



Full wwPDB EM Validation Report ⓘ

Jun 8, 2026 – 04:20 PM JST

PDB ID : 9VGF / pdb_00009vgf
EMDB ID : EMD-65048
Title : Cryo-EM structure of CagX-CagY complex with C17 symmetry
Authors : Mok, C.Y.; Chu, H.Y.; Au, S.W.N.
Deposited on : 2025-06-13
Resolution : 2.58 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 EMDB 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

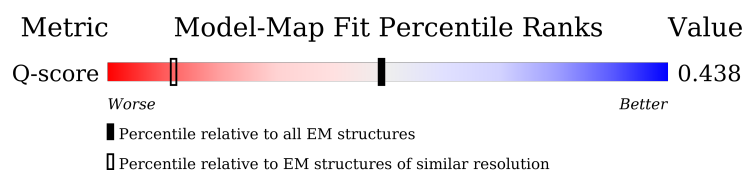
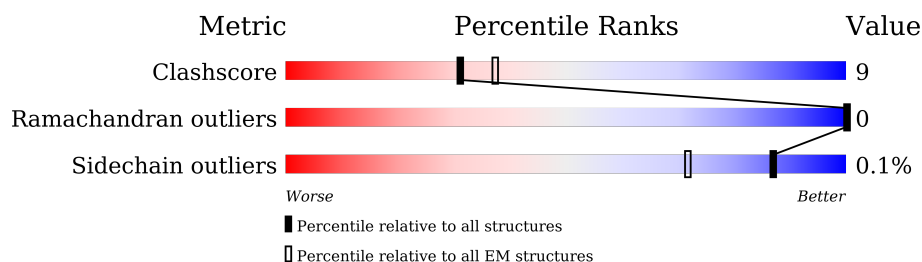
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY





The reported resolution of this entry is 2.58 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.








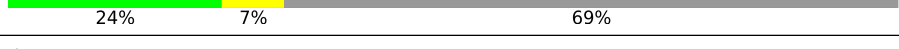

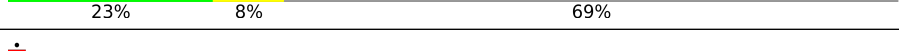
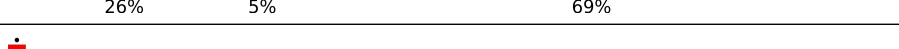
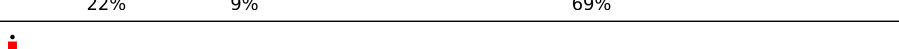















Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7675 (2.08 - 3.08)

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	AX	495	
1	BX	495	
1	CX	495	
1	DX	495	

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Mol	Chain	Length	Quality of chain
1	EX	495	
1	FX	495	
1	GX	495	
1	HX	495	
1	IX	495	
1	JX	495	
1	KX	495	
1	LX	495	
1	MX	495	
1	NX	495	
1	OX	495	
1	PX	495	
1	QX	495	
2	AY	441	
2	BY	441	
2	CY	441	
2	DY	441	
2	EY	441	
2	FY	441	
2	GY	441	
2	HY	441	
2	IY	441	
2	JY	441	
2	KY	441	
2	LY	441	

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Mol	Chain	Length	Quality of chain
2	MY	441	 15% 83%
2	NY	441	 14% 83%
2	OY	441	 14% 83%
2	PY	441	 15% 83%
2	QY	441	 15% 83%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 63274 atoms, of which 31569 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 X.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	AX	154	Total	C	H	N	O	S	0	0
			2513	803	1257	214	237	2		
1	BX	154	Total	C	H	N	O	S	0	0
			2513	803	1257	214	237	2		
1	CX	154	Total	C	H	N	O	S	0	0
			2513	803	1257	214	237	2		
1	DX	154	Total	C	H	N	O	S	0	0
			2513	803	1257	214	237	2		
1	EX	154	Total	C	H	N	O	S	0	0
			2513	803	1257	214	237	2		
1	FX	154	Total	C	H	N	O	S	0	0
			2513	803	1257	214	237	2		
1	GX	154	Total	C	H	N	O	S	0	0
			2513	803	1257	214	237	2		
1	HX	154	Total	C	H	N	O	S	0	0
			2513	803	1257	214	237	2		
1	IX	154	Total	C	H	N	O	S	0	0
			2513	803	1257	214	237	2		
1	JX	154	Total	C	H	N	O	S	0	0
			2513	803	1257	214	237	2		
1	KX	154	Total	C	H	N	O	S	0	0
			2513	803	1257	214	237	2		
1	LX	154	Total	C	H	N	O	S	0	0
			2513	803	1257	214	237	2		
1	MX	154	Total	C	H	N	O	S	0	0
			2513	803	1257	214	237	2		
1	NX	154	Total	C	H	N	O	S	0	0
			2513	803	1257	214	237	2		
1	OX	154	Total	C	H	N	O	S	0	0
			2513	803	1257	214	237	2		
1	PX	154	Total	C	H	N	O	S	0	0
			2513	803	1257	214	237	2		
1	QX	154	Total	C	H	N	O	S	0	0
			2513	803	1257	214	237	2		

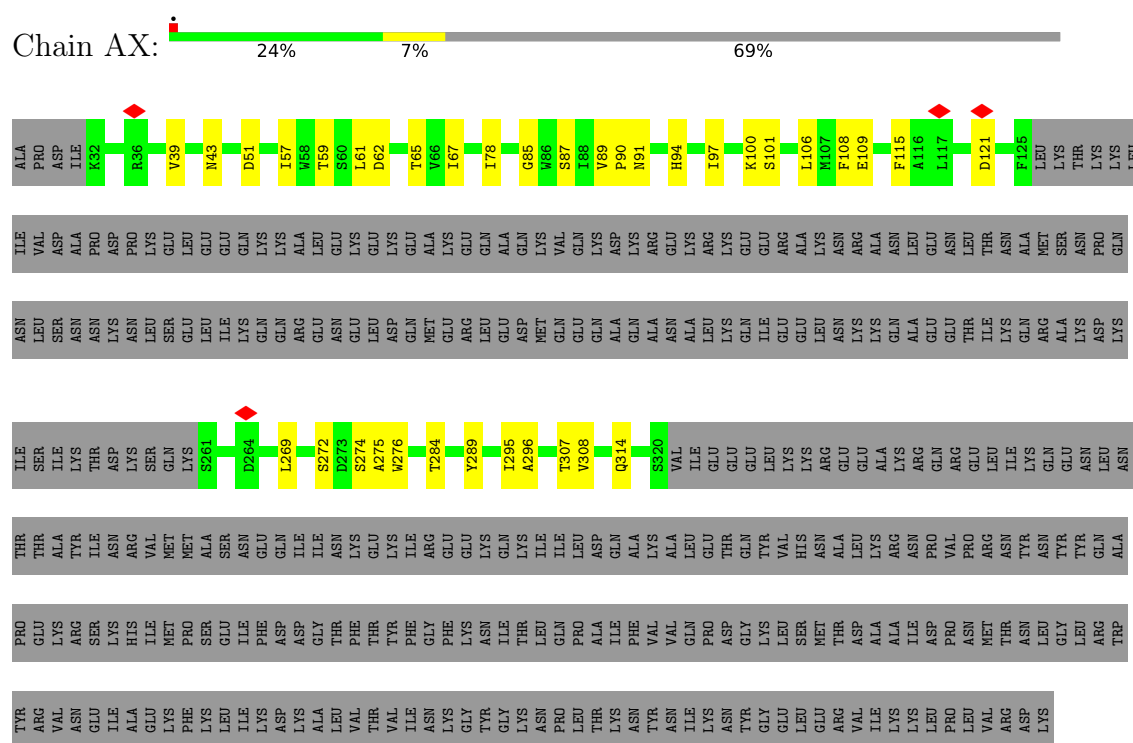
- Molecule 2 is a protein called Type IV secretion system apparatus protein CagY.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	AY	77	Total	C	H	N	O	S	0	0
			1209	374	600	105	126	4		
2	BY	77	Total	C	H	N	O	S	0	0
			1209	374	600	105	126	4		
2	CY	77	Total	C	H	N	O	S	0	0
			1209	374	600	105	126	4		
2	DY	77	Total	C	H	N	O	S	0	0
			1209	374	600	105	126	4		
2	EY	77	Total	C	H	N	O	S	0	0
			1209	374	600	105	126	4		
2	FY	77	Total	C	H	N	O	S	0	0
			1209	374	600	105	126	4		
2	GY	77	Total	C	H	N	O	S	0	0
			1209	374	600	105	126	4		
2	HY	77	Total	C	H	N	O	S	0	0
			1209	374	600	105	126	4		
2	IY	77	Total	C	H	N	O	S	0	0
			1209	374	600	105	126	4		
2	JY	77	Total	C	H	N	O	S	0	0
			1209	374	600	105	126	4		
2	KY	77	Total	C	H	N	O	S	0	0
			1209	374	600	105	126	4		
2	LY	77	Total	C	H	N	O	S	0	0
			1209	374	600	105	126	4		
2	MY	77	Total	C	H	N	O	S	0	0
			1209	374	600	105	126	4		
2	NY	77	Total	C	H	N	O	S	0	0
			1209	374	600	105	126	4		
2	OY	77	Total	C	H	N	O	S	0	0
			1209	374	600	105	126	4		
2	PY	77	Total	C	H	N	O	S	0	0
			1209	374	600	105	126	4		
2	QY	77	Total	C	H	N	O	S	0	0
			1209	374	600	105	126	4		

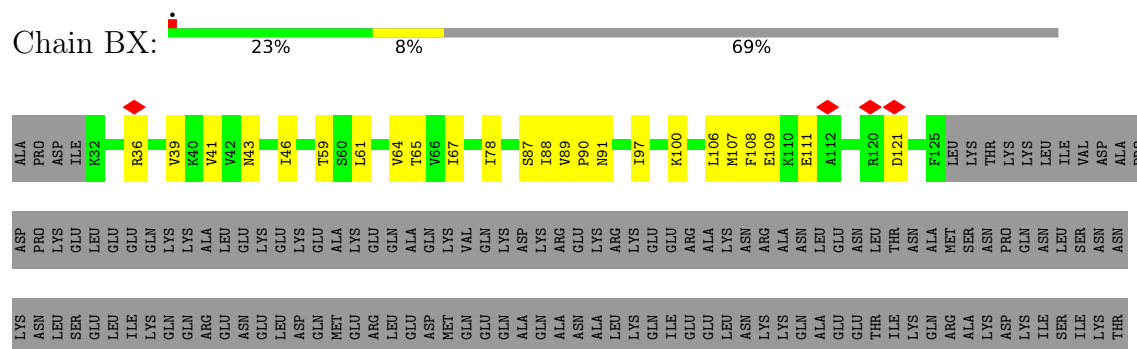
3 Residue-property plots [i](#)

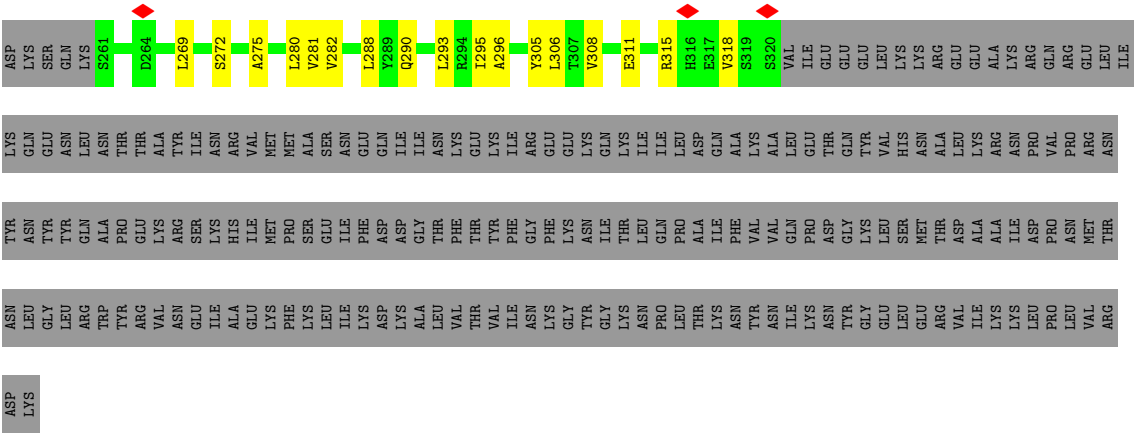
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

