



Full wwPDB EM Validation Report ⓘ

Nov 27, 2022 – 04:04 PM EST

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

This is a 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

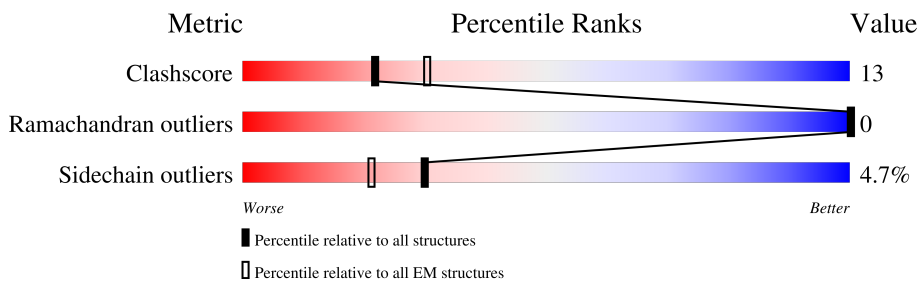
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






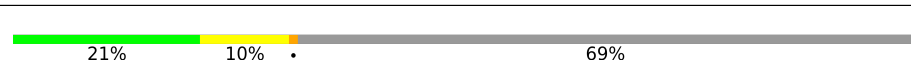


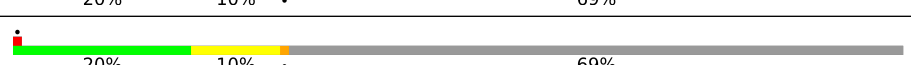
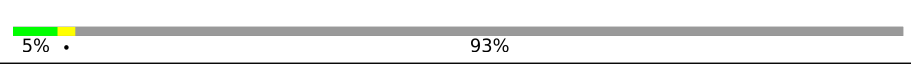
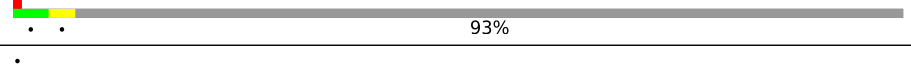
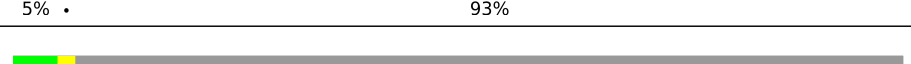
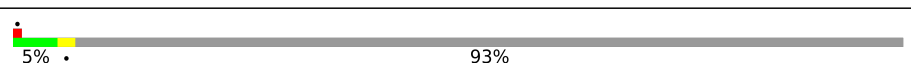
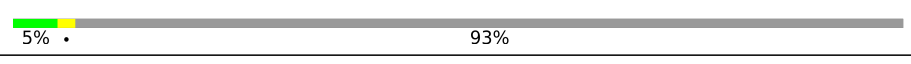
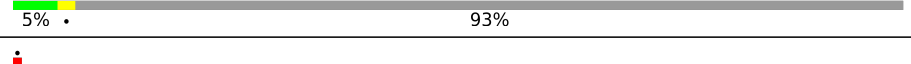
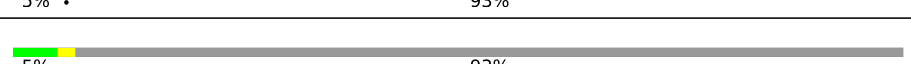
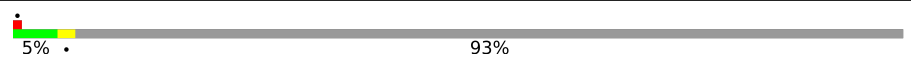
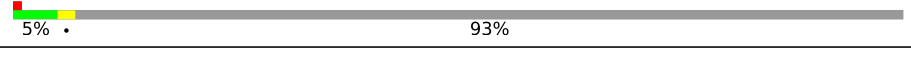
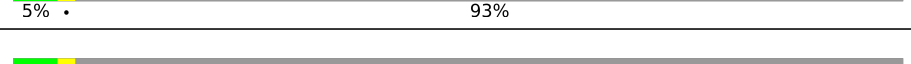
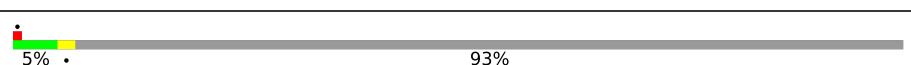
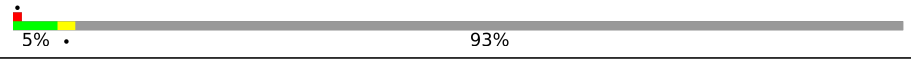
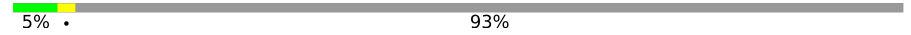



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	521	
1	BX	521	
1	CX	521	
1	DX	521	
1	EX	521	
1	FX	521	
1	GX	521	
1	HX	521	


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

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Mol	Chain	Length	Quality of chain
2	QY	1927	 5% • 93%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 40613 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cag pathogenicity island protein (Cag8).

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

There are 34 discrepancies between the modelled and reference sequences:

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

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

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

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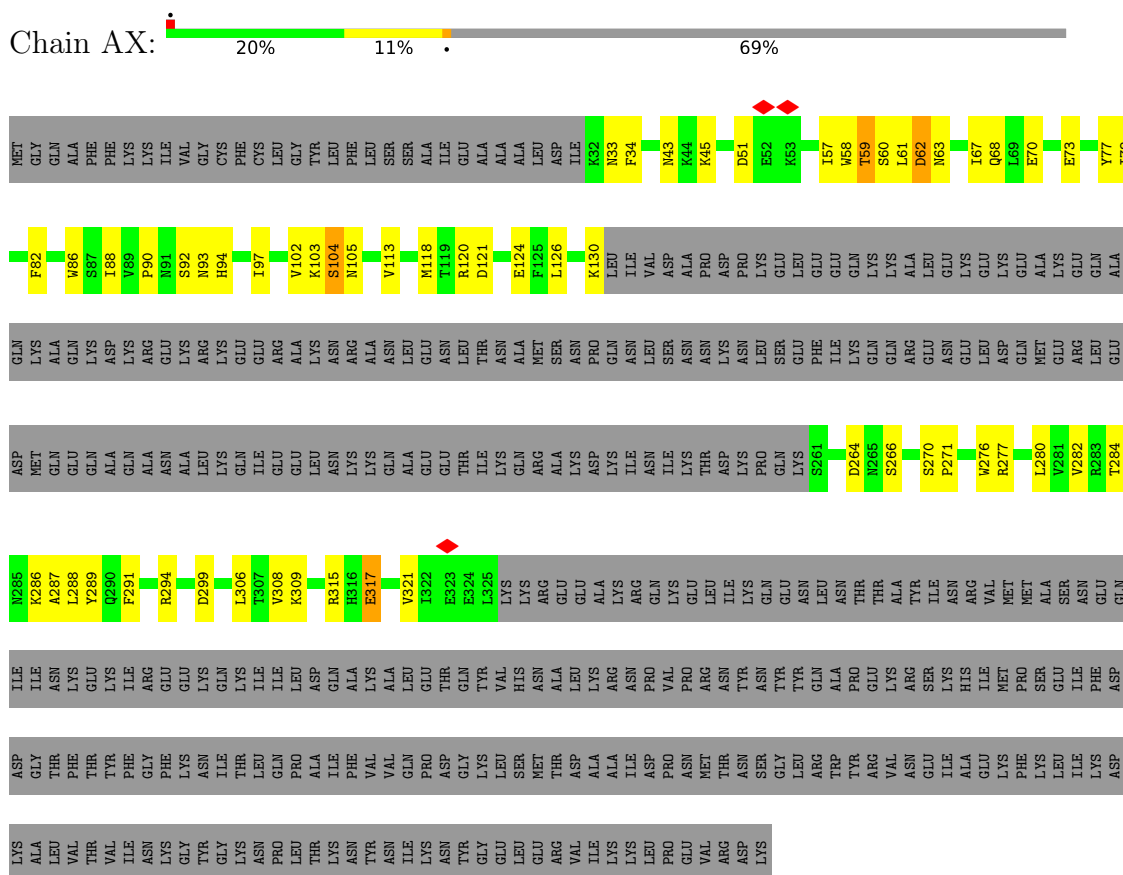
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	CY	135	Total	C	N	O	S	0	0
			1050	649	177	220	4		
2	DY	135	Total	C	N	O	S	0	0
			1050	649	177	220	4		
2	EY	135	Total	C	N	O	S	0	0
			1050	649	177	220	4		
2	FY	135	Total	C	N	O	S	0	0
			1050	649	177	220	4		
2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

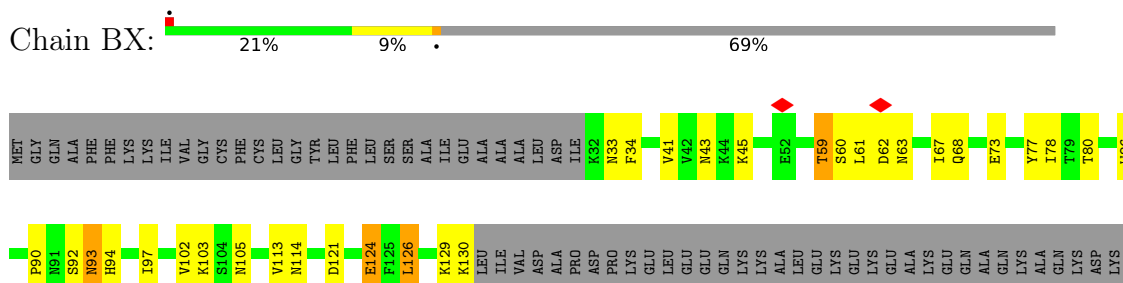
3 Residue-property plots [i](#)

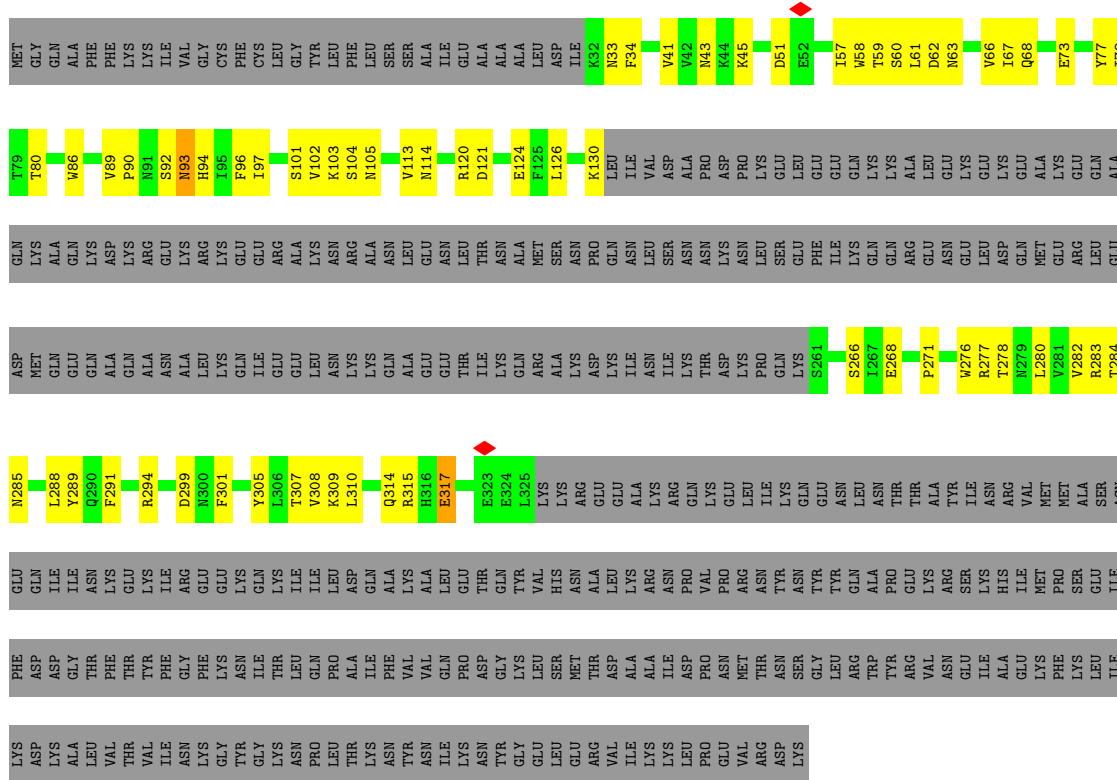
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 (Cag8)

