	GLN	N-CA-CB	5.57	119.48	110.40
1	AT	197	GLN	N-CA-CB	5.57	119.48	110.40
1	JT	73	TYR	N-CA-C	5.38	117.89	110.35
1	MT	73	TYR	N-CA-C	5.38	117.89	110.35
1	DT	73	TYR	N-CA-C	5.37	117.87	110.35
1	IT	73	TYR	N-CA-C	5.37	117.87	110.35
1	IT	197	GLN	CA-CB-CG	5.37	124.84	114.10
1	LT	73	TYR	N-CA-C	5.37	117.86	110.35
1	AT	197	GLN	CA-CB-CG	5.36	124.83	114.10
1	AT	73	TYR	N-CA-C	5.36	117.85	110.35
1	DT	197	GLN	CA-CB-CG	5.36	124.81	114.10
1	ET	197	GLN	CA-CB-CG	5.35	124.81	114.10
1	LT	197	GLN	CA-CB-CG	5.35	124.80	114.10
1	BT	73	TYR	N-CA-C	5.35	117.84	110.35
1	FT	197	GLN	CA-CB-CG	5.35	124.80	114.10
1	JT	197	GLN	CA-CB-CG	5.34	124.79	114.10
1	HT	73	TYR	N-CA-C	5.34	117.83	110.35
1	HT	197	GLN	CA-CB-CG	5.34	124.79	114.10
1	MT	197	GLN	CA-CB-CG	5.34	124.78	114.10
1	BT	197	GLN	CA-CB-CG	5.34	124.78	114.10
1	ET	73	TYR	N-CA-C	5.34	117.83	110.35
1	KT	197	GLN	CA-CB-CG	5.34	124.78	114.10
1	GT	73	TYR	N-CA-C	5.34	117.82	110.35
1	KT	73	TYR	N-CA-C	5.34	117.82	110.35
1	CT	197	GLN	CA-CB-CG	5.33	124.77	114.10
1	FT	73	TYR	N-CA-C	5.33	117.82	110.35
1	CT	73	TYR	N-CA-C	5.33	117.81	110.35
1	NT	197	GLN	CA-CB-CG	5.33	124.76	114.10
1	GT	197	GLN	CA-CB-CG	5.33	124.75	114.10
1	NT	73	TYR	N-CA-C	5.33	117.81	110.35
2	GX	379	GLN	CB-CA-C	-5.03	102.98	110.88
2	KX	379	GLN	CB-CA-C	-5.01	103.02	110.88
2	MX	379	GLN	CB-CA-C	-5.01	103.02	110.88
2	AX	379	GLN	CB-CA-C	-5.01	103.02	110.88
2	EX	379	GLN	CB-CA-C	-5.00	103.02	110.88
2	DX	379	GLN	CB-CA-C	-5.00	103.03	110.88

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AX	479	ILE	Peptide
2	BX	479	ILE	Peptide
2	CX	479	ILE	Peptide
2	DX	479	ILE	Peptide
2	EX	479	ILE	Peptide
2	FX	479	ILE	Peptide
2	GX	479	ILE	Peptide
2	HX	479	ILE	Peptide
2	IX	479	ILE	Peptide
2	JX	479	ILE	Peptide
2	KX	479	ILE	Peptide
2	LX	479	ILE	Peptide
2	MX	479	ILE	Peptide
2	NX	479	ILE	Peptide

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	AT	1502	0	1525	24	0
1	BT	1502	0	1525	25	0
1	CT	1502	0	1525	25	0
1	DT	1502	0	1525	26	0
1	ET	1502	0	1525	23	0
1	FT	1502	0	1525	29	0
1	GT	1502	0	1525	24	0
1	HT	1502	0	1525	25	0
1	IT	1502	0	1525	24	0
1	JT	1502	0	1525	24	0
1	KT	1502	0	1525	26	0
1	LT	1502	0	1525	26	0
1	MT	1502	0	1525	23	0
1	NT	1502	0	1525	21	0
2	AX	1275	0	1309	29	0
2	BX	1275	0	1309	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	CX	1275	0	1309	29	0
2	DX	1275	0	1309	27	0
2	EX	1275	0	1309	31	0
2	FX	1275	0	1309	31	0
2	GX	1275	0	1309	33	0
2	HX	1275	0	1309	32	0
2	IX	1275	0	1309	28	0
2	JX	1275	0	1309	30	0
2	KX	1275	0	1309	22	0
2	LX	1275	0	1309	29	0
2	MX	1275	0	1309	30	0
2	NX	1275	0	1309	29	0
3	AY	1578	0	1637	46	0
3	BY	1578	0	1637	46	0
3	CY	1578	0	1637	48	0
3	DY	1578	0	1637	44	0
3	EY	1578	0	1637	44	0
3	FY	1578	0	1637	46	0
3	GY	1578	0	1637	45	0
3	HY	1578	0	1637	45	0
3	IY	1578	0	1637	47	0
3	JY	1578	0	1637	44	0
3	KY	1578	0	1637	43	0
3	LY	1578	0	1637	41	0
3	MY	1578	0	1637	44	0
3	NY	1578	0	1637	43	0
All	All	60970	0	62594	1024	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 8.