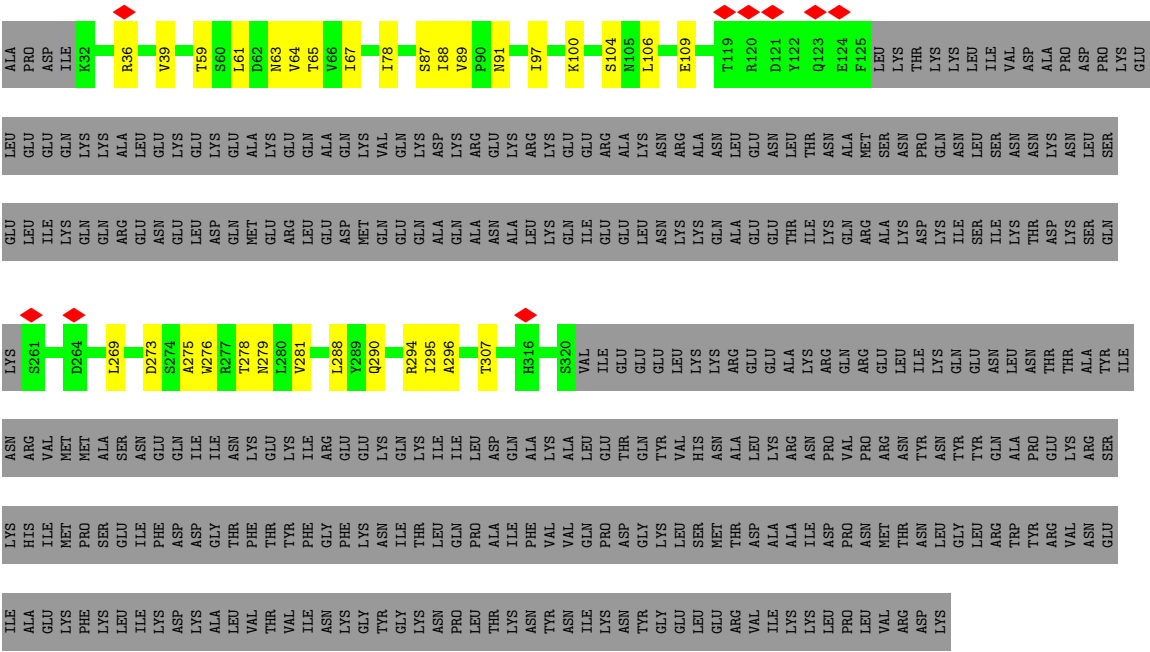


• Molecule 1: Cag pathogenicity island protein X

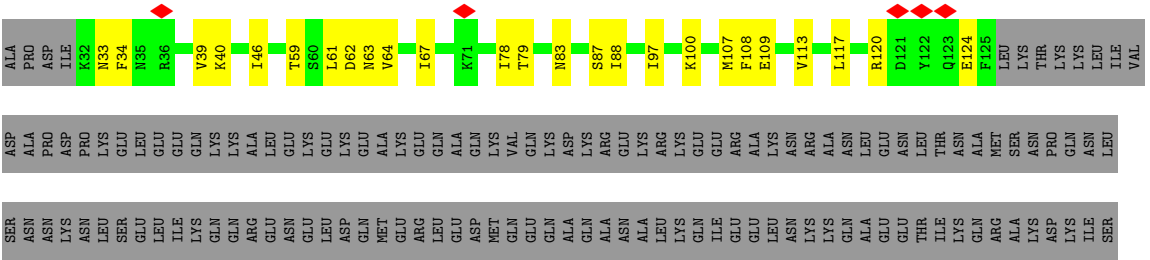


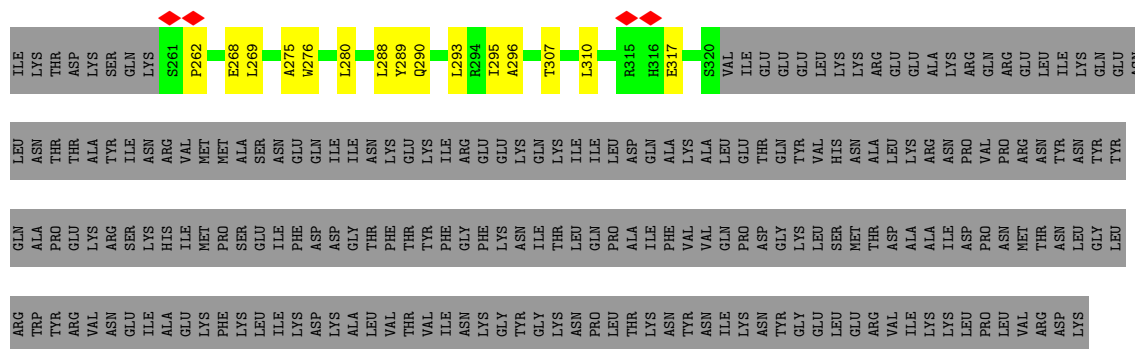


● Molecule 1: Cag pathogenicity island protein X

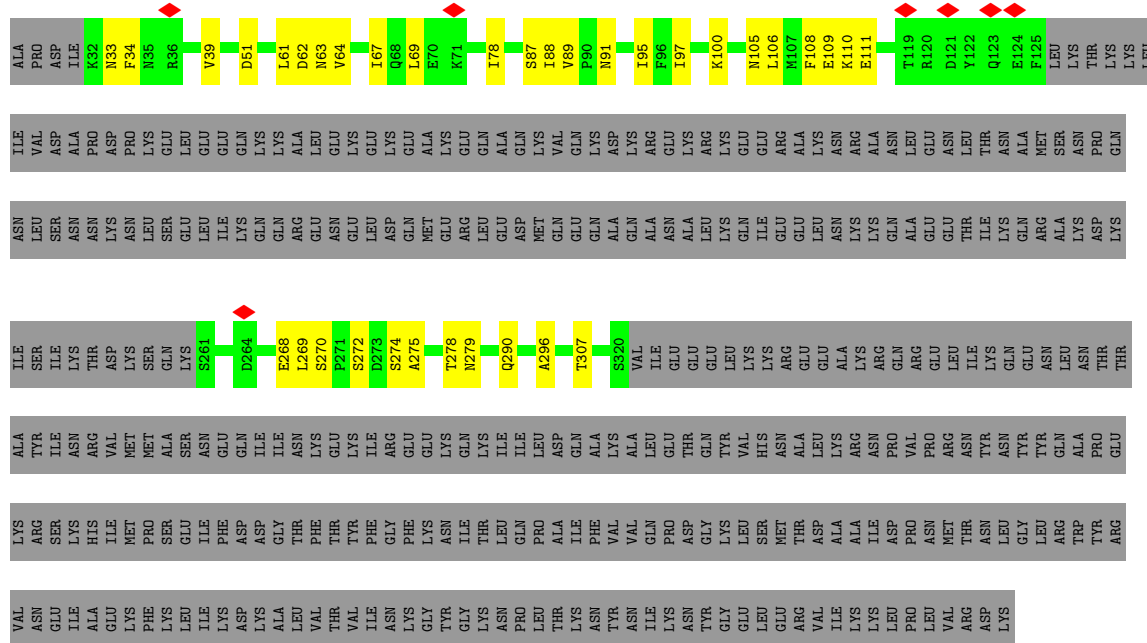


● Molecule 1: Cag pathogenicity island protein X

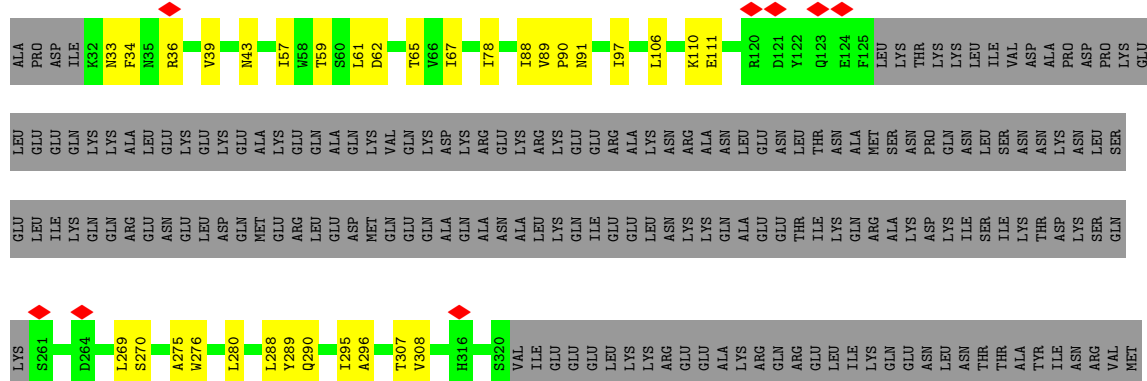


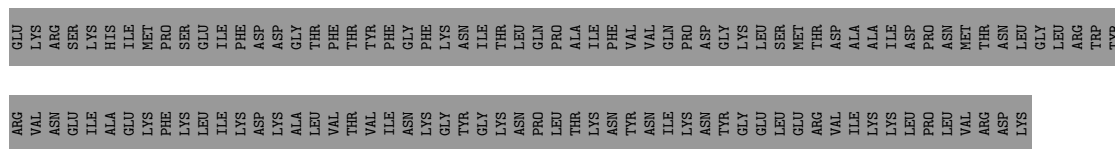


• Molecule 1: Cag pathogenicity island protein X

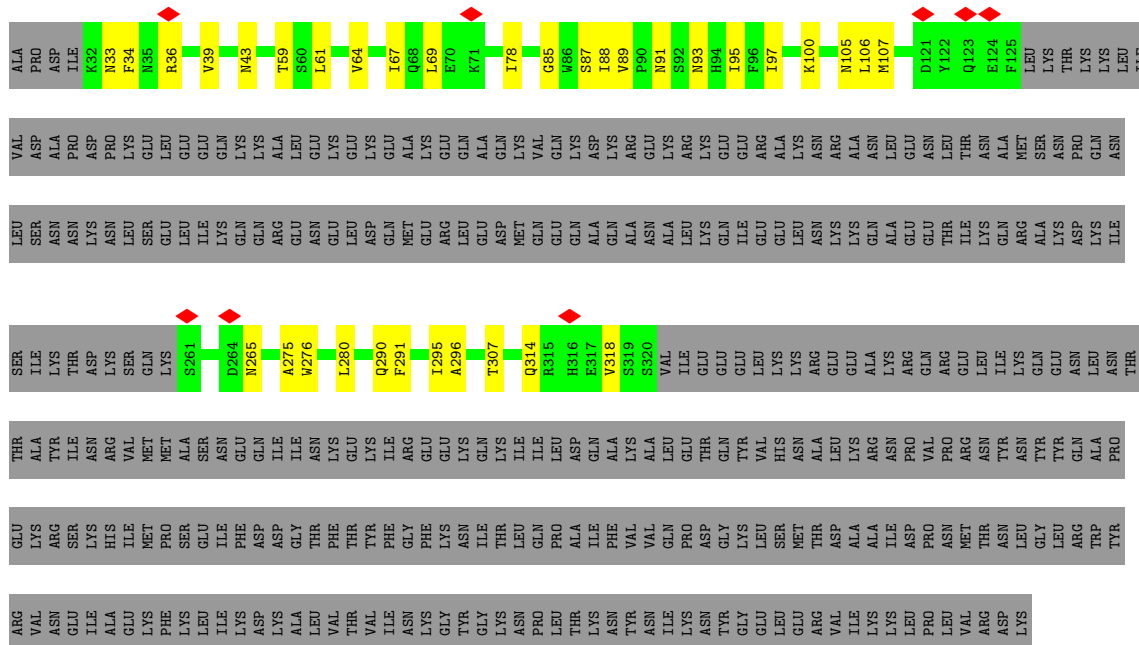


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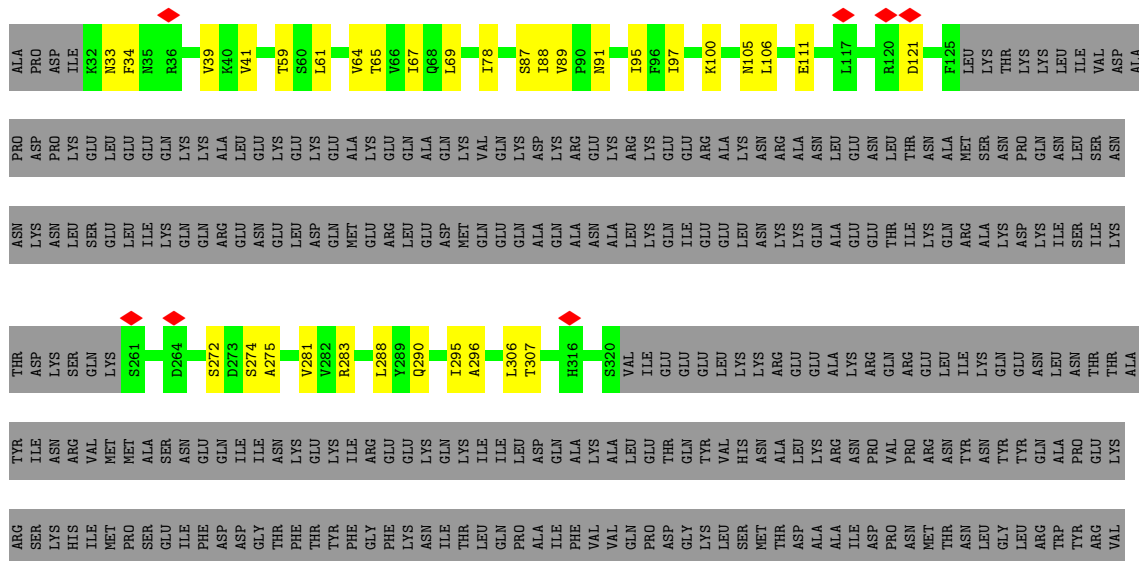




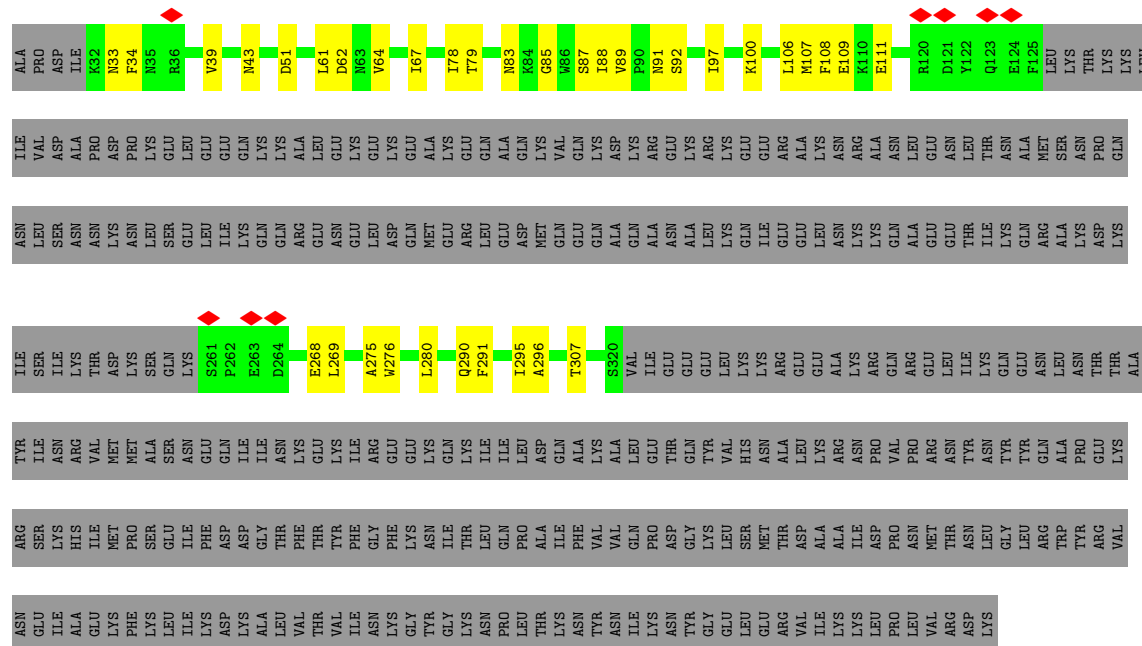
- Molecule 1: Cag pathogenicity island protein X



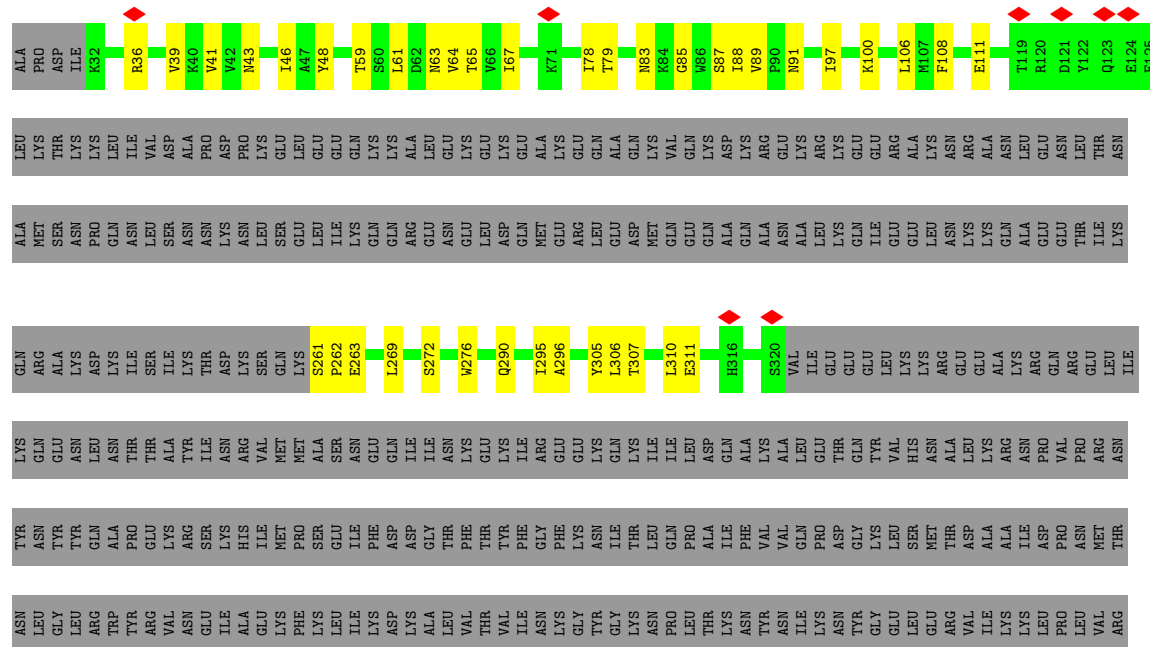
- Molecule 1: Cag pathogenicity island protein X



Chain KX:

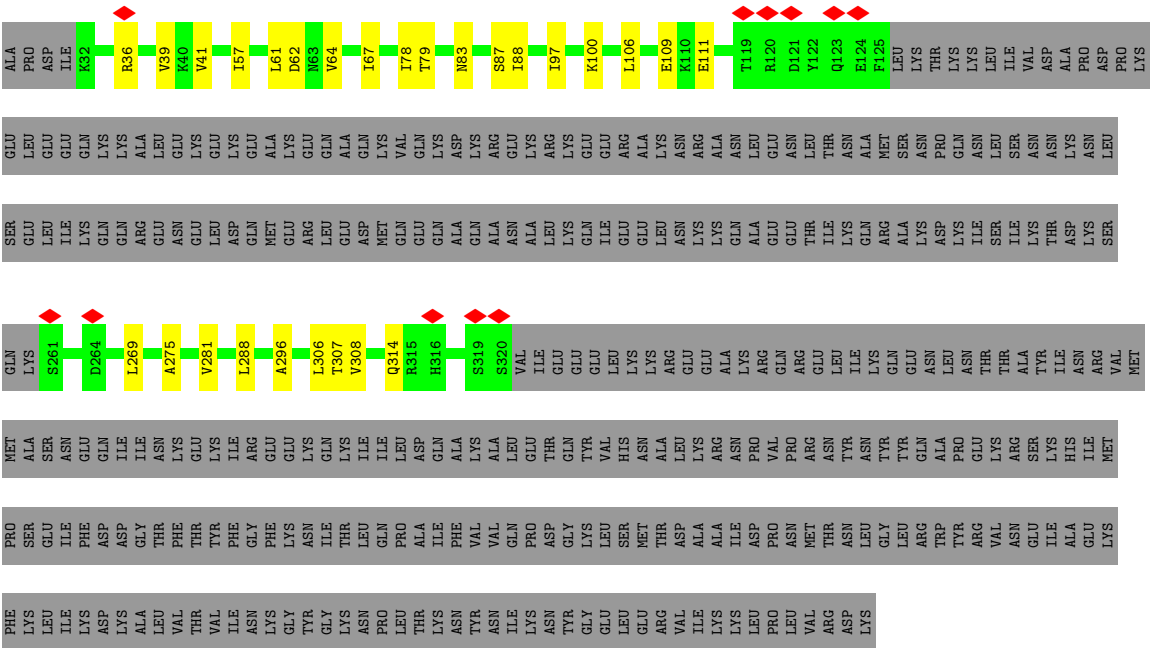


Chain LX:

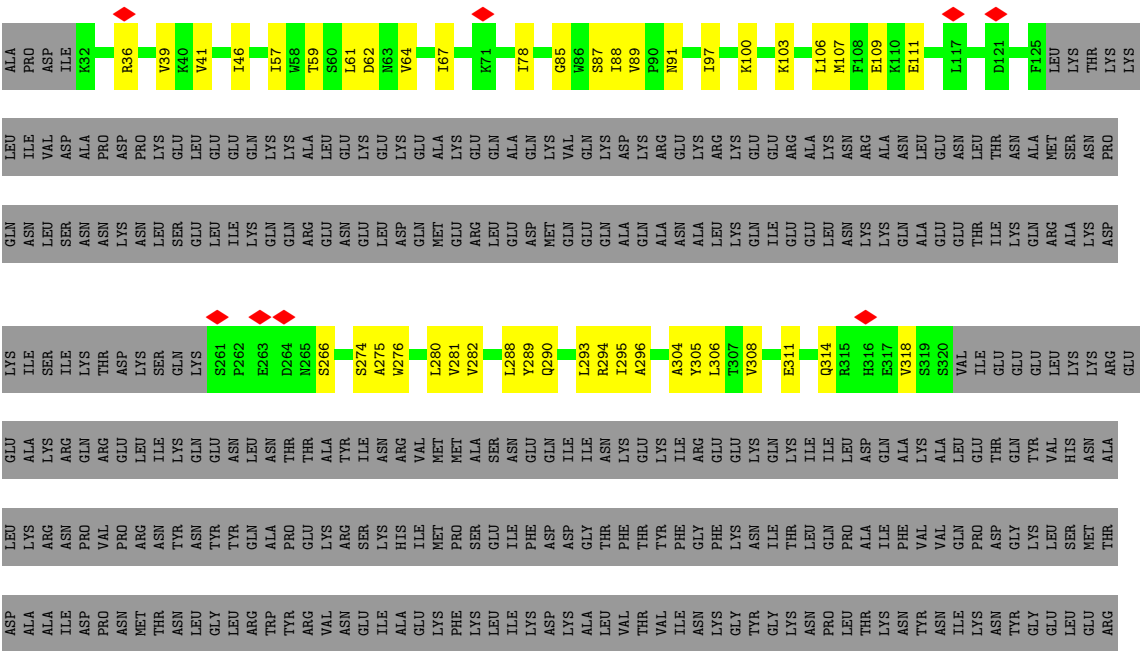


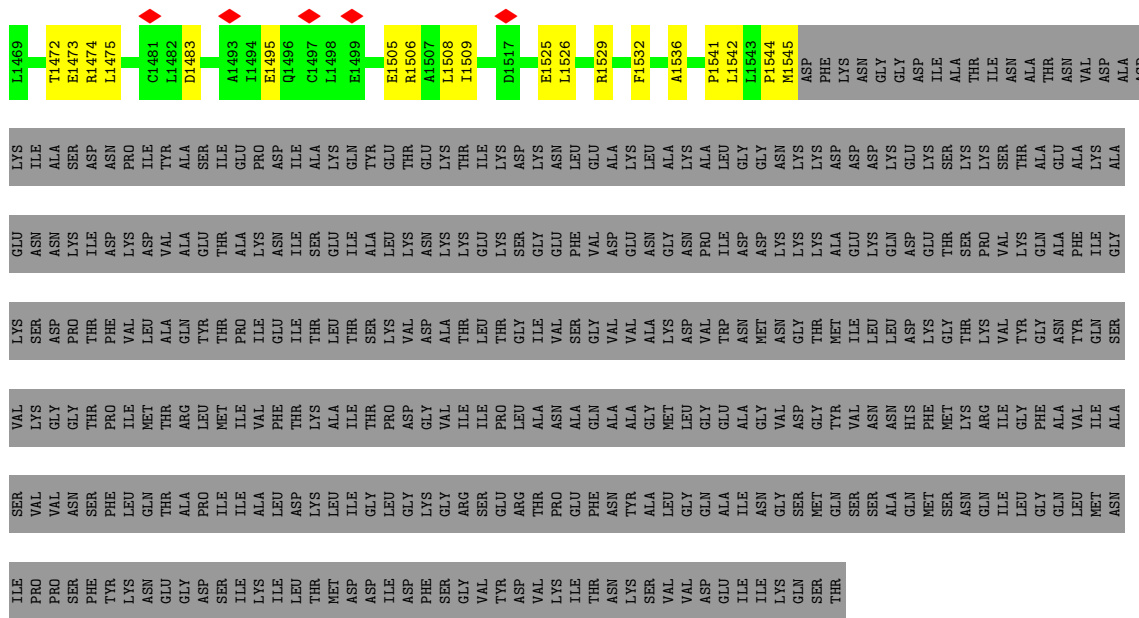
ASP
LYS

• Molecule 1: Cag pathogenicity island protein X

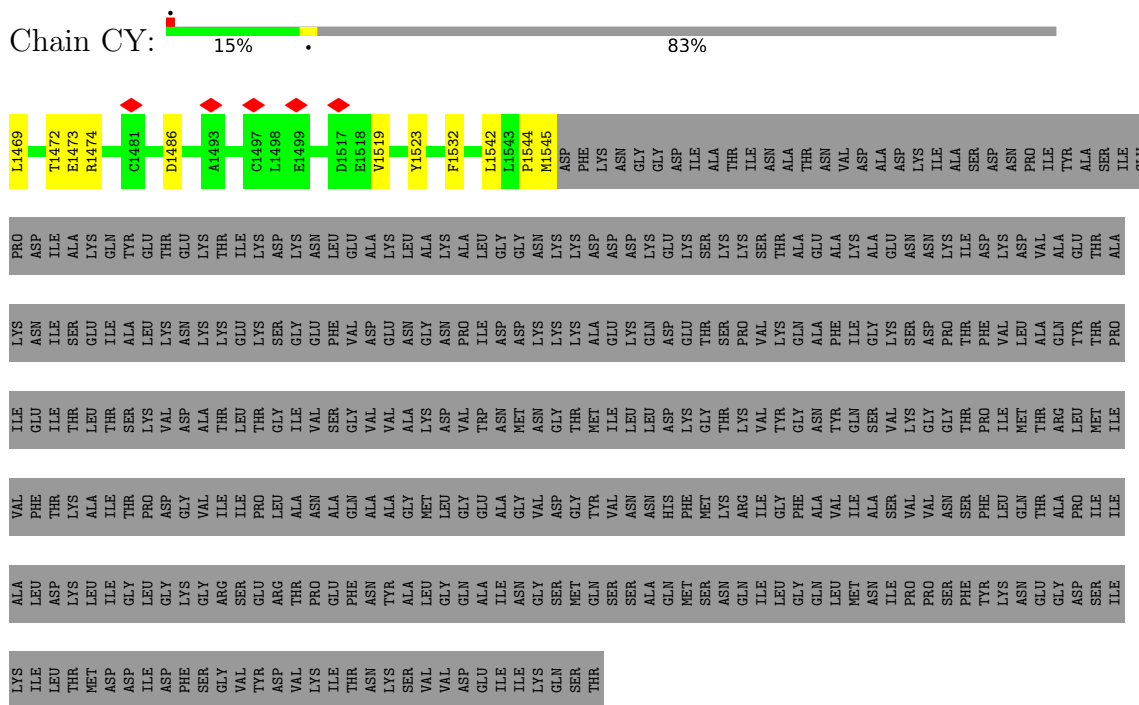


• Molecule 1: Cag pathogenicity island protein X

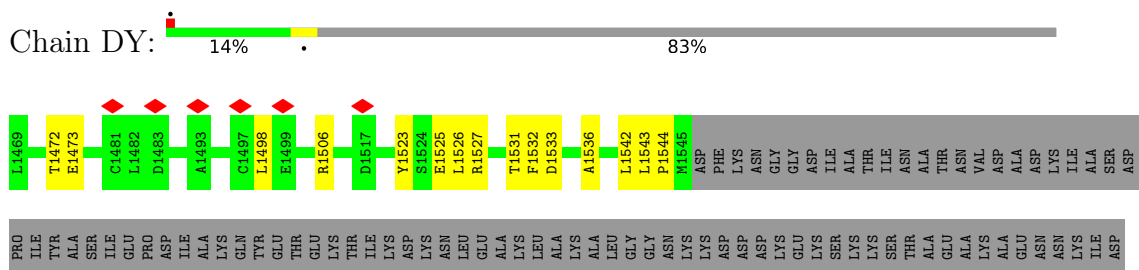




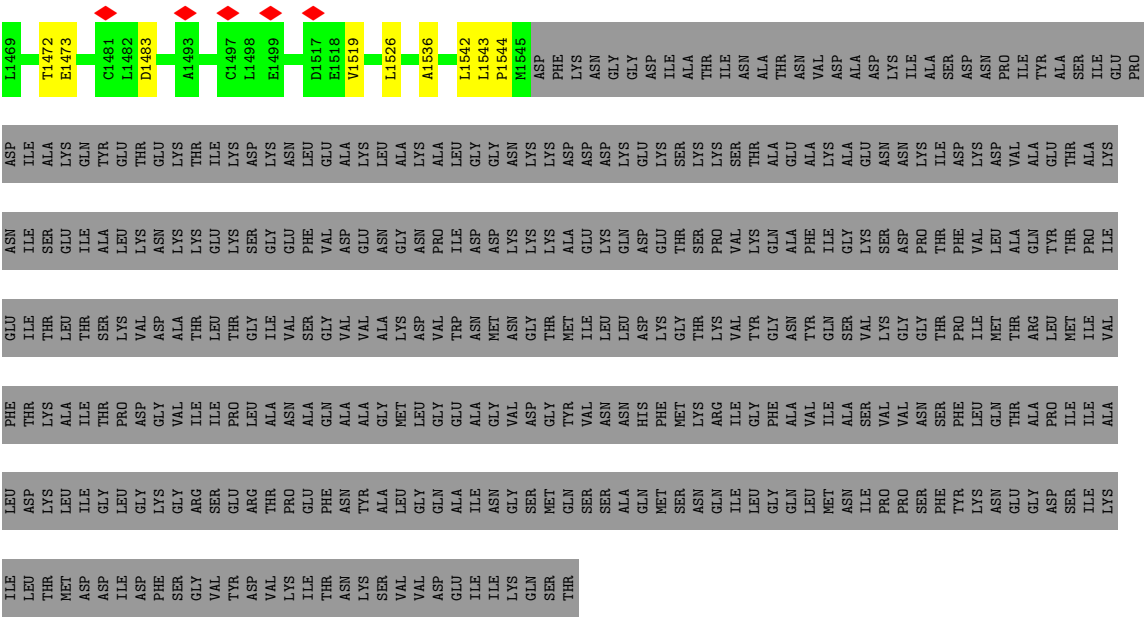
- Molecule 2: Type IV secretion system apparatus protein CagY



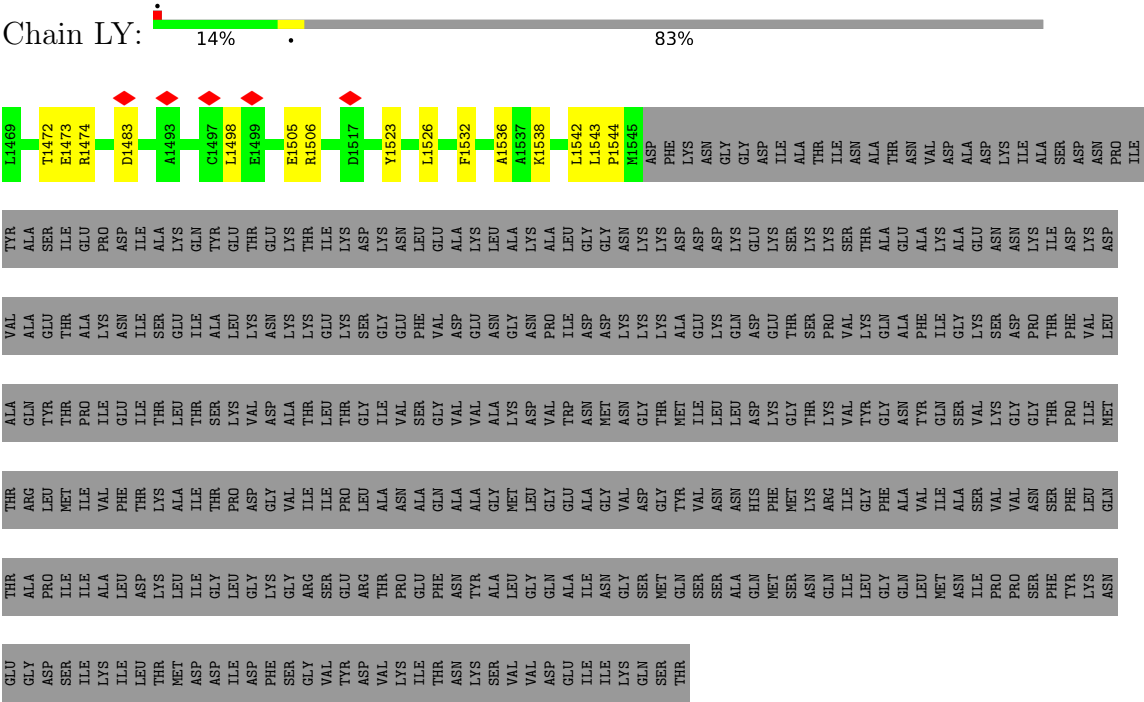
- Molecule 2: Type IV secretion system apparatus protein CagY



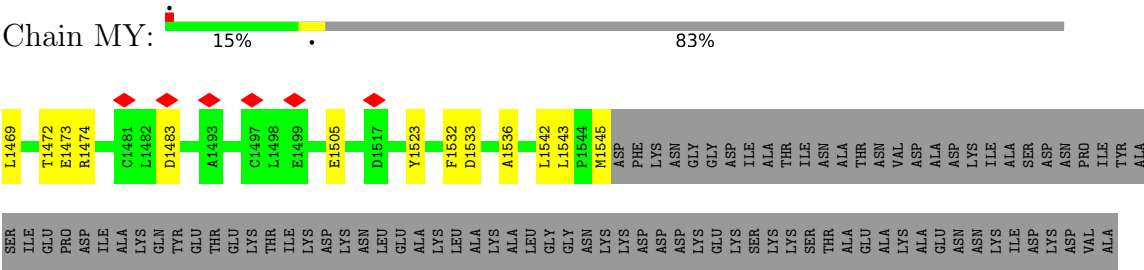




• Molecule 2: Type IV secretion system apparatus protein CagY



• Molecule 2: Type IV secretion system apparatus protein CagY



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

● Molecule 2: Type IV secretion system apparatus protein CagY



L1469	T1472	E1473	C1481	L1482	D1483	A1493	I1494	Q1496	C1497	L1498	E1499	R1506	D1517	F1518	V1519	Y1523	R1529	F1532	A1536	L1542	L1543	P1544	M1545	ASP	PHE	LYS	LYS	ASN	GLY	GLY	ILE	ALA	THR	ASN	ASN	VAL	ASP	ALA	GLY	THR	ASN	ASP	ASN		
PRO	ILE	TYR	SER	GLU	PRO	ALA	LYS	GLN	TYR	GLU	THR	GLY	THR	LYS	ASN	LEU	GLU	ALA	LYS	ALA	LEU	GLY	LYS	LYS	LYS	ASP	LYS	ASP	ASP	GLY	GLY	LYS	THR	ALA	GLU	ALA	VAL	ASP	LYS	GLY	THR	ASN	ASP	ASP	ASN
LYS	ASP	VAL	ALA	GLU	THR	ILE	ILE	GLY	THR	LYS	ALA	LYS	GLU	SER	GLY	PHE	VAL	ASP	GLY	PRO	ILE	ASP	LYS	LYS	LYS	ALA	GLU	LYS	LYS	GLN	THR	ALA	GLY	THR	PHE	THR	ILE	GLY	THR	ASN	ASP	THR	THR	PHE	
VAL	LEU	ALA	GLN	THR	PRO	ILE	THR	LEU	SER	VAL	ASP	ALA	LEU	THR	VAL	GLY	VAL	VAL	ASP	VAL	TRP	ASN	MET	ASN	GLY	THR	MET	ILE	LEU	LYS	ASP	GLY	GLY	ASN	VAL	TYR	THR	GLN	ILE	GLY	THR	ASN	GLY	PRO	
ILE	MET	THR	ARG	LEU	ILE	VAL	LYS	LYS	THR	ALA	ILE	THR	PRO	THR	ALA	ASN	GLN	ALA	GLY	LEU	GLY	VAL	VAL	ASP	GLY	GLY	THR	VAL	ASN	GLY	PHE	THR	VAL	VAL	VAL	THR	VAL	ILE	ILE	ALA	ASP	VAL	THR	PHE	
LEU	GLN	THR	ALA	PRO	ILE	ALA	ASP	LYS	LEU	GLY	ILE	GLY	LEU	GLY	LYS	ARG	SER	GLU	PHE	GLN	ALA	THR	GLY	GLN	GLY	GLN	SER	ASN	GLN	ALA	GLY	GLN	LEU	LEU	MET	ASN	GLY	THR	THR	THR	THR	THR	THR	THR	
LYS	ASN	GLY	ASP	SER	ILE	LYS	LEU	THR	MET	ASP	ILE	PHE	SER	GLY	VAL	GLY	VAL	THR	ILE	ASP	GLU	ILE	LYS	GLN	SER	THR	ASN	GLY	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR

● Molecule 2: Type IV secretion system apparatus protein CagY



L1469	T1472	E1473	R1474	L1475	D1483	E1495	Q1496	C1497	L1498	E1499	R1506	A1507	L1508	I1509	D1517	Y1523	R1527	F1532	A1536	L1542	L1543	P1544	M1545	ASP	PHE	LYS	ASN	GLY	GLY	ASP	ILE	ALA	THR	ASN	ASN	VAL	ASP	ALA	GLY	THR	ASN	ASP	ASN	PRO																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
ILE	TYR	ALA	SER	ILE	GLU	PRO	LYS	LYS	GLN	TYR	GLU	THR	LYS	LYS	LYS	ASN	GLU	LYS	ALA	LYS	GLY	LYS	ASN	LYS	LYS	ASP	ASP	ASP	LYS	LYS	LYS	THR	ILE	ASN	ALA	THR	ASN	ASN	VAL	ASP	ALA	GLY	THR	ASN	ASP	ASN	PRO																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
ASP	VAL	ALA	GLU	ALA	LYS	ASN	ILE	SER	GLU	LEU	LYS	ASN	GLY	GLU	SER	PHE	ASP	GLU	ASN	PRO	ILE	ASP	LYS	LYS	LYS	ALA	GLU	GLN	LYS	THR	SER	PRO	VAL	LYS	GLN	ALA	PHE	ILE	GLY	THR	THR	THR	THR	THR	THR	THR																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
LEU	ALA	GLN	TYR	THR	ILE	PRO	ILE	THR	LYS	VAL	ASP	ALA	THR	GLY	VAL	VAL	VAL	VAL	VAL	VAL	TRP	ASN	MET	ASN	GLY	THR	MET	ILE	LEU	LYS	ASP	LYS	THR	VAL	THR	GLY	ASN	TYR	GLN	SER	SER	VAL	LYS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GL



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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	373053	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS TALOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.673	Depositor
Minimum map value	-0.910	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.157	Depositor
Map size (Å)	292.16, 292.16, 292.16	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AX	0.18	0/1282	0.39	0/1735
1	BX	0.17	0/1282	0.37	0/1735
1	CX	0.17	0/1282	0.36	0/1735
1	DX	0.17	0/1282	0.37	0/1735
1	EX	0.17	0/1282	0.37	0/1735
1	FX	0.17	0/1282	0.36	0/1735
1	GX	0.18	0/1282	0.38	0/1735
1	HX	0.18	0/1282	0.39	0/1735
1	IX	0.18	0/1282	0.39	0/1735
1	JX	0.17	0/1282	0.39	0/1735
1	KX	0.17	0/1282	0.37	0/1735
1	LX	0.17	0/1282	0.37	0/1735
1	MX	0.17	0/1282	0.35	0/1735
1	NX	0.18	0/1282	0.37	0/1735
1	OX	0.17	0/1282	0.36	0/1735
1	PX	0.18	0/1282	0.37	0/1735
1	QX	0.18	0/1282	0.38	0/1735
2	AY	0.14	0/615	0.30	0/828
2	BY	0.15	0/615	0.34	0/828
2	CY	0.14	0/615	0.36	0/828
2	DY	0.14	0/615	0.30	0/828
2	EY	0.13	0/615	0.30	0/828
2	FY	0.13	0/615	0.30	0/828
2	GY	0.15	0/615	0.36	0/828
2	HY	0.13	0/615	0.32	0/828
2	IY	0.13	0/615	0.30	0/828
2	JY	0.14	0/615	0.33	0/828
2	KY	0.14	0/615	0.33	0/828
2	LY	0.15	0/615	0.36	0/828
2	MY	0.13	0/615	0.30	0/828
2	NY	0.14	0/615	0.31	0/828
2	OY	0.14	0/615	0.32	0/828
2	PY	0.15	0/615	0.35	0/828
2	QY	0.14	0/615	0.33	0/828

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.16	0/32249	0.36	0/43571

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AX	1256	1257	1255	33	0
1	BX	1256	1257	1255	34	0
1	CX	1256	1257	1255	26	0
1	DX	1256	1257	1255	32	0
1	EX	1256	1257	1255	31	0
1	FX	1256	1257	1255	30	0
1	GX	1256	1257	1255	29	0
1	HX	1256	1257	1255	29	0
1	IX	1256	1257	1255	26	0
1	JX	1256	1257	1255	25	0
1	KX	1256	1257	1255	31	0
1	LX	1256	1257	1255	33	0
1	MX	1256	1257	1255	20	0
1	NX	1256	1257	1255	36	0
1	OX	1256	1257	1255	31	0
1	PX	1256	1257	1255	28	0
1	QX	1256	1257	1255	27	0
2	AY	609	600	597	15	0
2	BY	609	600	597	16	0
2	CY	609	600	597	11	0
2	DY	609	600	597	15	0
2	EY	609	600	597	17	0
2	FY	609	600	597	12	0
2	GY	609	600	597	12	0
2	HY	609	600	597	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	IY	609	600	597	10	0
2	JY	609	600	597	15	0
2	KY	609	600	597	10	0
2	LY	609	600	597	13	0
2	MY	609	600	597	11	0
2	NY	609	600	597	14	0
2	OY	609	600	597	13	0
2	PY	609	600	597	10	0
2	QY	609	600	597	14	0
All	All	31705	31569	31484	558	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 9.