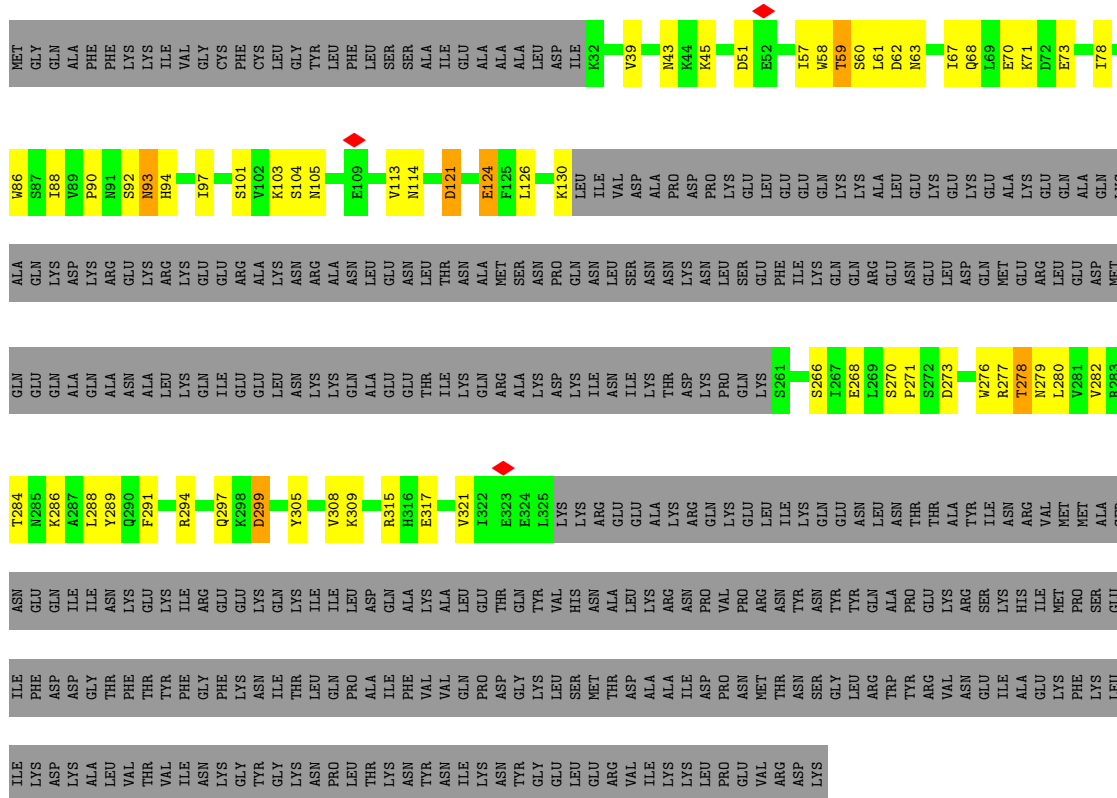


- Molecule 1: Cag pathogenicity island protein (Cag8)

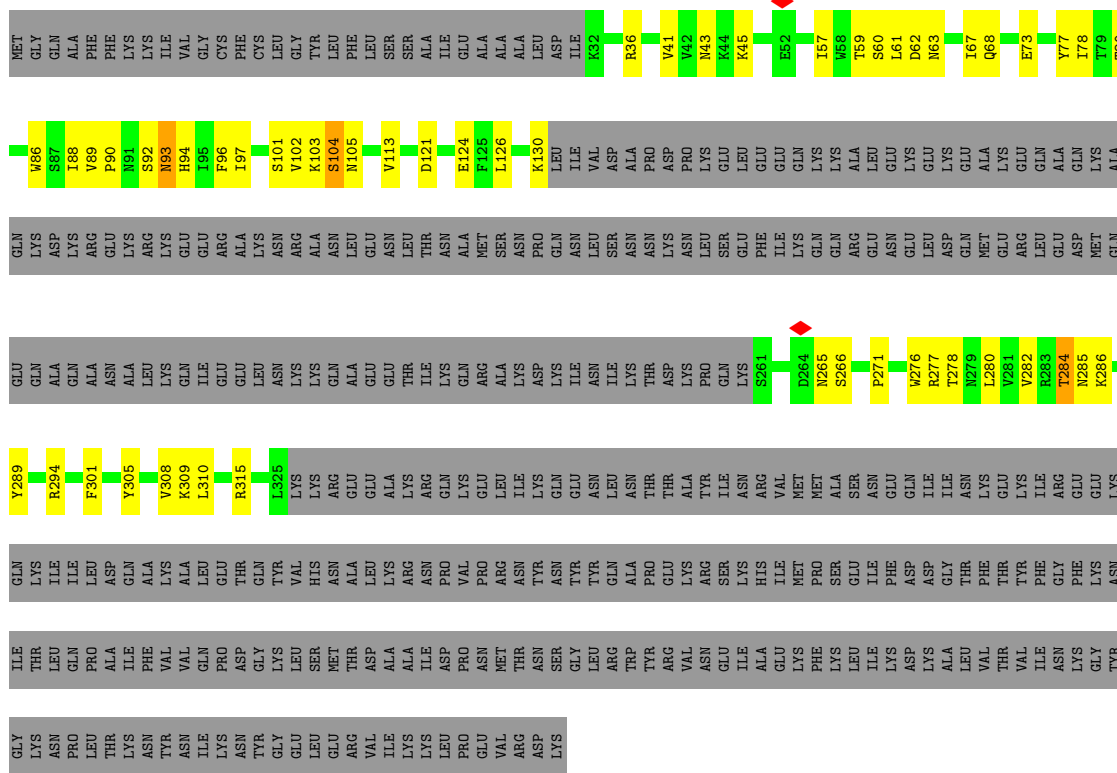




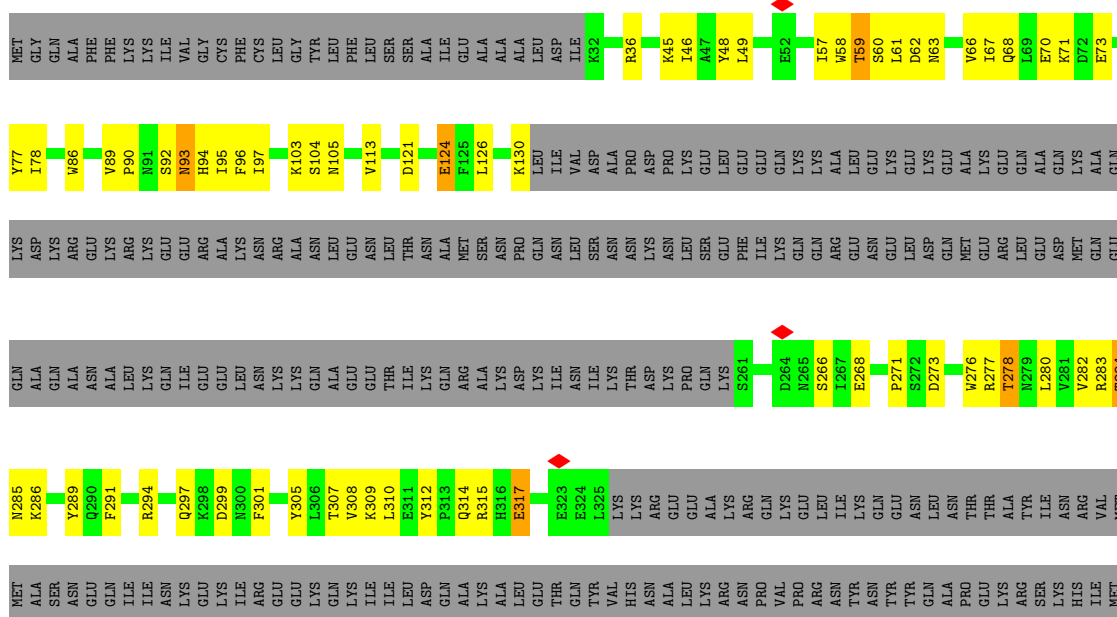
● Molecule 1: Cag pathogenicity island protein (Cag8)

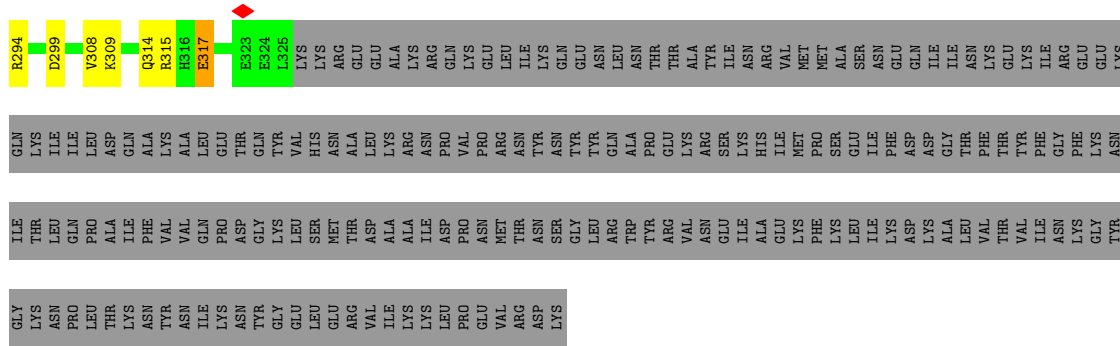


● Molecule 1: Cag pathogenicity island protein (Cag8)

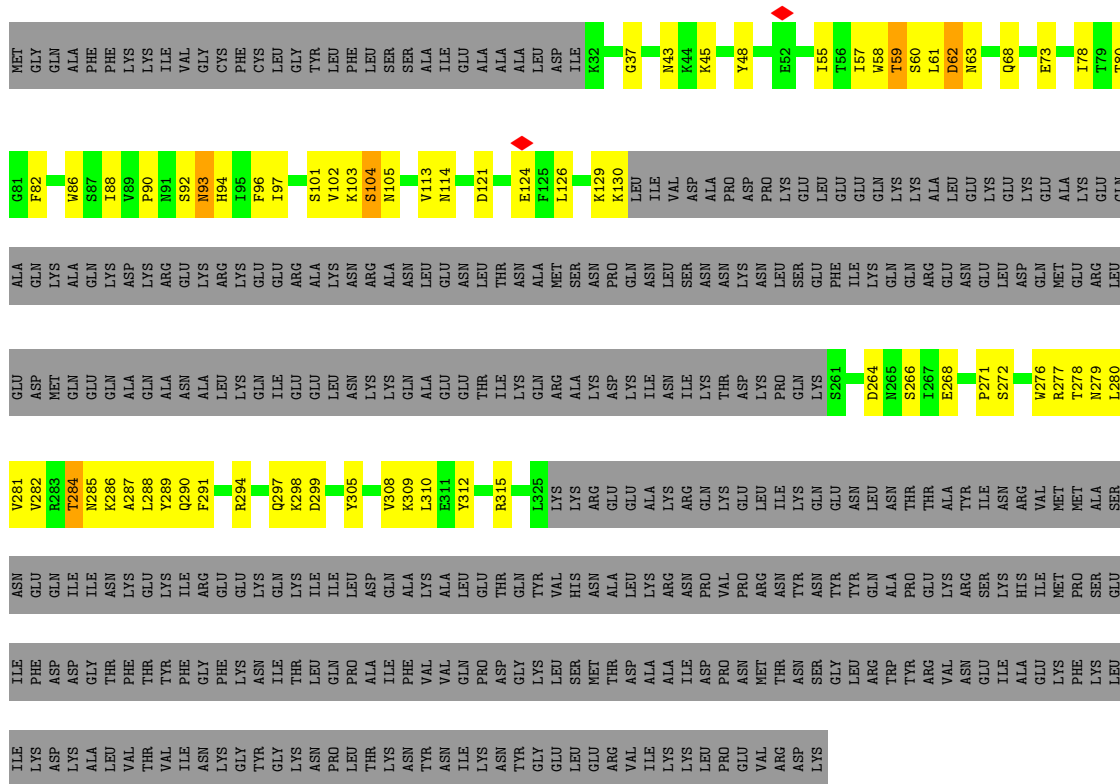


● Molecule 1: Cag pathogenicity island protein (Cag8)

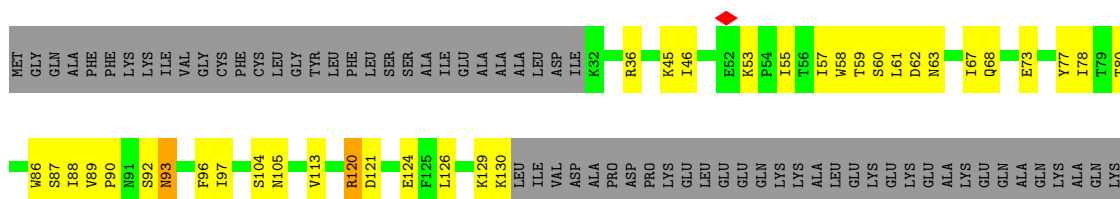


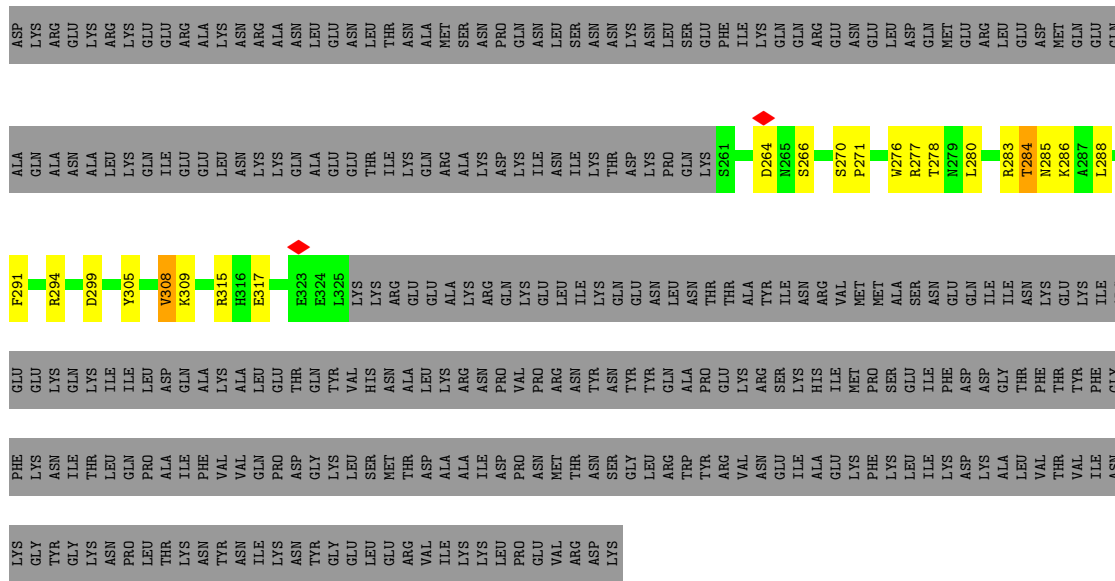


• Molecule 1: Cag pathogenicity island protein (Cag8)