All (1024) 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)
2:BX:444:PRO:O	2:CX:410:ARG:NH2	2.22	0.73
2:HX:444:PRO:O	2:IX:410:ARG:NH2	2.21	0.73
3:AY:1722:VAL:HB	3:AY:1732:LEU:HB2	1.72	0.72
3:DY:1722:VAL:HB	3:DY:1732:LEU:HB2	1.72	0.72
3:FY:1722:VAL:HB	3:FY:1732:LEU:HB2	1.72	0.72
3:CY:1722:VAL:HB	3:CY:1732:LEU:HB2	1.72	0.72
3:GY:1722:VAL:HB	3:GY:1732:LEU:HB2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BY:1722:VAL:HB	3:BY:1732:LEU:HB2	1.72	0.72
3:EY:1722:VAL:HB	3:EY:1732:LEU:HB2	1.72	0.72
3:IY:1722:VAL:HB	3:IY:1732:LEU:HB2	1.72	0.72
3:MY:1722:VAL:HB	3:MY:1732:LEU:HB2	1.72	0.72
3:NY:1722:VAL:HB	3:NY:1732:LEU:HB2	1.72	0.72
3:HY:1722:VAL:HB	3:HY:1732:LEU:HB2	1.72	0.71
3:KY:1700:ILE:O	3:KY:1876:SER:HA	1.90	0.71
3:NY:1700:ILE:O	3:NY:1876:SER:HA	1.91	0.71
3:KY:1722:VAL:HB	3:KY:1732:LEU:HB2	1.72	0.71
3:JY:1722:VAL:HB	3:JY:1732:LEU:HB2	1.72	0.71
3:LY:1700:ILE:O	3:LY:1876:SER:HA	1.91	0.71
3:LY:1722:VAL:HB	3:LY:1732:LEU:HB2	1.72	0.71
3:AY:1700:ILE:O	3:AY:1876:SER:HA	1.91	0.71
3:CY:1700:ILE:O	3:CY:1876:SER:HA	1.90	0.71
3:IY:1700:ILE:O	3:IY:1876:SER:HA	1.90	0.70
2:JX:480:LYS:HB2	2:JX:483:ALA:HB3	1.74	0.70
2:LX:480:LYS:HB2	2:LX:483:ALA:HB3	1.74	0.70
2:DX:480:LYS:HB2	2:DX:483:ALA:HB3	1.74	0.70
3:FY:1700:ILE:O	3:FY:1876:SER:HA	1.91	0.70
2:BX:480:LYS:HB2	2:BX:483:ALA:HB3	1.74	0.70
2:CX:480:LYS:HB2	2:CX:483:ALA:HB3	1.74	0.70
3:EY:1700:ILE:O	3:EY:1876:SER:HA	1.90	0.70
2:IX:480:LYS:HB2	2:IX:483:ALA:HB3	1.74	0.70
2:NX:480:LYS:HB2	2:NX:483:ALA:HB3	1.74	0.70
2:AX:480:LYS:HB2	2:AX:483:ALA:HB3	1.74	0.70
3:BY:1700:ILE:O	3:BY:1876:SER:HA	1.90	0.70
3:JY:1700:ILE:O	3:JY:1876:SER:HA	1.90	0.70
3:MY:1700:ILE:O	3:MY:1876:SER:HA	1.91	0.70
3:HY:1700:ILE:O	3:HY:1876:SER:HA	1.90	0.70
2:KX:480:LYS:HB2	2:KX:483:ALA:HB3	1.74	0.70
2:FX:480:LYS:HB2	2:FX:483:ALA:HB3	1.74	0.70
2:GX:480:LYS:HB2	2:GX:483:ALA:HB3	1.74	0.70
3:GY:1700:ILE:O	3:GY:1876:SER:HA	1.91	0.70
2:EX:480:LYS:HB2	2:EX:483:ALA:HB3	1.74	0.70
2:MX:480:LYS:HB2	2:MX:483:ALA:HB3	1.74	0.70
3:DY:1700:ILE:O	3:DY:1876:SER:HA	1.91	0.69
2:HX:480:LYS:HB2	2:HX:483:ALA:HB3	1.74	0.69
2:KX:439:ILE:HG12	2:KX:478:LEU:HG	1.77	0.67
2:EX:439:ILE:HG12	2:EX:478:LEU:HG	1.77	0.67
2:FX:439:ILE:HG12	2:FX:478:LEU:HG	1.77	0.67
2:LX:439:ILE:HG12	2:LX:478:LEU:HG	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HX:439:ILE:HG12	2:HX:478:LEU:HG	1.77	0.67
2:IX:439:ILE:HG12	2:IX:478:LEU:HG	1.77	0.67
2:NX:439:ILE:HG12	2:NX:478:LEU:HG	1.77	0.67
2:DX:439:ILE:HG12	2:DX:478:LEU:HG	1.77	0.67
2:KX:444:PRO:O	2:LX:410:ARG:NH2	2.28	0.67
2:BX:439:ILE:HG12	2:BX:478:LEU:HG	1.77	0.66
2:CX:439:ILE:HG12	2:CX:478:LEU:HG	1.77	0.66
2:MX:439:ILE:HG12	2:MX:478:LEU:HG	1.77	0.66
2:GX:439:ILE:HG12	2:GX:478:LEU:HG	1.77	0.66
2:JX:439:ILE:HG12	2:JX:478:LEU:HG	1.77	0.66
2:AX:439:ILE:HG12	2:AX:478:LEU:HG	1.77	0.66
3:EY:1857:GLN:NE2	3:FY:1856:ASN:OD1	2.30	0.65
3:IY:1857:GLN:NE2	3:JY:1856:ASN:OD1	2.30	0.64
3:KY:1857:GLN:NE2	3:LY:1856:ASN:OD1	2.30	0.64
3:GY:1857:GLN:NE2	3:HY:1856:ASN:OD1	2.31	0.64
3:HY:1857:GLN:NE2	3:IY:1856:ASN:OD1	2.31	0.64
2:AX:444:PRO:O	2:BX:410:ARG:NH2	2.30	0.64
3:LY:1857:GLN:NE2	3:MY:1856:ASN:OD1	2.30	0.64
3:DY:1857:GLN:NE2	3:EY:1856:ASN:OD1	2.31	0.64
3:AY:1856:ASN:OD1	3:NY:1857:GLN:NE2	2.30	0.63
1:ET:36:TYR:HB3	2:FX:404:TYR:HB3	1.78	0.63
2:FX:399:ARG:NH2	1:GT:169:HIS:O	2.31	0.63
3:FY:1857:GLN:NE2	3:GY:1856:ASN:OD1	2.31	0.63
3:JY:1857:GLN:NE2	3:KY:1856:ASN:OD1	2.32	0.63
3:BY:1857:GLN:NE2	3:CY:1856:ASN:OD1	2.31	0.63
3:AY:1857:GLN:NE2	3:BY:1856:ASN:OD1	2.31	0.62
2:JX:444:PRO:O	2:KX:410:ARG:NH2	2.32	0.62
3:MY:1857:GLN:NE2	3:NY:1856:ASN:OD1	2.32	0.62
3:CY:1857:GLN:NE2	3:DY:1856:ASN:OD1	2.32	0.61
1:JT:213:ARG:HH12	2:JX:364:ASN:HB3	1.64	0.61
1:LT:39:VAL:HG11	2:MX:419:ILE:HG13	1.82	0.61
2:EX:444:PRO:O	2:FX:410:ARG:NH2	2.33	0.61
3:NY:1714:VAL:HG21	3:NY:1757:ILE:HD13	1.82	0.61
1:CT:36:TYR:HB3	2:DX:404:TYR:HB3	1.83	0.61
3:LY:1714:VAL:HG21	3:LY:1757:ILE:HD13	1.82	0.61
3:MY:1714:VAL:HG21	3:MY:1757:ILE:HD13	1.83	0.61
3:KY:1714:VAL:HG21	3:KY:1757:ILE:HD13	1.82	0.61
1:IT:36:TYR:HB3	2:JX:404:TYR:HB3	1.82	0.60
1:LT:39:VAL:HG21	2:MX:419:ILE:HD12	1.82	0.60
1:MT:36:TYR:HB3	2:NX:404:TYR:HB3	1.82	0.60
3:AY:1714:VAL:HG21	3:AY:1757:ILE:HD13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:JY:1714:VAL:HG21	3:JY:1757:ILE:HD13	1.83	0.60
3:LY:1762:ALA:HB3	3:LY:1770:ILE:HB	1.84	0.60
3:BY:1714:VAL:HG21	3:BY:1757:ILE:HD13	1.83	0.60
1:GT:36:TYR:HB3	2:HX:404:TYR:HB3	1.81	0.60
2:MX:444:PRO:O	2:NX:410:ARG:NH2	2.35	0.60
3:NY:1762:ALA:HB3	3:NY:1770:ILE:HB	1.84	0.60
2:CX:444:PRO:O	2:DX:410:ARG:NH2	2.34	0.60
2:FX:444:PRO:O	2:GX:410:ARG:NH2	2.34	0.60
2:GX:444:PRO:O	2:HX:410:ARG:NH2	2.35	0.60
2:LX:444:PRO:O	2:MX:410:ARG:NH2	2.34	0.60
3:BY:1762:ALA:HB3	3:BY:1770:ILE:HB	1.84	0.60
3:IY:1714:VAL:HG21	3:IY:1757:ILE:HD13	1.83	0.60
1:AT:36:TYR:HB3	2:BX:404:TYR:HB3	1.83	0.60
3:JY:1762:ALA:HB3	3:JY:1770:ILE:HB	1.84	0.60
3:MY:1762:ALA:HB3	3:MY:1770:ILE:HB	1.84	0.60
3:CY:1714:VAL:HG21	3:CY:1757:ILE:HD13	1.83	0.59
3:EY:1714:VAL:HG21	3:EY:1757:ILE:HD13	1.82	0.59
3:HY:1714:VAL:HG21	3:HY:1757:ILE:HD13	1.83	0.59
3:KY:1762:ALA:HB3	3:KY:1770:ILE:HB	1.84	0.59
2:LX:399:ARG:NH2	1:MT:169:HIS:O	2.35	0.59
1:ET:39:VAL:HG11	2:FX:419:ILE:HG13	1.83	0.59
3:IY:1762:ALA:HB3	3:IY:1770:ILE:HB	1.84	0.59
1:LT:36:TYR:HB3	2:MX:404:TYR:HB3	1.84	0.59
3:AY:1762:ALA:HB3	3:AY:1770:ILE:HB	1.84	0.59
3:DY:1714:VAL:HG21	3:DY:1757:ILE:HD13	1.83	0.59
3:GY:1714:VAL:HG21	3:GY:1757:ILE:HD13	1.82	0.59
2:BX:399:ARG:NH2	1:CT:169:HIS:O	2.34	0.59
3:FY:1714:VAL:HG21	3:FY:1757:ILE:HD13	1.83	0.59
3:DY:1762:ALA:HB3	3:DY:1770:ILE:HB	1.84	0.59
3:GY:1762:ALA:HB3	3:GY:1770:ILE:HB	1.84	0.59
1:KT:36:TYR:HB3	2:LX:404:TYR:HB3	1.85	0.59
1:MT:39:VAL:HG11	2:NX:419:ILE:HG13	1.84	0.58
3:DY:1706:VAL:HB	3:DY:1871:LYS:HB3	1.86	0.58
2:AX:410:ARG:NH2	2:NX:444:PRO:O	2.36	0.58
3:AY:1706:VAL:HB	3:AY:1871:LYS:HB3	1.86	0.58
3:BY:1706:VAL:HB	3:BY:1871:LYS:HB3	1.86	0.58
3:EY:1762:ALA:HB3	3:EY:1770:ILE:HB	1.84	0.58
2:IX:444:PRO:O	2:JX:410:ARG:NH2	2.37	0.58
3:EY:1706:VAL:HB	3:EY:1871:LYS:HB3	1.86	0.58
3:FY:1762:ALA:HB3	3:FY:1770:ILE:HB	1.84	0.58
3:CY:1706:VAL:HB	3:CY:1871:LYS:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DT:36:TYR:HB3	2:EX:404:TYR:HB3	1.85	0.58
3:FY:1706:VAL:HB	3:FY:1871:LYS:HB3	1.86	0.58
2:AX:404:TYR:HB3	1:NT:36:TYR:HB3	1.84	0.58
3:HY:1762:ALA:HB3	3:HY:1770:ILE:HB	1.84	0.58
1:IT:81:VAL:HG21	2:IX:459:MET:HE3	1.84	0.58
1:IT:39:VAL:HG11	2:JX:419:ILE:HG13	1.84	0.57
3:MY:1706:VAL:HB	3:MY:1871:LYS:HB3	1.86	0.57
3:NY:1706:VAL:HB	3:NY:1871:LYS:HB3	1.86	0.57
1:AT:169:HIS:O	2:NX:399:ARG:NH2	2.37	0.57
1:ET:39:VAL:HG21	2:FX:419:ILE:HD12	1.86	0.57
3:GY:1706:VAL:HB	3:GY:1871:LYS:HB3	1.86	0.57
3:CY:1762:ALA:HB3	3:CY:1770:ILE:HB	1.84	0.57
1:BT:36:TYR:HB3	2:CX:404:TYR:HB3	1.86	0.57
1:AT:39:VAL:HG11	2:BX:419:ILE:HG13	1.87	0.57
1:MT:39:VAL:HG21	2:NX:419:ILE:HD12	1.86	0.57
1:BT:48:SER:OG	1:CT:170:GLY:O	2.22	0.57
2:DX:399:ARG:NH2	1:ET:169:HIS:O	2.37	0.57
3:KY:1706:VAL:HB	3:KY:1871:LYS:HB3	1.86	0.57
2:DX:444:PRO:O	2:EX:410:ARG:NH2	2.37	0.57
3:IY:1706:VAL:HB	3:IY:1871:LYS:HB3	1.86	0.57
3:HY:1706:VAL:HB	3:HY:1871:LYS:HB3	1.86	0.56
3:LY:1706:VAL:HB	3:LY:1871:LYS:HB3	1.86	0.56
3:JY:1706:VAL:HB	3:JY:1871:LYS:HB3	1.86	0.56
2:MX:399:ARG:NH2	1:NT:169:HIS:O	2.39	0.56
2:HX:399:ARG:NH2	1:IT:169:HIS:O	2.37	0.56
1:KT:39:VAL:HG11	2:LX:419:ILE:HG13	1.86	0.56
1:IT:39:VAL:HG21	2:JX:419:ILE:HD12	1.87	0.56
2:AX:419:ILE:HG13	1:NT:39:VAL:HG11	1.88	0.56
3:HY:1732:LEU:HD22	3:HY:1736:THR:HG21	1.89	0.55
3:IY:1732:LEU:HD22	3:IY:1736:THR:HG21	1.89	0.55
3:JY:1732:LEU:HD22	3:JY:1736:THR:HG21	1.89	0.55
2:KX:507:GLY:HA2	1:LT:168:LEU:HD11	1.87	0.55
2:AX:399:ARG:NH2	1:BT:169:HIS:O	2.38	0.55
2:EX:399:ARG:NH2	1:FT:169:HIS:O	2.39	0.55
3:LY:1732:LEU:HD22	3:LY:1736:THR:HG21	1.88	0.55
3:GY:1732:LEU:HD22	3:GY:1736:THR:HG21	1.89	0.55
3:KY:1732:LEU:HD22	3:KY:1736:THR:HG21	1.89	0.55
1:KT:81:VAL:HG21	2:KX:459:MET:HE3	1.88	0.55
3:MY:1732:LEU:HD22	3:MY:1736:THR:HG21	1.89	0.55
3:FY:1732:LEU:HD22	3:FY:1736:THR:HG21	1.89	0.54
3:NY:1732:LEU:HD22	3:NY:1736:THR:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LT:296:GLU:OE2	1:LT:300:ASN:ND2	2.41	0.54
3:AY:1732:LEU:HD22	3:AY:1736:THR:HG21	1.89	0.54
1:ET:296:GLU:OE2	1:ET:300:ASN:ND2	2.41	0.54
1:FT:296:GLU:OE2	1:FT:300:ASN:ND2	2.41	0.54
3:BY:1732:LEU:HD22	3:BY:1736:THR:HG21	1.88	0.54
1:IT:296:GLU:OE2	1:IT:300:ASN:ND2	2.41	0.54
1:MT:296:GLU:OE2	1:MT:300:ASN:ND2	2.41	0.54
3:DY:1732:LEU:HD22	3:DY:1736:THR:HG21	1.88	0.54
3:EY:1732:LEU:HD22	3:EY:1736:THR:HG21	1.89	0.54
1:KT:296:GLU:OE2	1:KT:300:ASN:ND2	2.41	0.54
1:FT:39:VAL:HG21	2:GX:419:ILE:HD12	1.89	0.54
1:CT:296:GLU:OE2	1:CT:300:ASN:ND2	2.41	0.54
3:CY:1732:LEU:HD22	3:CY:1736:THR:HG21	1.89	0.54
3:HY:1859:LEU:O	3:HY:1863:MET:CB	2.56	0.54
3:AY:1710:LEU:HD12	3:BY:1785:GLY:HA3	1.90	0.54
3:CY:1710:LEU:HD12	3:DY:1785:GLY:HA3	1.90	0.54
3:GY:1859:LEU:O	3:GY:1863:MET:CB	2.56	0.54
1:HT:296:GLU:OE2	1:HT:300:ASN:ND2	2.41	0.54
3:IY:1859:LEU:O	3:IY:1863:MET:CB	2.56	0.54
1:NT:296:GLU:OE2	1:NT:300:ASN:ND2	2.41	0.54
1:BT:296:GLU:OE2	1:BT:300:ASN:ND2	2.41	0.54
2:IX:399:ARG:NH2	1:JT:169:HIS:O	2.41	0.54
2:JX:399:ARG:NH2	1:KT:169:HIS:O	2.41	0.54
3:JY:1710:LEU:HD12	3:KY:1785:GLY:HA3	1.90	0.54
3:AY:1859:LEU:O	3:AY:1863:MET:CB	2.56	0.53
1:JT:296:GLU:OE2	1:JT:300:ASN:ND2	2.41	0.53
3:JY:1859:LEU:O	3:JY:1863:MET:CB	2.56	0.53
3:LY:1710:LEU:HD12	3:MY:1785:GLY:HA3	1.90	0.53
2:CX:399:ARG:NH2	1:DT:169:HIS:O	2.40	0.53
3:CY:1859:LEU:O	3:CY:1863:MET:CB	2.56	0.53
1:FT:39:VAL:HG11	2:GX:419:ILE:HG13	1.88	0.53
1:GT:296:GLU:OE2	1:GT:300:ASN:ND2	2.41	0.53
2:KX:399:ARG:NH2	1:LT:169:HIS:O	2.40	0.53
1:DT:39:VAL:HG11	2:EX:419:ILE:HG13	1.89	0.53
3:DY:1859:LEU:O	3:DY:1863:MET:CB	2.56	0.53
3:FY:1859:LEU:O	3:FY:1863:MET:CB	2.56	0.53
1:AT:296:GLU:OE2	1:AT:300:ASN:ND2	2.41	0.53
3:AY:1785:GLY:HA3	3:NY:1710:LEU:HD12	1.91	0.53
3:BY:1859:LEU:O	3:BY:1863:MET:CB	2.56	0.53
1:DT:296:GLU:OE2	1:DT:300:ASN:ND2	2.41	0.53
1:KT:39:VAL:HG21	2:LX:419:ILE:HD12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BX:507:GLY:HA2	1:CT:168:LEU:HD11	1.90	0.53
3:KY:1710:LEU:HD12	3:LY:1785:GLY:HA3	1.91	0.53
3:KY:1859:LEU:O	3:KY:1863:MET:CB	2.56	0.53
2:GX:376:ILE:HA	2:GX:379:GLN:HG2	1.91	0.53
3:MY:1859:LEU:O	3:MY:1863:MET:CB	2.56	0.53
2:AX:376:ILE:HA	2:AX:379:GLN:HG2	1.91	0.53
2:BX:376:ILE:HA	2:BX:379:GLN:HG2	1.91	0.53
1:FT:81:VAL:HG21	2:FX:459:MET:HE3	1.91	0.53
2:FX:376:ILE:HA	2:FX:379:GLN:HG2	1.91	0.53
2:GX:399:ARG:NH2	1:HT:169:HIS:O	2.42	0.53
3:GY:1710:LEU:HD12	3:HY:1785:GLY:HA3	1.90	0.53
1:HT:39:VAL:HG11	2:IX:419:ILE:HG13	1.90	0.53
3:HY:1858:ILE:HG13	3:IY:1859:LEU:HD21	1.91	0.53
2:MX:376:ILE:HA	2:MX:379:GLN:HG2	1.91	0.53
3:MY:1710:LEU:HD12	3:NY:1785:GLY:HA3	1.91	0.53
2:DX:376:ILE:HA	2:DX:379:GLN:HG2	1.91	0.53
2:EX:376:ILE:HA	2:EX:379:GLN:HG2	1.91	0.53
1:HT:111:ALA:O	1:IT:167:ASN:ND2	2.42	0.53
1:LT:114:ALA:HB1	1:LT:118:ILE:HD11	1.91	0.53
1:CT:114:ALA:HB1	1:CT:118:ILE:HD11	1.91	0.52
1:DT:114:ALA:HB1	1:DT:118:ILE:HD11	1.92	0.52
3:HY:1710:LEU:HD12	3:IY:1785:GLY:HA3	1.90	0.52
2:IX:376:ILE:HA	2:IX:379:GLN:HG2	1.91	0.52
1:JT:210:TYR:CD1	2:JX:368:ILE:HG13	2.45	0.52
2:KX:376:ILE:HA	2:KX:379:GLN:HG2	1.91	0.52
2:LX:376:ILE:HA	2:LX:379:GLN:HG2	1.91	0.52
2:CX:376:ILE:HA	2:CX:379:GLN:HG2	1.91	0.52
3:DY:1710:LEU:HD12	3:EY:1785:GLY:HA3	1.90	0.52
3:EY:1859:LEU:O	3:EY:1863:MET:CB	2.56	0.52
1:FT:114:ALA:HB1	1:FT:118:ILE:HD11	1.92	0.52
2:HX:376:ILE:HA	2:HX:379:GLN:HG2	1.91	0.52
3:LY:1859:LEU:O	3:LY:1863:MET:CB	2.56	0.52
1:NT:114:ALA:HB1	1:NT:118:ILE:HD11	1.92	0.52
2:NX:376:ILE:HA	2:NX:379:GLN:HG2	1.91	0.52
3:NY:1859:LEU:O	3:NY:1863:MET:CB	2.56	0.52
1:AT:114:ALA:HB1	1:AT:118:ILE:HD11	1.92	0.52
1:BT:111:ALA:O	1:CT:167:ASN:ND2	2.43	0.52
1:ET:114:ALA:HB1	1:ET:118:ILE:HD11	1.91	0.52
1:FT:36:TYR:HB3	2:GX:404:TYR:HB3	1.91	0.52
1:GT:90:SER:HA	1:GT:137:ASN:HB2	1.92	0.52
1:HT:90:SER:HA	1:HT:137:ASN:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:MT:114:ALA:HB1	1:MT:118:ILE:HD11	1.91	0.52
3:EY:1858:ILE:HG13	3:FY:1859:LEU:HD21	1.92	0.52
1:GT:39:VAL:HG11	2:HX:419:ILE:HG13	1.91	0.52
1:HT:114:ALA:HB1	1:HT:118:ILE:HD11	1.91	0.52
1:JT:90:SER:HA	1:JT:137:ASN:HB2	1.92	0.52
1:JT:114:ALA:HB1	1:JT:118:ILE:HD11	1.92	0.52
2:JX:376:ILE:HA	2:JX:379:GLN:HG2	1.91	0.52
1:KT:90:SER:HA	1:KT:137:ASN:HB2	1.92	0.52
3:LY:1858:ILE:HG13	3:MY:1859:LEU:HD21	1.92	0.52
3:EY:1710:LEU:HD12	3:FY:1785:GLY:HA3	1.91	0.52
3:AY:1859:LEU:HD21	3:NY:1858:ILE:HG13	1.92	0.52
3:AY:1858:ILE:HG13	3:BY:1859:LEU:HD21	1.92	0.52
3:BY:1710:LEU:HD12	3:CY:1785:GLY:HA3	1.92	0.52
1:GT:114:ALA:HB1	1:GT:118:ILE:HD11	1.91	0.52
1:KT:114:ALA:HB1	1:KT:118:ILE:HD11	1.92	0.52
1:BT:114:ALA:HB1	1:BT:118:ILE:HD11	1.92	0.52
1:ET:111:ALA:O	1:FT:167:ASN:ND2	2.43	0.52
1:IT:114:ALA:HB1	1:IT:118:ILE:HD11	1.91	0.52
1:MT:90:SER:HA	1:MT:137:ASN:HB2	1.92	0.52
1:FT:90:SER:HA	1:FT:137:ASN:HB2	1.92	0.52
1:IT:90:SER:HA	1:IT:137:ASN:HB2	1.92	0.52
1:ET:90:SER:HA	1:ET:137:ASN:HB2	1.92	0.52
1:ET:193:GLU:HA	1:ET:196:ASN:HD22	1.75	0.52
2:KX:439:ILE:HD12	2:KX:467:TYR:HD1	1.75	0.52
1:LT:90:SER:HA	1:LT:137:ASN:HB2	1.92	0.52
1:AT:39:VAL:HG21	2:BX:419:ILE:HD12	1.91	0.51
3:KY:1858:ILE:HG13	3:LY:1859:LEU:HD21	1.92	0.51
2:MX:439:ILE:HD12	2:MX:467:TYR:HD1	1.76	0.51
1:BT:81:VAL:HG21	2:BX:459:MET:HE3	1.91	0.51
1:FT:193:GLU:HA	1:FT:196:ASN:HD22	1.75	0.51
1:IT:213:ARG:HH12	2:IX:364:ASN:HB3	1.76	0.51
1:KT:193:GLU:HA	1:KT:196:ASN:HD22	1.75	0.51
1:DT:193:GLU:HA	1:DT:196:ASN:HD22	1.75	0.51
3:GY:1858:ILE:HG13	3:HY:1859:LEU:HD21	1.93	0.51
3:IY:1710:LEU:HD12	3:JY:1785:GLY:HA3	1.92	0.51
1:KT:111:ALA:O	1:LT:167:ASN:ND2	2.44	0.51
2:AX:439:ILE:HD12	2:AX:467:TYR:HD1	1.76	0.51
1:DT:90:SER:HA	1:DT:137:ASN:HB2	1.92	0.51
1:JT:193:GLU:HA	1:JT:196:ASN:HD22	1.75	0.51
1:NT:90:SER:HA	1:NT:137:ASN:HB2	1.92	0.51
1:CT:90:SER:HA	1:CT:137:ASN:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:FY:1710:LEU:HD12	3:GY:1785:GLY:HA3	1.92	0.51
3:FY:1858:ILE:HG13	3:GY:1859:LEU:HD21	1.93	0.51
1:GT:193:GLU:HA	1:GT:196:ASN:HD22	1.75	0.51
2:IX:436:GLN:HB2	3:IY:1734:LYS:HG2	1.93	0.51
3:IY:1858:ILE:HG13	3:JY:1859:LEU:HD21	1.93	0.51
1:AT:193:GLU:HA	1:AT:196:ASN:HD22	1.75	0.51
3:DY:1858:ILE:HG13	3:EY:1859:LEU:HD21	1.92	0.51
1:GT:81:VAL:HG21	2:GX:459:MET:HE3	1.93	0.51
2:IX:439:ILE:HD12	2:IX:467:TYR:HD1	1.76	0.51
1:JT:48:SER:OG	1:KT:170:GLY:O	2.28	0.51
1:MT:81:VAL:HG21	2:MX:459:MET:HE3	1.92	0.51
1:AT:90:SER:HA	1:AT:137:ASN:HB2	1.92	0.51
2:AX:419:ILE:HD12	1:NT:39:VAL:HG21	1.91	0.51
1:BT:193:GLU:HA	1:BT:196:ASN:HD22	1.75	0.51
1:CT:193:GLU:HA	1:CT:196:ASN:HD22	1.75	0.51
1:IT:210:TYR:CD1	2:IX:368:ILE:HG13	2.46	0.51
1:LT:81:VAL:HG21	2:LX:459:MET:HE3	1.91	0.51
1:MT:111:ALA:O	1:NT:167:ASN:ND2	2.44	0.51
3:MY:1858:ILE:HG13	3:NY:1859:LEU:HD21	1.93	0.51
1:DT:39:VAL:HG21	2:EX:419:ILE:HD12	1.92	0.51
1:LT:193:GLU:HA	1:LT:196:ASN:HD22	1.75	0.51
1:AT:111:ALA:O	1:BT:167:ASN:ND2	2.44	0.50
1:IT:193:GLU:HA	1:IT:196:ASN:HD22	1.75	0.50
1:BT:90:SER:HA	1:BT:137:ASN:HB2	1.92	0.50
3:CY:1858:ILE:HG13	3:DY:1859:LEU:HD21	1.93	0.50
1:DT:111:ALA:O	1:ET:167:ASN:ND2	2.44	0.50
2:EX:439:ILE:HD12	2:EX:467:TYR:HD1	1.75	0.50
1:DT:81:VAL:HG21	2:DX:459:MET:HE3	1.93	0.50
2:FX:439:ILE:HD12	2:FX:467:TYR:HD1	1.76	0.50
2:HX:439:ILE:HD12	2:HX:467:TYR:HD1	1.76	0.50
3:JY:1858:ILE:HG13	3:KY:1859:LEU:HD21	1.93	0.50
2:CX:439:ILE:HD12	2:CX:467:TYR:HD1	1.76	0.50
3:CY:1859:LEU:O	3:CY:1863:MET:HB2	2.11	0.50
1:HT:39:VAL:HG21	2:IX:419:ILE:HD12	1.92	0.50
1:JT:81:VAL:HG21	2:JX:459:MET:HE3	1.92	0.50
2:JX:439:ILE:HD12	2:JX:467:TYR:HD1	1.76	0.50
2:LX:439:ILE:HD12	2:LX:467:TYR:HD1	1.76	0.50
1:AT:81:VAL:HG21	2:AX:459:MET:HE3	1.93	0.50
3:BY:1858:ILE:HG13	3:CY:1859:LEU:HD21	1.93	0.50
1:HT:193:GLU:HA	1:HT:196:ASN:HD22	1.75	0.50
2:IX:507:GLY:HA2	1:JT:168:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:NY:1859:LEU:O	3:NY:1863:MET:HB2	2.11	0.50
2:AX:497:LEU:O	2:BX:432:ASN:ND2	2.37	0.50
3:BY:1859:LEU:O	3:BY:1863:MET:HB2	2.11	0.50
1:ET:81:VAL:HG21	2:EX:459:MET:HE3	1.94	0.50