All (558) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:OX:121:ASP:OD2	1:PX:261:SER:N	2.03	0.89
1:NX:280:LEU:HD12	1:NX:293:LEU:HD11	1.55	0.86
1:NX:290:GLN:NE2	1:OX:307:THR:OG1	2.09	0.86
1:IX:39:VAL:HG21	1:IX:296:ALA:HB1	1.65	0.77
1:BX:39:VAL:HG21	1:BX:296:ALA:HB1	1.67	0.76
2:AY:1542:LEU:HB3	1:BX:106:LEU:HD21	1.69	0.75
2:FY:1486:ASP:OD1	1:GX:40:LYS:NZ	2.21	0.73
1:JX:39:VAL:HG21	1:JX:296:ALA:HB1	1.70	0.73
1:LX:79:THR:OG1	1:LX:83:ASN:OD1	2.06	0.73
1:QX:39:VAL:HG21	1:QX:296:ALA:HB1	1.70	0.73
1:EX:110:LYS:O	2:EY:1529:ARG:NH2	2.23	0.72
1:FX:39:VAL:HG21	1:FX:296:ALA:HB1	1.72	0.71
1:NX:39:VAL:HG21	1:NX:296:ALA:HB1	1.71	0.71
1:FX:290:GLN:NE2	1:GX:307:THR:OG1	2.23	0.71
1:PX:281:VAL:HG13	1:PX:288:LEU:HD21	1.73	0.71
1:BX:111:GLU:OE2	2:BY:1529:ARG:NE	2.25	0.69
1:GX:79:THR:OG1	1:GX:83:ASN:OD1	2.11	0.69
2:LY:1498:LEU:O	2:LY:1506:ARG:NH1	2.25	0.69
1:QX:79:THR:OG1	1:QX:83:ASN:OD1	2.10	0.68
1:EX:67:ILE:HD11	1:EX:97:ILE:HD13	1.76	0.68
2:MY:1523:TYR:OH	1:NX:62:ASP:OD1	2.10	0.68
1:GX:284:THR:OG1	1:GX:287:ALA:O	2.09	0.68
1:LX:39:VAL:HG21	1:LX:296:ALA:HB1	1.74	0.68
1:BX:109:GLU:N	1:BX:109:GLU:OE1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KX:79:THR:OG1	1:KX:83:ASN:OD1	2.09	0.67
1:LX:290:GLN:NE2	1:MX:307:THR:OG1	2.27	0.67
1:JX:111:GLU:OE2	2:JY:1529:ARG:NE	2.28	0.66
1:EX:39:VAL:HG21	1:EX:296:ALA:HB1	1.76	0.66
2:BY:1545:MET:SD	1:CX:104:SER:OG	2.49	0.66
1:OX:310:LEU:HD23	1:OX:312:TYR:OH	1.94	0.66
1:MX:79:THR:OG1	1:MX:83:ASN:OD1	2.13	0.66
1:CX:39:VAL:HG21	1:CX:296:ALA:HB1	1.79	0.65
1:DX:79:THR:OG1	1:DX:83:ASN:OD1	2.14	0.65
2:JY:1474:ARG:NH1	2:JY:1505:GLU:OE2	2.29	0.65
1:MX:39:VAL:HG21	1:MX:296:ALA:HB1	1.79	0.65
1:PX:314:GLN:O	1:PX:318:VAL:HG23	1.97	0.65
1:HX:39:VAL:HG21	1:HX:296:ALA:HB1	1.79	0.64
1:PX:39:VAL:HG21	1:PX:296:ALA:HB1	1.80	0.64
2:AY:1542:LEU:CB	1:BX:106:LEU:HD21	2.26	0.64
1:OX:268:GLU:N	1:OX:268:GLU:OE1	2.31	0.64
1:OX:290:GLN:NE2	1:PX:307:THR:OG1	2.31	0.64
1:AX:39:VAL:HG21	1:AX:296:ALA:HB1	1.80	0.63
1:DX:39:VAL:HG21	1:DX:296:ALA:HB1	1.80	0.63
1:NX:111:GLU:OE2	2:NY:1529:ARG:NH1	2.31	0.62
1:EX:111:GLU:OE1	2:EY:1529:ARG:NE	2.33	0.62
2:MY:1533:ASP:OD2	1:NX:274:SER:OG	2.17	0.62
1:PX:67:ILE:HD11	1:PX:97:ILE:HD13	1.80	0.62
2:QY:1474:ARG:NH1	2:QY:1505:GLU:OE2	2.33	0.62
1:DX:280:LEU:HD12	1:DX:293:LEU:HD21	1.81	0.62
2:CY:1486:ASP:OD1	1:DX:40:LYS:NZ	2.32	0.62
1:CX:109:GLU:OE1	1:CX:109:GLU:N	2.33	0.61
1:IX:87:SER:OG	1:IX:100:LYS:NZ	2.24	0.61
1:IX:290:GLN:NE2	1:JX:307:THR:OG1	2.34	0.60
2:NY:1483:ASP:OD1	1:OX:36:ARG:NH2	2.34	0.60
1:NX:280:LEU:CD1	1:NX:293:LEU:HD11	2.28	0.60
1:OX:39:VAL:HG21	1:OX:296:ALA:HB1	1.83	0.60
1:QX:48:TYR:O	1:QX:314:GLN:NE2	2.35	0.60
1:FX:57:ILE:CD1	1:FX:308:VAL:HG11	2.32	0.60
1:MX:111:GLU:OE2	1:MX:111:GLU:N	2.34	0.60
1:DX:290:GLN:NE2	1:EX:307:THR:OG1	2.34	0.60
1:PX:311:GLU:OE2	1:PX:311:GLU:N	2.34	0.60
1:AX:307:THR:OG1	1:QX:290:GLN:NE2	2.35	0.59
2:FY:1523:TYR:OH	1:GX:62:ASP:OD1	2.19	0.59
1:HX:109:GLU:OE1	1:HX:109:GLU:N	2.34	0.59
1:AX:109:GLU:OE2	1:AX:109:GLU:N	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HY:1536:ALA:HB2	2:HY:1543:LEU:HD11	1.84	0.59
2:NY:1536:ALA:HB2	2:NY:1543:LEU:HD11	1.84	0.59
1:DX:109:GLU:N	1:DX:109:GLU:OE1	2.35	0.59
1:DX:67:ILE:HD11	1:DX:97:ILE:HD13	1.84	0.59
1:GX:85:GLY:O	1:GX:276:TRP:NE1	2.33	0.59
1:HX:290:GLN:NE2	1:IX:307:THR:OG1	2.35	0.59
1:IX:67:ILE:HD11	1:IX:97:ILE:HD13	1.84	0.59
2:HY:1545:MET:HB3	1:IX:107:MET:HE1	1.85	0.58
1:DX:87:SER:OG	1:DX:100:LYS:NZ	2.28	0.58
1:EX:78:ILE:HD11	1:EX:88:ILE:HG21	1.84	0.58
1:PX:290:GLN:NE2	1:QX:307:THR:OG1	2.36	0.58
2:PY:1542:LEU:CB	1:QX:106:LEU:HD11	2.33	0.58
1:KX:67:ILE:HD11	1:KX:97:ILE:HD13	1.83	0.58
1:AX:87:SER:OG	1:AX:100:LYS:NZ	2.30	0.58
1:AX:115:PHE:HD1	2:AY:1538:LYS:HZ3	1.51	0.58
2:CY:1542:LEU:HD11	1:DX:262:PRO:HB3	1.85	0.58
1:MX:67:ILE:HD11	1:MX:97:ILE:HD13	1.83	0.58
2:NY:1523:TYR:OH	1:OX:62:ASP:OD1	2.21	0.58
2:NY:1542:LEU:CB	1:OX:106:LEU:HD11	2.34	0.58
2:LY:1543:LEU:HD23	2:LY:1544:PRO:O	2.02	0.58
1:NX:109:GLU:OE2	1:NX:109:GLU:N	2.36	0.58
1:AX:106:LEU:HD11	2:QY:1542:LEU:CB	2.34	0.58
2:KY:1542:LEU:HD11	1:LX:262:PRO:HB3	1.86	0.58
2:KY:1544:PRO:HG2	1:LX:269:LEU:HD12	1.86	0.58
1:JX:105:ASN:OD1	1:JX:106:LEU:N	2.37	0.57
1:EX:290:GLN:NE2	1:FX:307:THR:OG1	2.36	0.57
2:FY:1542:LEU:CB	1:GX:106:LEU:HD21	2.34	0.57
1:HX:67:ILE:HD11	1:HX:97:ILE:HD13	1.85	0.57
2:JY:1495:GLU:OE1	2:JY:1506:ARG:NH2	2.37	0.57
2:DY:1542:LEU:CB	1:EX:106:LEU:HD11	2.35	0.57
2:GY:1495:GLU:OE1	2:GY:1506:ARG:NH2	2.37	0.57
1:MX:87:SER:OG	1:MX:100:LYS:NZ	2.26	0.57
1:CX:78:ILE:HD11	1:CX:88:ILE:HG21	1.86	0.57
1:AX:51:ASP:O	1:BX:43:ASN:ND2	2.37	0.57
1:CX:290:GLN:NE2	1:DX:307:THR:OG1	2.38	0.57
1:JX:78:ILE:HD11	1:JX:88:ILE:HG21	1.86	0.57
1:NX:87:SER:OG	1:NX:100:LYS:NZ	2.28	0.56
2:BY:1475:LEU:HD11	2:BY:1509:ILE:HG12	1.86	0.56
2:FY:1542:LEU:HB3	1:GX:106:LEU:HD21	1.87	0.56
1:KX:290:GLN:NE2	1:LX:307:THR:OG1	2.39	0.56
1:MX:57:ILE:CD1	1:MX:308:VAL:HG11	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:PY:1475:LEU:HD11	2:PY:1509:ILE:HG12	1.86	0.56
1:HX:78:ILE:HD11	1:HX:88:ILE:HG21	1.86	0.56
2:KY:1536:ALA:HB2	2:KY:1543:LEU:HD11	1.86	0.56
2:MY:1532:PHE:CE1	1:NX:275:ALA:HB2	2.41	0.56
1:NX:280:LEU:HD23	1:NX:282:VAL:HG23	1.87	0.56
2:OY:1532:PHE:CE1	1:PX:275:ALA:HB2	2.40	0.56
2:GY:1536:ALA:HB2	2:GY:1543:LEU:HD11	1.87	0.56
1:AX:275:ALA:HB2	2:QY:1532:PHE:CE1	2.41	0.56
1:FX:111:GLU:OE2	2:FY:1529:ARG:NE	2.38	0.56
2:LY:1536:ALA:HB2	2:LY:1543:LEU:HD11	1.88	0.56
1:KX:39:VAL:HG21	1:KX:296:ALA:HB1	1.88	0.56
2:IY:1532:PHE:CE1	1:JX:275:ALA:HB2	2.41	0.55
1:KX:87:SER:OG	1:KX:100:LYS:NZ	2.24	0.55
2:MY:1474:ARG:NH1	2:MY:1505:GLU:OE2	2.39	0.55
2:KY:1542:LEU:HD11	1:LX:262:PRO:CB	2.36	0.55
1:IX:78:ILE:HD11	1:IX:88:ILE:HG21	1.88	0.55
1:JX:67:ILE:HD11	1:JX:97:ILE:HD13	1.87	0.55
2:OY:1542:LEU:CB	1:PX:106:LEU:HD11	2.37	0.55
1:PX:87:SER:OG	1:PX:100:LYS:NZ	2.26	0.55
2:CY:1523:TYR:OH	1:DX:62:ASP:OD1	2.23	0.55
2:CY:1532:PHE:CZ	1:DX:275:ALA:HB2	2.42	0.55
1:QX:57:ILE:CD1	1:QX:308:VAL:HG11	2.36	0.55
1:AX:78:ILE:HG21	1:AX:90:PRO:HG3	1.88	0.55
2:BY:1542:LEU:CB	1:CX:106:LEU:HD11	2.37	0.55
2:GY:1483:ASP:OD1	1:HX:36:ARG:NH2	2.39	0.55
2:DY:1543:LEU:HD23	2:DY:1544:PRO:O	2.07	0.55
2:HY:1532:PHE:CE1	1:IX:275:ALA:HB2	2.41	0.55
2:LY:1542:LEU:CB	1:MX:106:LEU:HD11	2.36	0.55
1:JX:89:VAL:HG12	1:JX:91:ASN:OD1	2.07	0.55
2:EY:1544:PRO:CG	1:FX:269:LEU:HD12	2.37	0.54
1:LX:111:GLU:OE1	1:LX:111:GLU:N	2.35	0.54
2:OY:1545:MET:HB3	1:PX:107:MET:HE1	1.87	0.54
2:BY:1483:ASP:OD1	1:CX:36:ARG:NH2	2.39	0.54
1:FX:59:THR:HG22	1:FX:65:THR:CB	2.37	0.54
1:KX:61:LEU:HD12	1:KX:61:LEU:H	1.72	0.54
2:PY:1495:GLU:OE1	2:PY:1506:ARG:NH2	2.40	0.54
2:DY:1498:LEU:O	2:DY:1506:ARG:NH1	2.41	0.54
2:JY:1542:LEU:CB	1:KX:106:LEU:HD11	2.36	0.54
2:NY:1532:PHE:CZ	1:OX:275:ALA:HB2	2.42	0.54
1:LX:78:ILE:HD11	1:LX:88:ILE:HG21	1.89	0.54
2:GY:1538:LYS:HD2	2:GY:1538:LYS:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:OY:1495:GLU:OE1	2:OY:1506:ARG:NH2	2.40	0.54
1:EX:109:GLU:OE1	1:EX:109:GLU:N	2.38	0.54
2:GY:1542:LEU:CB	1:HX:106:LEU:HD11	2.37	0.54
1:AX:67:ILE:HD11	1:AX:97:ILE:HD13	1.90	0.54
1:HX:57:ILE:CD1	1:HX:308:VAL:HG11	2.37	0.54
1:FX:59:THR:HG22	1:FX:65:THR:OG1	2.08	0.54
1:EX:87:SER:OG	1:EX:100:LYS:NZ	2.32	0.53
2:JY:1536:ALA:HB2	2:JY:1543:LEU:HD11	1.90	0.53
2:FY:1532:PHE:CZ	1:GX:275:ALA:HB2	2.43	0.53
2:IY:1542:LEU:CB	1:JX:106:LEU:HD11	2.38	0.53
1:PX:57:ILE:CD1	1:PX:308:VAL:HG11	2.38	0.53
1:AX:269:LEU:HD12	2:QY:1544:PRO:HG2	1.90	0.53
1:BX:78:ILE:HD11	1:BX:88:ILE:HG21	1.88	0.53
1:EX:89:VAL:HG12	1:EX:91:ASN:OD1	2.08	0.53
1:HX:85:GLY:O	1:HX:276:TRP:NE1	2.39	0.53
2:QY:1543:LEU:HD23	2:QY:1544:PRO:O	2.09	0.53
1:BX:67:ILE:HD11	1:BX:97:ILE:HD13	1.91	0.53
1:IX:39:VAL:HG21	1:IX:296:ALA:CB	2.36	0.53
1:OX:51:ASP:O	1:PX:43:ASN:ND2	2.42	0.53
1:NX:41:VAL:CG2	1:NX:306:LEU:HD13	2.38	0.53
1:NX:67:ILE:HD11	1:NX:97:ILE:HD13	1.91	0.53
1:PX:109:GLU:N	1:PX:109:GLU:OE1	2.37	0.53
2:AY:1495:GLU:OE1	2:AY:1506:ARG:NH2	2.40	0.52
1:NX:39:VAL:HG21	1:NX:296:ALA:CB	2.39	0.52
1:KX:111:GLU:OE1	1:KX:111:GLU:N	2.34	0.52
2:MY:1545:MET:HB3	1:NX:107:MET:HE1	1.91	0.52
1:NX:46:ILE:O	1:NX:311:GLU:N	2.39	0.52
1:PX:89:VAL:HG12	1:PX:91:ASN:OD1	2.10	0.52
2:PY:1532:PHE:CE1	1:QX:275:ALA:HB2	2.45	0.52
1:DX:39:VAL:HG21	1:DX:296:ALA:CB	2.39	0.52
2:LY:1523:TYR:OH	1:MX:62:ASP:OD1	2.28	0.52
1:EX:108:PHE:O	2:EY:1526:LEU:HD11	2.09	0.52
2:LY:1538:LYS:HD2	2:LY:1538:LYS:O	2.09	0.52
1:AX:274:SER:OG	2:QY:1533:ASP:OD2	2.24	0.52
2:DY:1525:GLU:OE2	2:DY:1526:LEU:HD22	2.10	0.52
2:EY:1542:LEU:CB	1:FX:106:LEU:HD11	2.39	0.52
1:OX:46:ILE:O	1:OX:311:GLU:N	2.38	0.52
1:BX:282:VAL:O	1:BX:288:LEU:HD12	2.10	0.52
1:EX:51:ASP:O	1:FX:43:ASN:ND2	2.43	0.52
1:OX:57:ILE:CD1	1:OX:308:VAL:HG11	2.39	0.52
1:GX:67:ILE:HD11	1:GX:97:ILE:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GX:276:TRP:HB2	1:GX:295:ILE:HD11	1.92	0.51
2:JY:1532:PHE:CE2	1:KX:275:ALA:HB2	2.45	0.51
1:DX:78:ILE:HD11	1:DX:88:ILE:HG21	1.92	0.51
2:OY:1498:LEU:O	2:OY:1506:ARG:NH1	2.43	0.51
1:GX:290:GLN:HE21	1:HX:307:THR:HG1	1.57	0.51
1:KX:78:ILE:HD11	1:KX:88:ILE:HG21	1.93	0.51
1:LX:261:SER:OG	1:LX:263:GLU:OE2	2.26	0.51
2:PY:1532:PHE:CZ	1:QX:275:ALA:HB2	2.46	0.51
2:IY:1498:LEU:O	2:IY:1506:ARG:NH1	2.43	0.51
1:OX:78:ILE:HD11	1:OX:88:ILE:HG21	1.91	0.51
2:DY:1532:PHE:CE1	1:EX:275:ALA:HB2	2.46	0.51
1:EX:105:ASN:OD1	1:EX:106:LEU:N	2.43	0.51
2:OY:1475:LEU:HD11	2:OY:1509:ILE:HG12	1.93	0.51
1:BX:87:SER:OG	1:BX:100:LYS:NZ	2.31	0.51
1:NX:78:ILE:HD11	1:NX:88:ILE:HG21	1.93	0.51
1:GX:57:ILE:CD1	1:GX:308:VAL:HG11	2.41	0.51
2:GY:1532:PHE:CE1	1:HX:275:ALA:HB2	2.46	0.51
1:AX:314:GLN:OE1	1:AX:314:GLN:N	2.40	0.51
2:PY:1542:LEU:HB3	1:QX:106:LEU:HD11	1.93	0.51
1:LX:87:SER:OG	1:LX:100:LYS:NZ	2.31	0.50
2:BY:1495:GLU:OE1	2:BY:1506:ARG:NH2	2.43	0.50
2:CY:1469:LEU:HD21	2:CY:1474:ARG:HG3	1.93	0.50
1:BX:61:LEU:H	1:BX:61:LEU:HD12	1.75	0.50
1:BX:280:LEU:HD12	1:BX:293:LEU:HD11	1.91	0.50
1:HX:61:LEU:HD12	1:HX:61:LEU:H	1.76	0.50
1:IX:89:VAL:HG12	1:IX:91:ASN:OD1	2.10	0.50
2:PY:1544:PRO:HG2	1:QX:269:LEU:HD12	1.94	0.50
1:DX:280:LEU:CD1	1:DX:293:LEU:HD21	2.41	0.50
1:FX:67:ILE:HD11	1:FX:97:ILE:HD13	1.93	0.50
1:HX:314:GLN:O	1:HX:318:VAL:HG23	2.11	0.50
2:PY:1475:LEU:HD21	2:PY:1508:LEU:HD23	1.93	0.50
1:BX:89:VAL:HG12	1:BX:91:ASN:OD1	2.11	0.50
2:BY:1475:LEU:HD21	2:BY:1508:LEU:HD23	1.94	0.50
1:JX:281:VAL:CG1	1:JX:288:LEU:HD11	2.42	0.50
1:GX:59:THR:O	1:GX:296:ALA:N	2.40	0.50
1:GX:61:LEU:H	1:GX:61:LEU:HD12	1.76	0.50
2:HY:1483:ASP:OD1	1:IX:36:ARG:NH2	2.42	0.50
1:KX:276:TRP:HB2	1:KX:295:ILE:HD11	1.92	0.50
1:JX:61:LEU:HD12	1:JX:61:LEU:H	1.77	0.50
2:JY:1523:TYR:OH	1:KX:62:ASP:OD1	2.29	0.50
1:KX:268:GLU:OE1	1:KX:268:GLU:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BY:1544:PRO:HG2	1:CX:269:LEU:HD12	1.93	0.50
1:NX:89:VAL:HG12	1:NX:91:ASN:OD1	2.12	0.50
1:LX:85:GLY:O	1:LX:276:TRP:NE1	2.37	0.49
1:OX:61:LEU:HD12	1:OX:61:LEU:H	1.76	0.49
2:AY:1545:MET:HB3	1:BX:107:MET:HE1	1.93	0.49
2:JY:1498:LEU:O	2:JY:1506:ARG:NH1	2.45	0.49
1:QX:61:LEU:H	1:QX:61:LEU:HD12	1.77	0.49
1:QX:59:THR:HG21	1:QX:97:ILE:HD11	1.93	0.49
1:DX:61:LEU:HD12	1:DX:61:LEU:H	1.76	0.49
1:NX:59:THR:O	1:NX:296:ALA:N	2.39	0.49
2:BY:1474:ARG:NH1	2:BY:1505:GLU:OE2	2.46	0.49
1:FX:89:VAL:HG12	1:FX:91:ASN:OD1	2.11	0.49
1:GX:46:ILE:O	1:GX:311:GLU:N	2.43	0.49
1:EX:39:VAL:HG21	1:EX:296:ALA:CB	2.40	0.49
1:GX:78:ILE:HD11	1:GX:88:ILE:HG21	1.93	0.49
1:IX:276:TRP:HB2	1:IX:295:ILE:HD11	1.95	0.49
1:PX:61:LEU:HD12	1:PX:61:LEU:H	1.76	0.49
1:IX:59:THR:O	1:IX:296:ALA:N	2.40	0.49
2:JY:1544:PRO:HG2	1:KX:269:LEU:HD12	1.95	0.49
1:LX:67:ILE:HD11	1:LX:97:ILE:HD13	1.94	0.49
2:FY:1532:PHE:CE2	1:GX:275:ALA:HB2	2.48	0.48
1:IX:61:LEU:HD12	1:IX:61:LEU:H	1.78	0.48
1:QX:89:VAL:HG12	1:QX:91:ASN:OD1	2.12	0.48
1:QX:107:MET:SD	1:QX:107:MET:N	2.83	0.48
2:KY:1542:LEU:CB	1:LX:106:LEU:HD11	2.43	0.48
2:LY:1474:ARG:NH1	2:LY:1505:GLU:OE2	2.47	0.48
1:PX:288:LEU:HD23	1:PX:289:TYR:N	2.28	0.48
2:EY:1544:PRO:HG2	1:FX:269:LEU:HD12	1.95	0.48
2:AY:1532:PHE:CE1	1:BX:275:ALA:HB2	2.49	0.48
1:CX:89:VAL:HG12	1:CX:91:ASN:OD1	2.13	0.48
1:CX:276:TRP:HB2	1:CX:295:ILE:HD11	1.95	0.48
1:PX:33:ASN:OD1	1:PX:34:PHE:N	2.46	0.48
1:FX:61:LEU:HD12	1:FX:61:LEU:H	1.78	0.48
1:OX:33:ASN:OD1	1:OX:34:PHE:N	2.47	0.48
1:AX:57:ILE:CD1	1:AX:308:VAL:HG11	2.43	0.48
1:HX:57:ILE:HD13	1:HX:308:VAL:HG11	1.96	0.48
1:MX:314:GLN:OE1	1:MX:314:GLN:N	2.36	0.48
2:MY:1483:ASP:OD1	1:NX:36:ARG:NH2	2.47	0.48
1:OX:89:VAL:HG12	1:OX:91:ASN:OD1	2.14	0.48
1:PX:78:ILE:HD11	1:PX:88:ILE:HG21	1.94	0.48
1:AX:85:GLY:O	1:AX:276:TRP:NE1	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HX:41:VAL:HG21	1:HX:306:LEU:HD13	1.95	0.48
2:OY:1542:LEU:HB2	1:PX:106:LEU:HD11	1.96	0.48
1:CX:67:ILE:HD11	1:CX:97:ILE:HD13	1.95	0.47
2:JY:1542:LEU:HB2	1:KX:106:LEU:HD11	1.96	0.47
1:CX:281:VAL:HG13	1:CX:288:LEU:HD11	1.95	0.47
2:DY:1523:TYR:OH	1:EX:62:ASP:OD1	2.31	0.47
1:DX:120:ARG:NE	1:DX:124:GLU:OE2	2.48	0.47
2:EY:1536:ALA:HB2	2:EY:1543:LEU:HD11	1.96	0.47
1:HX:41:VAL:CG2	1:HX:306:LEU:HD13	2.44	0.47
1:MX:61:LEU:HD12	1:MX:61:LEU:H	1.79	0.47
1:CX:281:VAL:CG1	1:CX:288:LEU:HD11	2.44	0.47
1:BX:39:VAL:HG21	1:BX:296:ALA:CB	2.42	0.47
2:FY:1474:ARG:NH1	2:FY:1505:GLU:OE2	2.48	0.47
2:HY:1532:PHE:CZ	1:IX:275:ALA:HB2	2.49	0.47
1:NX:41:VAL:HG21	1:NX:306:LEU:HD13	1.96	0.47
1:OX:85:GLY:O	1:OX:276:TRP:NE1	2.39	0.47
1:AX:272:SER:C	1:AX:295:ILE:HD12	2.39	0.47
2:BY:1542:LEU:HB3	1:CX:106:LEU:HD11	1.97	0.47
1:CX:61:LEU:HD12	1:CX:61:LEU:H	1.80	0.47
1:DX:113:VAL:O	1:DX:117:LEU:HD13	2.15	0.47
2:DY:1533:ASP:OD2	1:EX:274:SER:OG	2.30	0.47
1:GX:86:TRP:CH2	1:GX:293:LEU:HB3	2.49	0.47
1:KX:108:PHE:O	2:KY:1526:LEU:HD11	2.15	0.47
1:KX:109:GLU:OE1	1:KX:109:GLU:N	2.40	0.47
1:NX:276:TRP:HB2	1:NX:295:ILE:HD11	1.97	0.47
1:OX:280:LEU:N	1:OX:291:PHE:O	2.48	0.47
2:OY:1523:TYR:OH	1:PX:62:ASP:OD1	2.32	0.47
1:BX:272:SER:C	1:BX:295:ILE:HD12	2.40	0.47
1:EX:61:LEU:H	1:EX:61:LEU:HD12	1.80	0.47
2:EY:1474:ARG:NH1	2:EY:1505:GLU:OE2	2.48	0.47
1:JX:33:ASN:OD1	1:JX:34:PHE:N	2.48	0.47
2:NY:1542:LEU:HB2	1:OX:106:LEU:HD11	1.96	0.47
1:AX:108:PHE:O	2:AY:1526:LEU:HD11	2.15	0.47
2:EY:1483:ASP:OD1	1:FX:36:ARG:NH2	2.48	0.47
2:GY:1542:LEU:HD13	1:HX:262:PRO:HB3	1.97	0.47
1:IX:85:GLY:O	1:IX:276:TRP:NE1	2.41	0.47
1:NX:281:VAL:HG22	1:NX:290:GLN:OE1	2.15	0.47
1:LX:61:LEU:H	1:LX:61:LEU:HD12	1.81	0.46
1:PX:268:GLU:N	1:PX:268:GLU:OE2	2.48	0.46
2:IY:1495:GLU:OE1	2:IY:1506:ARG:NH2	2.49	0.46
1:AX:59:THR:O	1:AX:296:ALA:N	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AX:106:LEU:HD11	2:QY:1542:LEU:HB2	1.98	0.46
1:BX:108:PHE:O	2:BY:1526:LEU:HD11	2.16	0.46
2:OY:1527:ARG:NE	1:PX:62:ASP:OD2	2.48	0.46
1:CX:39:VAL:HG21	1:CX:296:ALA:CB	2.45	0.46
1:HX:87:SER:OG	1:HX:100:LYS:NZ	2.31	0.46
1:LX:41:VAL:HG21	1:LX:306:LEU:HD13	1.97	0.46
2:LY:1472:THR:HG23	2:LY:1473:GLU:N	2.31	0.46
1:QX:59:THR:O	1:QX:296:ALA:N	2.42	0.46