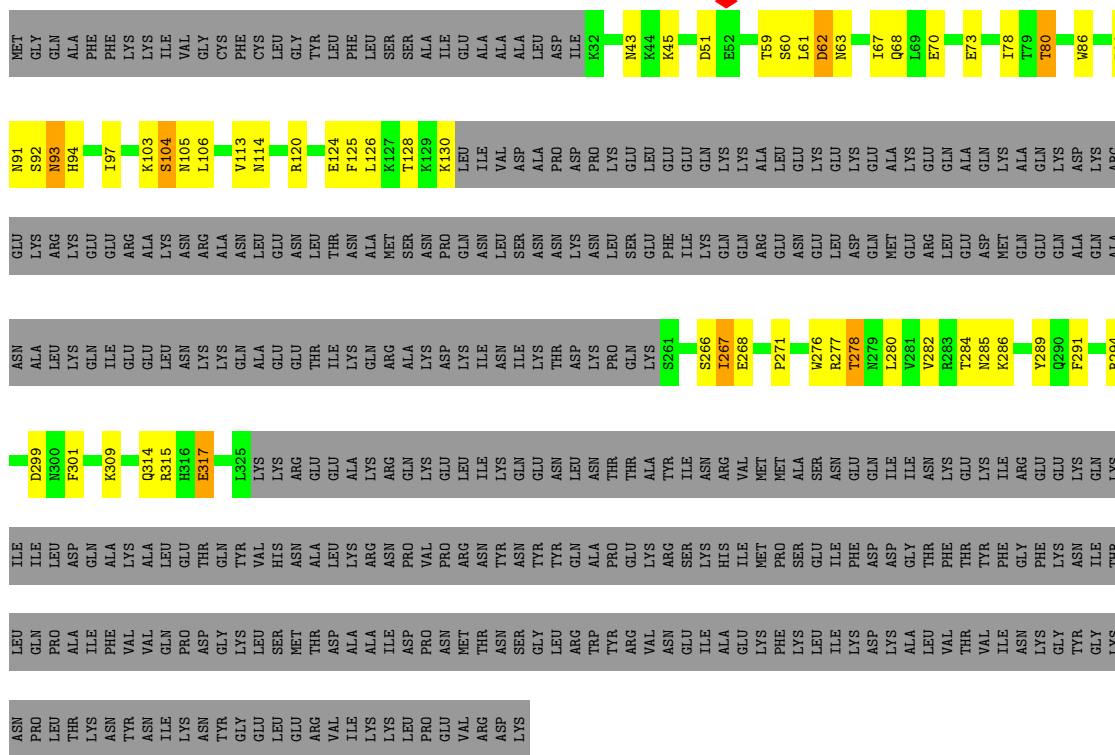


• Molecule 1: Cag pathogenicity island protein (Cag8)





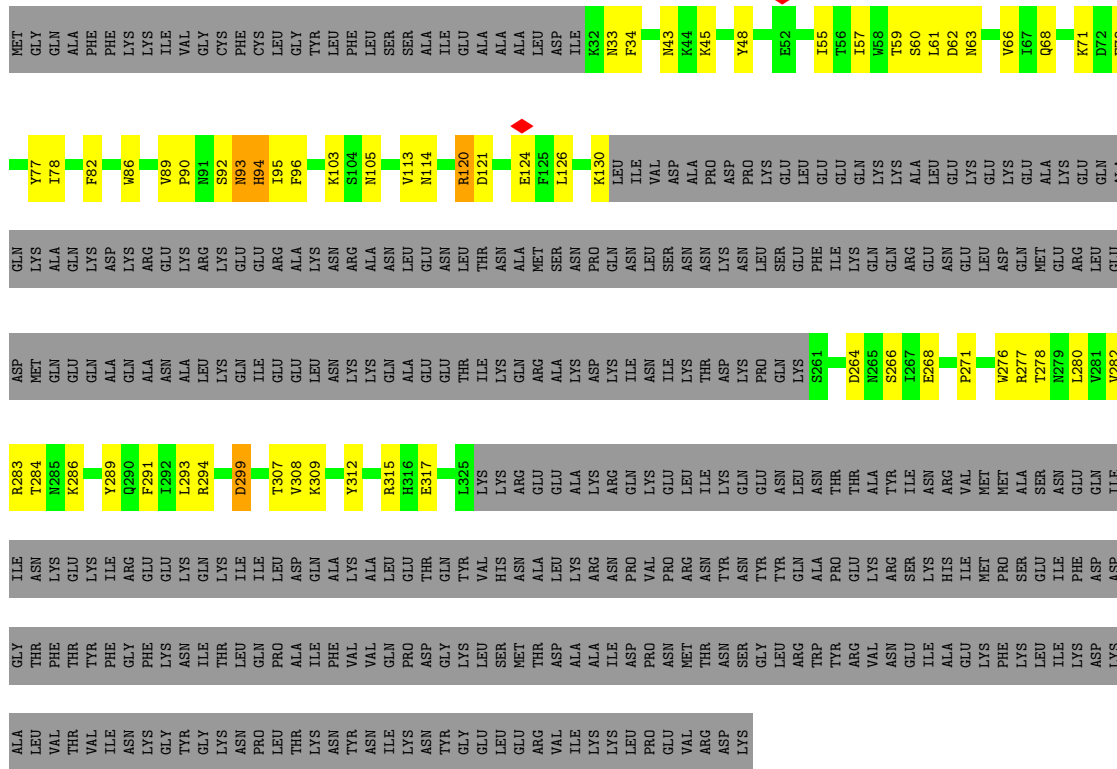
● Molecule 1: Cag pathogenicity island protein (Cag8)



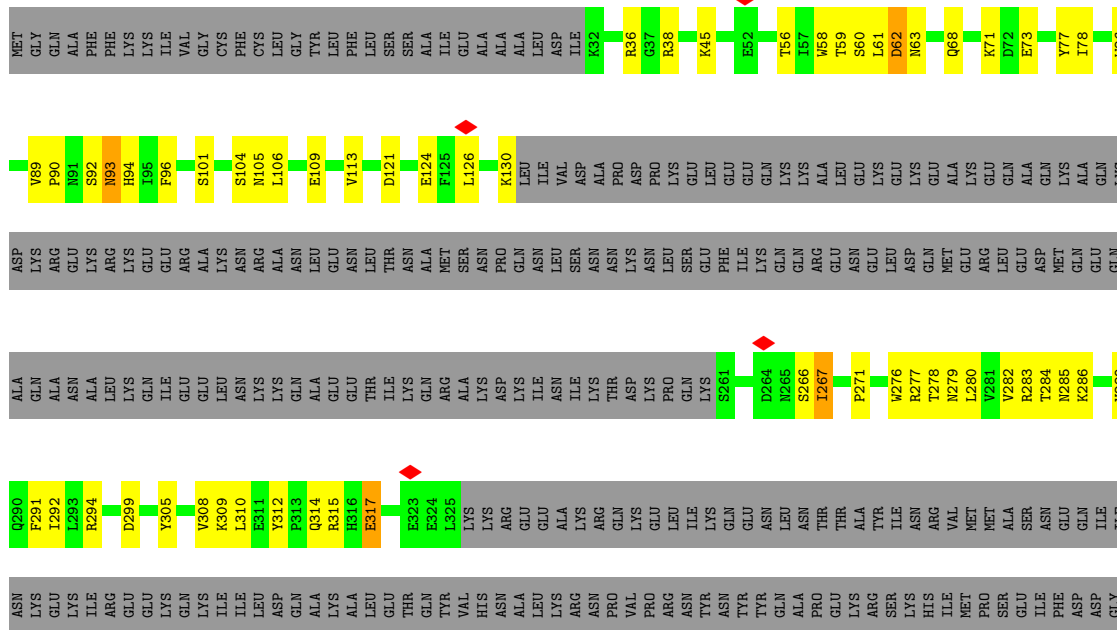
● Molecule 1: Cag pathogenicity island protein (Cag8)

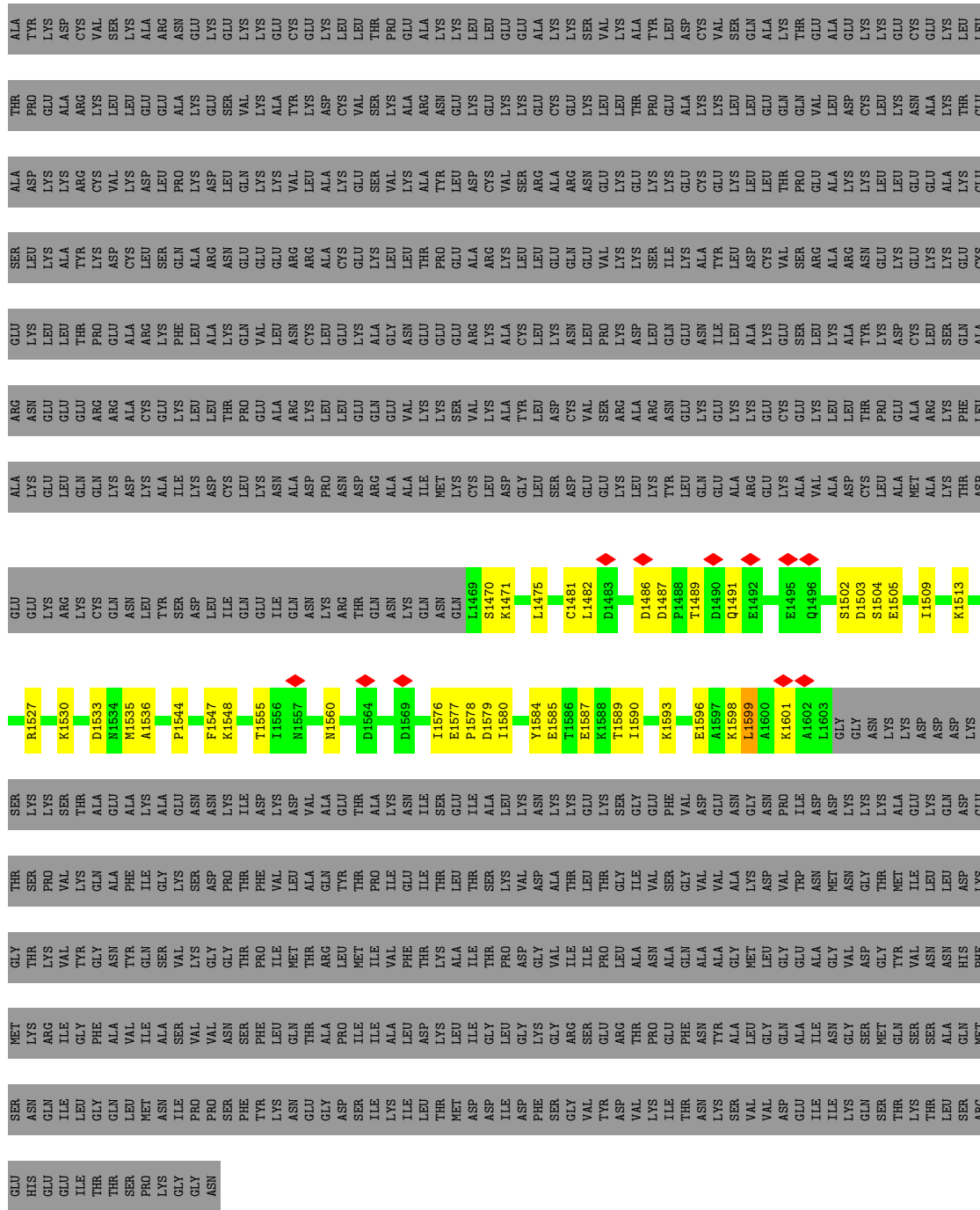


● Molecule 1: Cag pathogenicity island protein (Cag8)