1:FT:111:ALA:O	1:GT:167:ASN:ND2	2.45	0.50
3:FY:1740:GLY:HA2	3:FY:1759:PHE:HA	1.94	0.50
3:HY:1859:LEU:O	3:HY:1863:MET:HB2	2.11	0.50
3:IY:1763:ILE:HG12	3:IY:1769:ILE:HG22	1.94	0.50
3:JY:1859:LEU:O	3:JY:1863:MET:HB2	2.11	0.50
3:KY:1859:LEU:O	3:KY:1863:MET:HB2	2.11	0.50
1:NT:193:GLU:HA	1:NT:196:ASN:HD22	1.75	0.50
3:AY:1859:LEU:O	3:AY:1863:MET:HB2	2.11	0.50
3:EY:1740:GLY:HA2	3:EY:1759:PHE:HA	1.94	0.50
3:GY:1740:GLY:HA2	3:GY:1759:PHE:HA	1.94	0.50
3:GY:1763:ILE:HG12	3:GY:1769:ILE:HG22	1.94	0.50
3:KY:1763:ILE:HG12	3:KY:1769:ILE:HG22	1.94	0.50
3:AY:1740:GLY:HA2	3:AY:1759:PHE:HA	1.94	0.50
1:BT:39:VAL:HG11	2:CX:419:ILE:HG13	1.93	0.50
2:BX:436:GLN:HB2	3:BY:1734:LYS:HG2	1.93	0.50
2:DX:439:ILE:HD12	2:DX:467:TYR:HD1	1.76	0.50
3:EY:1763:ILE:HG12	3:EY:1769:ILE:HG22	1.94	0.50
2:NX:439:ILE:HD12	2:NX:467:TYR:HD1	1.76	0.50
3:NY:1740:GLY:HA2	3:NY:1759:PHE:HA	1.94	0.50
1:AT:167:ASN:ND2	1:NT:111:ALA:O	2.45	0.49
3:BY:1740:GLY:HA2	3:BY:1759:PHE:HA	1.94	0.49
3:DY:1740:GLY:HA2	3:DY:1759:PHE:HA	1.94	0.49
1:HT:81:VAL:HG21	2:HX:459:MET:HE3	1.93	0.49
3:HY:1740:GLY:HA2	3:HY:1759:PHE:HA	1.94	0.49
3:HY:1763:ILE:HG12	3:HY:1769:ILE:HG22	1.94	0.49
3:IY:1859:LEU:O	3:IY:1863:MET:HB2	2.12	0.49
3:LY:1859:LEU:O	3:LY:1863:MET:HB2	2.12	0.49
3:MY:1740:GLY:HA2	3:MY:1759:PHE:HA	1.94	0.49
1:AT:28:VAL:HG23	1:AT:29:VAL:H	1.78	0.49
3:CY:1740:GLY:HA2	3:CY:1759:PHE:HA	1.94	0.49
1:FT:48:SER:OG	1:GT:170:GLY:O	2.29	0.49
2:FX:399:ARG:NH1	2:FX:495:ASN:OD1	2.46	0.49
1:HT:36:TYR:HB3	2:IX:404:TYR:HB3	1.92	0.49
2:IX:455:ILE:HB	3:IY:1765:PRO:HB3	1.93	0.49
2:IX:481:ASP:HB3	3:IY:1875:ASP:HA	1.95	0.49
3:JY:1763:ILE:HG12	3:JY:1769:ILE:HG22	1.94	0.49
3:LY:1763:ILE:HG12	3:LY:1769:ILE:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:MX:399:ARG:NH1	2:MX:495:ASN:OD1	2.46	0.49
1:NT:81:VAL:HG21	2:NX:459:MET:HE3	1.94	0.49
2:EX:399:ARG:NH1	2:EX:495:ASN:OD1	2.46	0.49
3:EY:1859:LEU:O	3:EY:1863:MET:HB2	2.11	0.49
2:GX:439:ILE:HD12	2:GX:467:TYR:HD1	1.75	0.49
3:LY:1740:GLY:HA2	3:LY:1759:PHE:HA	1.94	0.49
3:FY:1763:ILE:HG12	3:FY:1769:ILE:HG22	1.94	0.49
2:GX:399:ARG:NH1	2:GX:495:ASN:OD1	2.46	0.49
1:IT:111:ALA:O	1:JT:167:ASN:ND2	2.45	0.49
3:IY:1740:GLY:HA2	3:IY:1759:PHE:HA	1.94	0.49
1:LT:111:ALA:O	1:MT:167:ASN:ND2	2.45	0.49
3:NY:1763:ILE:HG12	3:NY:1769:ILE:HG22	1.94	0.49
1:BT:28:VAL:HG23	1:BT:29:VAL:H	1.78	0.49
2:BX:399:ARG:NH1	2:BX:495:ASN:OD1	2.46	0.49
2:BX:439:ILE:HD12	2:BX:467:TYR:HD1	1.76	0.49
2:CX:399:ARG:NH1	2:CX:495:ASN:OD1	2.46	0.49
3:CY:1763:ILE:HG12	3:CY:1769:ILE:HG22	1.94	0.49
1:FT:28:VAL:HG23	1:FT:29:VAL:H	1.78	0.49
1:MT:193:GLU:HA	1:MT:196:ASN:HD22	1.75	0.49
1:NT:28:VAL:HG23	1:NT:29:VAL:H	1.78	0.49
2:NX:399:ARG:NH1	2:NX:495:ASN:OD1	2.46	0.49
2:GX:400:ASN:HB3	2:GX:421:ASP:OD1	2.13	0.49
2:JX:399:ARG:NH1	2:JX:495:ASN:OD1	2.46	0.49
3:KY:1740:GLY:HA2	3:KY:1759:PHE:HA	1.94	0.49
3:MY:1859:LEU:O	3:MY:1863:MET:HB2	2.12	0.49
2:DX:400:ASN:HB3	2:DX:421:ASP:OD1	2.13	0.49
1:GT:39:VAL:HG21	2:HX:419:ILE:HD12	1.95	0.49
3:GY:1859:LEU:O	3:GY:1863:MET:HB2	2.11	0.49
2:HX:400:ASN:HB3	2:HX:421:ASP:OD1	2.13	0.49
3:JY:1740:GLY:HA2	3:JY:1759:PHE:HA	1.94	0.49
1:KT:196:ASN:OD1	3:LY:1907:GLN:NE2	2.46	0.49
2:DX:399:ARG:NH1	2:DX:495:ASN:OD1	2.46	0.49
1:ET:28:VAL:HG23	1:ET:29:VAL:H	1.78	0.49
2:CX:481:ASP:HB3	3:CY:1875:ASP:HA	1.94	0.49
3:EY:1699:GLU:HG2	3:EY:1719:ALA:HB3	1.95	0.49
3:FY:1699:GLU:HG2	3:FY:1719:ALA:HB3	1.95	0.49
3:GY:1699:GLU:HG2	3:GY:1719:ALA:HB3	1.95	0.49
2:KX:399:ARG:NH1	2:KX:495:ASN:OD1	2.46	0.49
1:CT:28:VAL:HG23	1:CT:29:VAL:H	1.78	0.49
3:FY:1859:LEU:O	3:FY:1863:MET:HB2	2.11	0.49
1:GT:28:VAL:HG23	1:GT:29:VAL:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HX:399:ARG:NH1	2:HX:495:ASN:OD1	2.46	0.49
1:JT:99:ALA:HB2	1:JT:124:PRO:HB3	1.95	0.49
1:JT:213:ARG:NH1	2:JX:364:ASN:HB3	2.28	0.49
1:KT:28:VAL:HG23	1:KT:29:VAL:H	1.78	0.49
3:MY:1698:ILE:HG23	3:MY:1722:VAL:HG21	1.95	0.49
3:AY:1698:ILE:HG23	3:AY:1722:VAL:HG21	1.95	0.48
2:CX:400:ASN:HB3	2:CX:421:ASP:OD1	2.13	0.48
3:DY:1699:GLU:HG2	3:DY:1719:ALA:HB3	1.95	0.48
3:HY:1699:GLU:HG2	3:HY:1719:ALA:HB3	1.95	0.48
2:JX:507:GLY:HA2	1:KT:168:LEU:HD11	1.94	0.48
2:LX:399:ARG:NH1	2:LX:495:ASN:OD1	2.46	0.48
3:CY:1698:ILE:HG23	3:CY:1722:VAL:HG21	1.95	0.48
3:EY:1698:ILE:HG23	3:EY:1722:VAL:HG21	1.95	0.48
1:HT:99:ALA:HB2	1:HT:124:PRO:HB3	1.95	0.48
3:HY:1698:ILE:HG23	3:HY:1722:VAL:HG21	1.95	0.48
1:JT:28:VAL:HG23	1:JT:29:VAL:H	1.78	0.48
3:KY:1698:ILE:HG23	3:KY:1722:VAL:HG21	1.95	0.48
2:MX:400:ASN:HB3	2:MX:421:ASP:OD1	2.13	0.48
2:NX:400:ASN:HB3	2:NX:421:ASP:OD1	2.13	0.48
3:DY:1859:LEU:O	3:DY:1863:MET:HB2	2.12	0.48
2:EX:400:ASN:HB3	2:EX:421:ASP:OD1	2.13	0.48
3:FY:1698:ILE:HG23	3:FY:1722:VAL:HG21	1.95	0.48
1:IT:28:VAL:HG23	1:IT:29:VAL:H	1.78	0.48
3:IY:1699:GLU:HG2	3:IY:1719:ALA:HB3	1.95	0.48
2:JX:364:ASN:HA	2:JX:367:LYS:HG2	1.96	0.48
2:LX:400:ASN:HB3	2:LX:421:ASP:OD1	2.13	0.48
3:LY:1873:GLU:HG2	3:MY:1781:LEU:HD22	1.95	0.48
2:AX:400:ASN:HB3	2:AX:421:ASP:OD1	2.13	0.48
3:BY:1763:ILE:HG12	3:BY:1769:ILE:HG22	1.94	0.48
2:DX:364:ASN:HA	2:DX:367:LYS:HG2	1.96	0.48
1:FT:99:ALA:HB2	1:FT:124:PRO:HB3	1.95	0.48
2:KX:400:ASN:HB3	2:KX:421:ASP:OD1	2.13	0.48
2:AX:364:ASN:HA	2:AX:367:LYS:HG2	1.96	0.48
2:AX:399:ARG:NH1	2:AX:495:ASN:OD1	2.46	0.48
3:CY:1699:GLU:HG2	3:CY:1719:ALA:HB3	1.95	0.48
2:FX:364:ASN:HA	2:FX:367:LYS:HG2	1.96	0.48
2:HX:364:ASN:HA	2:HX:367:LYS:HG2	1.96	0.48
2:HX:497:LEU:O	2:IX:432:ASN:ND2	2.38	0.48
2:IX:400:ASN:HB3	2:IX:421:ASP:OD1	2.13	0.48
3:IY:1873:GLU:HG2	3:JY:1781:LEU:HD22	1.95	0.48
3:JY:1698:ILE:HG23	3:JY:1722:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:MT:28:VAL:HG23	1:MT:29:VAL:H	1.78	0.48
3:EY:1792:ASN:O	3:EY:1797:ARG:NH1	2.46	0.48
2:FX:400:ASN:HB3	2:FX:421:ASP:OD1	2.13	0.48
3:FY:1792:ASN:O	3:FY:1797:ARG:NH1	2.46	0.48
3:JY:1699:GLU:HG2	3:JY:1719:ALA:HB3	1.95	0.48
1:LT:99:ALA:HB2	1:LT:124:PRO:HB3	1.95	0.48
2:LX:364:ASN:HA	2:LX:367:LYS:HG2	1.96	0.48
3:MY:1763:ILE:HG12	3:MY:1769:ILE:HG22	1.94	0.48
2:BX:400:ASN:HB3	2:BX:421:ASP:OD1	2.13	0.48
3:JY:1792:ASN:O	3:JY:1797:ARG:NH1	2.46	0.48
3:AY:1713:ILE:HD11	3:BY:1880:LEU:HD23	1.96	0.48
3:CY:1873:GLU:HG2	3:DY:1781:LEU:HD22	1.95	0.48
3:GY:1698:ILE:HG23	3:GY:1722:VAL:HG21	1.95	0.48
3:HY:1713:ILE:HD11	3:IY:1880:LEU:HD23	1.96	0.48
2:IX:399:ARG:NH1	2:IX:495:ASN:OD1	2.46	0.48
2:JX:400:ASN:HB3	2:JX:421:ASP:OD1	2.13	0.48
3:MY:1792:ASN:O	3:MY:1797:ARG:NH1	2.46	0.48
3:BY:1699:GLU:HG2	3:BY:1719:ALA:HB3	1.95	0.48
2:CX:364:ASN:HA	2:CX:367:LYS:HG2	1.96	0.48
3:DY:1698:ILE:HG23	3:DY:1722:VAL:HG21	1.95	0.48
3:GY:1792:ASN:O	3:GY:1797:ARG:NH1	2.46	0.48
2:MX:364:ASN:HA	2:MX:367:LYS:HG2	1.96	0.48
3:NY:1792:ASN:O	3:NY:1797:ARG:NH1	2.46	0.48
3:AY:1763:ILE:HG12	3:AY:1769:ILE:HG22	1.94	0.48
2:IX:450:MET:HE1	3:JY:1880:LEU:HD11	1.95	0.48
3:KY:1699:GLU:HG2	3:KY:1719:ALA:HB3	1.95	0.48
3:LY:1792:ASN:O	3:LY:1797:ARG:NH1	2.46	0.48
3:DY:1792:ASN:O	3:DY:1797:ARG:NH1	2.46	0.47
3:EY:1873:GLU:HG2	3:FY:1781:LEU:HD22	1.96	0.47
1:LT:28:VAL:HG23	1:LT:29:VAL:H	1.78	0.47
3:LY:1707:ASP:HB2	3:MY:1783:GLU:HB2	1.96	0.47
3:AY:1781:LEU:HD22	3:NY:1873:GLU:HG2	1.95	0.47
3:AY:1792:ASN:O	3:AY:1797:ARG:NH1	2.46	0.47
3:KY:1792:ASN:O	3:KY:1797:ARG:NH1	2.46	0.47
2:BX:364:ASN:HA	2:BX:367:LYS:HG2	1.96	0.47
3:BY:1698:ILE:HG23	3:BY:1722:VAL:HG21	1.95	0.47
1:DT:28:VAL:HG23	1:DT:29:VAL:H	1.78	0.47
3:DY:1763:ILE:HG12	3:DY:1769:ILE:HG22	1.94	0.47
1:HT:28:VAL:HG23	1:HT:29:VAL:H	1.78	0.47
2:IX:364:ASN:HA	2:IX:367:LYS:HG2	1.96	0.47
3:IY:1698:ILE:HG23	3:IY:1722:VAL:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:LY:1698:ILE:HG23	3:LY:1722:VAL:HG21	1.95	0.47
1:NT:52:LEU:HD12	1:NT:89:HIS:CD2	2.49	0.47
3:NY:1698:ILE:HG23	3:NY:1722:VAL:HG21	1.95	0.47
1:AT:99:ALA:HB2	1:AT:124:PRO:HB3	1.95	0.47
3:AY:1699:GLU:HG2	3:AY:1719:ALA:HB3	1.95	0.47
3:BY:1873:GLU:HG2	3:CY:1781:LEU:HD22	1.95	0.47
1:CT:99:ALA:HB2	1:CT:124:PRO:HB3	1.95	0.47
2:CX:450:MET:HE1	3:DY:1880:LEU:HD11	1.96	0.47
1:DT:48:SER:OG	1:ET:170:GLY:O	2.31	0.47
1:IT:306:LEU:HD22	2:IX:384:GLU:HB2	1.97	0.47
3:IY:1792:ASN:O	3:IY:1797:ARG:NH1	2.46	0.47
3:LY:1699:GLU:HG2	3:LY:1719:ALA:HB3	1.95	0.47
1:MT:52:LEU:HD12	1:MT:89:HIS:CD2	2.49	0.47
3:AY:1783:GLU:HB2	3:NY:1707:ASP:HB2	1.96	0.47
1:CT:52:LEU:HD12	1:CT:89:HIS:CD2	2.49	0.47
2:GX:364:ASN:HA	2:GX:367:LYS:HG2	1.96	0.47
3:GY:1713:ILE:HD11	3:HY:1880:LEU:HD23	1.97	0.47
3:JY:1873:GLU:HG2	3:KY:1781:LEU:HD22	1.96	0.47
1:LT:33:ASN:ND2	2:MX:407:PRO:O	2.47	0.47
1:AT:52:LEU:HD12	1:AT:89:HIS:CD2	2.49	0.47
3:BY:1713:ILE:HD11	3:CY:1880:LEU:HD23	1.97	0.47
3:BY:1792:ASN:O	3:BY:1797:ARG:NH1	2.46	0.47
1:CT:81:VAL:HG21	2:CX:459:MET:HE3	1.95	0.47
1:DT:52:LEU:HD12	1:DT:89:HIS:CD2	2.49	0.47
2:EX:364:ASN:HA	2:EX:367:LYS:HG2	1.96	0.47
1:LT:52:LEU:HD12	1:LT:89:HIS:CD2	2.49	0.47
1:BT:52:LEU:HD12	1:BT:89:HIS:CD2	2.49	0.47
1:BT:99:ALA:HB2	1:BT:124:PRO:HB3	1.95	0.47
1:ET:52:LEU:HD12	1:ET:89:HIS:CD2	2.49	0.47
1:FT:199:TYR:HB3	2:FX:379:GLN:OE1	2.15	0.47
3:FY:1873:GLU:HG2	3:GY:1781:LEU:HD22	1.96	0.47
1:GT:99:ALA:HB2	1:GT:124:PRO:HB3	1.95	0.47
1:IT:52:LEU:HD12	1:IT:89:HIS:CD2	2.49	0.47
1:IT:99:ALA:HB2	1:IT:124:PRO:HB3	1.95	0.47
1:KT:52:LEU:HD12	1:KT:89:HIS:CD2	2.50	0.47
3:MY:1699:GLU:HG2	3:MY:1719:ALA:HB3	1.95	0.47
1:NT:99:ALA:HB2	1:NT:124:PRO:HB3	1.95	0.47
3:NY:1699:GLU:HG2	3:NY:1719:ALA:HB3	1.95	0.47
1:DT:99:ALA:HB2	1:DT:124:PRO:HB3	1.95	0.47
1:FT:52:LEU:HD12	1:FT:89:HIS:CD2	2.49	0.47
1:FT:60:PRO:HA	1:FT:137:ASN:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GT:60:PRO:HA	1:GT:137:ASN:O	2.15	0.47
1:HT:52:LEU:HD12	1:HT:89:HIS:CD2	2.49	0.47
1:IT:60:PRO:HA	1:IT:137:ASN:O	2.15	0.47
1:JT:52:LEU:HD12	1:JT:89:HIS:CD2	2.49	0.47
1:KT:99:ALA:HB2	1:KT:124:PRO:HB3	1.95	0.47
2:BX:480:LYS:NZ	3:BY:1699:GLU:OE2	2.38	0.47
3:DY:1713:ILE:HD11	3:EY:1880:LEU:HD23	1.96	0.47
1:ET:60:PRO:HA	1:ET:137:ASN:O	2.15	0.47
1:ET:99:ALA:HB2	1:ET:124:PRO:HB3	1.95	0.47
2:GX:477:LYS:HD3	2:GX:484:LEU:HD11	1.96	0.47
1:HT:60:PRO:HA	1:HT:137:ASN:O	2.15	0.47
3:HY:1792:ASN:O	3:HY:1797:ARG:NH1	2.46	0.47
1:MT:99:ALA:HB2	1:MT:124:PRO:HB3	1.95	0.47
3:MY:1873:GLU:HG2	3:NY:1781:LEU:HD22	1.97	0.47
3:CY:1713:ILE:HD11	3:DY:1880:LEU:HD23	1.97	0.47
3:CY:1792:ASN:O	3:CY:1797:ARG:NH1	2.46	0.47
1:DT:60:PRO:HA	1:DT:137:ASN:O	2.15	0.47
2:EX:507:GLY:HA2	1:FT:168:LEU:HD11	1.97	0.47
1:GT:52:LEU:HD12	1:GT:89:HIS:CD2	2.49	0.47
2:HX:477:LYS:HD3	2:HX:484:LEU:HD11	1.96	0.47
1:JT:60:PRO:HA	1:JT:137:ASN:O	2.15	0.47
3:JY:1707:ASP:HB2	3:KY:1783:GLU:HB2	1.96	0.47
2:KX:364:ASN:HA	2:KX:367:LYS:HG2	1.96	0.47
2:NX:364:ASN:HA	2:NX:367:LYS:HG2	1.96	0.47
1:CT:60:PRO:HA	1:CT:137:ASN:O	2.15	0.46
3:GY:1707:ASP:HB2	3:HY:1783:GLU:HB2	1.96	0.46
2:IX:477:LYS:HD3	2:IX:484:LEU:HD11	1.96	0.46
1:LT:60:PRO:HA	1:LT:137:ASN:O	2.15	0.46
1:GT:291:GLU:O	1:GT:295:ASN:HB2	2.16	0.46
2:JX:477:LYS:HD3	2:JX:484:LEU:HD11	1.96	0.46
3:MY:1707:ASP:HB2	3:NY:1783:GLU:HB2	1.97	0.46
2:FX:417:SER:N	2:FX:429:GLY:O	2.44	0.46
2:FX:477:LYS:HD3	2:FX:484:LEU:HD11	1.96	0.46
3:FY:1713:ILE:HD11	3:GY:1880:LEU:HD23	1.97	0.46
2:IX:450:MET:HE3	3:JY:1697:PRO:HB3	1.97	0.46
3:IY:1713:ILE:HD11	3:JY:1880:LEU:HD23	1.97	0.46
1:KT:291:GLU:O	1:KT:295:ASN:HB2	2.16	0.46
1:LT:291:GLU:O	1:LT:295:ASN:HB2	2.16	0.46
1:AT:60:PRO:HA	1:AT:137:ASN:O	2.15	0.46
1:CT:111:ALA:O	1:DT:167:ASN:ND2	2.49	0.46
3:CY:1707:ASP:HB2	3:DY:1783:GLU:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EX:477:LYS:HD3	2:EX:484:LEU:HD11	1.96	0.46
1:FT:291:GLU:O	1:FT:295:ASN:HB2	2.16	0.46
3:GY:1873:GLU:HG2	3:HY:1781:LEU:HD22	1.96	0.46
1:HT:199:TYR:HB3	2:HX:379:GLN:OE1	2.16	0.46
1:KT:60:PRO:HA	1:KT:137:ASN:O	2.15	0.46
2:KX:477:LYS:HD3	2:KX:484:LEU:HD11	1.96	0.46
1:BT:39:VAL:HG21	2:CX:419:ILE:HD12	1.97	0.46
1:ET:291:GLU:O	1:ET:295:ASN:HB2	2.16	0.46
2:MX:477:LYS:HD3	2:MX:484:LEU:HD11	1.96	0.46
2:NX:477:LYS:HD3	2:NX:484:LEU:HD11	1.96	0.46
1:HT:291:GLU:O	1:HT:295:ASN:HB2	2.16	0.46
1:KT:51:PRO:HD3	2:KX:495:ASN:HB2	1.97	0.46
1:KT:200:LYS:HD3	1:KT:200:LYS:HA	1.76	0.46
2:LX:477:LYS:HD3	2:LX:484:LEU:HD11	1.96	0.46
2:BX:455:ILE:HB	3:BY:1765:PRO:HB3	1.98	0.46
3:FY:1707:ASP:HB2	3:GY:1783:GLU:HB2	1.97	0.46
3:KY:1707:ASP:HB2	3:LY:1783:GLU:HB2	1.98	0.46
3:KY:1873:GLU:HG2	3:LY:1781:LEU:HD22	1.98	0.46
1:MT:291:GLU:O	1:MT:295:ASN:HB2	2.16	0.46
2:MX:392:LEU:HD22	3:NY:1728:THR:HB	1.98	0.46
2:AX:392:LEU:HD22	3:BY:1728:THR:HB	1.98	0.46
1:BT:60:PRO:HA	1:BT:137:ASN:O	2.15	0.46
2:DX:477:LYS:HD3	2:DX:484:LEU:HD11	1.96	0.46
3:DY:1873:GLU:HG2	3:EY:1781:LEU:HD22	1.98	0.46
1:MT:60:PRO:HA	1:MT:137:ASN:O	2.15	0.46
2:AX:477:LYS:HD3	2:AX:484:LEU:HD11	1.96	0.46
2:CX:436:GLN:HB2	3:CY:1734:LYS:HG2	1.98	0.46
2:CX:477:LYS:HD3	2:CX:484:LEU:HD11	1.96	0.46
1:DT:291:GLU:O	1:DT:295:ASN:HB2	2.16	0.46
3:IY:1707:ASP:HB2	3:JY:1783:GLU:HB2	1.97	0.46
3:JY:1713:ILE:HD11	3:KY:1880:LEU:HD23	1.97	0.46
2:BX:477:LYS:HD3	2:BX:484:LEU:HD11	1.96	0.46
3:KY:1713:ILE:HD11	3:LY:1880:LEU:HD23	1.97	0.46
1:AT:48:SER:OG	1:BT:170:GLY:O	2.32	0.45
1:JT:291:GLU:O	1:JT:295:ASN:HB2	2.16	0.45
1:NT:60:PRO:HA	1:NT:137:ASN:O	2.15	0.45
3:AY:1880:LEU:HD23	3:NY:1713:ILE:HD11	1.98	0.45
1:CT:291:GLU:O	1:CT:295:ASN:HB2	2.16	0.45
2:IX:480:LYS:NZ	3:IY:1699:GLU:OE2	2.41	0.45
3:MY:1713:ILE:HD11	3:NY:1880:LEU:HD23	1.97	0.45
2:AX:459:MET:HE2	2:AX:459:MET:HB3	1.88	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AY:1707:ASP:HB2	3:BY:1783:GLU:HB2	1.98	0.45
3:DY:1707:ASP:HB2	3:EY:1783:GLU:HB2	1.98	0.45
1:NT:200:LYS:HA	1:NT:200:LYS:HD3	1.76	0.45
3:BY:1707:ASP:HB2	3:CY:1783:GLU:HB2	1.97	0.45
3:EY:1707:ASP:HB2	3:FY:1783:GLU:HB2	1.96	0.45
3:EY:1713:ILE:HD11	3:FY:1880:LEU:HD23	1.98	0.45
1:NT:291:GLU:O	1:NT:295:ASN:HB2	2.16	0.45
1:BT:291:GLU:O	1:BT:295:ASN:HB2	2.16	0.45
2:HX:392:LEU:HD22	3:IY:1728:THR:HB	1.97	0.45
1:IT:291:GLU:O	1:IT:295:ASN:HB2	2.16	0.45
1:LT:200:LYS:HD3	1:LT:200:LYS:HA	1.76	0.45
2:AX:432:ASN:ND2	2:NX:497:LEU:O	2.38	0.45
3:AY:1873:GLU:HG2	3:BY:1781:LEU:HD22	1.98	0.45
1:CT:38:PRO:HG2	1:DT:55:LYS:HB2	1.97	0.45
3:FY:1690:PHE:O	3:FY:1887:PHE:N	2.45	0.45
3:HY:1873:GLU:HG2	3:IY:1781:LEU:HD22	1.97	0.45
2:JX:481:ASP:HB3	3:JY:1875:ASP:HA	1.98	0.45
1:AT:170:GLY:O	1:NT:48:SER:OG	2.32	0.45
1:CT:51:PRO:HD3	2:CX:495:ASN:HB2	1.99	0.45
3:EY:1900:VAL:HA	3:EY:1903:GLU:HG3	1.99	0.45
1:AT:291:GLU:O	1:AT:295:ASN:HB2	2.16	0.45
3:AY:1900:VAL:HA	3:AY:1903:GLU:HG3	1.99	0.45
1:GT:111:ALA:O	1:HT:167:ASN:ND2	2.50	0.45
1:JT:36:TYR:HB3	2:KX:404:TYR:HB3	1.98	0.45
2:CX:459:MET:HE2	2:CX:459:MET:HB3	1.88	0.45
3:FY:1900:VAL:HA	3:FY:1903:GLU:HG3	1.99	0.45
2:LX:392:LEU:HD22	3:MY:1728:THR:HB	1.99	0.45
3:NY:1690:PHE:O	3:NY:1887:PHE:N	2.45	0.45
3:NY:1900:VAL:HA	3:NY:1903:GLU:HG3	1.99	0.45
1:AT:200:LYS:HD3	1:AT:200:LYS:HA	1.76	0.45
2:DX:459:MET:HE2	2:DX:459:MET:HB3	1.88	0.45
2:BX:392:LEU:HD22	3:CY:1728:THR:HB	1.99	0.44
2:KX:417:SER:N	2:KX:429:GLY:O	2.44	0.44
2:LX:497:LEU:O	2:MX:432:ASN:ND2	2.40	0.44
3:LY:1713:ILE:HD11	3:MY:1880:LEU:HD23	1.98	0.44
3:AY:1690:PHE:O	3:AY:1887:PHE:N	2.45	0.44
3:DY:1900:VAL:HA	3:DY:1903:GLU:HG3	1.99	0.44
3:HY:1707:ASP:HB2	3:IY:1783:GLU:HB2	1.98	0.44
3:MY:1900:VAL:HA	3:MY:1903:GLU:HG3	1.99	0.44
1:AT:75:LEU:HD23	1:AT:75:LEU:HA	1.86	0.44
3:AY:1728:THR:HB	2:NX:392:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EX:497:LEU:O	2:FX:432:ASN:ND2	2.41	0.44
3:KY:1732:LEU:HA	3:KY:1732:LEU:HD23	1.84	0.44
2:NX:480:LYS:NZ	3:NY:1699:GLU:OE2	2.48	0.44
2:AX:507:GLY:HA2	1:BT:168:LEU:HD11	1.99	0.44
1:FT:33:ASN:ND2	2:GX:407:PRO:O	2.50	0.44
2:FX:392:LEU:HD22	3:GY:1728:THR:HB	1.98	0.44
1:LT:196:ASN:OD1	3:MY:1907:GLN:NE2	2.50	0.44
1:MT:75:LEU:HA	1:MT:75:LEU:HD23	1.86	0.44
3:LY:1900:VAL:HA	3:LY:1903:GLU:HG3	1.99	0.44
3:BY:1900:VAL:HA	3:BY:1903:GLU:HG3	1.99	0.44
1:GT:48:SER:OG	1:HT:170:GLY:O	2.35	0.44
2:GX:417:SER:N	2:GX:429:GLY:O	2.45	0.44
1:HT:213:ARG:HH12	2:HX:364:ASN:HB3	1.83	0.44
2:JX:436:GLN:HB2	3:JY:1734:LYS:HG2	1.99	0.44
2:CX:455:ILE:HB	3:CY:1765:PRO:HB3	1.99	0.44
3:GY:1900:VAL:HA	3:GY:1903:GLU:HG3	1.99	0.44
1:AT:33:ASN:HD22	2:BX:406:ALA:HB1	1.83	0.44
2:EX:481:ASP:OD1	2:EX:481:ASP:N	2.50	0.44
1:MT:200:LYS:HD3	1:MT:200:LYS:HA	1.76	0.44
3:MY:1690:PHE:O	3:MY:1887:PHE:N	2.45	0.44