1:AX:89:VAL:HG12	1:AX:91:ASN:OD1	2.15	0.46
2:KY:1542:LEU:HB2	1:LX:106:LEU:HD11	1.97	0.46
1:LX:272:SER:C	1:LX:295:ILE:HD12	2.41	0.46
1:FX:78:ILE:HD11	1:FX:88:ILE:HG21	1.97	0.46
1:GX:276:TRP:CB	1:GX:295:ILE:HD11	2.44	0.46
1:IX:280:LEU:N	1:IX:291:PHE:O	2.48	0.46
1:JX:290:GLN:NE2	1:KX:307:THR:OG1	2.49	0.46
1:DX:317:GLU:N	1:DX:317:GLU:OE1	2.49	0.46
2:GY:1472:THR:HG23	2:GY:1473:GLU:N	2.31	0.46
1:JX:87:SER:OG	1:JX:100:LYS:NZ	2.38	0.46
1:PX:64:VAL:O	1:PX:64:VAL:HG13	2.15	0.46
1:QX:87:SER:OG	1:QX:100:LYS:NZ	2.29	0.46
1:FX:39:VAL:HG21	1:FX:296:ALA:CB	2.42	0.46
2:IY:1472:THR:HG23	2:IY:1473:GLU:N	2.31	0.46
1:NX:85:GLY:O	1:NX:276:TRP:NE1	2.42	0.46
2:AY:1469:LEU:HD23	2:AY:1474:ARG:HG3	1.98	0.45
1:DX:268:GLU:CD	1:DX:268:GLU:H	2.24	0.45
2:GY:1542:LEU:HB3	1:HX:106:LEU:HD11	1.97	0.45
2:IY:1532:PHE:CZ	1:JX:275:ALA:HB2	2.50	0.45
1:NX:61:LEU:HD12	1:NX:61:LEU:H	1.81	0.45
1:CX:276:TRP:CB	1:CX:295:ILE:HD11	2.45	0.45
1:NX:39:VAL:HG11	1:NX:304:ALA:HB2	1.97	0.45
2:AY:1544:PRO:HG2	1:BX:269:LEU:HD12	1.99	0.45
2:FY:1472:THR:HG23	2:FY:1473:GLU:N	2.32	0.45
1:LX:48:TYR:HB2	1:LX:310:LEU:HD22	1.98	0.45
2:QY:1536:ALA:HB2	2:QY:1543:LEU:HD11	1.97	0.45
1:BX:41:VAL:HG21	1:BX:306:LEU:HD13	1.99	0.45
2:JY:1545:MET:HB3	1:KX:107:MET:HE1	1.99	0.45
1:KX:89:VAL:HG12	1:KX:91:ASN:OD1	2.17	0.45
2:LY:1542:LEU:HB2	1:MX:106:LEU:HD11	1.97	0.45
1:AX:61:LEU:HD12	1:AX:61:LEU:H	1.82	0.45
2:DY:1542:LEU:HB2	1:EX:106:LEU:HD11	1.99	0.45
2:EY:1472:THR:HG23	2:EY:1473:GLU:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EY:1532:PHE:CE1	1:FX:275:ALA:HB2	2.51	0.45
2:GY:1474:ARG:NH1	2:GY:1505:GLU:OE2	2.49	0.45
1:JX:121:ASP:OD1	1:JX:121:ASP:C	2.60	0.45
1:KX:51:ASP:O	1:LX:43:ASN:ND2	2.49	0.45
2:NY:1532:PHE:CE1	1:OX:275:ALA:HB2	2.52	0.45
2:DY:1472:THR:HG23	2:DY:1473:GLU:N	2.31	0.45
1:OX:67:ILE:HD11	1:OX:97:ILE:HD13	1.98	0.45
2:EY:1469:LEU:HD12	2:EY:1469:LEU:O	2.17	0.45
2:LY:1483:ASP:OD1	1:MX:36:ARG:NH2	2.49	0.45
2:GY:1544:PRO:HG2	1:HX:269:LEU:HD12	1.98	0.45
2:DY:1536:ALA:HB2	2:DY:1543:LEU:HD11	1.99	0.45
1:LX:89:VAL:HG12	1:LX:91:ASN:OD1	2.16	0.45
1:QX:268:GLU:H	1:QX:268:GLU:CD	2.25	0.45
2:EY:1523:TYR:OH	1:FX:62:ASP:OD1	2.31	0.45
1:HX:268:GLU:CD	1:HX:268:GLU:H	2.25	0.45
1:LX:59:THR:O	1:LX:296:ALA:N	2.42	0.45
1:MX:64:VAL:HG13	1:MX:64:VAL:O	2.17	0.45
2:KY:1472:THR:HG23	2:KY:1473:GLU:N	2.33	0.44
1:OX:276:TRP:CB	1:OX:295:ILE:HD11	2.46	0.44
1:HX:89:VAL:HG12	1:HX:91:ASN:OD1	2.18	0.44
2:OY:1472:THR:HG23	2:OY:1473:GLU:N	2.33	0.44
1:GX:87:SER:OG	1:GX:100:LYS:NZ	2.38	0.44
2:IY:1536:ALA:HB2	2:IY:1543:LEU:HD11	1.99	0.44
1:AX:106:LEU:HD11	2:QY:1542:LEU:HB3	1.99	0.44
1:CX:59:THR:HG22	1:CX:65:THR:CB	2.47	0.44
1:BX:41:VAL:CG2	1:BX:306:LEU:HD13	2.48	0.44
2:BY:1525:GLU:OE2	2:BY:1526:LEU:HD22	2.17	0.44
2:HY:1472:THR:HG23	2:HY:1473:GLU:N	2.33	0.44
1:KX:276:TRP:CB	1:KX:295:ILE:HD11	2.48	0.44
2:KY:1483:ASP:OD1	1:LX:36:ARG:NH2	2.50	0.44
1:DX:33:ASN:OD1	1:DX:34:PHE:N	2.50	0.44
2:FY:1495:GLU:OE1	2:FY:1506:ARG:NH2	2.51	0.44
1:IX:105:ASN:OD1	1:IX:106:LEU:N	2.50	0.44
1:LX:39:VAL:HG21	1:LX:296:ALA:CB	2.44	0.44
2:MY:1472:THR:HG23	2:MY:1473:GLU:N	2.33	0.44
1:FX:59:THR:O	1:FX:296:ALA:N	2.45	0.43
1:FX:276:TRP:CB	1:FX:295:ILE:HD11	2.48	0.43
1:IX:314:GLN:O	1:IX:318:VAL:HG23	2.18	0.43
1:KX:268:GLU:H	1:KX:268:GLU:CD	2.26	0.43
1:MX:109:GLU:OE2	1:MX:109:GLU:N	2.37	0.43
1:NX:64:VAL:O	1:NX:64:VAL:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EY:1495:GLU:OE1	2:EY:1506:ARG:NH2	2.50	0.43
1:NX:103:LYS:NZ	1:NX:266:SER:OG	2.34	0.43
1:NX:288:LEU:HD23	1:NX:289:TYR:N	2.33	0.43
1:LX:59:THR:HG22	1:LX:65:THR:CB	2.48	0.43
2:NY:1472:THR:HG23	2:NY:1473:GLU:N	2.33	0.43
1:BX:290:GLN:NE2	1:CX:307:THR:OG1	2.51	0.43
2:DY:1544:PRO:HG2	1:EX:269:LEU:HD12	2.01	0.43
2:FY:1545:MET:HB3	1:GX:107:MET:HE1	2.00	0.43
2:JY:1472:THR:HG23	2:JY:1473:GLU:N	2.33	0.43
2:PY:1483:ASP:OD1	1:QX:36:ARG:NH2	2.51	0.43
2:QY:1472:THR:HG23	2:QY:1473:GLU:N	2.33	0.43
1:AX:43:ASN:ND2	1:QX:51:ASP:O	2.52	0.43
2:AY:1483:ASP:OD1	1:BX:36:ARG:NH2	2.52	0.43
1:GX:59:THR:HG22	1:GX:65:THR:CB	2.49	0.43
1:GX:89:VAL:HG12	1:GX:91:ASN:OD1	2.19	0.43
2:IY:1532:PHE:HZ	1:JX:274:SER:HG	1.65	0.43
1:LX:41:VAL:CG2	1:LX:306:LEU:HD13	2.48	0.43
2:MY:1542:LEU:CB	1:NX:106:LEU:HD11	2.49	0.43
1:AX:106:LEU:HD12	2:QY:1543:LEU:C	2.44	0.43
1:BX:64:VAL:O	1:BX:64:VAL:HG13	2.18	0.43
1:EX:268:GLU:OE2	1:EX:268:GLU:N	2.49	0.43
1:NX:305:TYR:HB2	1:NX:308:VAL:HG22	2.00	0.43
1:BX:59:THR:HG22	1:BX:65:THR:CB	2.47	0.43
1:EX:268:GLU:H	1:EX:268:GLU:CD	2.27	0.43
1:IX:33:ASN:OD1	1:IX:34:PHE:N	2.52	0.43
1:PX:268:GLU:CD	1:PX:268:GLU:H	2.27	0.43
1:CX:87:SER:OG	1:CX:100:LYS:NZ	2.35	0.43
2:DY:1531:THR:N	1:EX:270:SER:OG	2.52	0.43
1:JX:64:VAL:O	1:JX:64:VAL:HG13	2.19	0.43
1:KX:33:ASN:OD1	1:KX:34:PHE:N	2.51	0.43
1:AX:109:GLU:O	2:AY:1529:ARG:NH2	2.52	0.43
1:BX:315:ARG:O	1:BX:318:VAL:HG12	2.19	0.43
2:DY:1533:ASP:OD1	1:EX:272:SER:OG	2.34	0.43
1:FX:110:LYS:O	2:FY:1529:ARG:NH2	2.51	0.43
1:AX:272:SER:OG	2:QY:1533:ASP:OD1	2.36	0.42
2:CY:1545:MET:HB3	1:DX:107:MET:HE1	2.00	0.42
1:EX:64:VAL:HG13	1:EX:64:VAL:O	2.19	0.42
2:IY:1474:ARG:NH1	2:IY:1505:GLU:OE2	2.52	0.42
1:JX:41:VAL:HG21	1:JX:306:LEU:HD13	2.01	0.42
1:KX:85:GLY:O	1:KX:276:TRP:NE1	2.41	0.42
1:BX:59:THR:HG22	1:BX:65:THR:OG1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BY:1532:PHE:CE1	1:CX:275:ALA:HB2	2.54	0.42
1:FX:288:LEU:HD23	1:FX:289:TYR:N	2.35	0.42
1:GX:43:ASN:OD1	1:GX:43:ASN:C	2.62	0.42
1:HX:281:VAL:CG1	1:HX:288:LEU:HD11	2.50	0.42
2:OY:1543:LEU:HD23	2:OY:1544:PRO:HD2	2.00	0.42
1:AX:101:SER:O	1:AX:101:SER:OG	2.36	0.42
1:DX:288:LEU:HD23	1:DX:289:TYR:N	2.35	0.42
2:MY:1536:ALA:HB3	2:NY:1519:VAL:HG22	2.01	0.42
1:NX:280:LEU:CD2	1:NX:282:VAL:HG23	2.48	0.42
2:NY:1495:GLU:OE1	2:NY:1506:ARG:NH2	2.50	0.42
1:OX:276:TRP:HB2	1:OX:295:ILE:HD11	2.02	0.42
1:AX:94:HIS:ND1	1:QX:283:ARG:HD2	2.34	0.42
1:BX:78:ILE:HG21	1:BX:90:PRO:HG3	2.01	0.42
1:DX:64:VAL:O	1:DX:64:VAL:HG13	2.19	0.42
1:JX:272:SER:C	1:JX:295:ILE:HD12	2.45	0.42
1:OX:279:ASN:ND2	1:OX:290:GLN:OE1	2.43	0.42
1:CX:64:VAL:O	1:CX:64:VAL:HG13	2.19	0.42
2:CY:1532:PHE:CE1	1:DX:275:ALA:HB2	2.55	0.42
1:HX:66:VAL:HG12	1:HX:306:LEU:O	2.20	0.42
2:HY:1532:PHE:HA	2:HY:1535:MET:HE3	2.01	0.42
1:LX:63:ASN:OD1	1:LX:64:VAL:N	2.53	0.42
1:OX:57:ILE:HD13	1:OX:308:VAL:HG11	2.00	0.42
2:OY:1475:LEU:HD21	2:OY:1508:LEU:HD23	2.02	0.42
1:QX:59:THR:HG22	1:QX:65:THR:HG21	2.01	0.42
1:AX:62:ASP:OD1	2:QY:1523:TYR:OH	2.36	0.42
2:CY:1544:PRO:CG	1:DX:269:LEU:HD12	2.50	0.42
1:DX:46:ILE:HB	1:DX:310:LEU:HD23	2.01	0.42
1:EX:33:ASN:OD1	1:EX:34:PHE:N	2.52	0.42
2:EY:1542:LEU:C	1:FX:106:LEU:HD11	2.44	0.42
2:GY:1542:LEU:HB2	1:HX:106:LEU:HD11	2.02	0.42
1:OX:43:ASN:OD1	1:OX:43:ASN:C	2.63	0.42
2:OY:1544:PRO:HG2	1:PX:269:LEU:HD12	2.01	0.42
2:AY:1472:THR:HG23	2:AY:1473:GLU:N	2.34	0.42
2:AY:1543:LEU:HD23	2:AY:1544:PRO:O	2.20	0.42
1:BX:281:VAL:HG12	1:BX:288:LEU:HD11	2.01	0.42
2:DY:1527:ARG:HE	1:EX:61:LEU:HB2	1.85	0.42
1:JX:283:ARG:NH1	1:KX:92:SER:OG	2.53	0.42
2:JY:1532:PHE:CZ	1:KX:275:ALA:HB2	2.55	0.42
1:KX:88:ILE:CD1	1:KX:97:ILE:HG22	2.49	0.42
1:PX:276:TRP:HB2	1:PX:295:ILE:HD11	2.01	0.42
2:BY:1541:PRO:O	2:BY:1542:LEU:HD23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CY:1542:LEU:HD11	1:DX:262:PRO:CB	2.47	0.42
1:DX:108:PHE:O	2:DY:1526:LEU:HD11	2.20	0.42
1:GX:39:VAL:HG21	1:GX:296:ALA:HB1	2.02	0.42
2:HY:1542:LEU:CB	1:IX:106:LEU:HD11	2.50	0.42
2:JY:1533:ASP:OD1	2:JY:1533:ASP:N	2.52	0.42
2:MY:1536:ALA:HB2	2:MY:1543:LEU:HD11	2.01	0.42
1:QX:46:ILE:O	1:QX:311:GLU:N	2.43	0.42
1:AX:121:ASP:OD2	1:AX:121:ASP:C	2.63	0.42
1:BX:46:ILE:O	1:BX:311:GLU:N	2.46	0.42
1:FX:33:ASN:OD1	1:FX:34:PHE:N	2.53	0.42
1:IX:43:ASN:OD1	1:IX:43:ASN:C	2.63	0.42
1:IX:69:LEU:HD13	1:IX:95:ILE:HD12	2.02	0.42
2:IY:1542:LEU:HB3	1:JX:106:LEU:HD11	2.01	0.42
1:JX:59:THR:HG22	1:JX:65:THR:CB	2.49	0.42
1:JX:69:LEU:HD13	1:JX:95:ILE:HD12	2.01	0.42
2:BY:1472:THR:HG23	2:BY:1473:GLU:N	2.35	0.41
1:DX:59:THR:O	1:DX:296:ALA:N	2.45	0.41
1:GX:63:ASN:OD1	1:GX:64:VAL:N	2.53	0.41
1:HX:39:VAL:HG21	1:HX:296:ALA:CB	2.47	0.41
1:NX:57:ILE:O	1:NX:294:ARG:N	2.43	0.41
1:OX:64:VAL:O	1:OX:64:VAL:HG13	2.20	0.41
1:QX:64:VAL:O	1:QX:64:VAL:HG13	2.20	0.41
1:AX:43:ASN:C	1:AX:43:ASN:OD1	2.64	0.41
2:AY:1536:ALA:HB2	2:AY:1543:LEU:HD11	2.02	0.41
1:FX:59:THR:HG21	1:FX:97:ILE:HD11	2.02	0.41
1:MX:78:ILE:HD11	1:MX:88:ILE:HG21	2.01	0.41
1:QX:264:ASP:O	1:QX:266:SER:N	2.53	0.41
1:CX:278:THR:HG22	1:CX:279:ASN:N	2.35	0.41
1:HX:272:SER:C	1:HX:295:ILE:HD12	2.45	0.41
1:KX:64:VAL:O	1:KX:64:VAL:HG13	2.20	0.41
1:GX:261:SER:N	1:GX:262:PRO:CD	2.84	0.41
1:IX:64:VAL:O	1:IX:64:VAL:HG13	2.20	0.41
2:MY:1469:LEU:HD21	2:MY:1474:ARG:HG3	2.02	0.41
1:AX:59:THR:HG22	1:AX:65:THR:CB	2.50	0.41
2:AY:1485:LEU:HD21	2:AY:1493:ALA:HB1	2.03	0.41
1:LX:59:THR:HG21	1:LX:97:ILE:HD11	2.01	0.41
1:NX:314:GLN:O	1:NX:318:VAL:HG23	2.21	0.41
2:QY:1538:LYS:HD2	2:QY:1538:LYS:O	2.19	0.41
2:EY:1542:LEU:HB2	1:FX:106:LEU:HD11	2.01	0.41
1:HX:64:VAL:O	1:HX:64:VAL:HG13	2.21	0.41
1:CX:63:ASN:OD1	1:CX:64:VAL:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CY:1472:THR:HG23	2:CY:1473:GLU:N	2.35	0.41
2:EY:1531:THR:N	1:FX:270:SER:OG	2.54	0.41
1:FX:78:ILE:HG21	1:FX:90:PRO:HG3	2.02	0.41
2:JY:1536:ALA:HB3	2:KY:1519:VAL:HG22	2.03	0.41
1:BX:121:ASP:OD2	1:BX:121:ASP:C	2.64	0.41
1:EX:63:ASN:OD1	1:EX:64:VAL:N	2.54	0.41
1:FX:78:ILE:HG13	1:FX:280:LEU:HD11	2.03	0.41
1:HX:268:GLU:OE2	1:HX:268:GLU:N	2.51	0.41
1:IX:265:ASN:OD1	1:IX:265:ASN:O	2.38	0.41
1:JX:41:VAL:CG2	1:JX:306:LEU:HD13	2.51	0.41
1:LX:43:ASN:OD1	1:LX:43:ASN:C	2.64	0.41
1:LX:64:VAL:O	1:LX:64:VAL:HG13	2.21	0.41
1:LX:108:PHE:O	2:LY:1526:LEU:HD11	2.21	0.41
2:LY:1532:PHE:CE1	1:MX:275:ALA:HB2	2.56	0.41
2:LY:1544:PRO:HG2	1:MX:269:LEU:HD12	2.03	0.41
1:BX:305:TYR:CB	1:BX:308:VAL:HG22	2.51	0.41
2:BY:1536:ALA:HB3	2:CY:1519:VAL:HG22	2.01	0.41
1:LX:46:ILE:O	1:LX:311:GLU:N	2.45	0.41
2:NY:1545:MET:HG2	1:OX:107:MET:HE1	2.03	0.41
1:BX:281:VAL:CG1	1:BX:288:LEU:HD11	2.51	0.40
1:CX:59:THR:HG22	1:CX:65:THR:OG1	2.21	0.40
1:DX:276:TRP:CB	1:DX:295:ILE:HD11	2.51	0.40
1:IX:69:LEU:O	1:IX:93:ASN:ND2	2.52	0.40
1:KX:280:LEU:N	1:KX:291:PHE:O	2.55	0.40
1:MX:281:VAL:CG1	1:MX:288:LEU:HD11	2.50	0.40
2:NY:1542:LEU:HB3	1:OX:106:LEU:HD11	2.03	0.40
1:BX:318:VAL:O	1:BX:318:VAL:HG22	2.20	0.40
1:CX:273:ASP:OD2	1:CX:294:ARG:NH2	2.48	0.40
1:GX:59:THR:HG22	1:GX:65:THR:OG1	2.21	0.40
1:QX:272:SER:C	1:QX:295:ILE:HD12	2.46	0.40
1:AX:284:THR:HG21	1:AX:289:TYR:CE1	2.56	0.40
1:EX:278:THR:HG22	1:EX:279:ASN:N	2.37	0.40
1:KX:43:ASN:C	1:KX:43:ASN:OD1	2.64	0.40
2:PY:1472:THR:HG23	2:PY:1473:GLU:N	2.36	0.40
1:EX:69:LEU:HD13	1:EX:95:ILE:HD12	2.03	0.40
1:LX:65:THR:HG23	1:LX:305:TYR:O	2.22	0.40
1:NX:57:ILE:CD1	1:NX:308:VAL:HG11	2.52	0.40
2:NY:1544:PRO:HG2	1:OX:269:LEU:HD12	2.04	0.40
1:QX:63:ASN:OD1	1:QX:64:VAL:N	2.55	0.40
1:DX:63:ASN:OD1	1:DX:64:VAL:N	2.54	0.40
1:MX:41:VAL:HG21	1:MX:306:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NX:305:TYR:CB	1:NX:308:VAL:HG22	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AX	150/495 (30%)	140 (93%)	10 (7%)	0	100	100
1	BX	150/495 (30%)	140 (93%)	10 (7%)	0	100	100
1	CX	150/495 (30%)	143 (95%)	7 (5%)	0	100	100
1	DX	150/495 (30%)	139 (93%)	11 (7%)	0	100	100
1	EX	150/495 (30%)	141 (94%)	9 (6%)	0	100	100
1	FX	150/495 (30%)	143 (95%)	7 (5%)	0	100	100
1	GX	150/495 (30%)	140 (93%)	10 (7%)	0	100	100
1	HX	150/495 (30%)	138 (92%)	12 (8%)	0	100	100
1	IX	150/495 (30%)	142 (95%)	8 (5%)	0	100	100
1	JX	150/495 (30%)	141 (94%)	9 (6%)	0	100	100
1	KX	150/495 (30%)	141 (94%)	9 (6%)	0	100	100
1	LX	150/495 (30%)	141 (94%)	9 (6%)	0	100	100
1	MX	150/495 (30%)	142 (95%)	8 (5%)	0	100	100
1	NX	150/495 (30%)	142 (95%)	8 (5%)	0	100	100
1	OX	150/495 (30%)	138 (92%)	12 (8%)	0	100	100
1	PX	150/495 (30%)	141 (94%)	9 (6%)	0	100	100
1	QX	150/495 (30%)	138 (92%)	12 (8%)	0	100	100
2	AY	75/441 (17%)	72 (96%)	3 (4%)	0	100	100
2	BY	75/441 (17%)	72 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	CY	75/441 (17%)	72 (96%)	3 (4%)	0	100	100
2	DY	75/441 (17%)	74 (99%)	1 (1%)	0	100	100
2	EY	75/441 (17%)	73 (97%)	2 (3%)	0	100	100
2	FY	75/441 (17%)	74 (99%)	1 (1%)	0	100	100
2	GY	75/441 (17%)	74 (99%)	1 (1%)	0	100	100
2	HY	75/441 (17%)	74 (99%)	1 (1%)	0	100	100
2	IY	75/441 (17%)	74 (99%)	1 (1%)	0	100	100
2	JY	75/441 (17%)	74 (99%)	1 (1%)	0	100	100
2	KY	75/441 (17%)	74 (99%)	1 (1%)	0	100	100
2	LY	75/441 (17%)	73 (97%)	2 (3%)	0	100	100
2	MY	75/441 (17%)	74 (99%)	1 (1%)	0	100	100
2	NY	75/441 (17%)	73 (97%)	2 (3%)	0	100	100
2	OY	75/441 (17%)	74 (99%)	1 (1%)	0	100	100
2	PY	75/441 (17%)	73 (97%)	2 (3%)	0	100	100
2	QY	75/441 (17%)	75 (100%)	0	0	100	100
All	All	3825/15912 (24%)	3639 (95%)	186 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AX	142/451 (32%)	142 (100%)	0	100	100
1	BX	142/451 (32%)	142 (100%)	0	100	100
1	CX	142/451 (32%)	142 (100%)	0	100	100
1	DX	142/451 (32%)	142 (100%)	0	100	100
1	EX	142/451 (32%)	142 (100%)	0	100	100
1	FX	142/451 (32%)	142 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	GX	142/451 (32%)	141 (99%)	1 (1%)	76	88
1	HX	142/451 (32%)	142 (100%)	0	100	100
1	IX	142/451 (32%)	142 (100%)	0	100	100
1	JX	142/451 (32%)	142 (100%)	0	100	100
1	KX	142/451 (32%)	142 (100%)	0	100	100
1	LX	142/451 (32%)	142 (100%)	0	100	100
1	MX	142/451 (32%)	142 (100%)	0	100	100
1	NX	142/451 (32%)	142 (100%)	0	100	100
1	OX	142/451 (32%)	141 (99%)	1 (1%)	76	88
1	PX	142/451 (32%)	142 (100%)	0	100	100
1	QX	142/451 (32%)	142 (100%)	0	100	100
2	AY	68/371 (18%)	68 (100%)	0	100	100
2	BY	68/371 (18%)	68 (100%)	0	100	100
2	CY	68/371 (18%)	68 (100%)	0	100	100
2	DY	68/371 (18%)	68 (100%)	0	100	100
2	EY	68/371 (18%)	68 (100%)	0	100	100
2	FY	68/371 (18%)	67 (98%)	1 (2%)	57	78
2	GY	68/371 (18%)	68 (100%)	0	100	100
2	HY	68/371 (18%)	68 (100%)	0	100	100
2	IY	68/371 (18%)	68 (100%)	0	100	100
2	JY	68/371 (18%)	68 (100%)	0	100	100
2	KY	68/371 (18%)	68 (100%)	0	100	100
2	LY	68/371 (18%)	68 (100%)	0	100	100
2	MY	68/371 (18%)	68 (100%)	0	100	100
2	NY	68/371 (18%)	68 (100%)	0	100	100
2	OY	68/371 (18%)	68 (100%)	0	100	100
2	PY	68/371 (18%)	68 (100%)	0	100	100
2	QY	68/371 (18%)	68 (100%)	0	100	100
All	All	3570/13974 (26%)	3567 (100%)	3 (0%)	87	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	FY	1483	ASP
1	GX	283	ARG
1	OX	83	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	BX	68	GLN
1	BX	98	GLN
1	BX	114	ASN
1	BX	314	GLN
2	BY	1534	ASN
1	CX	114	ASN
2	CY	1484	ASN
1	DX	98	GLN
1	DX	297	GLN
1	EX	114	ASN
1	EX	123	GLN
1	EX	265	ASN
1	GX	114	ASN
1	HX	114	ASN
1	IX	94	HIS
1	IX	114	ASN
1	JX	83	ASN
1	JX	285	ASN
1	KX	114	ASN
1	LX	94	HIS
1	LX	98	GLN
1	LX	114	ASN
1	MX	98	GLN
1	NX	114	ASN
1	OX	98	GLN
1	OX	114	ASN
1	OX	297	GLN
1	PX	98	GLN
1	PX	114	ASN
1	PX	314	GLN
1	PX	316	HIS
1	QX	114	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