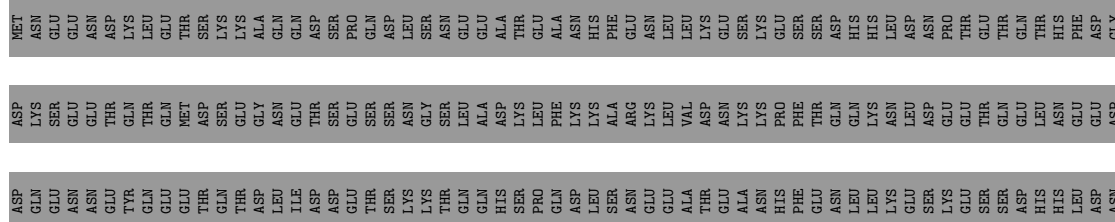
● Molecule 1: Cag pathogenicity island protein (Cag8)

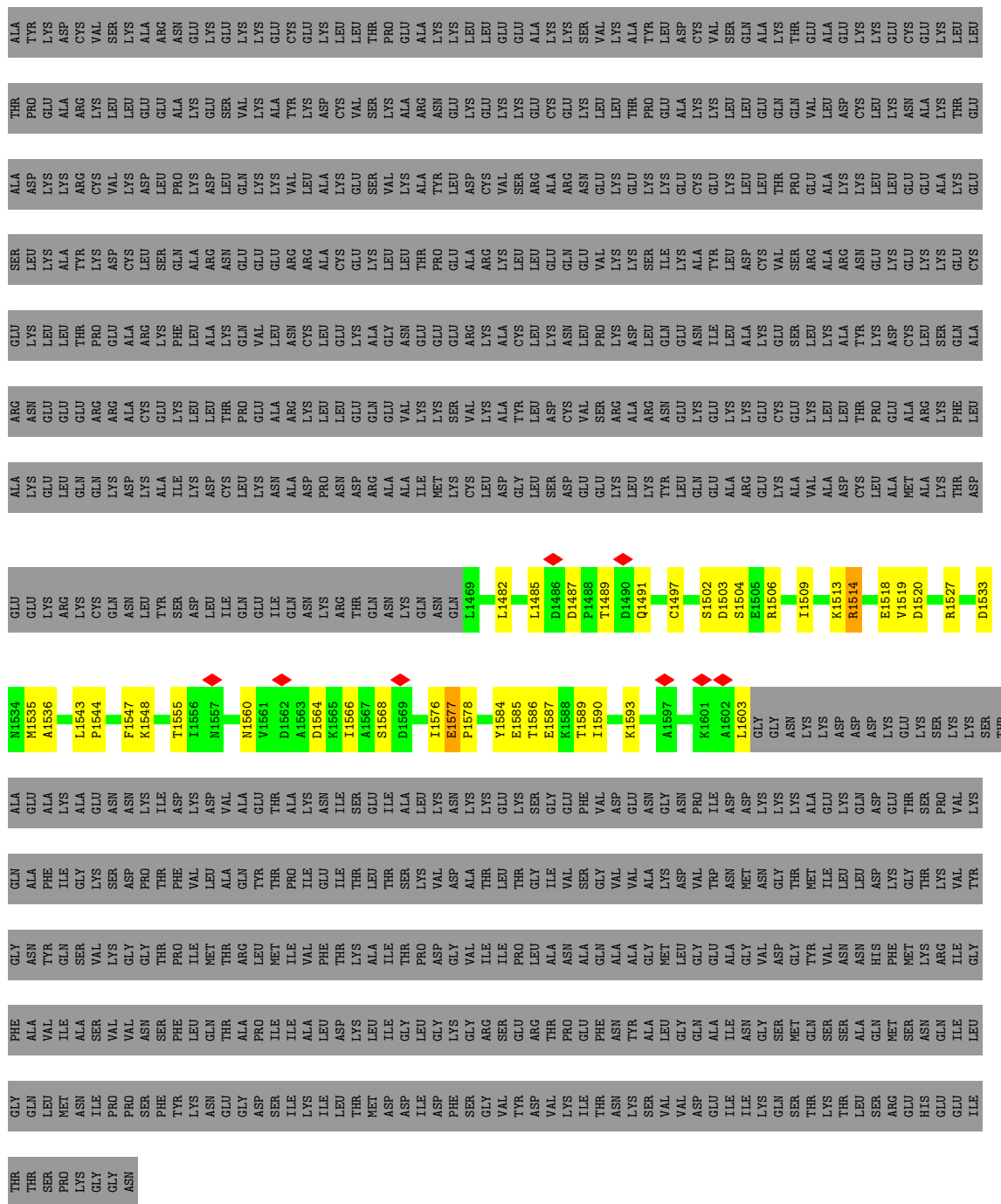




• Molecule 2: Cag pathogenicity island protein (Cag7)

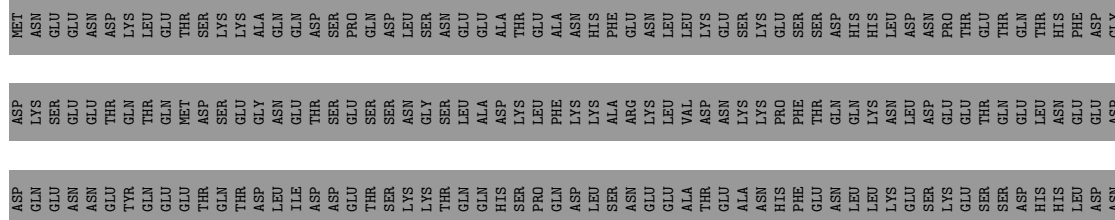
Chain DY: 5% 93%





● Molecule 2: Cag pathogenicity island protein (Cag7)

Chain NY: 5% . 93%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20929	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	59.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.148	Depositor
Minimum map value	-0.069	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	836.39996, 836.39996, 836.39996	wwPDB
Map dimensions	510, 510, 510	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.64, 1.64, 1.64	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AX	0.39	0/1365	0.46	0/1845
1	BX	0.39	0/1365	0.46	0/1845
1	CX	0.39	0/1365	0.46	0/1845
1	DX	0.40	0/1365	0.46	0/1845
1	EX	0.39	0/1365	0.46	0/1845
1	FX	0.39	0/1365	0.46	0/1845
1	GX	0.39	0/1365	0.46	0/1845
1	HX	0.40	0/1365	0.46	0/1845
1	IX	0.39	0/1365	0.46	0/1845
1	JX	0.40	0/1365	0.46	0/1845
1	KX	0.39	0/1365	0.46	0/1845
1	LX	0.39	0/1365	0.46	0/1845
1	MX	0.39	0/1365	0.46	0/1845
1	NX	0.39	0/1365	0.46	0/1845
1	OX	0.39	0/1365	0.46	0/1845
1	PX	0.39	0/1365	0.46	0/1845
1	QX	0.40	0/1365	0.46	0/1845
2	AY	0.30	0/1061	0.41	0/1432
2	BY	0.30	0/1061	0.42	0/1432
2	CY	0.31	0/1061	0.43	0/1432
2	DY	0.31	0/1061	0.42	0/1432
2	EY	0.30	0/1061	0.42	0/1432
2	FY	0.30	0/1061	0.41	0/1432
2	GY	0.30	0/1061	0.42	0/1432
2	HY	0.33	0/1061	0.45	0/1432
2	IY	0.30	0/1061	0.41	0/1432
2	JY	0.31	0/1061	0.43	0/1432
2	KY	0.30	0/1061	0.42	0/1432
2	LY	0.30	0/1061	0.42	0/1432
2	MY	0.30	0/1061	0.42	0/1432
2	NY	0.30	0/1061	0.42	0/1432
2	OY	0.31	0/1061	0.42	0/1432
2	PY	0.30	0/1061	0.41	0/1432
2	QY	0.30	0/1061	0.41	0/1432