3:AY:1729:MET:HB3	2:NX:503:ILE:HG13	2.00	0.44
1:FT:75:LEU:HD23	1:FT:75:LEU:HA	1.86	0.44
1:JT:38:PRO:HG2	1:KT:55:LYS:HB2	2.00	0.44
3:JY:1900:VAL:HA	3:JY:1903:GLU:HG3	1.99	0.44
1:KT:48:SER:OG	1:LT:170:GLY:O	2.34	0.44
3:KY:1900:VAL:HA	3:KY:1903:GLU:HG3	1.99	0.44
2:CX:450:MET:HE3	3:DY:1697:PRO:HB3	2.00	0.43
2:HX:459:MET:HE2	2:HX:459:MET:HB3	1.88	0.43
3:IY:1900:VAL:HA	3:IY:1903:GLU:HG3	1.99	0.43
2:JX:450:MET:HE1	3:KY:1880:LEU:HD11	2.00	0.43
1:NT:75:LEU:HD23	1:NT:75:LEU:HA	1.86	0.43
3:CY:1900:VAL:HA	3:CY:1903:GLU:HG3	1.99	0.43
2:DX:503:ILE:HG13	3:EY:1729:MET:HB3	2.01	0.43
1:FT:200:LYS:HA	1:FT:200:LYS:HD3	1.76	0.43
2:GX:392:LEU:HD22	3:HY:1728:THR:HB	1.99	0.43
2:DX:455:ILE:HB	3:DY:1765:PRO:HB3	2.00	0.43
1:ET:200:LYS:HA	1:ET:200:LYS:HD3	1.76	0.43
3:EY:1690:PHE:O	3:EY:1887:PHE:N	2.45	0.43
2:FX:507:GLY:HA2	1:GT:168:LEU:HD11	2.00	0.43
3:HY:1900:VAL:HA	3:HY:1903:GLU:HG3	1.99	0.43
1:JT:111:ALA:O	1:KT:167:ASN:ND2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:JY:1732:LEU:HA	3:JY:1732:LEU:HD23	1.84	0.43
1:LT:38:PRO:HA	2:MX:404:TYR:HA	2.00	0.43
3:DY:1690:PHE:O	3:DY:1887:PHE:N	2.45	0.43
3:GY:1708:ALA:HB3	3:GY:1869:PHE:HB3	2.01	0.43
1:JT:199:TYR:HB3	2:JX:379:GLN:OE1	2.19	0.43
2:JX:459:MET:HE2	2:JX:459:MET:HB3	1.88	0.43
3:MY:1708:ALA:HB3	3:MY:1869:PHE:HB3	2.01	0.43
1:CT:48:SER:OG	1:DT:170:GLY:O	2.29	0.43
2:DX:503:ILE:HA	3:EY:1729:MET:HA	2.00	0.43
1:FT:196:ASN:OD1	3:GY:1907:GLN:NE2	2.52	0.43
3:FY:1732:LEU:HD23	3:FY:1732:LEU:HA	1.84	0.43
1:GT:200:LYS:HA	1:GT:200:LYS:HD3	1.76	0.43
2:KX:481:ASP:HB3	3:KY:1875:ASP:HA	2.01	0.43
3:MY:1906:LYS:HA	3:MY:1909:THR:HG22	2.01	0.43
3:AY:1729:MET:HA	2:NX:503:ILE:HA	2.00	0.43
3:AY:1906:LYS:HA	3:AY:1909:THR:HG22	2.01	0.43
3:BY:1708:ALA:HB3	3:BY:1869:PHE:HB3	2.01	0.43
3:DY:1708:ALA:HB3	3:DY:1869:PHE:HB3	2.01	0.43
3:KY:1708:ALA:HB3	3:KY:1869:PHE:HB3	2.01	0.43
3:KY:1906:LYS:HA	3:KY:1909:THR:HG22	2.01	0.43
2:AX:394:ARG:HE	2:AX:394:ARG:HB3	1.67	0.43
3:BY:1690:PHE:O	3:BY:1887:PHE:N	2.45	0.43
3:CY:1690:PHE:O	3:CY:1887:PHE:N	2.45	0.43
3:CY:1906:LYS:HA	3:CY:1909:THR:HG22	2.01	0.43
2:DX:497:LEU:O	2:EX:432:ASN:ND2	2.39	0.43
2:FX:481:ASP:OD1	2:FX:481:ASP:N	2.50	0.43
1:GT:196:ASN:OD1	3:HY:1907:GLN:NE2	2.51	0.43
2:GX:497:LEU:O	2:HX:432:ASN:ND2	2.39	0.43
2:GX:507:GLY:HA2	1:HT:168:LEU:HD11	2.01	0.43
1:HT:200:LYS:HA	1:HT:200:LYS:HD3	1.76	0.43
3:IY:1708:ALA:HB3	3:IY:1869:PHE:HB3	2.01	0.43
3:AY:1708:ALA:HB3	3:AY:1869:PHE:HB3	2.01	0.43
1:BT:306:LEU:HD22	2:BX:384:GLU:HB2	2.00	0.43
3:EY:1708:ALA:HB3	3:EY:1869:PHE:HB3	2.01	0.43
1:HT:48:SER:OG	1:IT:170:GLY:O	2.34	0.43
2:HX:507:GLY:HA2	1:IT:168:LEU:HD11	2.01	0.43
2:LX:417:SER:N	2:LX:429:GLY:O	2.44	0.43
1:BT:200:LYS:HA	1:BT:200:LYS:HD3	1.76	0.43
1:DT:200:LYS:HA	1:DT:200:LYS:HD3	1.76	0.43
2:DX:392:LEU:HD22	3:EY:1728:THR:HB	1.99	0.43
1:ET:51:PRO:HD3	2:EX:495:ASN:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:GY:1732:LEU:HA	3:GY:1732:LEU:HD23	1.84	0.43
3:NY:1906:LYS:HA	3:NY:1909:THR:HG22	2.01	0.43
3:BY:1906:LYS:HA	3:BY:1909:THR:HG22	2.01	0.42
1:CT:39:VAL:HG11	2:DX:419:ILE:HG13	2.00	0.42
2:EX:459:MET:HE2	2:EX:459:MET:HB3	1.88	0.42
3:EY:1906:LYS:HA	3:EY:1909:THR:HG22	2.01	0.42
3:HY:1906:LYS:HA	3:HY:1909:THR:HG22	2.01	0.42
3:IY:1732:LEU:HA	3:IY:1732:LEU:HD23	1.84	0.42
2:JX:455:ILE:HB	3:JY:1765:PRO:HB3	2.00	0.42
3:JY:1906:LYS:HA	3:JY:1909:THR:HG22	2.01	0.42
3:LY:1906:LYS:HA	3:LY:1909:THR:HG22	2.01	0.42
2:MX:503:ILE:HA	3:NY:1729:MET:HA	2.01	0.42
2:DX:450:MET:HE1	3:EY:1880:LEU:HD11	2.01	0.42
3:FY:1720:LYS:HA	3:FY:1734:LYS:HE2	2.01	0.42
3:HY:1732:LEU:HA	3:HY:1732:LEU:HD23	1.84	0.42
3:NY:1708:ALA:HB3	3:NY:1869:PHE:HB3	2.01	0.42
2:AX:436:GLN:HB2	3:AY:1734:LYS:HG2	2.01	0.42
3:EY:1720:LYS:HA	3:EY:1734:LYS:HE2	2.01	0.42
2:FX:503:ILE:HA	3:GY:1729:MET:HA	2.01	0.42
3:FY:1708:ALA:HB3	3:FY:1869:PHE:HB3	2.01	0.42
3:GY:1720:LYS:HA	3:GY:1734:LYS:HE2	2.01	0.42
2:LX:507:GLY:HA2	1:MT:168:LEU:HD11	2.00	0.42
3:DY:1720:LYS:HA	3:DY:1734:LYS:HE2	2.00	0.42
2:EX:392:LEU:HD22	3:FY:1728:THR:HB	1.99	0.42
3:GY:1903:GLU:HA	3:GY:1906:LYS:HG3	2.02	0.42
3:HY:1720:LYS:HA	3:HY:1734:LYS:HE2	2.00	0.42
2:JX:392:LEU:HD22	3:KY:1728:THR:HB	2.01	0.42
2:LX:394:ARG:HE	2:LX:394:ARG:HB3	1.68	0.42
2:MX:497:LEU:O	2:NX:432:ASN:ND2	2.40	0.42
2:NX:440:PHE:CZ	3:NY:1873:GLU:HB3	2.55	0.42
3:NY:1786:VAL:HG22	3:NY:1871:LYS:HE2	2.01	0.42
3:IY:1903:GLU:HA	3:IY:1906:LYS:HG3	2.02	0.42
3:KY:1786:VAL:HG22	3:KY:1871:LYS:HE2	2.01	0.42
3:KY:1903:GLU:HA	3:KY:1906:LYS:HG3	2.02	0.42
3:MY:1786:VAL:HG22	3:MY:1871:LYS:HE2	2.01	0.42
2:BX:503:ILE:HG13	3:CY:1729:MET:HB3	2.02	0.42
2:DX:436:GLN:HB2	3:DY:1734:LYS:HG2	2.01	0.42
2:DX:507:GLY:HA2	1:ET:168:LEU:HD11	2.02	0.42
2:EX:436:GLN:HB2	3:EY:1734:LYS:HG2	2.02	0.42
3:EY:1903:GLU:HA	3:EY:1906:LYS:HG3	2.02	0.42
2:FX:503:ILE:HG13	3:GY:1729:MET:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:JY:1689:THR:O	3:JY:1724:ASN:ND2	2.34	0.42
2:LX:450:MET:HE1	3:MY:1880:LEU:HD11	2.01	0.42
3:MY:1720:LYS:HA	3:MY:1734:LYS:HE2	2.00	0.42
3:NY:1720:LYS:HA	3:NY:1734:LYS:HE2	2.00	0.42
2:CX:440:PHE:CZ	3:CY:1873:GLU:HB3	2.54	0.42
2:EX:503:ILE:HG13	3:FY:1729:MET:HB3	2.02	0.42
2:GX:440:PHE:CZ	3:GY:1873:GLU:HB3	2.55	0.42
3:IY:1720:LYS:HA	3:IY:1734:LYS:HE2	2.00	0.42
3:LY:1786:VAL:HG22	3:LY:1871:LYS:HE2	2.01	0.42
2:AX:455:ILE:HB	3:AY:1765:PRO:HB3	2.01	0.42
3:AY:1880:LEU:HD11	2:NX:450:MET:HE1	2.01	0.42
2:EX:450:MET:HE1	3:FY:1880:LEU:HD11	2.01	0.42
1:IT:200:LYS:HA	1:IT:200:LYS:HD3	1.76	0.42
2:IX:479:ILE:HG22	3:IY:1874:GLY:HA3	2.02	0.42
3:AY:1720:LYS:HA	3:AY:1734:LYS:HE2	2.01	0.42
3:CY:1720:LYS:HA	3:CY:1734:LYS:HE2	2.01	0.42
2:DX:481:ASP:HB3	3:DY:1875:ASP:HA	2.01	0.42
3:FY:1906:LYS:HA	3:FY:1909:THR:HG22	2.01	0.42
2:GX:436:GLN:HB2	3:GY:1734:LYS:HG2	2.02	0.42
2:GX:450:MET:HE1	3:HY:1880:LEU:HD11	2.02	0.42
1:JT:56:LEU:HD12	1:JT:59:THR:HB	2.02	0.42
2:KX:459:MET:HE2	2:KX:459:MET:HB3	1.88	0.42
3:KY:1689:THR:O	3:KY:1724:ASN:ND2	2.34	0.42
1:LT:199:TYR:HB3	2:LX:379:GLN:OE1	2.20	0.42
3:LY:1708:ALA:HB3	3:LY:1869:PHE:HB3	2.01	0.42
2:MX:503:ILE:HG13	3:NY:1729:MET:HB3	2.02	0.42
2:AX:503:ILE:HA	3:BY:1729:MET:HA	2.01	0.42
3:BY:1903:GLU:HA	3:BY:1906:LYS:HG3	2.01	0.42
3:DY:1903:GLU:HA	3:DY:1906:LYS:HG3	2.02	0.42
3:HY:1903:GLU:HA	3:HY:1906:LYS:HG3	2.02	0.42
1:KT:75:LEU:HD23	1:KT:75:LEU:HA	1.86	0.42
2:LX:503:ILE:HG13	3:MY:1729:MET:HB3	2.02	0.42
3:LY:1720:LYS:HA	3:LY:1734:LYS:HE2	2.01	0.42
3:MY:1903:GLU:HA	3:MY:1906:LYS:HG3	2.02	0.42
3:AY:1786:VAL:HG22	3:AY:1871:LYS:HE2	2.01	0.41
3:AY:1859:LEU:O	3:AY:1863:MET:HB3	2.20	0.41
3:BY:1786:VAL:HG22	3:BY:1871:LYS:HE2	2.01	0.41
1:CT:200:LYS:HA	1:CT:200:LYS:HD3	1.76	0.41
2:CX:392:LEU:HD22	3:DY:1728:THR:HB	2.01	0.41
2:CX:479:ILE:HG22	3:CY:1874:GLY:HA3	2.02	0.41
2:GX:481:ASP:OD1	2:GX:481:ASP:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GX:503:ILE:HG13	3:HY:1729:MET:HB3	2.02	0.41
3:HY:1708:ALA:HB3	3:HY:1869:PHE:HB3	2.01	0.41
3:HY:1859:LEU:O	3:HY:1863:MET:HB3	2.20	0.41
3:IY:1859:LEU:O	3:IY:1863:MET:HB3	2.20	0.41
3:JY:1786:VAL:HG22	3:JY:1871:LYS:HE2	2.01	0.41
3:JY:1903:GLU:HA	3:JY:1906:LYS:HG3	2.02	0.41
2:KX:392:LEU:HD22	3:LY:1728:THR:HB	2.02	0.41
2:LX:440:PHE:CZ	3:LY:1873:GLU:HB3	2.55	0.41
2:LX:480:LYS:NZ	3:LY:1699:GLU:OE2	2.48	0.41
3:MY:1898:LYS:HA	3:MY:1901:VAL:HG12	2.02	0.41
3:NY:1859:LEU:O	3:NY:1863:MET:HB3	2.20	0.41
3:AY:1732:LEU:HA	3:AY:1732:LEU:HD23	1.84	0.41
2:BX:394:ARG:HE	2:BX:394:ARG:HB3	1.68	0.41
3:CY:1708:ALA:HB3	3:CY:1869:PHE:HB3	2.01	0.41
2:FX:371:GLU:HA	2:FX:374:LYS:HG2	2.02	0.41
3:FY:1903:GLU:HA	3:FY:1906:LYS:HG3	2.02	0.41
3:IY:1890:VAL:HG12	3:JY:1683:ILE:HG13	2.02	0.41
3:IY:1906:LYS:HA	3:IY:1909:THR:HG22	2.01	0.41
3:JY:1720:LYS:HA	3:JY:1734:LYS:HE2	2.01	0.41
1:KT:56:LEU:HD12	1:KT:59:THR:HB	2.02	0.41
1:BT:51:PRO:HD3	2:BX:495:ASN:HB2	2.02	0.41
3:BY:1720:LYS:HA	3:BY:1734:LYS:HE2	2.00	0.41
2:CX:435:LEU:HD11	3:CY:1720:LYS:HE3	2.02	0.41
3:EY:1859:LEU:O	3:EY:1863:MET:HB3	2.20	0.41
2:FX:501:TYR:OH	1:GT:168:LEU:HB2	2.20	0.41
1:GT:56:LEU:HD12	1:GT:59:THR:HB	2.02	0.41
1:HT:56:LEU:HD12	1:HT:59:THR:HB	2.02	0.41
2:HX:371:GLU:HA	2:HX:374:LYS:HG2	2.03	0.41
1:IT:56:LEU:HD12	1:IT:59:THR:HB	2.02	0.41
3:IY:1689:THR:O	3:IY:1724:ASN:ND2	2.34	0.41
2:MX:417:SER:N	2:MX:429:GLY:O	2.44	0.41
3:NY:1797:ARG:HG3	3:NY:1865:ILE:HB	2.03	0.41
1:BT:167:ASN:HB3	1:BT:173:VAL:HG11	2.03	0.41
3:BY:1859:LEU:O	3:BY:1863:MET:HB3	2.20	0.41
3:BY:1898:LYS:HA	3:BY:1901:VAL:HG12	2.02	0.41
2:EX:503:ILE:HA	3:FY:1729:MET:HA	2.02	0.41
1:FT:213:ARG:HH12	2:FX:364:ASN:HB3	1.86	0.41
3:FY:1859:LEU:O	3:FY:1863:MET:HB3	2.20	0.41
3:IY:1786:VAL:HG22	3:IY:1871:LYS:HE2	2.01	0.41
3:JY:1708:ALA:HB3	3:JY:1869:PHE:HB3	2.01	0.41
3:JY:1859:LEU:O	3:JY:1863:MET:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:KY:1797:ARG:HG3	3:KY:1865:ILE:HB	2.03	0.41
1:MT:51:PRO:HD3	2:MX:495:ASN:HB2	2.03	0.41
2:MX:507:GLY:HA2	1:NT:168:LEU:HD11	2.02	0.41
1:CT:167:ASN:HB3	1:CT:173:VAL:HG11	2.03	0.41
1:DT:213:ARG:HH12	2:DX:364:ASN:HB3	1.85	0.41
1:FT:56:LEU:HD12	1:FT:59:THR:HB	2.02	0.41
2:FX:450:MET:HE1	3:GY:1880:LEU:HD11	2.03	0.41
2:GX:394:ARG:HE	2:GX:394:ARG:HB3	1.68	0.41
3:GY:1906:LYS:HA	3:GY:1909:THR:HG22	2.01	0.41
1:JT:298:LEU:HD13	2:JX:373:GLN:HE22	1.86	0.41
3:JY:1797:ARG:HG3	3:JY:1865:ILE:HB	2.03	0.41
3:KY:1720:LYS:HA	3:KY:1734:LYS:HE2	2.01	0.41
3:MY:1797:ARG:HG3	3:MY:1865:ILE:HB	2.03	0.41
1:AT:167:ASN:HB3	1:AT:173:VAL:HG11	2.03	0.41
3:CY:1797:ARG:HG3	3:CY:1865:ILE:HB	2.03	0.41
2:HX:417:SER:N	2:HX:429:GLY:O	2.45	0.41
3:KY:1898:LYS:HA	3:KY:1901:VAL:HG12	2.03	0.41
1:LT:56:LEU:HD12	1:LT:59:THR:HB	2.02	0.41
2:LX:503:ILE:HA	3:MY:1729:MET:HA	2.02	0.41
3:LY:1890:VAL:HG12	3:MY:1683:ILE:HG13	2.03	0.41
3:NY:1700:ILE:HG13	3:NY:1879:ILE:HG12	2.02	0.41
3:NY:1898:LYS:HA	3:NY:1901:VAL:HG12	2.02	0.41
3:AY:1797:ARG:HG3	3:AY:1865:ILE:HB	2.03	0.41
2:BX:503:ILE:HA	3:CY:1729:MET:HA	2.02	0.41
3:BY:1700:ILE:HG13	3:BY:1879:ILE:HG12	2.02	0.41
3:BY:1797:ARG:HG3	3:BY:1865:ILE:HB	2.03	0.41
3:CY:1732:LEU:HD23	3:CY:1732:LEU:HA	1.84	0.41
1:DT:167:ASN:HB3	1:DT:173:VAL:HG11	2.03	0.41
2:DX:371:GLU:HA	2:DX:374:LYS:HG2	2.02	0.41
2:EX:440:PHE:CZ	3:EY:1873:GLU:HB3	2.56	0.41
2:FX:440:PHE:CZ	3:FY:1873:GLU:HB3	2.55	0.41
2:GX:503:ILE:HA	3:HY:1729:MET:HA	2.02	0.41
3:GY:1786:VAL:HG22	3:GY:1871:LYS:HE2	2.01	0.41
3:HY:1797:ARG:HG3	3:HY:1865:ILE:HB	2.03	0.41
1:IT:51:PRO:HD3	2:IX:495:ASN:HB2	2.03	0.41
2:JX:371:GLU:HA	2:JX:374:LYS:HG2	2.02	0.41
3:JY:1700:ILE:HG13	3:JY:1879:ILE:HG12	2.02	0.41
3:LY:1797:ARG:HG3	3:LY:1865:ILE:HB	2.03	0.41
2:MX:440:PHE:CZ	3:MY:1873:GLU:HB3	2.55	0.41
3:MY:1859:LEU:O	3:MY:1863:MET:HB3	2.20	0.41
2:AX:450:MET:HE1	3:BY:1880:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AY:1700:ILE:HG13	3:AY:1879:ILE:HG12	2.02	0.41
3:AY:1898:LYS:HA	3:AY:1901:VAL:HG12	2.02	0.41
2:BX:435:LEU:HD11	3:BY:1720:LYS:HE3	2.02	0.41
1:CT:75:LEU:HD23	1:CT:75:LEU:HA	1.86	0.41
1:CT:213:ARG:HH12	2:CX:364:ASN:HB3	1.85	0.41
3:CY:1786:VAL:HG22	3:CY:1871:LYS:HE2	2.01	0.41
3:DY:1859:LEU:O	3:DY:1863:MET:HB3	2.20	0.41
3:DY:1906:LYS:HA	3:DY:1909:THR:HG22	2.01	0.41
2:EX:455:ILE:HB	3:EY:1765:PRO:HB3	2.03	0.41
3:EY:1890:VAL:HG12	3:FY:1683:ILE:HG13	2.02	0.41
2:FX:436:GLN:HB2	3:FY:1734:LYS:HG2	2.02	0.41
2:FX:459:MET:HE2	2:FX:459:MET:HB3	1.88	0.41
3:FY:1786:VAL:HG22	3:FY:1871:LYS:HE2	2.01	0.41
3:IY:1797:ARG:HG3	3:IY:1865:ILE:HB	2.03	0.41
3:KY:1700:ILE:HG13	3:KY:1879:ILE:HG12	2.02	0.41
3:LY:1700:ILE:HG13	3:LY:1879:ILE:HG12	2.02	0.41
2:MX:459:MET:HE2	2:MX:459:MET:HB3	1.88	0.41
1:NT:167:ASN:HB3	1:NT:173:VAL:HG11	2.03	0.41
2:NX:394:ARG:HE	2:NX:394:ARG:HB3	1.68	0.41
1:BT:75:LEU:HA	1:BT:75:LEU:HD23	1.86	0.41
2:BX:440:PHE:CZ	3:BY:1873:GLU:HB3	2.56	0.41
3:CY:1694:GLN:N	3:CY:1884:ASP:OD2	2.54	0.41
3:CY:1700:ILE:HG13	3:CY:1879:ILE:HG12	2.02	0.41
3:CY:1903:GLU:HA	3:CY:1906:LYS:HG3	2.02	0.41
1:DT:298:LEU:HD12	1:DT:298:LEU:HA	1.88	0.41
3:DY:1694:GLN:N	3:DY:1884:ASP:OD2	2.54	0.41
1:ET:48:SER:OG	1:FT:170:GLY:O	2.31	0.41
1:ET:167:ASN:HB3	1:ET:173:VAL:HG11	2.03	0.41
2:EX:480:LYS:NZ	3:EY:1699:GLU:OE2	2.49	0.41
3:EY:1786:VAL:HG22	3:EY:1871:LYS:HE2	2.01	0.41
1:FT:38:PRO:HA	2:GX:404:TYR:HA	2.03	0.41
3:FY:1689:THR:O	3:FY:1724:ASN:ND2	2.34	0.41
1:GT:199:TYR:HB3	2:GX:379:GLN:OE1	2.21	0.41
2:GX:455:ILE:HB	3:GY:1765:PRO:HB3	2.02	0.41
2:GX:481:ASP:HB3	3:GY:1875:ASP:HA	2.02	0.41
3:GY:1694:GLN:N	3:GY:1884:ASP:OD2	2.54	0.41
1:HT:298:LEU:HA	1:HT:298:LEU:HD12	1.88	0.41
2:HX:436:GLN:HB2	3:HY:1734:LYS:HG2	2.02	0.41
2:HX:440:PHE:CZ	3:HY:1873:GLU:HB3	2.56	0.41
2:HX:503:ILE:HA	3:IY:1729:MET:HA	2.02	0.41
3:HY:1786:VAL:HG22	3:HY:1871:LYS:HE2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:IY:1700:ILE:HG13	3:IY:1879:ILE:HG12	2.02	0.41
1:JT:200:LYS:HA	1:JT:200:LYS:HD3	1.76	0.41
2:JX:440:PHE:CZ	3:JY:1873:GLU:HB3	2.56	0.41
2:JX:497:LEU:O	2:KX:432:ASN:ND2	2.40	0.41
3:JY:1898:LYS:HA	3:JY:1901:VAL:HG12	2.02	0.41
2:KX:436:GLN:HB2	3:KY:1734:LYS:HG2	2.02	0.41
2:KX:455:ILE:HB	3:KY:1765:PRO:HB3	2.01	0.41
3:KY:1859:LEU:O	3:KY:1863:MET:HB3	2.20	0.41
1:MT:56:LEU:HD12	1:MT:59:THR:HB	2.02	0.41
1:MT:167:ASN:HB3	1:MT:173:VAL:HG11	2.03	0.41
1:MT:199:TYR:HB3	2:MX:379:GLN:OE1	2.21	0.41
2:MX:450:MET:HE1	3:NY:1880:LEU:HD11	2.03	0.41
3:MY:1700:ILE:HG13	3:MY:1879:ILE:HG12	2.02	0.41
2:NX:436:GLN:HB2	3:NY:1734:LYS:HG2	2.02	0.41
3:NY:1903:GLU:HA	3:NY:1906:LYS:HG3	2.02	0.41
2:AX:440:PHE:CZ	3:AY:1873:GLU:HB3	2.56	0.41
1:BT:56:LEU:HD12	1:BT:59:THR:HB	2.02	0.41
3:BY:1890:VAL:HG12	3:CY:1683:ILE:HG13	2.02	0.41
2:CX:480:LYS:NZ	3:CY:1699:GLU:OE2	2.45	0.41
2:CX:507:GLY:HA2	1:DT:168:LEU:HD11	2.03	0.41
3:DY:1797:ARG:HG3	3:DY:1865:ILE:HB	2.03	0.41
1:ET:56:LEU:HD12	1:ET:59:THR:HB	2.02	0.41
3:FY:1694:GLN:N	3:FY:1884:ASP:OD2	2.54	0.41
3:FY:1797:ARG:HG3	3:FY:1865:ILE:HB	2.03	0.41
2:HX:365:LYS:HE2	2:HX:365:LYS:HB2	1.98	0.41
1:LT:75:LEU:HD23	1:LT:75:LEU:HA	1.86	0.41
3:LY:1689:THR:O	3:LY:1724:ASN:ND2	2.34	0.41
2:AX:503:ILE:HG13	3:BY:1729:MET:HB3	2.03	0.40
1:CT:56:LEU:HD12	1:CT:59:THR:HB	2.02	0.40
1:DT:75:LEU:HD23	1:DT:75:LEU:HA	1.86	0.40
3:DY:1898:LYS:HA	3:DY:1901:VAL:HG12	2.03	0.40
2:EX:365:LYS:HE2	2:EX:365:LYS:HB2	1.98	0.40
2:HX:455:ILE:HB	3:HY:1765:PRO:HB3	2.02	0.40
1:LT:167:ASN:HB3	1:LT:173:VAL:HG11	2.03	0.40
2:MX:436:GLN:HB2	3:MY:1734:LYS:HG2	2.02	0.40
2:NX:394:ARG:HD2	2:NX:394:ARG:HA	1.93	0.40
2:NX:417:SER:N	2:NX:429:GLY:O	2.45	0.40
1:AT:168:LEU:HD11	2:NX:507:GLY:HA2	2.03	0.40
3:CY:1859:LEU:O	3:CY:1863:MET:HB3	2.20	0.40
3:EY:1797:ARG:HG3	3:EY:1865:ILE:HB	2.03	0.40
3:GY:1859:LEU:O	3:GY:1863:MET:HB3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:HY:1700:ILE:HG13	3:HY:1879:ILE:HG12	2.02	0.40
1:KT:167:ASN:HB3	1:KT:173:VAL:HG11	2.03	0.40
1:AT:56:LEU:HD12	1:AT:59:THR:HB	2.02	0.40
2:AX:417:SER:N	2:AX:429:GLY:O	2.45	0.40
1:DT:56:LEU:HD12	1:DT:59:THR:HB	2.02	0.40
3:DY:1786:VAL:HG22	3:DY:1871:LYS:HE2	2.01	0.40
3:FY:1879:ILE:HD13	3:FY:1879:ILE:HA	1.86	0.40
2:GX:365:LYS:HE2	2:GX:365:LYS:HB2	1.98	0.40
3:GY:1797:ARG:HG3	3:GY:1865:ILE:HB	2.03	0.40
3:IY:1694:GLN:N	3:IY:1884:ASP:OD2	2.54	0.40
3:KY:1890:VAL:HG12	3:LY:1683:ILE:HG13	2.03	0.40
2:LX:436:GLN:HB2	3:LY:1734:LYS:HG2	2.02	0.40
2:AX:481:ASP:HB3	3:AY:1875:ASP:HA	2.02	0.40
3:AY:1694:GLN:N	3:AY:1884:ASP:OD2	2.54	0.40
2:DX:440:PHE:CZ	3:DY:1873:GLU:HB3	2.57	0.40
2:EX:394:ARG:HE	2:EX:394:ARG:HB3	1.68	0.40
3:EY:1879:ILE:HD13	3:EY:1879:ILE:HA	1.86	0.40
1:FT:167:ASN:HB3	1:FT:173:VAL:HG11	2.03	0.40
1:FT:202:LEU:HD13	2:FX:375:ILE:HD11	2.04	0.40
2:GX:371:GLU:HA	2:GX:374:LYS:HG2	2.03	0.40
2:HX:481:ASP:HB3	3:HY:1875:ASP:HA	2.02	0.40
2:LX:459:MET:HE2	2:LX:459:MET:HB3	1.88	0.40
3:LY:1898:LYS:HA	3:LY:1901:VAL:HG12	2.02	0.40
3:AY:1903:GLU:HA	3:AY:1906:LYS:HG3	2.02	0.40
3:DY:1700:ILE:HG13	3:DY:1879:ILE:HG12	2.02	0.40
3:FY:1898:LYS:HA	3:FY:1901:VAL:HG12	2.02	0.40
3:GY:1879:ILE:HD13	3:GY:1879:ILE:HA	1.86	0.40
1:HT:51:PRO:HD3	2:HX:495:ASN:HB2	2.04	0.40
2:HX:450:MET:HE1	3:IY:1880:LEU:HD11	2.03	0.40
3:HY:1898:LYS:HA	3:HY:1901:VAL:HG12	2.03	0.40
3:IY:1898:LYS:HA	3:IY:1901:VAL:HG12	2.03	0.40
2:LX:394:ARG:HD2	2:LX:394:ARG:HA	1.93	0.40
2:NX:371:GLU:HA	2:NX:374:LYS:HG2	2.02	0.40