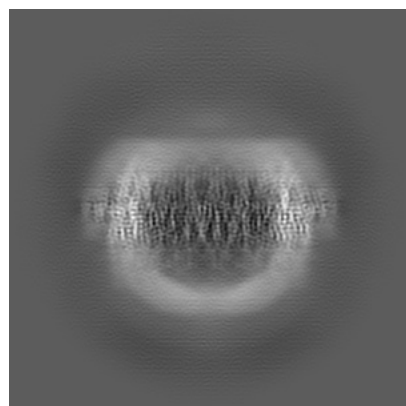
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65048. These allow visual inspection of the internal detail of the map and identification of artifacts.

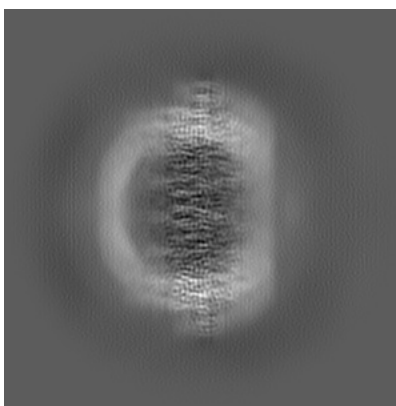
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

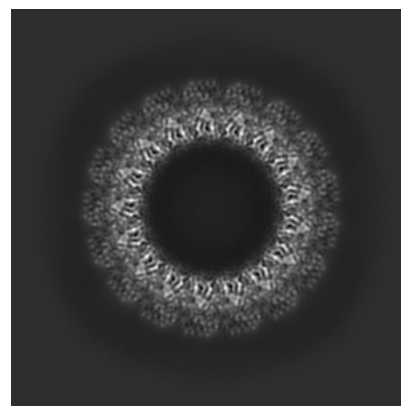
6.1.1 Primary map



X

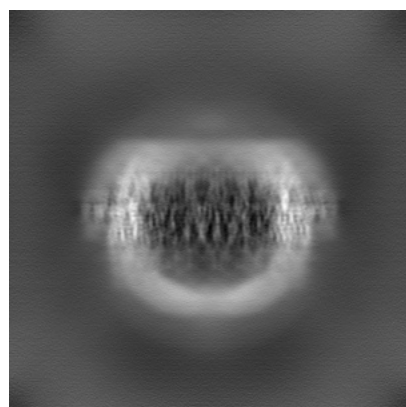


Y

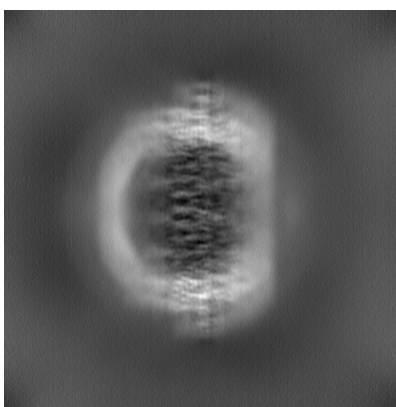


Z

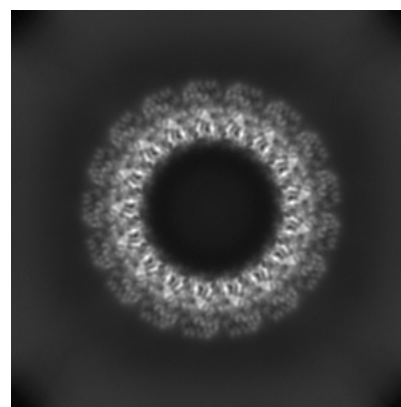
6.1.2 Raw map



X



Y

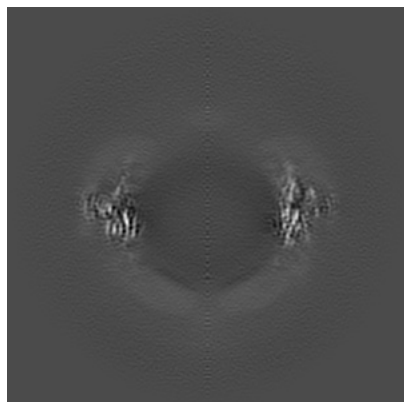


Z

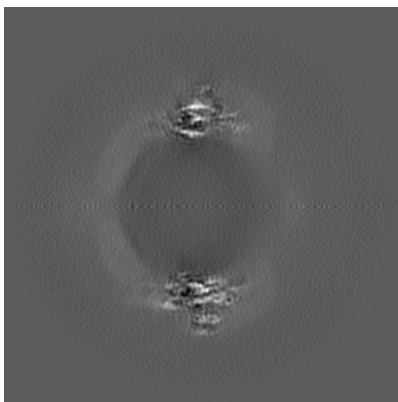
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