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (1048) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LX:126:LEU:O	1:LX:130:LYS:HB2	1.65	0.96
1:MX:126:LEU:O	1:MX:130:LYS:HB2	1.68	0.93
1:QX:126:LEU:O	1:QX:130:LYS:HB2	1.68	0.93
1:NX:126:LEU:O	1:NX:130:LYS:HB2	1.71	0.91
1:JX:126:LEU:O	1:JX:130:LYS:HB2	1.71	0.91
1:HX:126:LEU:O	1:HX:130:LYS:HB2	1.71	0.90
1:KX:126:LEU:O	1:KX:130:LYS:HB2	1.73	0.89
1:AX:126:LEU:O	1:AX:130:LYS:HB2	1.73	0.88
1:IX:126:LEU:O	1:IX:130:LYS:HB2	1.74	0.87
1:GX:126:LEU:O	1:GX:130:LYS:HB2	1.75	0.87
1:DX:126:LEU:O	1:DX:130:LYS:HB2	1.74	0.87
1:CX:126:LEU:O	1:CX:130:LYS:HB2	1.74	0.86
1:BX:126:LEU:O	1:BX:130:LYS:HB2	1.74	0.86
1:FX:126:LEU:O	1:FX:130:LYS:HB2	1.79	0.83
1:OX:126:LEU:O	1:OX:130:LYS:HB2	1.79	0.82
2:GY:1576:ILE:HG21	2:HY:1584:TYR:HE1	1.45	0.81
1:PX:126:LEU:O	1:PX:130:LYS:HB2	1.80	0.81
2:HY:1482:LEU:HD13	2:HY:1513:LYS:HD2	1.61	0.80
2:OY:1576:ILE:HG21	2:PY:1584:TYR:HE1	1.48	0.79
2:NY:1576:ILE:HG21	2:OY:1584:TYR:HE1	1.49	0.78
1:QX:77:TYR:HB2	1:QX:283:ARG:HH21	1.49	0.78
2:PY:1576:ILE:HG21	2:QY:1584:TYR:HE1	1.49	0.77
2:LY:1576:ILE:HG21	2:MY:1584:TYR:HE1	1.50	0.77
2:MY:1576:ILE:HG21	2:NY:1584:TYR:HE1	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:OX:284:THR:HG23	1:OX:286:LYS:H	1.50	0.76
2:KY:1576:ILE:HG21	2:LY:1584:TYR:HE1	1.49	0.76
1:DX:73:GLU:OE2	1:DX:315:ARG:NH1	2.17	0.76
1:FX:277:ARG:HD2	1:FX:294:ARG:HH11	1.49	0.76
1:EX:126:LEU:O	1:EX:130:LYS:HB2	1.85	0.76
1:AX:104:SER:HB2	2:QY:1547:PHE:HB3	1.67	0.75
2:CY:1482:LEU:HD13	2:CY:1513:LYS:HD2	1.67	0.75
1:NX:73:GLU:OE2	1:NX:315:ARG:NH1	2.18	0.75
2:BY:1576:ILE:HG21	2:CY:1584:TYR:HE1	1.50	0.75
1:KX:104:SER:HB2	2:JY:1547:PHE:HB3	1.69	0.74
1:BX:277:ARG:HD2	1:BX:294:ARG:HH11	1.52	0.74
1:QX:73:GLU:OE2	1:QX:315:ARG:NH1	2.20	0.73
2:HY:1576:ILE:HG21	2:IY:1584:TYR:HE1	1.52	0.73
1:HX:73:GLU:OE2	1:HX:315:ARG:NH1	2.16	0.73
1:NX:104:SER:HB2	2:MY:1547:PHE:HB3	1.70	0.72
2:AY:1584:TYR:HE1	2:QY:1576:ILE:HG21	1.54	0.72
1:EX:73:GLU:OE2	1:EX:315:ARG:NH1	2.21	0.72
2:DY:1576:ILE:HG21	2:EY:1584:TYR:HE1	1.52	0.72
1:LX:73:GLU:OE2	1:LX:315:ARG:NH1	2.23	0.72
1:MX:73:GLU:OE2	1:MX:315:ARG:NH1	2.23	0.72
1:BX:73:GLU:OE2	1:BX:315:ARG:NH1	2.19	0.72
1:PX:104:SER:HB2	2:OY:1547:PHE:HB3	1.72	0.71
2:OY:1482:LEU:HD13	2:OY:1513:LYS:HD2	1.71	0.71
1:FX:104:SER:HB2	2:EY:1547:PHE:HB3	1.72	0.71
1:OX:277:ARG:HD2	1:OX:294:ARG:HH11	1.53	0.70
1:MX:104:SER:HB2	2:LY:1547:PHE:HB3	1.73	0.70
1:LX:78:ILE:HG21	1:LX:90:PRO:HG3	1.72	0.70
1:IX:73:GLU:OE2	1:IX:315:ARG:NH1	2.19	0.70
1:JX:104:SER:HB2	2:IY:1547:PHE:HB3	1.71	0.70
2:FY:1533:ASP:HA	2:GY:1519:VAL:HG21	1.72	0.70
2:IY:1576:ILE:HG21	2:JY:1584:TYR:HE1	1.55	0.70
1:AX:277:ARG:HD2	1:AX:294:ARG:HH11	1.57	0.69
1:IX:78:ILE:HG21	1:IX:90:PRO:HG3	1.75	0.69
1:AX:73:GLU:OE2	1:AX:315:ARG:NH1	2.25	0.69
1:KX:277:ARG:HD2	1:KX:294:ARG:HH11	1.56	0.69
1:LX:104:SER:HB2	2:KY:1547:PHE:HB3	1.73	0.69
2:EY:1576:ILE:HG21	2:FY:1584:TYR:HE1	1.57	0.69
1:MX:78:ILE:HG21	1:MX:90:PRO:HG3	1.74	0.68
1:EX:277:ARG:HD2	1:EX:294:ARG:HH11	1.58	0.68
2:KY:1533:ASP:HA	2:LY:1519:VAL:HG21	1.76	0.68
1:HX:68:GLN:HA	1:HX:94:HIS:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:JY:1482:LEU:HD13	2:JY:1513:LYS:HD2	1.76	0.67
1:JX:68:GLN:HB3	1:JX:309:LYS:HA	1.77	0.67
1:HX:277:ARG:HD2	1:HX:294:ARG:HH11	1.59	0.67
1:KX:73:GLU:OE2	1:KX:315:ARG:NH1	2.25	0.67
1:JX:73:GLU:OE2	1:JX:315:ARG:NH1	2.23	0.67
2:CY:1576:ILE:HG21	2:DY:1584:TYR:HE1	1.60	0.67
1:PX:277:ARG:HD2	1:PX:294:ARG:HH11	1.60	0.66
1:NX:277:ARG:HD2	1:NX:294:ARG:HH11	1.60	0.66
1:CX:73:GLU:OE2	1:CX:315:ARG:NH1	2.28	0.66
1:JX:277:ARG:HD2	1:JX:294:ARG:HH11	1.60	0.66
1:NX:78:ILE:HG21	1:NX:90:PRO:HG3	1.77	0.66
2:JY:1576:ILE:HG21	2:KY:1584:TYR:HE1	1.61	0.66
1:FX:61:LEU:HD22	1:FX:271:PRO:HG2	1.76	0.66
1:CX:104:SER:HB2	2:BY:1547:PHE:HB3	1.78	0.65
1:QX:67:ILE:HA	1:QX:308:VAL:HG23	1.78	0.65
1:LX:61:LEU:HD22	1:LX:271:PRO:HG2	1.78	0.65
1:FX:78:ILE:HG21	1:FX:90:PRO:HG3	1.79	0.65
1:IX:51:ASP:O	1:JX:43:ASN:ND2	2.29	0.65
1:OX:68:GLN:HB3	1:OX:309:LYS:HA	1.79	0.65
1:OX:61:LEU:HD22	1:OX:271:PRO:HG2	1.79	0.65
2:GY:1598:LYS:HA	2:GY:1601:LYS:HE3	1.80	0.64
1:GX:77:TYR:HB2	1:GX:283:ARG:HH21	1.62	0.64
1:KX:67:ILE:HA	1:KX:308:VAL:HG23	1.79	0.64
1:JX:78:ILE:HG21	1:JX:90:PRO:HG3	1.80	0.64
1:DX:104:SER:HB2	2:CY:1547:PHE:HB3	1.79	0.64
2:AY:1533:ASP:HA	2:BY:1519:VAL:HG21	1.80	0.64
1:KX:62:ASP:OD1	2:IY:1548:LYS:NZ	2.31	0.63
1:PX:78:ILE:HG21	1:PX:90:PRO:HG3	1.80	0.63
2:BY:1533:ASP:HA	2:CY:1519:VAL:HG21	1.79	0.63
1:GX:104:SER:HB2	2:FY:1547:PHE:HB3	1.80	0.63
1:BX:62:ASP:OD1	2:QY:1548:LYS:NZ	2.30	0.63
1:CX:129:LYS:O	1:DX:120:ARG:NH1	2.31	0.63
2:JY:1489:THR:O	2:JY:1491:GLN:NE2	2.31	0.63
1:DX:62:ASP:OD2	2:BY:1548:LYS:NZ	2.31	0.63
1:LX:277:ARG:HD2	1:LX:294:ARG:HH11	1.63	0.63
1:BX:105:ASN:OD1	1:BX:266:SER:OG	2.17	0.63
1:PX:105:ASN:OD1	1:PX:266:SER:OG	2.16	0.63
1:CX:51:ASP:O	1:DX:43:ASN:ND2	2.31	0.62
1:IX:77:TYR:HB2	1:IX:283:ARG:HH21	1.64	0.62
1:HX:78:ILE:HG21	1:HX:90:PRO:HG3	1.82	0.62
1:QX:105:ASN:OD1	1:QX:266:SER:OG	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GY:1587:GLU:HA	2:GY:1590:ILE:HD12	1.82	0.62
1:OX:282:VAL:HG13	1:OX:289:TYR:HB2	1.82	0.61
1:PX:73:GLU:OE2	1:PX:315:ARG:NH1	2.21	0.61
2:FY:1536:ALA:HB3	2:GY:1519:VAL:HG23	1.82	0.61
2:IY:1587:GLU:HA	2:IY:1590:ILE:HD12	1.81	0.61
1:AX:78:ILE:HG21	1:AX:90:PRO:HG3	1.82	0.61
1:CX:299:ASP:OD1	1:CX:299:ASP:N	2.30	0.61
1:HX:104:SER:HB2	2:GY:1547:PHE:HB3	1.82	0.61
1:FX:45:LYS:HD3	1:FX:309:LYS:HB3	1.83	0.61
1:GX:61:LEU:HD22	1:GX:271:PRO:HG2	1.83	0.61
1:AX:43:ASN:HD21	1:QX:52:GLU:HA	1.64	0.61
2:CY:1587:GLU:HA	2:CY:1590:ILE:HD12	1.81	0.61
1:GX:73:GLU:OE2	1:GX:315:ARG:NH1	2.21	0.61
1:QX:277:ARG:HD2	1:QX:294:ARG:HH11	1.66	0.61
2:NY:1536:ALA:HB3	2:OY:1519:VAL:HG23	1.81	0.61
2:HY:1470:SER:OG	2:HY:1471:LYS:N	2.34	0.61
1:DX:277:ARG:HD2	1:DX:294:ARG:HH11	1.66	0.61
1:LX:92:SER:O	1:LX:93:ASN:ND2	2.34	0.61
1:CX:45:LYS:HD3	1:CX:309:LYS:HB3	1.83	0.60
1:MX:61:LEU:HD12	2:LY:1527:ARG:HD3	1.83	0.60
1:PX:284:THR:HG23	1:PX:286:LYS:H	1.65	0.60
1:MX:299:ASP:OD1	1:MX:299:ASP:N	2.32	0.60
2:DY:1587:GLU:HA	2:DY:1590:ILE:HD12	1.82	0.60
1:MX:105:ASN:OD1	1:MX:266:SER:OG	2.18	0.60
1:HX:92:SER:O	1:HX:93:ASN:ND2	2.34	0.60
2:AY:1519:VAL:HG23	2:QY:1536:ALA:HB3	1.83	0.60
1:AX:120:ARG:NH1	1:QX:129:LYS:O	2.34	0.60
1:OX:73:GLU:OE2	1:OX:315:ARG:NH1	2.19	0.60
1:DX:51:ASP:O	1:EX:43:ASN:ND2	2.35	0.60
2:BY:1587:GLU:OE1	2:BY:1591:LYS:NZ	2.34	0.60
1:BX:282:VAL:HG13	1:BX:289:TYR:HB2	1.83	0.60
1:QX:61:LEU:HD22	1:QX:271:PRO:HG2	1.84	0.59
2:BY:1489:THR:O	2:BY:1491:GLN:NE2	2.34	0.59
2:MY:1533:ASP:HA	2:NY:1519:VAL:HG21	1.84	0.59
1:DX:92:SER:HB2	2:CY:1560:ASN:HA	1.85	0.59
1:GX:92:SER:O	1:GX:93:ASN:ND2	2.35	0.59
1:CX:77:TYR:HB2	1:CX:283:ARG:HH21	1.67	0.59
1:JX:299:ASP:HB2	2:JY:1512:ILE:HD13	1.84	0.59
2:JY:1587:GLU:HA	2:JY:1590:ILE:HD12	1.84	0.59
1:AX:45:LYS:HD3	1:AX:309:LYS:HB3	1.84	0.59
1:BX:288:LEU:HD22	1:CX:68:GLN:HE21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CX:277:ARG:HD2	1:CX:294:ARG:HH11	1.67	0.59
2:HY:1533:ASP:HA	2:IY:1519:VAL:HG21	1.85	0.59
1:LX:51:ASP:O	1:MX:43:ASN:ND2	2.35	0.59
2:LY:1587:GLU:HA	2:LY:1590:ILE:HD12	1.84	0.59
1:FX:73:GLU:OE2	1:FX:315:ARG:NH1	2.20	0.59
1:HX:36:ARG:HH11	2:GY:1488:PRO:HD3	1.67	0.59
1:BX:80:THR:HG22	1:BX:280:LEU:HD13	1.85	0.59
1:FX:80:THR:HG22	1:FX:280:LEU:HA	1.84	0.59
1:PX:61:LEU:HD22	1:PX:271:PRO:HG2	1.83	0.59
2:BY:1587:GLU:HA	2:BY:1590:ILE:HD12	1.83	0.59