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 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	AT	171/278 (62%)	160 (94%)	11 (6%)	0	100	100
1	BT	171/278 (62%)	160 (94%)	11 (6%)	0	100	100
1	CT	171/278 (62%)	160 (94%)	11 (6%)	0	100	100
1	DT	171/278 (62%)	160 (94%)	11 (6%)	0	100	100
1	ET	171/278 (62%)	160 (94%)	11 (6%)	0	100	100
1	FT	171/278 (62%)	160 (94%)	11 (6%)	0	100	100
1	GT	171/278 (62%)	160 (94%)	11 (6%)	0	100	100
1	HT	171/278 (62%)	160 (94%)	11 (6%)	0	100	100
1	IT	171/278 (62%)	160 (94%)	11 (6%)	0	100	100
1	JT	171/278 (62%)	160 (94%)	11 (6%)	0	100	100
1	KT	171/278 (62%)	160 (94%)	11 (6%)	0	100	100
1	LT	171/278 (62%)	160 (94%)	11 (6%)	0	100	100
1	MT	171/278 (62%)	160 (94%)	11 (6%)	0	100	100
1	NT	171/278 (62%)	160 (94%)	11 (6%)	0	100	100
2	AX	153/522 (29%)	145 (95%)	8 (5%)	0	100	100
2	BX	153/522 (29%)	145 (95%)	8 (5%)	0	100	100
2	CX	153/522 (29%)	145 (95%)	8 (5%)	0	100	100
2	DX	153/522 (29%)	145 (95%)	8 (5%)	0	100	100
2	EX	153/522 (29%)	145 (95%)	8 (5%)	0	100	100
2	FX	153/522 (29%)	145 (95%)	8 (5%)	0	100	100
2	GX	153/522 (29%)	145 (95%)	8 (5%)	0	100	100
2	HX	153/522 (29%)	145 (95%)	8 (5%)	0	100	100
2	IX	153/522 (29%)	145 (95%)	8 (5%)	0	100	100
2	JX	153/522 (29%)	145 (95%)	8 (5%)	0	100	100
2	KX	153/522 (29%)	145 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	LX	153/522 (29%)	145 (95%)	8 (5%)	0	100	100
2	MX	153/522 (29%)	145 (95%)	8 (5%)	0	100	100
2	NX	153/522 (29%)	145 (95%)	8 (5%)	0	100	100
3	AY	205/1927 (11%)	195 (95%)	10 (5%)	0	100	100
3	BY	205/1927 (11%)	195 (95%)	10 (5%)	0	100	100
3	CY	205/1927 (11%)	195 (95%)	10 (5%)	0	100	100
3	DY	205/1927 (11%)	195 (95%)	10 (5%)	0	100	100
3	EY	205/1927 (11%)	195 (95%)	10 (5%)	0	100	100
3	FY	205/1927 (11%)	195 (95%)	10 (5%)	0	100	100
3	GY	205/1927 (11%)	195 (95%)	10 (5%)	0	100	100
3	HY	205/1927 (11%)	195 (95%)	10 (5%)	0	100	100
3	IY	205/1927 (11%)	195 (95%)	10 (5%)	0	100	100
3	JY	205/1927 (11%)	195 (95%)	10 (5%)	0	100	100
3	KY	205/1927 (11%)	195 (95%)	10 (5%)	0	100	100
3	LY	205/1927 (11%)	195 (95%)	10 (5%)	0	100	100
3	MY	205/1927 (11%)	195 (95%)	10 (5%)	0	100	100
3	NY	205/1927 (11%)	195 (95%)	10 (5%)	0	100	100
All	All	7406/38178 (19%)	7000 (94%)	406 (6%)	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	AT	169/254 (66%)	169 (100%)	0	100	100
1	BT	169/254 (66%)	169 (100%)	0	100	100
1	CT	169/254 (66%)	169 (100%)	0	100	100
1	DT	169/254 (66%)	169 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	ET	169/254 (66%)	169 (100%)	0	100	100
1	FT	169/254 (66%)	169 (100%)	0	100	100
1	GT	169/254 (66%)	169 (100%)	0	100	100
1	HT	169/254 (66%)	169 (100%)	0	100	100
1	IT	169/254 (66%)	169 (100%)	0	100	100
1	JT	169/254 (66%)	169 (100%)	0	100	100
1	KT	169/254 (66%)	169 (100%)	0	100	100
1	LT	169/254 (66%)	169 (100%)	0	100	100
1	MT	169/254 (66%)	169 (100%)	0	100	100
1	NT	169/254 (66%)	169 (100%)	0	100	100
2	AX	139/470 (30%)	139 (100%)	0	100	100
2	BX	139/470 (30%)	139 (100%)	0	100	100
2	CX	139/470 (30%)	139 (100%)	0	100	100
2	DX	139/470 (30%)	139 (100%)	0	100	100
2	EX	139/470 (30%)	139 (100%)	0	100	100
2	FX	139/470 (30%)	139 (100%)	0	100	100
2	GX	139/470 (30%)	139 (100%)	0	100	100
2	HX	139/470 (30%)	139 (100%)	0	100	100
2	IX	139/470 (30%)	139 (100%)	0	100	100
2	JX	139/470 (30%)	139 (100%)	0	100	100
2	KX	139/470 (30%)	139 (100%)	0	100	100
2	LX	139/470 (30%)	139 (100%)	0	100	100
2	MX	139/470 (30%)	139 (100%)	0	100	100
2	NX	139/470 (30%)	139 (100%)	0	100	100
3	AY	177/1724 (10%)	177 (100%)	0	100	100
3	BY	177/1724 (10%)	177 (100%)	0	100	100
3	CY	177/1724 (10%)	177 (100%)	0	100	100
3	DY	177/1724 (10%)	177 (100%)	0	100	100
3	EY	177/1724 (10%)	177 (100%)	0	100	100
3	FY	177/1724 (10%)	177 (100%)	0	100	100
3	GY	177/1724 (10%)	177 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	HY	177/1724 (10%)	177 (100%)	0	100	100
3	IY	177/1724 (10%)	177 (100%)	0	100	100
3	JY	177/1724 (10%)	177 (100%)	0	100	100
3	KY	177/1724 (10%)	177 (100%)	0	100	100
3	LY	177/1724 (10%)	177 (100%)	0	100	100
3	MY	177/1724 (10%)	177 (100%)	0	100	100
3	NY	177/1724 (10%)	177 (100%)	0	100	100
All	All	6790/34272 (20%)	6790 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	AT	77	ASN
1	AT	196	ASN
2	AX	373	GLN
3	AY	1741	ASN
3	AY	1864	ASN
3	AY	1907	GLN
1	BT	77	ASN
1	BT	169	HIS
2	BX	373	GLN
2	BX	389	HIS
3	BY	1741	ASN
3	BY	1864	ASN
3	BY	1907	GLN
1	CT	77	ASN
1	CT	196	ASN
2	CX	373	GLN
3	CY	1741	ASN
3	CY	1864	ASN
3	CY	1907	GLN
1	DT	77	ASN
1	DT	196	ASN
2	DX	373	GLN
2	DX	389	HIS
3	DY	1741	ASN
3	DY	1864	ASN