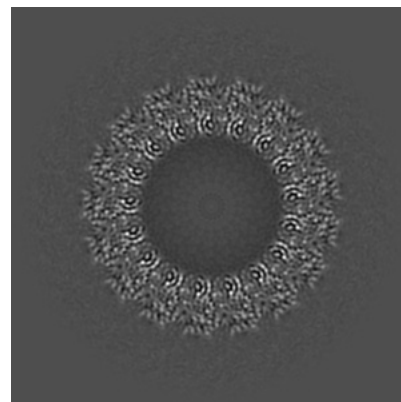
6.2.1 Primary map



X Index: 176

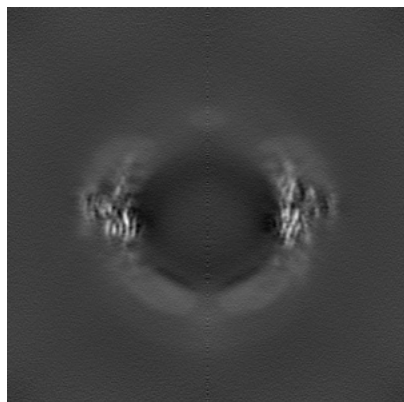


Y Index: 176

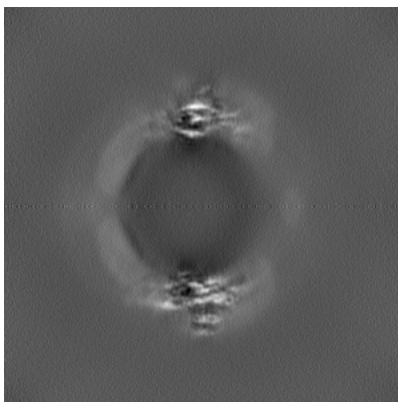


Z Index: 176

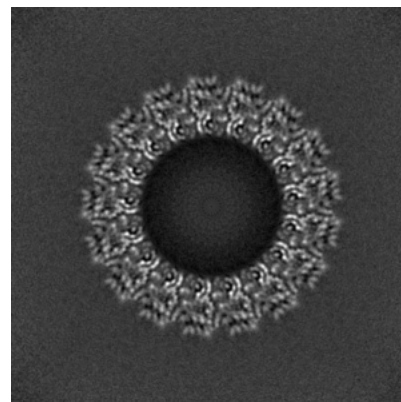
6.2.2 Raw map



X Index: 176



Y Index: 176

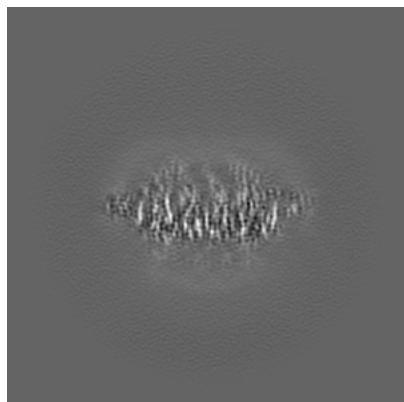


Z Index: 176

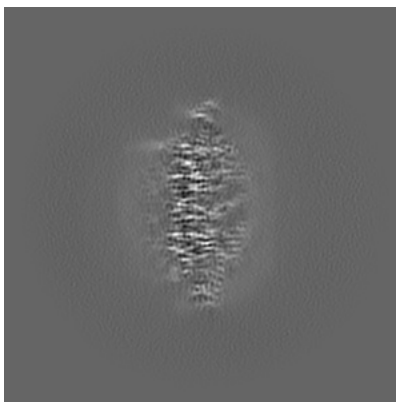
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

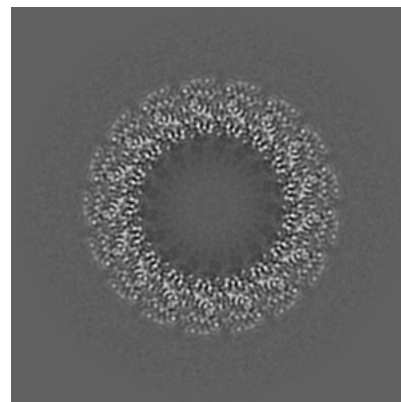
6.3.1 Primary map



X Index: 241

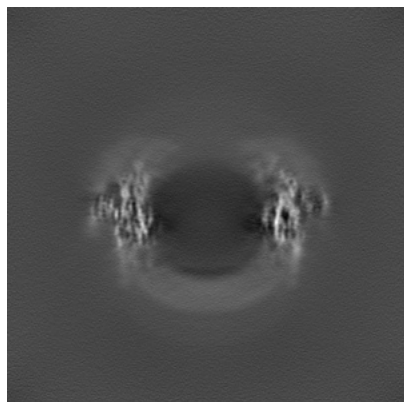


Y Index: 242

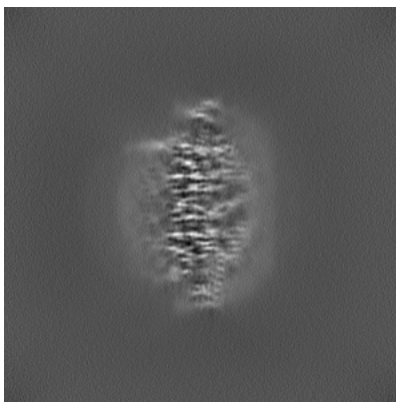


Z Index: 172

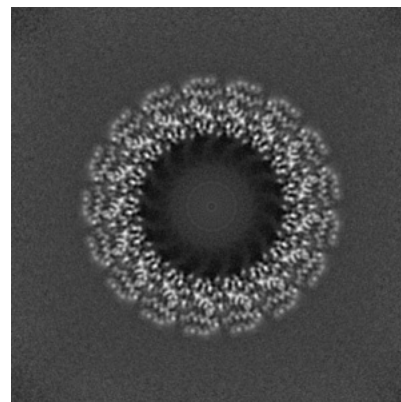
6.3.2 Raw map



X Index: 139



Y Index: 242

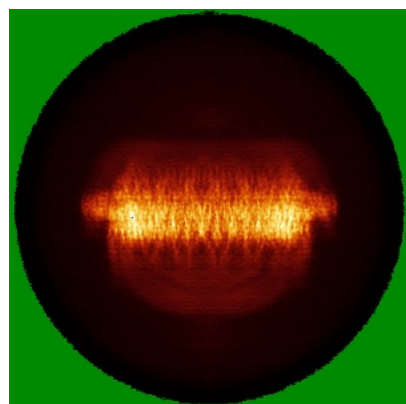


Z Index: 172

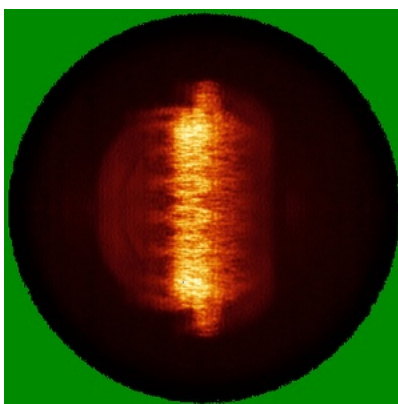
The images above show the largest variance slices of the map in three orthogonal directions.

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

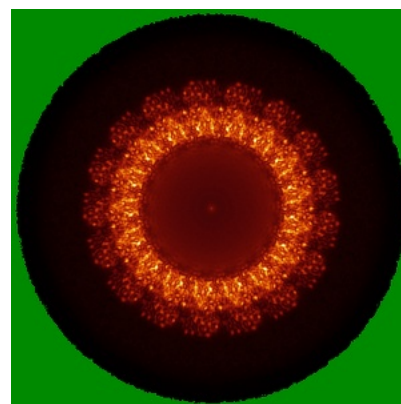
6.4.1 Primary map



X

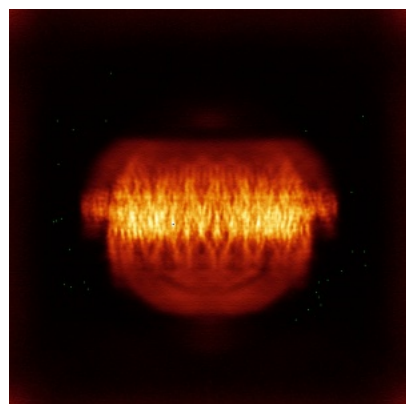


Y

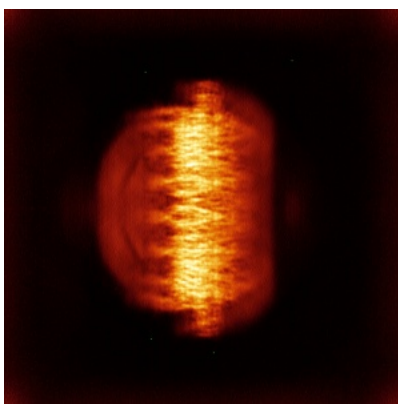


Z

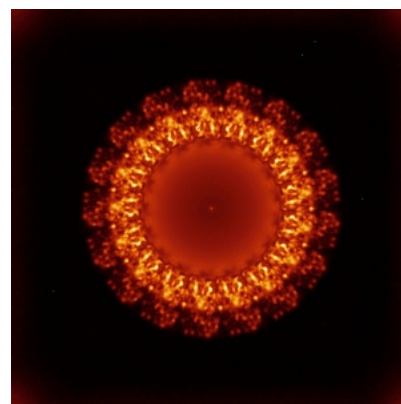
6.4.2 Raw map



X



Y

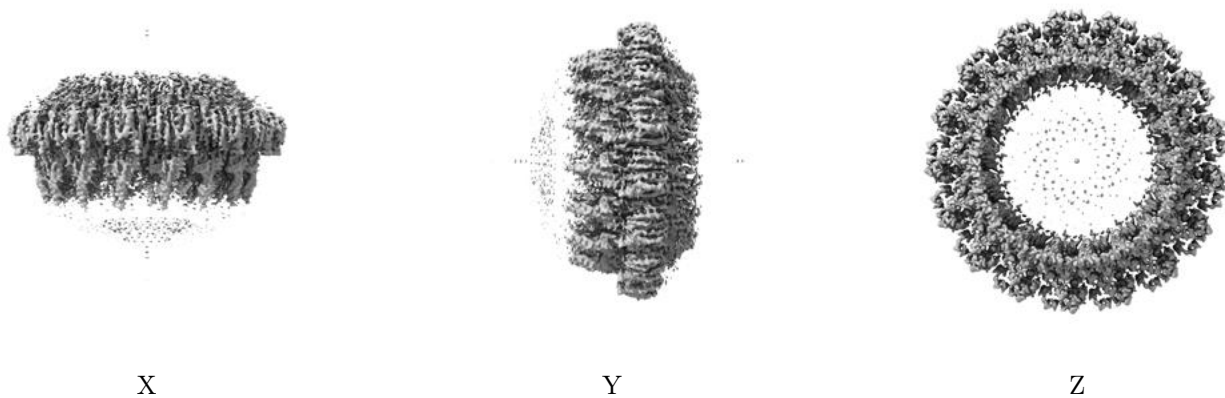


Z

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.

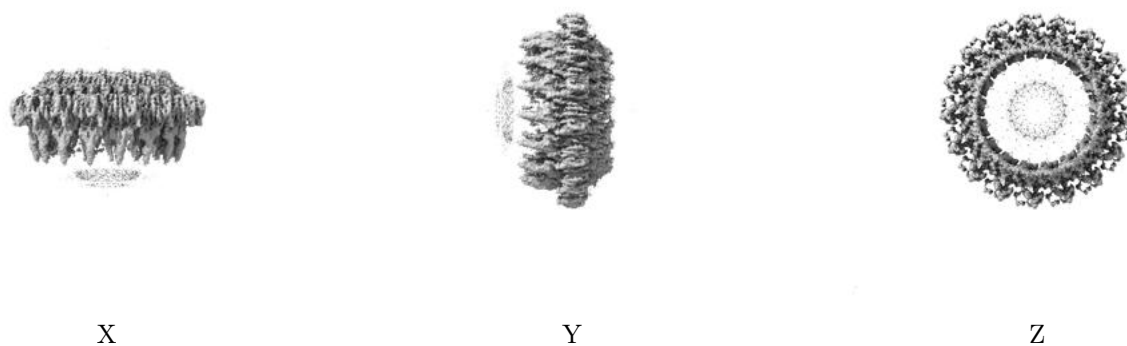
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.157. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

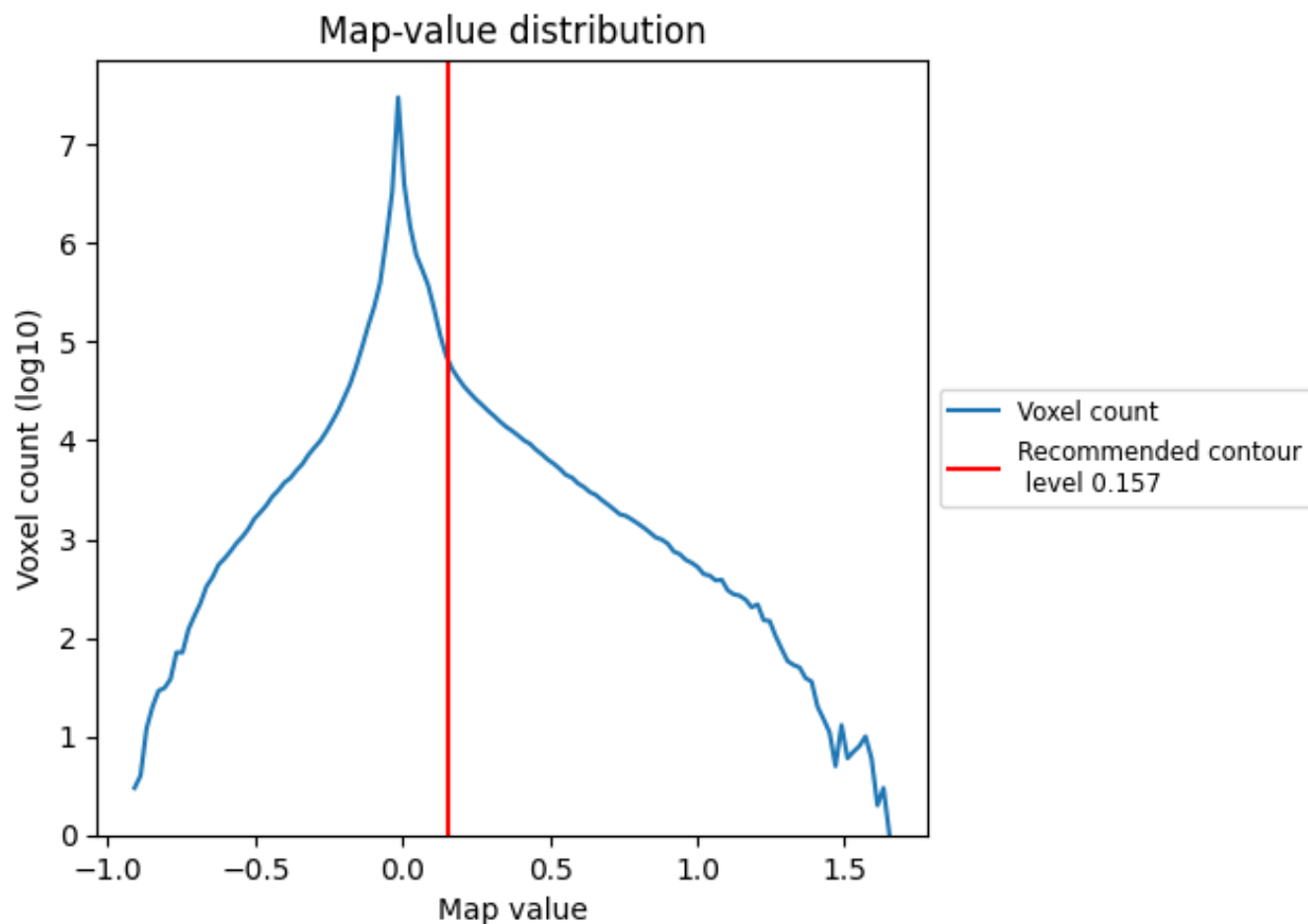
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

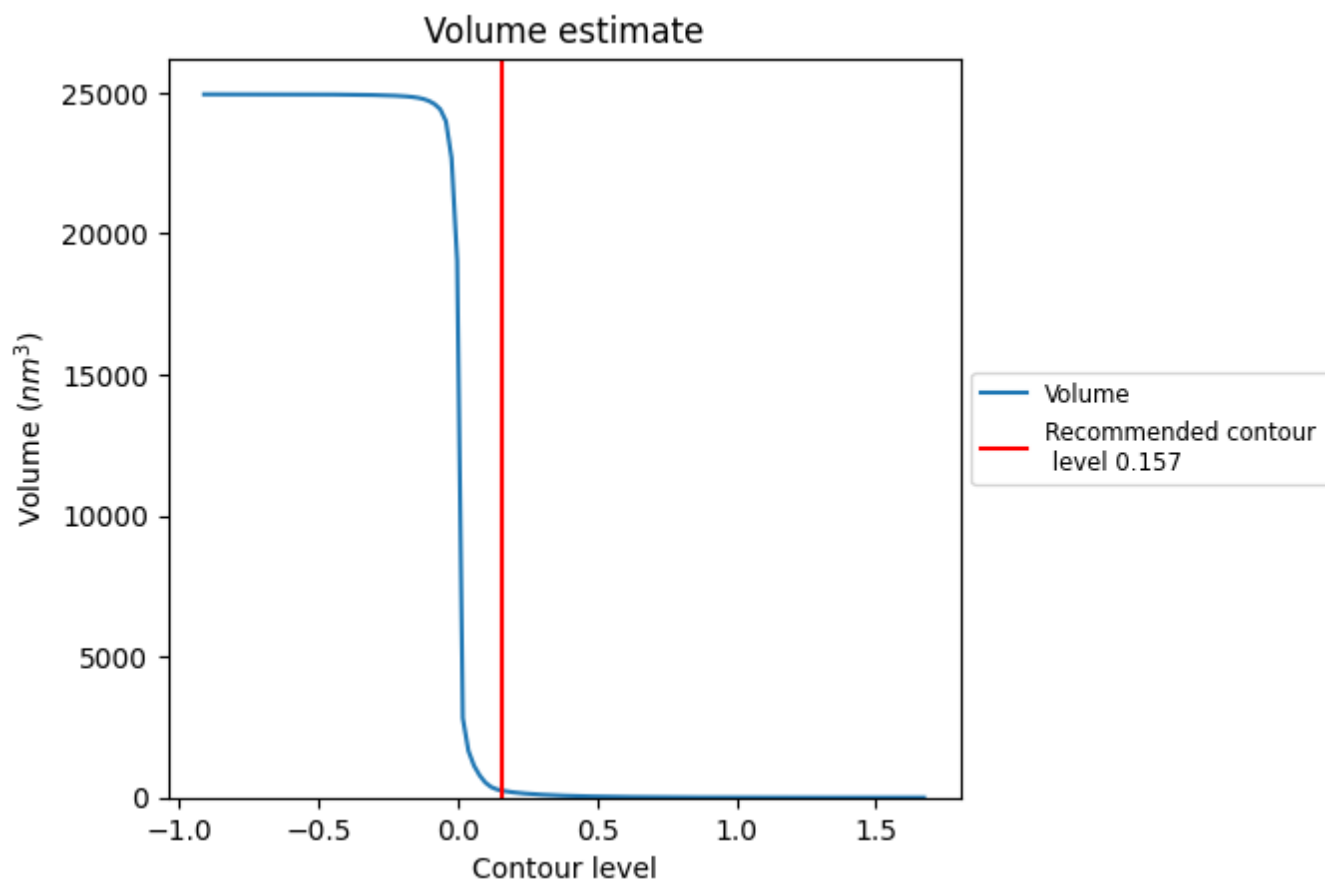
This section contains the results of statistical analysis of the map.