2:DY:1482:LEU:HD13	2:DY:1513:LYS:HD2	1.85	0.59
1:LX:61:LEU:HD12	2:KY:1527:ARG:HD3	1.85	0.58
1:OX:62:ASP:OD2	2:MY:1548:LYS:NZ	2.36	0.58
2:AY:1489:THR:O	2:AY:1491:GLN:NE2	2.35	0.58
2:LY:1489:THR:O	2:LY:1491:GLN:NE2	2.36	0.58
1:EX:92:SER:O	1:EX:93:ASN:ND2	2.36	0.58
1:IX:61:LEU:HD22	1:IX:271:PRO:HG2	1.85	0.58
2:EY:1587:GLU:HA	2:EY:1590:ILE:HD12	1.84	0.58
1:DX:61:LEU:HD22	1:DX:271:PRO:HG2	1.84	0.58
2:AY:1470:SER:OG	2:AY:1471:LYS:N	2.35	0.58
2:AY:1587:GLU:HA	2:AY:1590:ILE:HD12	1.84	0.58
2:PY:1470:SER:OG	2:PY:1471:LYS:N	2.34	0.58
1:BX:67:ILE:HD11	1:BX:97:ILE:HD13	1.85	0.58
1:NX:284:THR:HG23	1:NX:286:LYS:H	1.68	0.58
1:PX:92:SER:O	1:PX:93:ASN:ND2	2.37	0.58
2:PY:1587:GLU:HA	2:PY:1590:ILE:HD12	1.85	0.58
1:AX:61:LEU:HD12	2:QY:1527:ARG:HD3	1.83	0.58
1:JX:288:LEU:HD22	1:KX:68:GLN:HE21	1.68	0.58
2:KY:1564:ASP:OD1	2:KY:1564:ASP:N	2.31	0.58
1:BX:280:LEU:N	1:BX:291:PHE:O	2.30	0.58
1:CX:92:SER:O	1:CX:93:ASN:ND2	2.36	0.58
1:EX:288:LEU:HD22	1:FX:68:GLN:HE21	1.68	0.58
1:FX:67:ILE:HD11	1:FX:97:ILE:HD13	1.86	0.58
1:LX:105:ASN:OD1	1:LX:266:SER:OG	2.19	0.58
1:EX:105:ASN:OD1	1:EX:266:SER:OG	2.21	0.58
1:IX:93:ASN:HD22	2:HY:1566:ILE:HD13	1.69	0.58
1:GX:105:ASN:OD1	1:GX:266:SER:OG	2.19	0.58
2:DY:1536:ALA:HB3	2:EY:1519:VAL:HG23	1.86	0.58
2:FY:1534:ASN:OD1	2:FY:1538:LYS:NZ	2.30	0.58
2:AY:1536:ALA:HB3	2:BY:1519:VAL:HG23	1.86	0.57
2:BY:1482:LEU:HD13	2:BY:1513:LYS:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GY:1503:ASP:OD2	2:GY:1504:SER:N	2.36	0.57
1:FX:105:ASN:OD1	1:FX:266:SER:OG	2.20	0.57
1:CX:105:ASN:OD1	1:CX:266:SER:OG	2.20	0.57
1:DX:77:TYR:HA	2:CY:1555:THR:HG23	1.85	0.57
1:JX:277:ARG:HD2	1:JX:294:ARG:NH1	2.19	0.57
1:JX:282:VAL:HG13	1:JX:289:TYR:HB2	1.86	0.57
1:MX:67:ILE:HA	1:MX:308:VAL:HG13	1.85	0.57
2:HY:1489:THR:O	2:HY:1491:GLN:NE2	2.36	0.57
1:CX:289:TYR:HH	1:CX:312:TYR:HH	1.53	0.57
1:BX:67:ILE:HA	1:BX:308:VAL:HG23	1.85	0.57
1:BX:92:SER:O	1:BX:93:ASN:ND2	2.37	0.57
1:FX:59:THR:OG1	1:FX:60:SER:N	2.37	0.57
1:KX:45:LYS:HD3	1:KX:309:LYS:HB3	1.86	0.57
1:DX:61:LEU:HD12	2:CY:1527:ARG:HD3	1.87	0.57
1:EX:71:LYS:HE2	2:DY:1566:ILE:HB	1.87	0.57
2:JY:1533:ASP:HA	2:KY:1519:VAL:HG21	1.86	0.57
2:QY:1587:GLU:HA	2:QY:1590:ILE:HD12	1.86	0.57
1:CX:62:ASP:OD1	2:AY:1548:LYS:NZ	2.37	0.57
1:NX:61:LEU:HD22	1:NX:271:PRO:HG2	1.87	0.57
2:CY:1533:ASP:HA	2:DY:1519:VAL:HG21	1.87	0.57
2:HY:1536:ALA:HB3	2:IY:1519:VAL:HG23	1.86	0.57
1:CX:101:SER:OG	2:AY:1549:ASN:ND2	2.38	0.57
1:OX:45:LYS:HD3	1:OX:309:LYS:HB3	1.87	0.57
1:HX:45:LYS:HD3	1:HX:309:LYS:HB3	1.87	0.56
1:HX:67:ILE:HA	1:HX:308:VAL:HG23	1.87	0.56
1:GX:59:THR:OG1	1:GX:60:SER:N	2.38	0.56
1:HX:77:TYR:HA	2:GY:1555:THR:HG23	1.86	0.56
1:QX:78:ILE:HG21	1:QX:90:PRO:HG3	1.86	0.56
1:AX:59:THR:HG21	1:AX:86:TRP:CZ3	2.40	0.56
1:CX:61:LEU:HD22	1:CX:271:PRO:HG2	1.86	0.56
1:AX:105:ASN:OD1	1:AX:266:SER:OG	2.20	0.56
1:QX:289:TYR:HH	1:QX:312:TYR:HH	1.53	0.56
2:NY:1482:LEU:HD13	2:NY:1513:LYS:HD2	1.87	0.56
1:JX:59:THR:OG1	1:JX:60:SER:N	2.38	0.56
1:OX:92:SER:O	1:OX:93:ASN:ND2	2.38	0.56
2:FY:1489:THR:O	2:FY:1491:GLN:NE2	2.39	0.56
2:MY:1543:LEU:HD12	2:NY:1526:LEU:HD11	1.87	0.56
1:AX:92:SER:O	1:AX:93:ASN:ND2	2.39	0.56
1:EX:78:ILE:HG21	1:EX:90:PRO:HG3	1.88	0.56
1:IX:271:PRO:HB3	1:IX:276:TRP:CE2	2.40	0.56
1:OX:57:ILE:HD12	1:OX:308:VAL:HG11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BY:1503:ASP:OD2	2:BY:1504:SER:N	2.38	0.56
2:DY:1489:THR:O	2:DY:1491:GLN:NE2	2.39	0.56
1:CX:280:LEU:N	1:CX:291:PHE:O	2.36	0.56
1:PX:77:TYR:HB2	1:PX:283:ARG:HH21	1.71	0.56
2:NY:1533:ASP:HA	2:OY:1519:VAL:HG21	1.87	0.56
1:HX:80:THR:HG22	1:HX:280:LEU:HD13	1.88	0.56
1:PX:45:LYS:HD3	1:PX:309:LYS:HB3	1.88	0.56
1:DX:45:LYS:HD3	1:DX:309:LYS:HB3	1.87	0.56
1:DX:277:ARG:HD2	1:DX:294:ARG:NH1	2.20	0.56
1:EX:104:SER:HB2	2:DY:1547:PHE:HB3	1.88	0.56
1:KX:92:SER:O	1:KX:93:ASN:ND2	2.39	0.56
1:BX:284:THR:HG23	1:BX:286:LYS:H	1.71	0.56
2:LY:1503:ASP:OD2	2:LY:1504:SER:N	2.39	0.56
1:LX:45:LYS:HD3	1:LX:309:LYS:HB3	1.87	0.55
1:NX:289:TYR:OH	1:NX:312:TYR:OH	2.22	0.55
2:FY:1487:ASP:OD2	2:FY:1489:THR:OG1	2.21	0.55
1:MX:59:THR:OG1	1:MX:60:SER:N	2.40	0.55
1:OX:78:ILE:HG21	1:OX:90:PRO:HG3	1.87	0.55
1:CX:282:VAL:HG13	1:CX:289:TYR:HB2	1.88	0.55
1:HX:61:LEU:HD22	1:HX:271:PRO:HG2	1.88	0.55
1:LX:282:VAL:HG13	1:LX:289:TYR:HB2	1.87	0.55
2:LY:1495:GLU:OE2	2:LY:1506:ARG:NH2	2.39	0.55
1:EX:45:LYS:HD3	1:EX:309:LYS:HB3	1.87	0.55
1:GX:282:VAL:HG13	1:GX:289:TYR:HB2	1.88	0.55
2:GY:1579:ASP:HB3	2:GY:1582:LYS:HD3	1.88	0.55
1:IX:59:THR:OG1	1:IX:60:SER:N	2.40	0.55
2:GY:1470:SER:OG	2:GY:1471:LYS:N	2.40	0.55
2:KY:1489:THR:O	2:KY:1491:GLN:NE2	2.39	0.55
2:PY:1533:ASP:HA	2:QY:1519:VAL:HG21	1.88	0.55
1:GX:46:ILE:HG23	1:GX:310:LEU:HD23	1.88	0.55
1:JX:271:PRO:HA	1:JX:276:TRP:CZ3	2.42	0.55
1:MX:45:LYS:HD3	1:MX:309:LYS:HB3	1.88	0.55
1:NX:45:LYS:HD3	1:NX:309:LYS:HB3	1.89	0.55
1:AX:51:ASP:O	1:BX:43:ASN:ND2	2.39	0.55
1:KX:284:THR:OG1	1:KX:285:ASN:N	2.38	0.55
1:KX:288:LEU:HD22	1:LX:68:GLN:HE21	1.71	0.55
1:QX:282:VAL:HG13	1:QX:289:TYR:HB2	1.87	0.55
2:HY:1587:GLU:HA	2:HY:1590:ILE:HD12	1.88	0.55
2:OY:1587:GLU:HA	2:OY:1590:ILE:HD12	1.88	0.55
1:CX:73:GLU:HG2	1:CX:286:LYS:HB2	1.88	0.55
1:FX:62:ASP:OD1	2:DY:1548:LYS:NZ	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AX:94:HIS:NE2	1:QX:283:ARG:HD3	2.22	0.55
2:LY:1533:ASP:HA	2:MY:1519:VAL:HG21	1.88	0.55
1:CX:283:ARG:HD3	1:DX:94:HIS:NE2	2.22	0.54
1:JX:289:TYR:OH	1:JX:312:TYR:OH	2.23	0.54
1:MX:61:LEU:HD22	1:MX:271:PRO:HG2	1.87	0.54
2:QY:1482:LEU:HD13	2:QY:1513:LYS:HD2	1.89	0.54
1:GX:89:VAL:HG13	1:GX:96:PHE:HB2	1.88	0.54
1:NX:92:SER:O	1:NX:93:ASN:ND2	2.41	0.54
1:IX:282:VAL:HG13	1:IX:289:TYR:HB2	1.89	0.54
2:IY:1533:ASP:HA	2:JY:1519:VAL:HG21	1.88	0.54
2:JY:1495:GLU:OE2	2:JY:1506:ARG:NH2	2.41	0.54
2:MY:1587:GLU:HA	2:MY:1590:ILE:HD12	1.88	0.54
1:KX:105:ASN:OD1	1:KX:266:SER:OG	2.19	0.54
2:IY:1482:LEU:HD13	2:IY:1513:LYS:HD2	1.88	0.54
2:LY:1536:ALA:HB3	2:MY:1519:VAL:HG23	1.88	0.54
1:JX:48:TYR:HD1	1:JX:55:ILE:HD11	1.71	0.54
1:FX:284:THR:OG1	1:FX:285:ASN:N	2.39	0.54
1:MX:277:ARG:HD2	1:MX:294:ARG:HH11	1.72	0.54
1:QX:92:SER:HB2	2:PY:1560:ASN:HA	1.88	0.54
2:QY:1489:THR:O	2:QY:1491:GLN:NE2	2.40	0.54
1:JX:61:LEU:HD22	1:JX:271:PRO:HG2	1.90	0.54
2:GY:1482:LEU:HD13	2:GY:1513:LYS:HD2	1.89	0.54
1:EX:271:PRO:HB3	1:EX:276:TRP:CE2	2.43	0.54
1:KX:129:LYS:O	1:LX:120:ARG:NH1	2.41	0.54
1:OX:105:ASN:OD1	1:OX:266:SER:OG	2.20	0.54
1:PX:282:VAL:HG13	1:PX:289:TYR:HB2	1.89	0.54
2:NY:1587:GLU:HA	2:NY:1590:ILE:HD12	1.89	0.54
1:BX:45:LYS:HD3	1:BX:309:LYS:HB3	1.90	0.53
1:CX:67:ILE:HA	1:CX:308:VAL:HG23	1.88	0.53
1:GX:284:THR:OG1	1:GX:285:ASN:N	2.40	0.53
1:KX:61:LEU:HD22	1:KX:271:PRO:HG2	1.90	0.53
2:IY:1536:ALA:HB3	2:JY:1519:VAL:HG23	1.90	0.53
1:EX:51:ASP:O	1:FX:43:ASN:ND2	2.41	0.53
1:GX:299:ASP:OD1	1:GX:299:ASP:N	2.31	0.53
2:FY:1587:GLU:HA	2:FY:1590:ILE:HD12	1.90	0.53
1:IX:283:ARG:HD3	1:JX:94:HIS:NE2	2.23	0.53
1:JX:37:GLY:HA2	1:JX:298:LYS:HB2	1.91	0.53
1:HX:271:PRO:HB3	1:HX:276:TRP:CE2	2.43	0.53
1:LX:277:ARG:HD2	1:LX:294:ARG:NH1	2.24	0.53
1:NX:43:ASN:OD1	1:NX:43:ASN:N	2.38	0.53
2:GY:1587:GLU:OE1	2:GY:1591:LYS:NZ	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AY:1519:VAL:HG21	2:QY:1533:ASP:HA	1.91	0.53
2:KY:1536:ALA:HB3	2:LY:1519:VAL:HG23	1.91	0.53
1:BX:59:THR:OG1	1:BX:60:SER:N	2.41	0.53
2:GY:1579:ASP:OD1	2:GY:1582:LYS:N	2.34	0.53
1:BX:68:GLN:HE22	1:BX:94:HIS:CD2	2.27	0.53
1:NX:282:VAL:HG13	1:NX:289:TYR:HB2	1.91	0.53
1:PX:59:THR:OG1	1:PX:60:SER:N	2.41	0.53
1:QX:45:LYS:HD3	1:QX:309:LYS:HB3	1.90	0.53