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Mol	Chain	Res	Type
3	DY	1907	GLN
1	ET	77	ASN
1	ET	196	ASN
2	EX	373	GLN
2	EX	389	HIS
3	EY	1741	ASN
3	EY	1864	ASN
3	EY	1907	GLN
1	FT	77	ASN
1	FT	169	HIS
2	FX	373	GLN
2	FX	389	HIS
3	FY	1741	ASN
3	FY	1864	ASN
3	FY	1907	GLN
1	GT	77	ASN
2	GX	373	GLN
2	GX	389	HIS
3	GY	1741	ASN
3	GY	1864	ASN
3	GY	1907	GLN
1	HT	77	ASN
1	HT	169	HIS
2	HX	373	GLN
2	HX	389	HIS
3	HY	1741	ASN
3	HY	1864	ASN
3	HY	1907	GLN
1	IT	77	ASN
2	IX	373	GLN
3	IY	1741	ASN
3	IY	1864	ASN
3	IY	1907	GLN
1	JT	77	ASN
1	JT	290	GLN
2	JX	373	GLN
3	JY	1741	ASN
3	JY	1864	ASN
3	JY	1907	GLN
1	KT	53	ASN
1	KT	77	ASN
2	KX	373	GLN

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Mol	Chain	Res	Type
2	KX	389	HIS
3	KY	1741	ASN
3	KY	1864	ASN
3	KY	1907	GLN
1	LT	77	ASN
2	LX	373	GLN
2	LX	389	HIS
3	LY	1741	ASN
3	LY	1864	ASN
3	LY	1907	GLN
1	MT	77	ASN
2	MX	373	GLN
3	MY	1741	ASN
3	MY	1864	ASN
3	MY	1907	GLN
1	NT	77	ASN
1	NT	169	HIS
2	NX	373	GLN
2	NX	389	HIS
3	NY	1726	ASN
3	NY	1741	ASN
3	NY	1864	ASN
3	NY	1907	GLN