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.

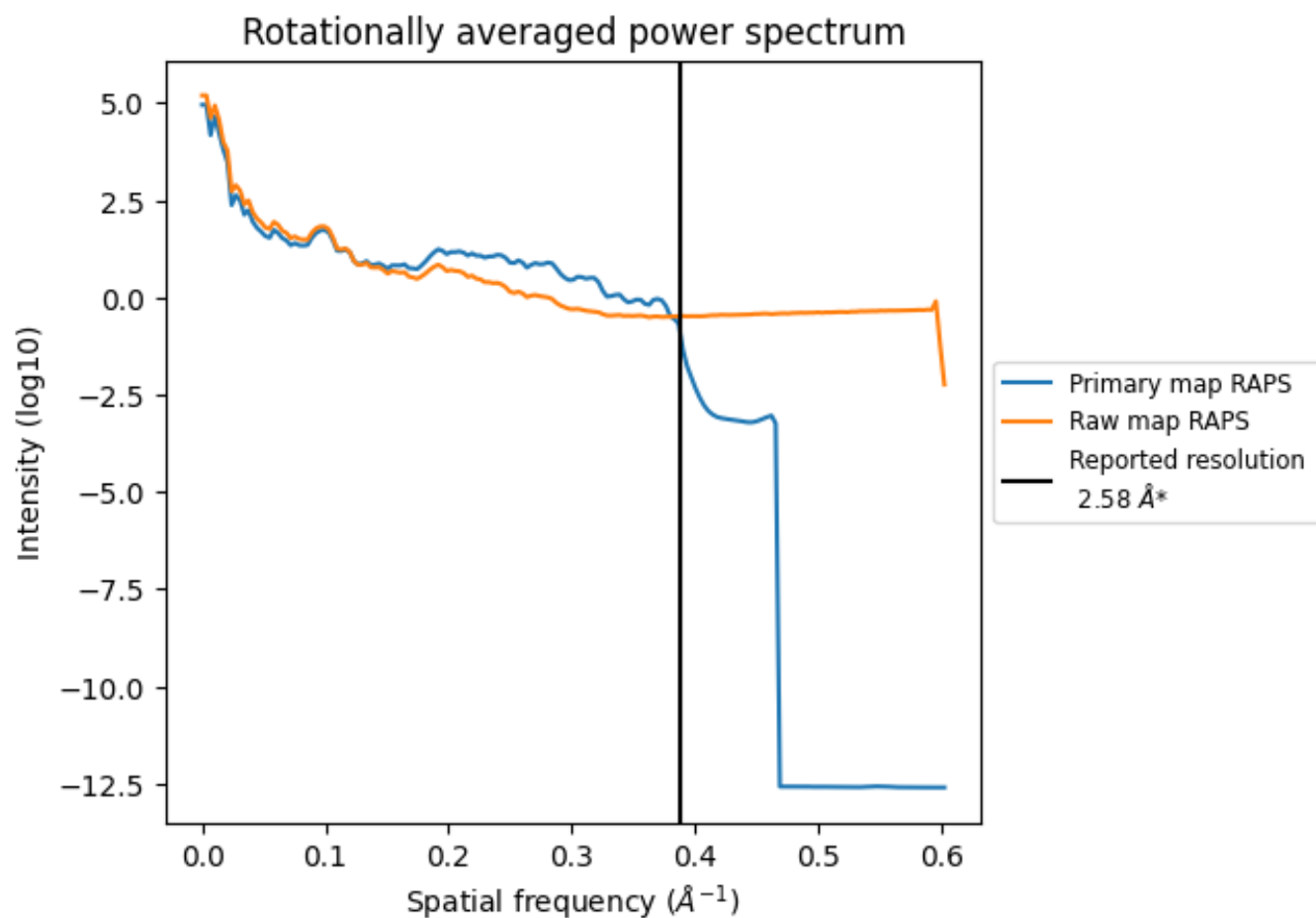
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 251 nm³; this corresponds to an approximate mass of 226 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 ⓘ

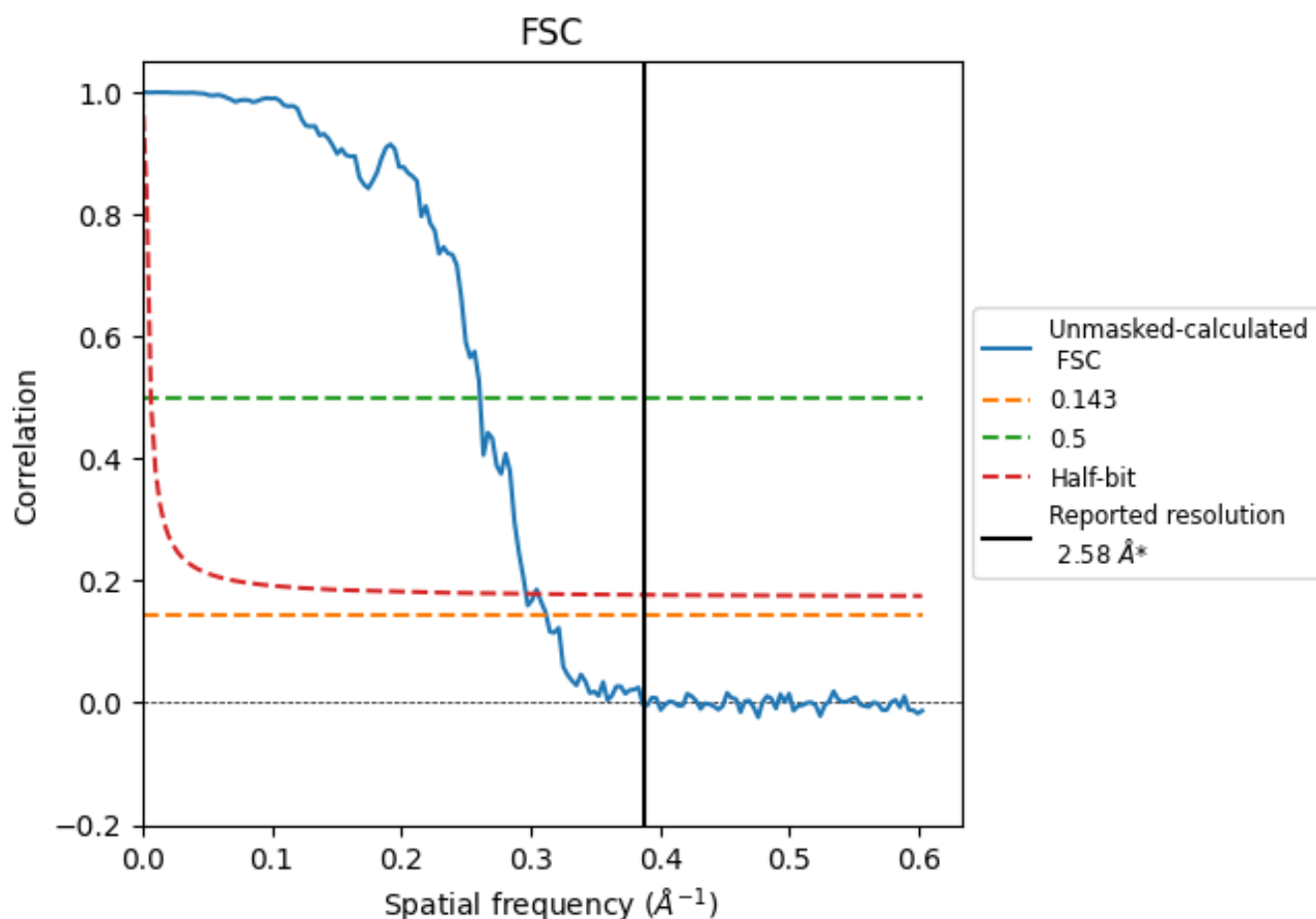


*Reported resolution corresponds to spatial frequency of 0.388 \AA^{-1}

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 0.388 \AA^{-1}

8.2 Resolution estimates [i](#)

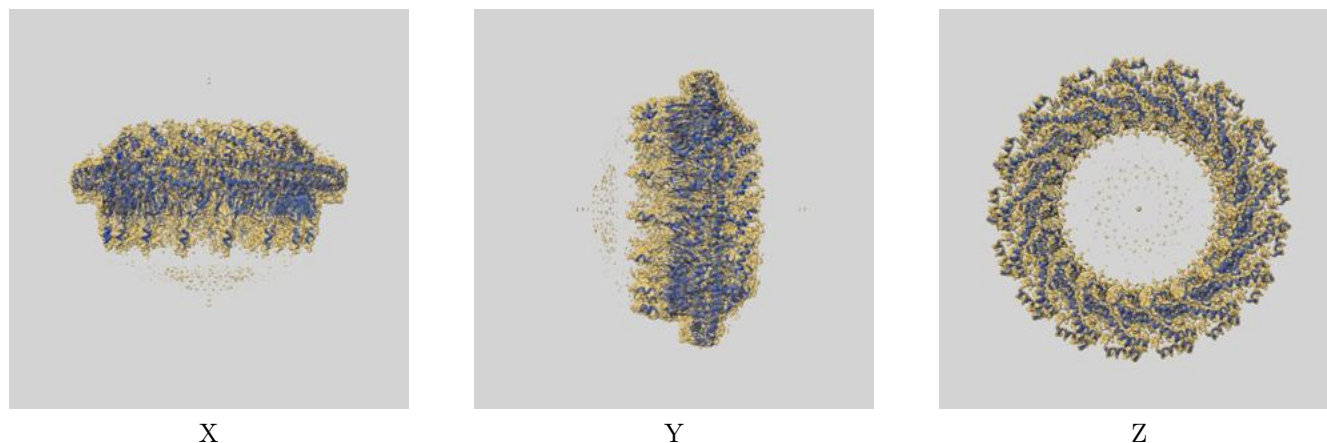
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.58	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.21	3.83	3.37

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.21 differs from the reported value 2.58 by more than 10 %

9 Map-model fit [i](#)

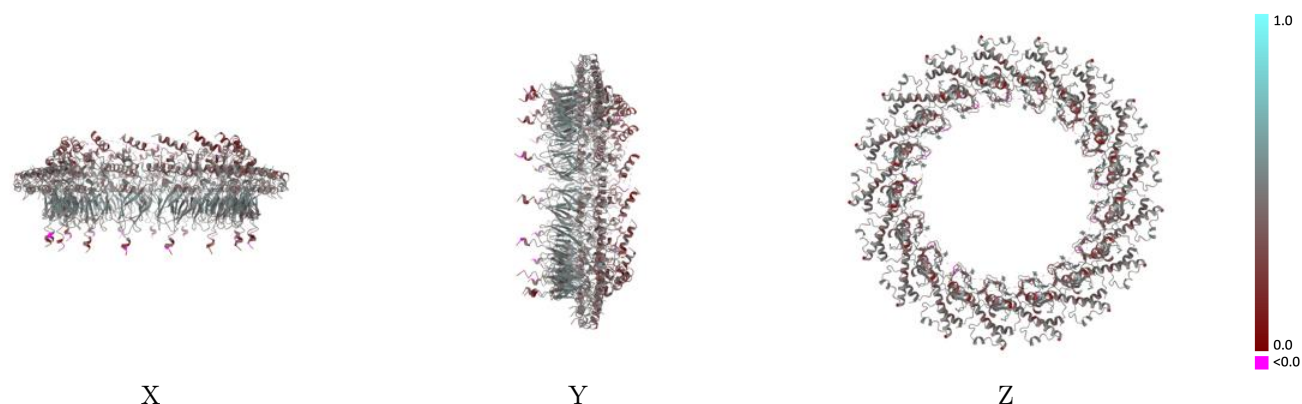
This section contains information regarding the fit between EMDB map EMD-65048 and PDB model 9VGF. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



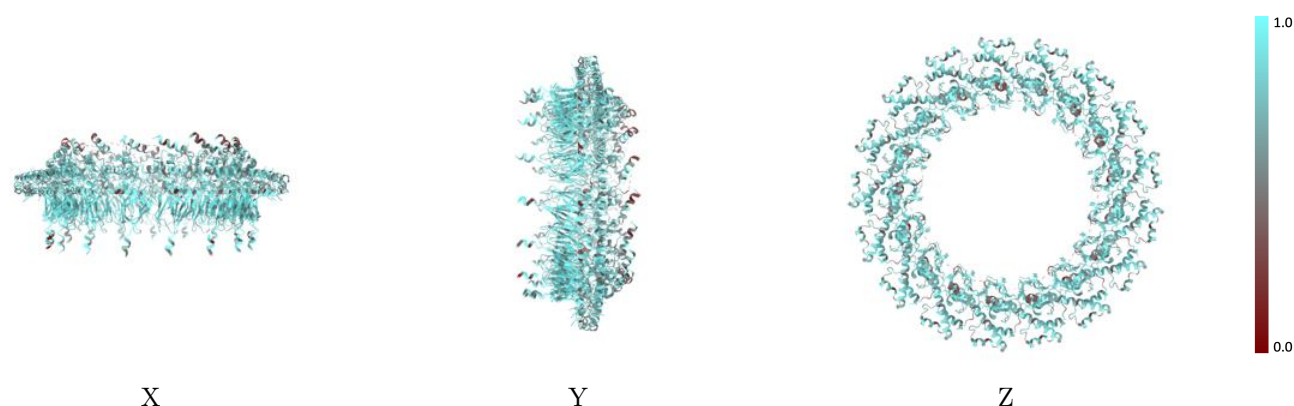
The images above show the 3D surface view of the map at the recommended contour level 0.157 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



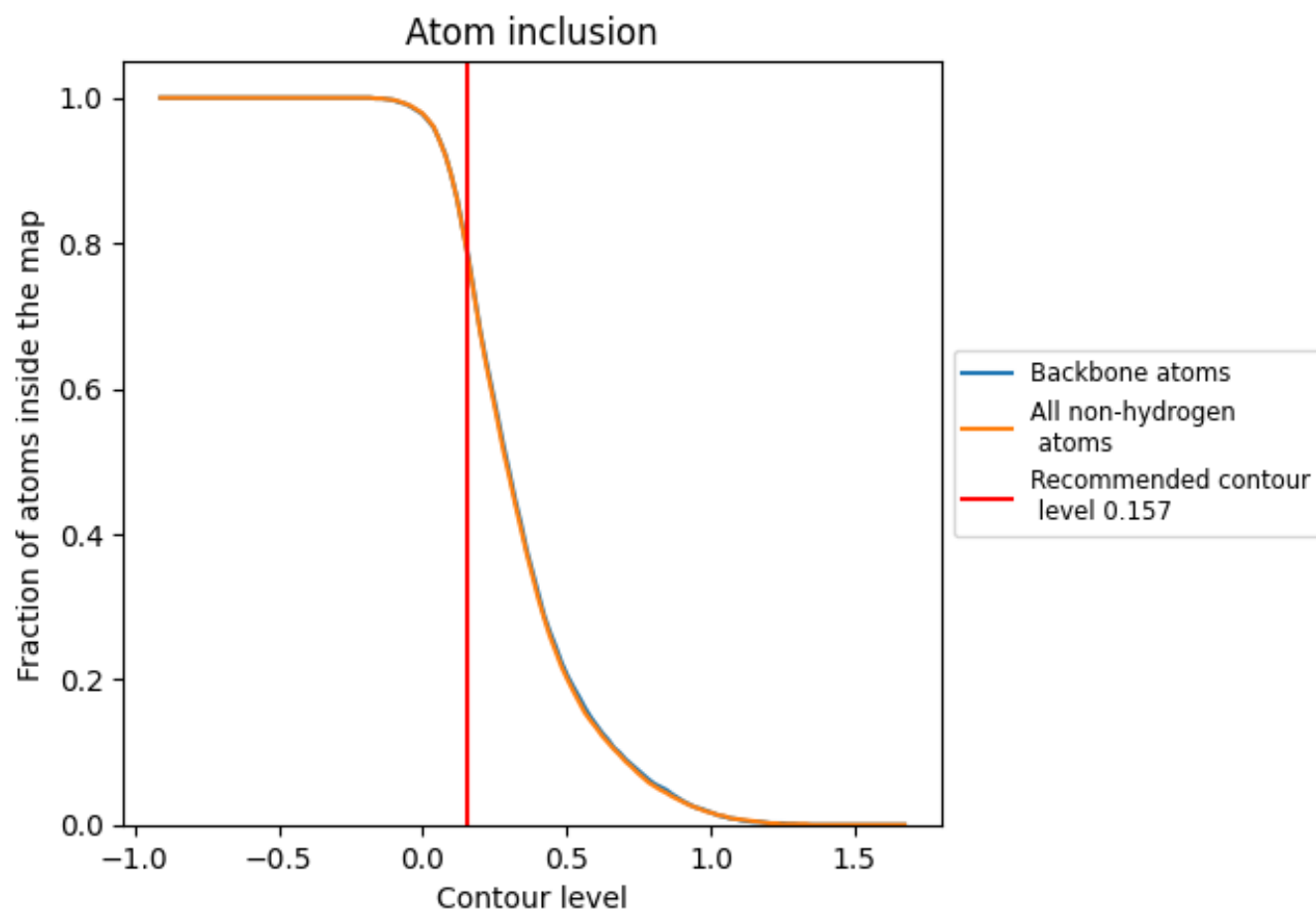
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.157).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 78% 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 (0.157) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7820	 0.4380
AX	 0.8110	 0.4450
AY	 0.7390	 0.4280
BX	 0.8100	 0.4490
BY	 0.7490	 0.4250
CX	 0.8080	 0.4410
CY	 0.7400	 0.4270
DX	 0.8050	 0.4460
DY	 0.7350	 0.4240
EX	 0.8000	 0.4450
EY	 0.7420	 0.4230
FX	 0.8060	 0.4380
FY	 0.7440	 0.4250
GX	 0.8190	 0.4430
GY	 0.7450	 0.4260
HX	 0.8090	 0.4450
HY	 0.7450	 0.4310
IX	 0.8020	 0.4410
IY	 0.7440	 0.4290
JX	 0.8220	 0.4480
JY	 0.7420	 0.4290
KX	 0.8090	 0.4400
KY	 0.7400	 0.4250
LX	 0.8110	 0.4430
LY	 0.7350	 0.4250
MX	 0.8010	 0.4430
MY	 0.7420	 0.4300
NX	 0.8090	 0.4400
NY	 0.7500	 0.4260
OX	 0.8130	 0.4460
OY	 0.7440	 0.4280
PX	 0.8090	 0.4450
PY	 0.7370	 0.4290
QX	 0.8060	 0.4420
QY	 0.7420	 0.4300