2:CY:1596:GLU:HA	2:CY:1599:LEU:HD23	1.91	0.53
2:GY:1536:ALA:HB3	2:HY:1519:VAL:HG23	1.90	0.53
1:EX:39:VAL:HG11	1:EX:60:SER:HB2	1.91	0.53
2:JY:1470:SER:OG	2:JY:1471:LYS:N	2.42	0.53
2:PY:1585:GLU:O	2:PY:1589:THR:HG23	2.09	0.53
1:AX:59:THR:OG1	1:AX:60:SER:N	2.41	0.52
1:CX:58:TRP:H	1:CX:305:TYR:HD2	1.57	0.52
1:DX:271:PRO:HB3	1:DX:276:TRP:CE2	2.42	0.52
1:LX:68:GLN:HA	1:LX:94:HIS:HB3	1.90	0.52
1:BX:129:LYS:O	1:CX:120:ARG:NH1	2.42	0.52
1:GX:57:ILE:HD12	1:GX:308:VAL:HG21	1.91	0.52
1:GX:67:ILE:HA	1:GX:308:VAL:HG23	1.92	0.52
1:IX:45:LYS:HD3	1:IX:309:LYS:HB3	1.91	0.52
1:IX:68:GLN:HE22	1:IX:94:HIS:CD2	2.27	0.52
1:LX:80:THR:HG22	1:LX:280:LEU:HD13	1.92	0.52
1:OX:59:THR:OG1	1:OX:60:SER:N	2.41	0.52
2:KY:1470:SER:OG	2:KY:1471:LYS:N	2.40	0.52
1:EX:282:VAL:HG13	1:EX:289:TYR:HB2	1.92	0.52
1:GX:67:ILE:HD11	1:GX:97:ILE:HD13	1.91	0.52
1:GX:71:LYS:HE2	2:FY:1566:ILE:HB	1.91	0.52
1:KX:59:THR:OG1	1:KX:60:SER:N	2.42	0.52
2:HY:1503:ASP:OD1	2:HY:1504:SER:N	2.42	0.52
2:JY:1503:ASP:OD2	2:JY:1504:SER:N	2.42	0.52
1:DX:283:ARG:HD3	1:EX:94:HIS:NE2	2.25	0.52
1:GX:277:ARG:HD2	1:GX:294:ARG:HH11	1.74	0.52
1:JX:129:LYS:O	1:KX:120:ARG:NH1	2.42	0.52
2:DY:1503:ASP:OD1	2:DY:1504:SER:N	2.43	0.52
2:GY:1489:THR:O	2:GY:1491:GLN:NE2	2.42	0.52
1:FX:73:GLU:HG2	1:FX:286:LYS:HB2	1.92	0.52
1:BX:78:ILE:HG21	1:BX:90:PRO:HG3	1.91	0.52
2:EY:1489:THR:O	2:EY:1491:GLN:NE2	2.41	0.52
2:MY:1487:ASP:OD1	2:MY:1489:THR:OG1	2.24	0.52
1:AX:282:VAL:HG13	1:AX:289:TYR:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FX:89:VAL:HG13	1:FX:96:PHE:HB2	1.90	0.52
1:FX:101:SER:OG	2:DY:1549:ASN:ND2	2.42	0.52
1:GX:45:LYS:HD3	1:GX:309:LYS:HB3	1.91	0.52
1:HX:59:THR:OG1	1:HX:60:SER:N	2.43	0.52
1:PX:36:ARG:HG2	1:PX:38:ARG:H	1.75	0.52
2:IY:1470:SER:OG	2:IY:1471:LYS:N	2.43	0.52
2:NY:1503:ASP:OD2	2:NY:1504:SER:N	2.43	0.52
1:CX:61:LEU:HD12	2:BY:1527:ARG:HD3	1.91	0.52
1:QX:68:GLN:HG2	1:QX:309:LYS:HG3	1.91	0.52
2:BY:1536:ALA:HB3	2:CY:1519:VAL:HG23	1.91	0.52
2:OY:1470:SER:OG	2:OY:1471:LYS:N	2.41	0.52
2:QY:1577:GLU:HG2	2:QY:1578:PRO:O	2.10	0.52
1:GX:78:ILE:HG21	1:GX:90:PRO:HG3	1.91	0.52
2:AY:1577:GLU:HG2	2:AY:1578:PRO:O	2.10	0.52
2:EY:1495:GLU:OE2	2:EY:1506:ARG:NH2	2.42	0.52
2:EY:1585:GLU:O	2:EY:1589:THR:HG23	2.10	0.52
1:AX:61:LEU:HD22	1:AX:271:PRO:HG2	1.91	0.52
1:DX:68:GLN:HB3	1:DX:309:LYS:HA	1.92	0.52
1:DX:282:VAL:HG13	1:DX:289:TYR:HB2	1.90	0.52
1:PX:289:TYR:HH	1:PX:312:TYR:HH	1.54	0.52
2:CY:1585:GLU:O	2:CY:1589:THR:HG23	2.10	0.52
2:EY:1470:SER:OG	2:EY:1471:LYS:N	2.43	0.52
2:FY:1482:LEU:HD13	2:FY:1513:LYS:HD2	1.91	0.52
1:CX:92:SER:HB2	2:BY:1560:ASN:HA	1.92	0.51
1:FX:93:ASN:HD22	2:EY:1566:ILE:HD13	1.75	0.51
1:NX:59:THR:OG1	1:NX:60:SER:N	2.43	0.51
2:AY:1585:GLU:O	2:AY:1589:THR:HG23	2.10	0.51
2:LY:1585:GLU:O	2:LY:1589:THR:HG23	2.11	0.51
1:GX:48:TYR:HB2	1:GX:310:LEU:HD22	1.93	0.51
1:NX:80:THR:HG22	1:NX:280:LEU:HD13	1.92	0.51
1:QX:271:PRO:HB3	1:QX:276:TRP:CE2	2.44	0.51
2:EY:1564:ASP:OD1	2:EY:1564:ASP:N	2.44	0.51
2:IY:1585:GLU:O	2:IY:1589:THR:HG23	2.10	0.51
1:AX:77:TYR:HA	2:QY:1555:THR:HG23	1.92	0.51
1:DX:67:ILE:HA	1:DX:308:VAL:HG23	1.90	0.51
1:FX:88:ILE:HG12	1:FX:97:ILE:HG22	1.93	0.51
1:IX:61:LEU:HD12	2:HY:1527:ARG:HD3	1.93	0.51
1:NX:60:SER:OG	1:NX:63:ASN:ND2	2.43	0.51
1:PX:71:LYS:HE2	2:OY:1566:ILE:HB	1.91	0.51
2:AY:1587:GLU:OE2	2:AY:1591:LYS:NZ	2.43	0.51
2:BY:1470:SER:OG	2:BY:1471:LYS:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:OY:1585:GLU:O	2:OY:1589:THR:HG23	2.10	0.51
1:DX:67:ILE:HD11	1:DX:97:ILE:HD13	1.92	0.51
1:EX:59:THR:OG1	1:EX:60:SER:N	2.43	0.51
1:GX:68:GLN:HE22	1:GX:94:HIS:CD2	2.28	0.51
1:LX:299:ASP:OD1	1:LX:299:ASP:N	2.33	0.51
2:FY:1503:ASP:OD2	2:FY:1504:SER:N	2.43	0.51
2:MY:1535:MET:HE2	2:MY:1544:PRO:HD3	1.91	0.51
1:NX:68:GLN:HA	1:NX:94:HIS:HB3	1.92	0.51
2:OY:1577:GLU:HG2	2:OY:1578:PRO:O	2.10	0.51
2:PY:1577:GLU:HG2	2:PY:1578:PRO:O	2.11	0.51
2:PY:1586:THR:HG22	2:QY:1599:LEU:HB2	1.92	0.51
2:QY:1585:GLU:O	2:QY:1589:THR:HG23	2.11	0.51
1:MX:68:GLN:HG2	1:MX:309:LYS:HG3	1.93	0.51
1:HX:33:ASN:OD1	1:HX:34:PHE:N	2.43	0.51
1:JX:284:THR:OG1	1:JX:285:ASN:N	2.42	0.51
1:MX:92:SER:O	1:MX:93:ASN:ND2	2.44	0.51
1:MX:282:VAL:HG13	1:MX:289:TYR:HB2	1.92	0.51
1:QX:68:GLN:HB3	1:QX:309:LYS:HA	1.92	0.51
2:HY:1534:ASN:OD1	2:HY:1538:LYS:NZ	2.31	0.51
2:NY:1534:ASN:OD1	2:NY:1538:LYS:NZ	2.31	0.51
1:JX:289:TYR:O	1:JX:290:GLN:NE2	2.44	0.51
1:LX:59:THR:OG1	1:LX:60:SER:N	2.42	0.51
2:FY:1585:GLU:O	2:FY:1589:THR:HG23	2.11	0.51
2:KY:1585:GLU:O	2:KY:1589:THR:HG23	2.10	0.51
2:MY:1593:LYS:HD2	2:NY:1603:LEU:HA	1.93	0.51
1:AX:59:THR:HG21	1:AX:86:TRP:HZ3	1.75	0.50
1:MX:73:GLU:HG2	1:MX:286:LYS:HB2	1.92	0.50
1:NX:277:ARG:HD2	1:NX:294:ARG:NH1	2.25	0.50
1:OX:68:GLN:HA	1:OX:94:HIS:HB3	1.93	0.50
2:DY:1585:GLU:O	2:DY:1589:THR:HG23	2.11	0.50
1:DX:57:ILE:HD12	1:DX:308:VAL:HG21	1.92	0.50
1:EX:62:ASP:OD1	2:CY:1548:LYS:NZ	2.44	0.50
1:QX:73:GLU:HG2	1:QX:286:LYS:HB2	1.93	0.50
2:BY:1585:GLU:O	2:BY:1589:THR:HG23	2.11	0.50
2:CY:1577:GLU:HG2	2:CY:1578:PRO:O	2.11	0.50
2:GY:1577:GLU:HG2	2:GY:1578:PRO:O	2.12	0.50
1:JX:68:GLN:HA	1:JX:94:HIS:HB3	1.94	0.50
1:LX:271:PRO:HB3	1:LX:276:TRP:CE2	2.47	0.50
1:MX:43:ASN:OD1	1:MX:43:ASN:N	2.42	0.50
1:PX:283:ARG:HD3	1:QX:94:HIS:NE2	2.26	0.50
1:QX:93:ASN:HD22	2:PY:1566:ILE:HD13	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CY:1576:ILE:HG21	2:DY:1584:TYR:CE1	2.45	0.50
2:DY:1577:GLU:HG2	2:DY:1578:PRO:O	2.12	0.50
1:IX:299:ASP:OD1	1:IX:299:ASP:N	2.32	0.50
1:JX:61:LEU:HD12	2:IY:1527:ARG:HD3	1.93	0.50
1:JX:105:ASN:OD1	1:JX:266:SER:OG	2.22	0.50
1:NX:129:LYS:O	1:OX:120:ARG:NH1	2.44	0.50
1:AX:68:GLN:HA	1:AX:94:HIS:HB3	1.93	0.50
1:DX:33:ASN:OD1	1:DX:34:PHE:N	2.44	0.50
1:GX:289:TYR:OH	1:GX:312:TYR:OH	2.24	0.50
1:IX:277:ARG:HD2	1:IX:294:ARG:HH11	1.75	0.50
2:EY:1503:ASP:OD1	2:EY:1504:SER:N	2.44	0.50
2:GY:1514:ARG:HG3	2:GY:1515:GLN:N	2.26	0.50
1:JX:289:TYR:HH	1:JX:312:TYR:HH	1.56	0.50
1:OX:71:LYS:HE2	2:NY:1566:ILE:HB	1.94	0.50
2:IY:1576:ILE:HG21	2:JY:1584:TYR:CE1	2.42	0.50
1:LX:73:GLU:HG2	1:LX:286:LYS:HB2	1.92	0.50
1:QX:92:SER:O	1:QX:93:ASN:ND2	2.45	0.50
2:OY:1533:ASP:HA	2:PY:1519:VAL:HG21	1.94	0.50
1:CX:290:GLN:NE2	1:DX:307:THR:OG1	2.45	0.50
2:CY:1503:ASP:OD1	2:CY:1504:SER:N	2.45	0.50
2:GY:1533:ASP:HA	2:HY:1519:VAL:HG21	1.94	0.50
2:IY:1564:ASP:OD1	2:IY:1564:ASP:N	2.33	0.50
2:NY:1585:GLU:O	2:NY:1589:THR:HG23	2.12	0.50
2:OY:1489:THR:O	2:OY:1491:GLN:NE2	2.42	0.50
1:EX:305:TYR:HB3	1:EX:308:VAL:HG13	1.94	0.50
2:HY:1585:GLU:O	2:HY:1589:THR:HG23	2.12	0.50
1:CX:271:PRO:HB3	1:CX:276:TRP:CE2	2.47	0.49
1:HX:277:ARG:HD2	1:HX:294:ARG:NH1	2.24	0.49
1:JX:280:LEU:N	1:JX:291:PHE:O	2.45	0.49
2:AY:1593:LYS:HD2	2:BY:1603:LEU:HD23	1.94	0.49
2:NY:1577:GLU:HG2	2:NY:1578:PRO:O	2.12	0.49
1:FX:282:VAL:HG13	1:FX:289:TYR:HB2	1.93	0.49
1:JX:92:SER:O	1:JX:93:ASN:ND2	2.45	0.49
2:BY:1577:GLU:HG2	2:BY:1578:PRO:O	2.12	0.49
2:JY:1536:ALA:HB3	2:KY:1519:VAL:HG23	1.93	0.49
2:JY:1577:GLU:HG2	2:JY:1578:PRO:O	2.12	0.49
2:JY:1585:GLU:O	2:JY:1589:THR:HG23	2.11	0.49
2:MY:1482:LEU:HD13	2:MY:1513:LYS:HD2	1.94	0.49
1:DX:78:ILE:HG21	1:DX:90:PRO:HG3	1.93	0.49
1:EX:284:THR:HG23	1:EX:286:LYS:H	1.77	0.49
1:HX:105:ASN:OD1	1:HX:266:SER:OG	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AX:271:PRO:HB3	1:AX:276:TRP:CE2	2.48	0.49
1:HX:282:VAL:HG13	1:HX:289:TYR:HB2	1.94	0.49
1:MX:278:THR:OG1	1:MX:279:ASN:N	2.46	0.49
2:EY:1536:ALA:HB3	2:FY:1519:VAL:HG23	1.95	0.49
2:JY:1486:ASP:OD1	2:JY:1487:ASP:N	2.45	0.49