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

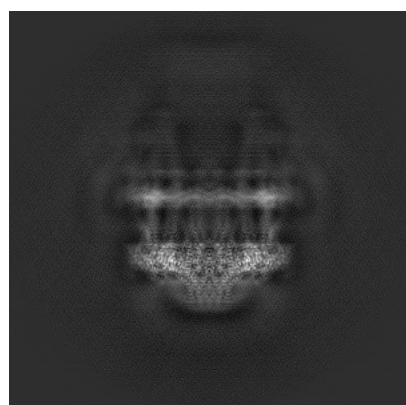
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22076. These allow visual inspection of the internal detail of the map and identification of artifacts.

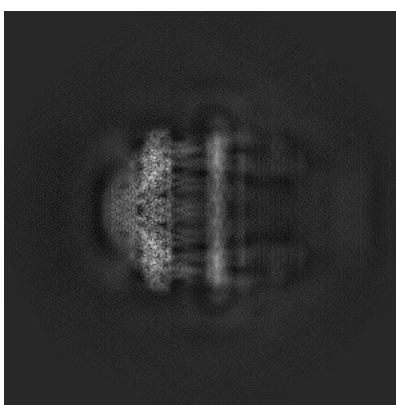
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

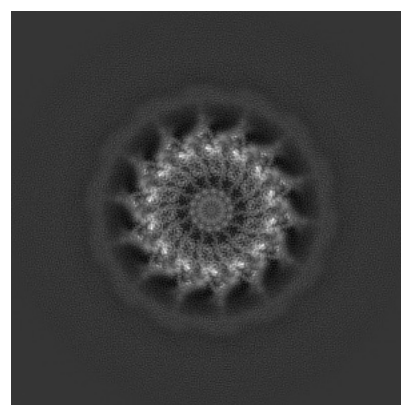
6.1.1 Primary map



X



Y



Z

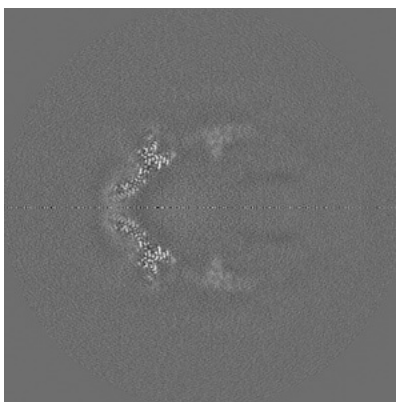
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

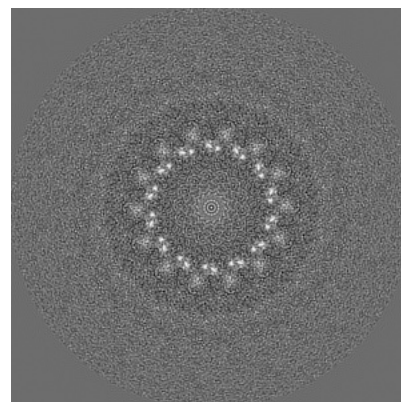
6.2.1 Primary map



X Index: 255



Y Index: 255

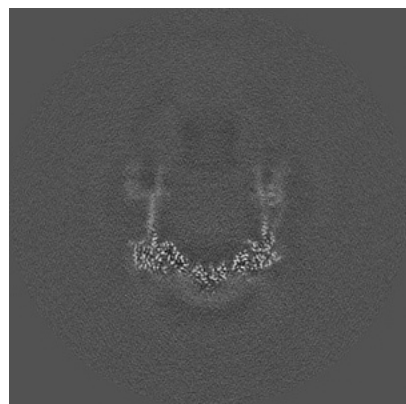


Z Index: 255

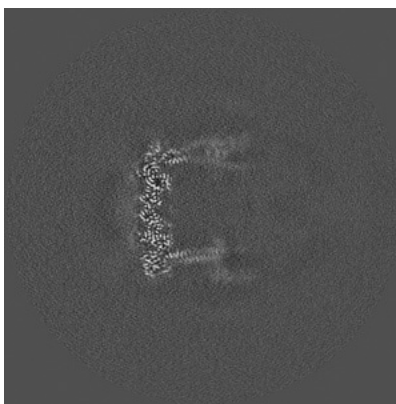
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

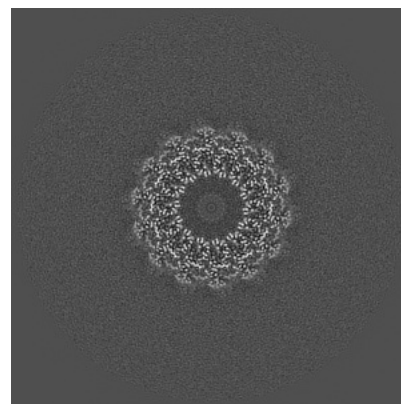
6.3.1 Primary map



X Index: 224



Y Index: 303

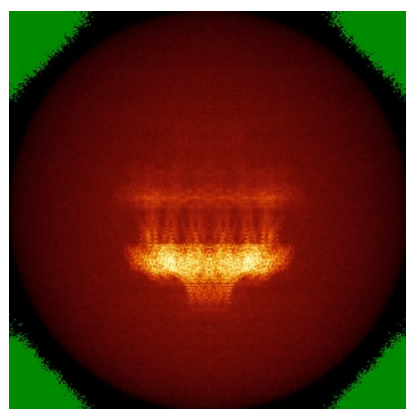


Z Index: 188

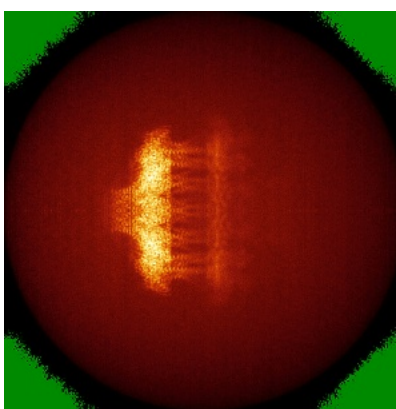
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

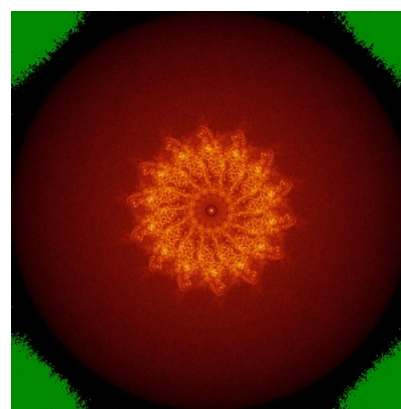
6.4.1 Primary map



X



Y

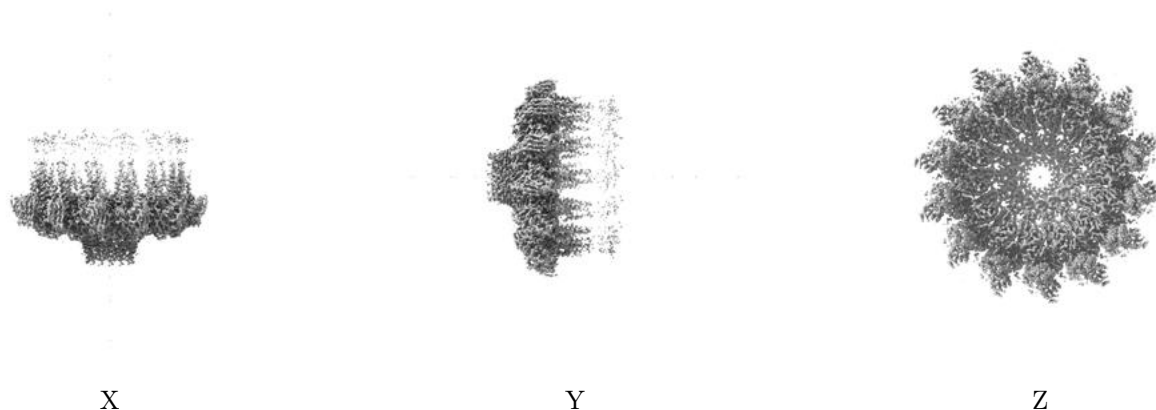


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

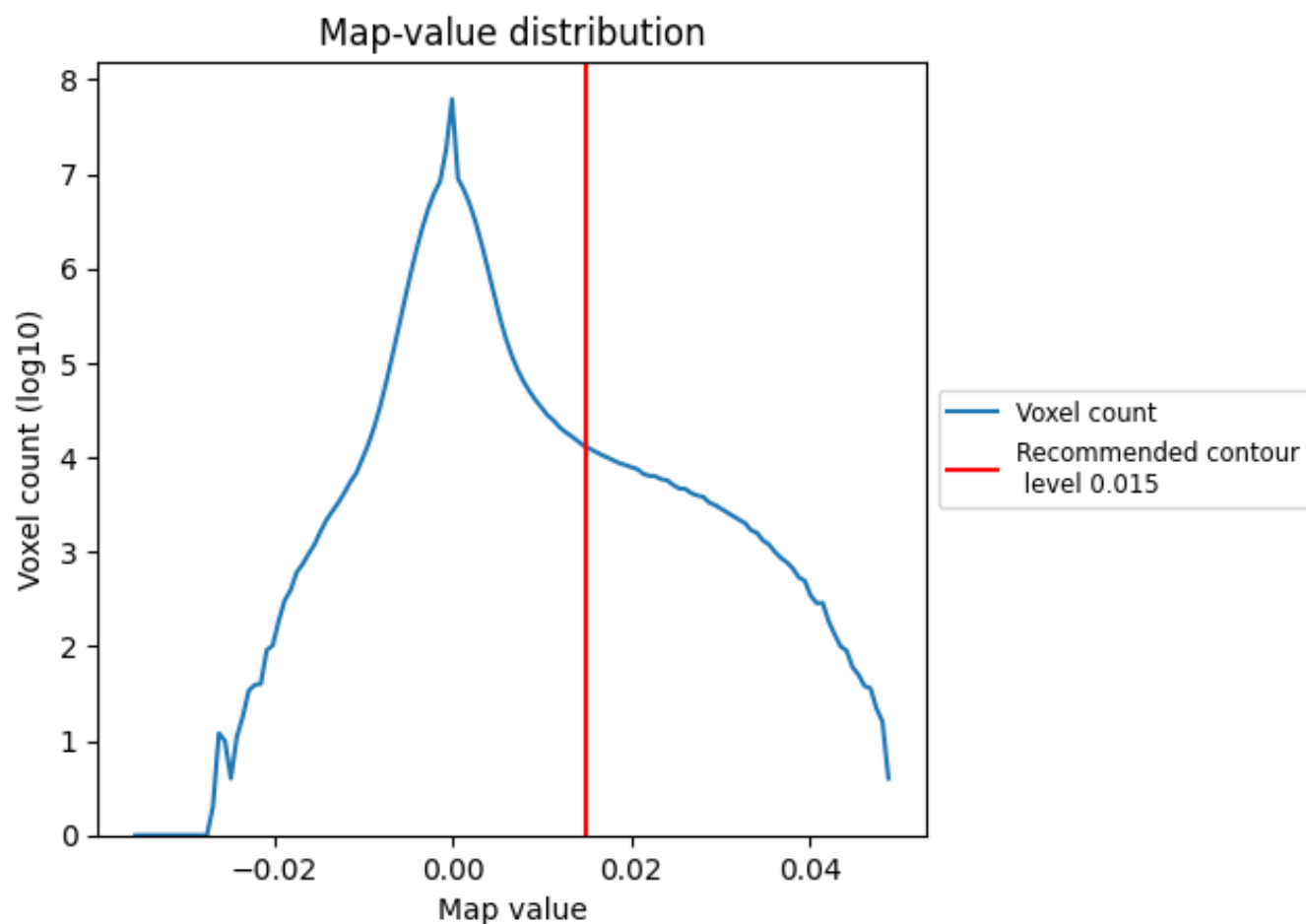
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

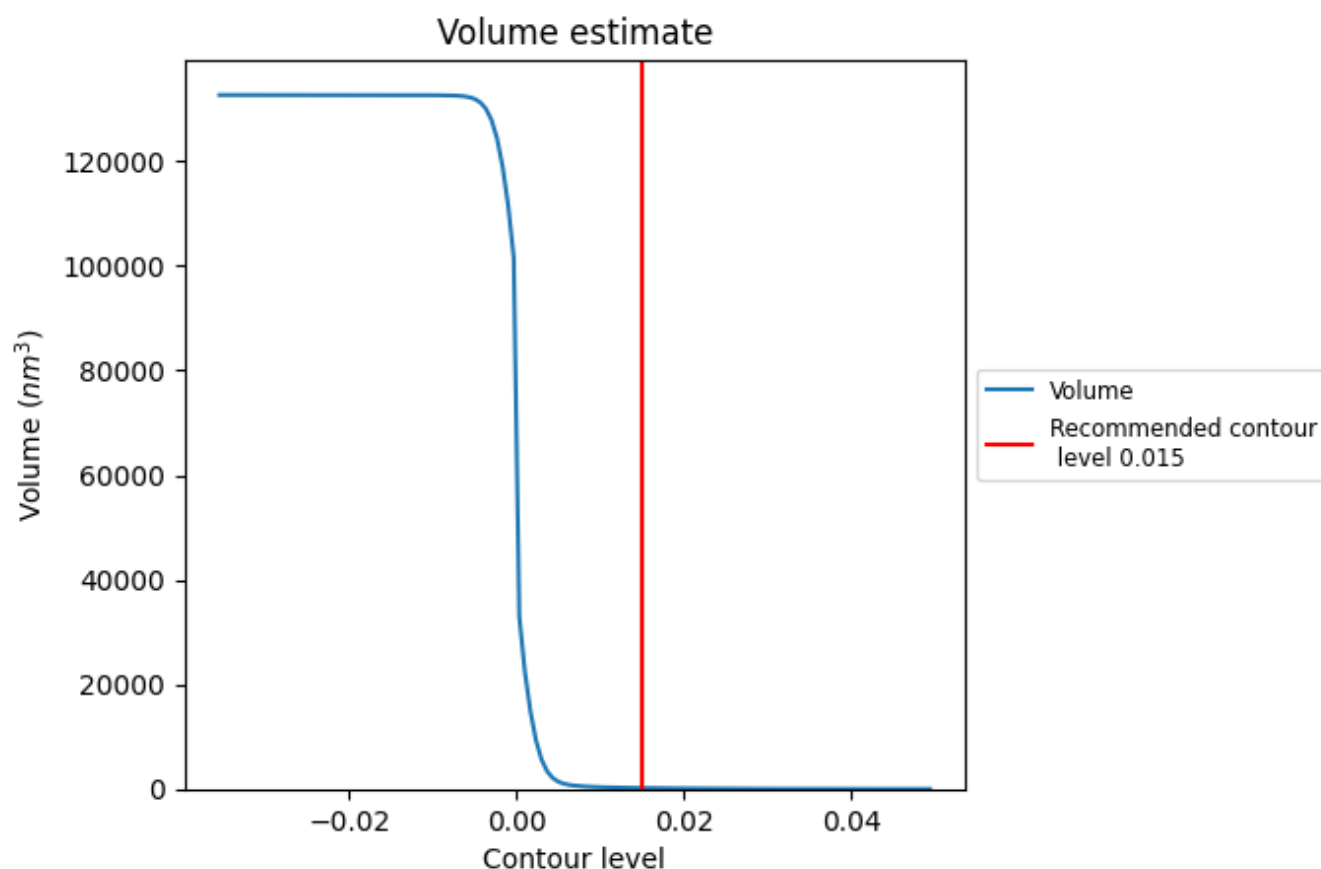
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

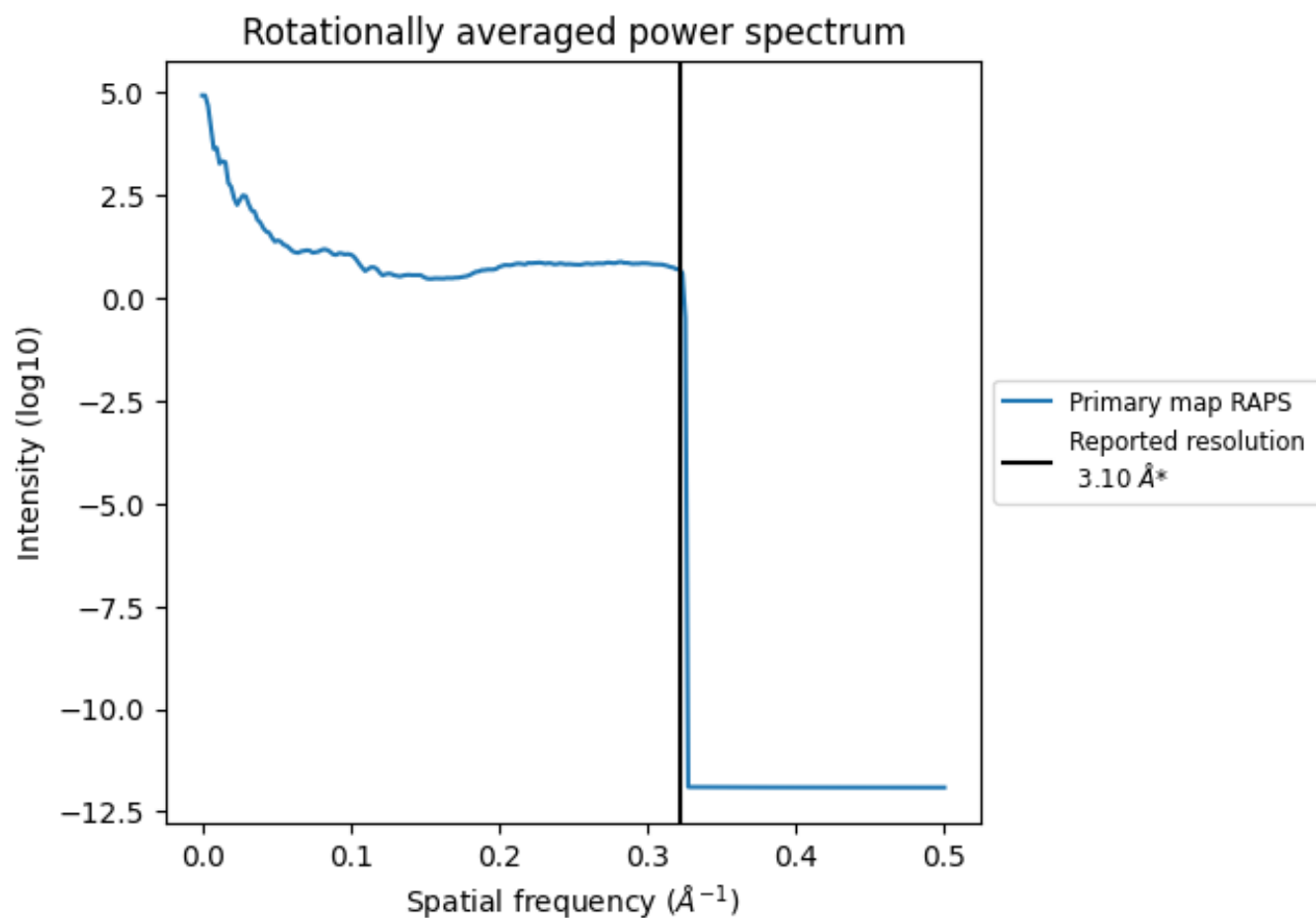
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 180 nm^3 ; this corresponds to an approximate mass of 163 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

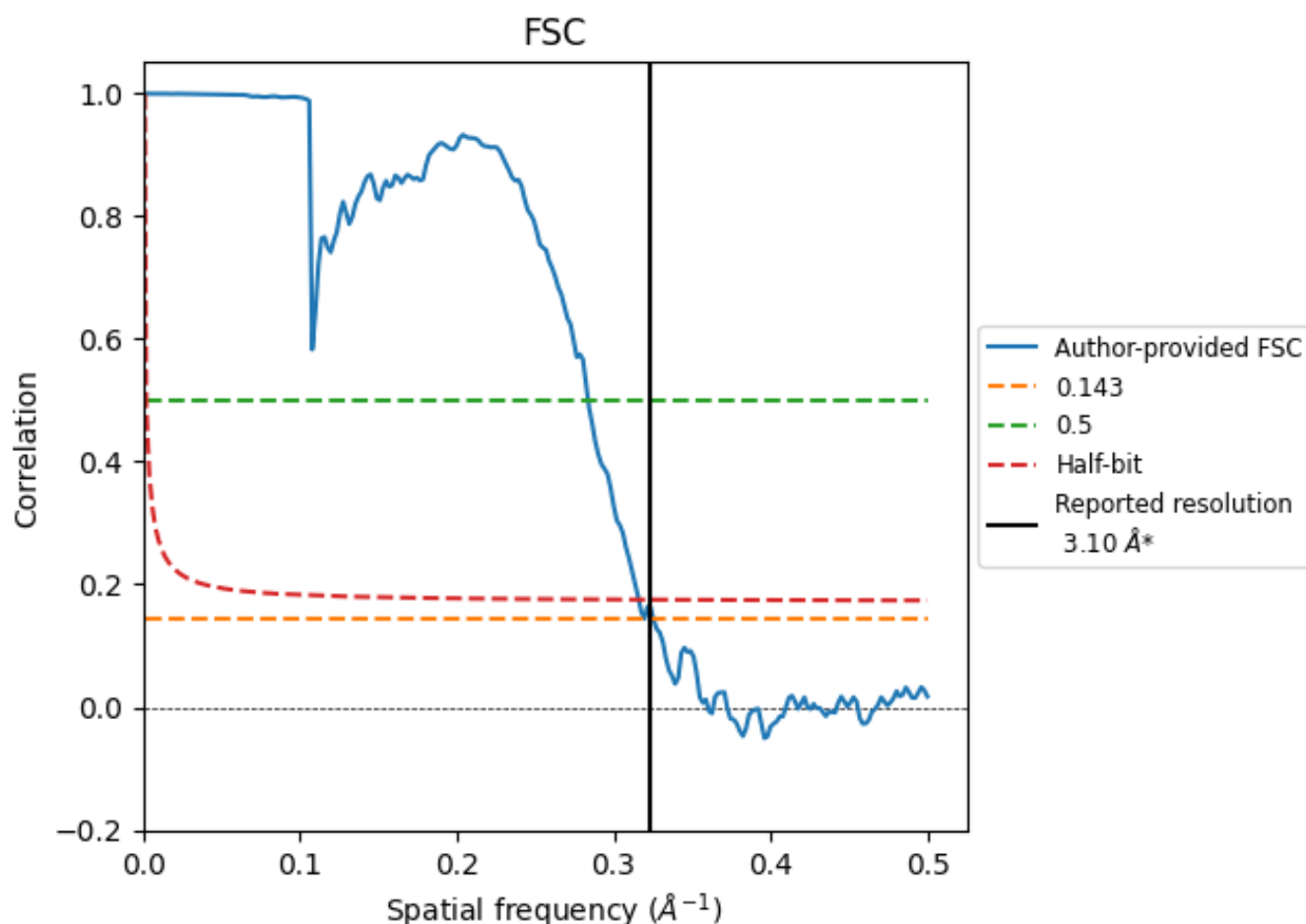


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

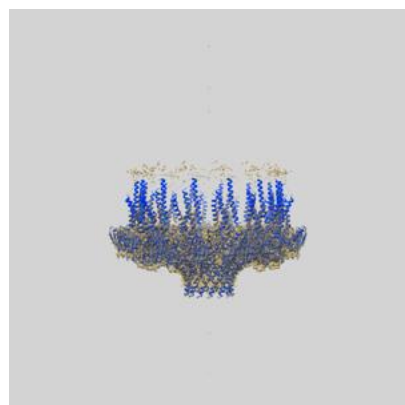
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.07	3.52	3.16
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

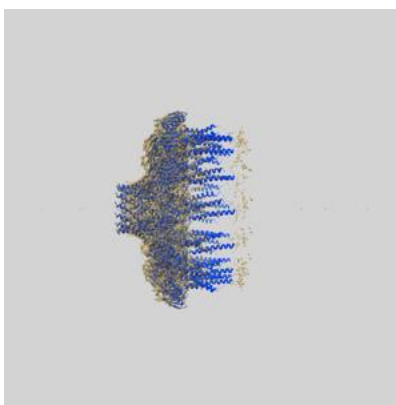
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22076 and PDB model 6X6K. Per-residue inclusion information can be found in section 3 on page 8.

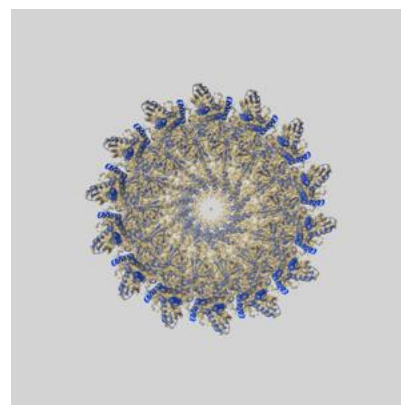
9.1 Map-model overlay [i](#)



X



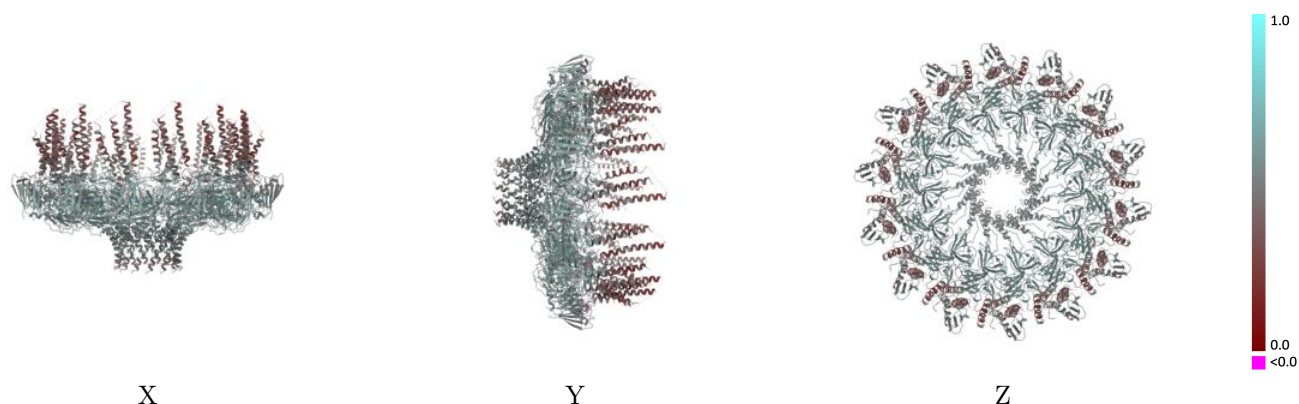
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)

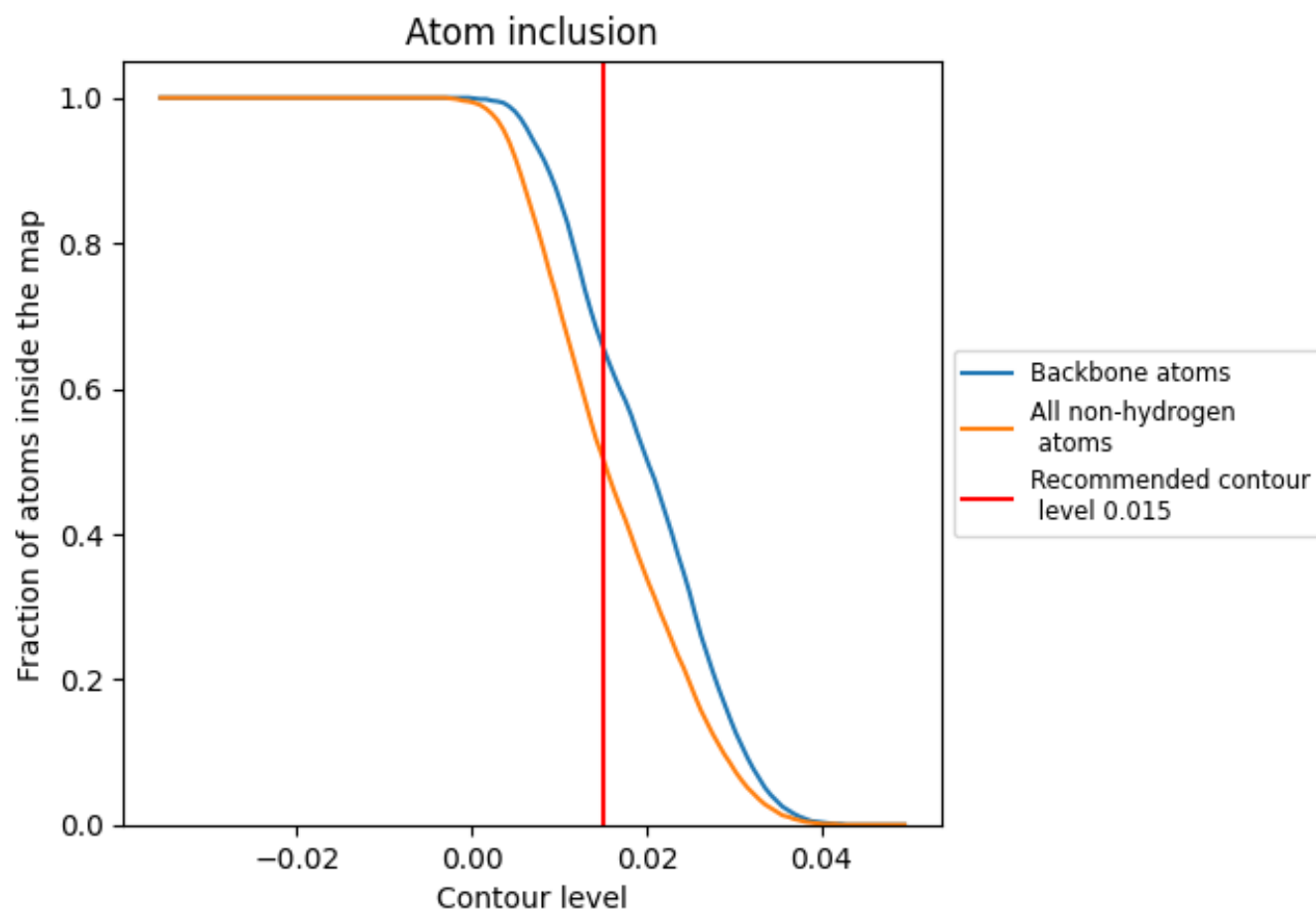


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5050	 0.5040
AT	 0.3380	 0.4550
AX	 0.5770	 0.5170
AY	 0.6070	 0.5400
BT	 0.3390	 0.4580
BX	 0.5750	 0.5160
BY	 0.6070	 0.5410
CT	 0.3350	 0.4550
CX	 0.5740	 0.5180
CY	 0.6040	 0.5410
DT	 0.3390	 0.4550
DX	 0.5720	 0.5190
DY	 0.6020	 0.5420
ET	 0.3400	 0.4550
EX	 0.5790	 0.5170
EY	 0.6040	 0.5430
FT	 0.3360	 0.4540
FX	 0.5780	 0.5190
FY	 0.6050	 0.5400
GT	 0.3330	 0.4530
GX	 0.5800	 0.5190
GY	 0.6090	 0.5410
HT	 0.3370	 0.4560
HX	 0.5770	 0.5170
HY	 0.6060	 0.5400
IT	 0.3370	 0.4560
IX	 0.5710	 0.5190
IY	 0.6070	 0.5400
JT	 0.3350	 0.4520
JX	 0.5740	 0.5170
JY	 0.6050	 0.5390
KT	 0.3360	 0.4550
KX	 0.5730	 0.5170
KY	 0.6020	 0.5400
LT	 0.3370	 0.4560



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Chain	Atom inclusion	Q-score
LX	 0.5790	 0.5170
LY	 0.6050	 0.5390
MT	 0.3350	 0.4570
MX	 0.5770	 0.5190
MY	 0.6050	 0.5390
NT	 0.3390	 0.4560
NX	 0.5790	 0.5170
NY	 0.6090	 0.5400