2:MY:1577:GLU:HG2	2:MY:1578:PRO:O	2.13	0.49
1:CX:277:ARG:HD2	1:CX:294:ARG:NH1	2.27	0.49
1:GX:59:THR:HG21	1:GX:86:TRP:CZ3	2.47	0.49
1:HX:121:ASP:HA	1:HX:124:GLU:HG3	1.94	0.49
1:PX:68:GLN:HA	1:PX:94:HIS:HB3	1.94	0.49
1:PX:101:SER:OG	2:NY:1549:ASN:ND2	2.45	0.49
1:CX:57:ILE:HG21	1:CX:97:ILE:HD11	1.94	0.49
1:DX:92:SER:O	1:DX:93:ASN:ND2	2.45	0.49
1:GX:283:ARG:HD3	1:HX:94:HIS:NE2	2.28	0.49
1:HX:57:ILE:HD12	1:HX:308:VAL:HG21	1.95	0.49
2:DY:1534:ASN:OD1	2:DY:1538:LYS:NZ	2.32	0.49
1:DX:80:THR:HG22	1:DX:280:LEU:HD13	1.95	0.49
1:FX:36:ARG:HH11	2:EY:1488:PRO:HD3	1.78	0.49
1:IX:105:ASN:OD1	1:IX:266:SER:OG	2.22	0.49
1:PX:106:LEU:HD21	1:PX:267:ILE:HD13	1.94	0.49
2:GY:1585:GLU:O	2:GY:1589:THR:HG23	2.11	0.49
2:HY:1577:GLU:HG2	2:HY:1578:PRO:O	2.12	0.49
1:EX:67:ILE:HD11	1:EX:97:ILE:HD13	1.94	0.49
1:HX:59:THR:HG21	1:HX:86:TRP:CZ3	2.48	0.49
1:NX:59:THR:HG21	1:NX:86:TRP:CZ3	2.48	0.49
2:EY:1533:ASP:HA	2:FY:1519:VAL:HG21	1.94	0.49
2:JY:1535:MET:HE2	2:JY:1544:PRO:HD3	1.95	0.49
2:KY:1479:SER:HB2	2:KY:1509:ILE:HD11	1.94	0.49
2:KY:1482:LEU:HD13	2:KY:1513:LYS:HD2	1.95	0.49
2:MY:1536:ALA:HB3	2:NY:1519:VAL:HG23	1.95	0.49
1:MX:68:GLN:HA	1:MX:94:HIS:HB3	1.94	0.49
2:FY:1577:GLU:HG2	2:FY:1578:PRO:O	2.13	0.49
2:KY:1503:ASP:OD1	2:KY:1504:SER:N	2.45	0.49
2:MY:1503:ASP:OD1	2:MY:1504:SER:N	2.46	0.49
2:MY:1585:GLU:O	2:MY:1589:THR:HG23	2.12	0.49
1:AX:280:LEU:N	1:AX:291:PHE:O	2.41	0.49
1:CX:281:VAL:HG12	1:CX:290:GLN:HE22	1.76	0.49
1:MX:284:THR:HG23	1:MX:286:LYS:H	1.77	0.49
1:PX:271:PRO:HB3	1:PX:276:TRP:CE2	2.48	0.49
1:HX:67:ILE:HD11	1:HX:97:ILE:HD13	1.94	0.48
2:BY:1535:MET:HE2	2:BY:1544:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:IY:1577:GLU:HG2	2:IY:1578:PRO:O	2.12	0.48
1:IX:262:PRO:HB2	2:HY:1542:LEU:HD11	1.93	0.48
2:AY:1503:ASP:OD2	2:AY:1504:SER:N	2.46	0.48
2:LY:1577:GLU:HG2	2:LY:1578:PRO:O	2.13	0.48
1:KX:78:ILE:HG21	1:KX:90:PRO:HG3	1.93	0.48
1:MX:59:THR:HG21	1:MX:86:TRP:CZ3	2.48	0.48
1:OX:45:LYS:HE3	1:OX:309:LYS:HD3	1.96	0.48
1:OX:68:GLN:HG2	1:OX:309:LYS:HG3	1.96	0.48
1:OX:289:TYR:OH	1:OX:312:TYR:OH	2.30	0.48
2:IY:1593:LYS:HD2	2:JY:1603:LEU:HA	1.94	0.48
2:PY:1482:LEU:HD13	2:PY:1513:LYS:HD2	1.96	0.48
1:DX:59:THR:HG21	1:DX:86:TRP:CZ3	2.47	0.48
2:BY:1495:GLU:OE2	2:BY:1506:ARG:NH2	2.46	0.48
2:NY:1499:GLU:OE1	2:NY:1500:GLY:N	2.46	0.48
1:CX:103:LYS:NZ	1:CX:268:GLU:HB3	2.29	0.48
1:DX:121:ASP:O	1:DX:124:GLU:HG3	2.13	0.48
1:GX:271:PRO:HA	1:GX:276:TRP:CZ3	2.49	0.48
1:OX:48:TYR:HD1	1:OX:55:ILE:HD11	1.78	0.48
2:JY:1499:GLU:OE1	2:JY:1500:GLY:N	2.46	0.48
2:QY:1503:ASP:OD2	2:QY:1504:SER:N	2.47	0.48
1:FX:67:ILE:HA	1:FX:308:VAL:HG23	1.95	0.48
1:QX:276:TRP:O	1:QX:278:THR:HG22	2.14	0.48
1:AX:299:ASP:OD1	1:AX:299:ASP:N	2.35	0.48
1:BX:61:LEU:HD22	1:BX:271:PRO:HG2	1.95	0.48
1:CX:59:THR:OG1	1:CX:60:SER:N	2.45	0.48
1:KX:271:PRO:HB3	1:KX:276:TRP:CE2	2.48	0.48
2:AY:1534:ASN:OD1	2:AY:1538:LYS:NZ	2.34	0.48
2:HY:1535:MET:HE2	2:HY:1544:PRO:HD3	1.95	0.48
2:KY:1495:GLU:OE2	2:KY:1506:ARG:NH2	2.47	0.48
2:OY:1503:ASP:OD1	2:OY:1504:SER:N	2.47	0.48
2:PY:1593:LYS:HD2	2:QY:1603:LEU:HD23	1.96	0.48
1:DX:299:ASP:OD1	1:DX:299:ASP:N	2.29	0.48
1:GX:276:TRP:O	1:GX:278:THR:HG22	2.14	0.48
1:IX:33:ASN:OD1	1:IX:34:PHE:N	2.46	0.48
1:LX:91:ASN:ND2	2:KY:1559:THR:OG1	2.46	0.48
1:OX:89:VAL:HG13	1:OX:96:PHE:HB2	1.95	0.48
1:OX:271:PRO:HB3	1:OX:276:TRP:CE2	2.49	0.48
2:KY:1577:GLU:HG2	2:KY:1578:PRO:O	2.13	0.48
1:EX:67:ILE:HA	1:EX:308:VAL:HG23	1.94	0.48
1:EX:88:ILE:HG12	1:EX:97:ILE:HG22	1.95	0.48
1:FX:276:TRP:O	1:FX:278:THR:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LX:59:THR:HG21	1:LX:86:TRP:CZ3	2.49	0.48
1:NX:280:LEU:N	1:NX:291:PHE:O	2.34	0.48
2:BY:1598:LYS:HA	2:BY:1601:LYS:HE3	1.95	0.48
1:DX:89:VAL:HG13	1:DX:96:PHE:HB2	1.95	0.47
1:IX:57:ILE:HD12	1:IX:308:VAL:HG11	1.96	0.47
1:JX:43:ASN:OD1	1:JX:43:ASN:N	2.34	0.47
1:QX:57:ILE:HD12	1:QX:308:VAL:HG21	1.96	0.47
1:QX:121:ASP:HA	1:QX:124:GLU:HG3	1.96	0.47
2:HY:1486:ASP:OD1	2:HY:1487:ASP:N	2.47	0.47
1:EX:68:GLN:HA	1:EX:94:HIS:HB3	1.94	0.47
1:NX:61:LEU:HD12	2:MY:1527:ARG:HD3	1.95	0.47
1:QX:80:THR:HG22	1:QX:280:LEU:HD13	1.94	0.47
2:MY:1564:ASP:OD1	2:MY:1564:ASP:N	2.45	0.47
2:QY:1495:GLU:OE2	2:QY:1506:ARG:NH2	2.47	0.47
1:AX:121:ASP:O	1:AX:124:GLU:HG3	2.14	0.47
1:CX:57:ILE:HD12	1:CX:308:VAL:HG21	1.95	0.47
1:HX:284:THR:OG1	1:HX:285:ASN:N	2.47	0.47
2:CY:1598:LYS:HA	2:CY:1601:LYS:HZ2	1.78	0.47
2:EY:1577:GLU:HG2	2:EY:1578:PRO:O	2.15	0.47
1:JX:57:ILE:HG21	1:JX:97:ILE:HD11	1.96	0.47
1:LX:301:PHE:O	2:LY:1476:HIS:HB2	2.14	0.47
2:EY:1514:ARG:O	2:EY:1518:GLU:HG2	2.15	0.47
2:IY:1503:ASP:OD2	2:IY:1504:SER:N	2.48	0.47
1:CX:276:TRP:O	1:CX:278:THR:HG22	2.15	0.47
1:FX:271:PRO:HB3	1:FX:276:TRP:CE2	2.50	0.47
1:KX:57:ILE:HD12	1:KX:308:VAL:HG21	1.95	0.47
1:QX:59:THR:HG21	1:QX:86:TRP:CZ3	2.49	0.47
2:NY:1470:SER:OG	2:NY:1471:LYS:N	2.45	0.47
1:BX:271:PRO:HA	1:BX:276:TRP:CZ3	2.50	0.47
1:LX:125:PHE:HA	1:LX:128:THR:HG22	1.97	0.47
1:AX:62:ASP:N	1:AX:62:ASP:OD2	2.47	0.47
1:DX:59:THR:OG1	1:DX:60:SER:N	2.47	0.47
1:GX:70:GLU:OE1	1:GX:315:ARG:NH1	2.46	0.47
1:KX:89:VAL:HG13	1:KX:96:PHE:HB2	1.96	0.47
1:OX:33:ASN:OD1	1:OX:34:PHE:N	2.48	0.47
2:EY:1534:ASN:OD1	2:EY:1538:LYS:NZ	2.34	0.47
2:KY:1487:ASP:OD2	2:KY:1489:THR:OG1	2.32	0.47
2:OY:1514:ARG:O	2:OY:1518:GLU:HG2	2.15	0.47
2:PY:1514:ARG:O	2:PY:1518:GLU:HG2	2.15	0.47
2:QY:1514:ARG:O	2:QY:1518:GLU:HG2	2.15	0.47
1:BX:33:ASN:OD1	1:BX:34:PHE:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CX:281:VAL:HG12	1:CX:290:GLN:NE2	2.30	0.47
1:DX:301:PHE:O	2:DY:1476:HIS:HB2	2.15	0.47
1:GX:103:LYS:NZ	1:GX:268:GLU:HB3	2.29	0.47
1:JX:284:THR:HG23	1:JX:287:ALA:H	1.79	0.47
1:KX:276:TRP:O	1:KX:278:THR:HG22	2.15	0.47
1:NX:58:TRP:H	1:NX:305:TYR:HD2	1.62	0.47
1:OX:276:TRP:O	1:OX:278:THR:HG22	2.14	0.47
1:QX:305:TYR:HB3	1:QX:308:VAL:HG13	1.96	0.47
2:PY:1536:ALA:HB3	2:QY:1519:VAL:HG23	1.97	0.47
1:HX:68:GLN:HG2	1:HX:309:LYS:HG3	1.97	0.47
1:JX:305:TYR:HB3	1:JX:308:VAL:HG23	1.97	0.47
1:MX:44:LYS:HD3	1:MX:46:ILE:HG12	1.96	0.47
1:NX:73:GLU:O	1:NX:93:ASN:HA	2.15	0.47
1:BX:277:ARG:HH11	1:BX:294:ARG:NH1	2.13	0.47
1:GX:277:ARG:HD2	1:GX:294:ARG:NH1	2.29	0.47
1:HX:106:LEU:HD21	1:HX:267:ILE:HD13	1.97	0.47
1:MX:51:ASP:O	1:NX:43:ASN:ND2	2.48	0.47
1:MX:101:SER:OG	2:KY:1549:ASN:ND2	2.47	0.47
1:BX:277:ARG:HD2	1:BX:294:ARG:NH1	2.27	0.46
1:CX:68:GLN:HE22	1:CX:94:HIS:CD2	2.33	0.46
1:CX:88:ILE:HG12	1:CX:97:ILE:HG22	1.96	0.46
1:GX:78:ILE:HD13	1:GX:90:PRO:HB3	1.97	0.46
1:KX:277:ARG:HH11	1:KX:294:ARG:NH1	2.12	0.46
1:CX:68:GLN:HB3	1:CX:309:LYS:HA	1.97	0.46
1:NX:36:ARG:NH1	2:MY:1485:LEU:O	2.36	0.46
2:MY:1489:THR:O	2:MY:1491:GLN:NE2	2.45	0.46
1:HX:276:TRP:O	1:HX:278:THR:HG22	2.15	0.46
1:KX:59:THR:HG21	1:KX:86:TRP:CZ3	2.50	0.46
1:OX:77:TYR:HA	2:NY:1555:THR:HG23	1.98	0.46
1:OX:103:LYS:NZ	1:OX:268:GLU:HB3	2.31	0.46
1:OX:121:ASP:O	1:OX:124:GLU:HG3	2.16	0.46
2:AY:1576:ILE:HD13	2:BY:1584:TYR:CE1	2.50	0.46
1:EX:61:LEU:HD22	1:EX:271:PRO:HG2	1.98	0.46
1:GX:271:PRO:HB3	1:GX:276:TRP:CE2	2.50	0.46
1:IX:276:TRP:O	1:IX:278:THR:HG22	2.16	0.46
1:PX:280:LEU:N	1:PX:291:PHE:O	2.29	0.46
2:LY:1487:ASP:OD1	2:LY:1489:THR:OG1	2.31	0.46
1:AX:120:ARG:HH22	1:QX:130:LYS:HA	1.80	0.46
1:CX:36:ARG:NH1	2:BY:1485:LEU:O	2.40	0.46
1:FX:73:GLU:CD	1:FX:289:TYR:HH	2.17	0.46
2:BY:1593:LYS:HE3	2:BY:1593:LYS:HB3	1.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DX:280:LEU:N	1:DX:291:PHE:O	2.37	0.46
1:EX:59:THR:HG21	1:EX:86:TRP:CZ3	2.50	0.46
1:QX:46:ILE:HG21	1:QX:55:ILE:HG21	1.98	0.46
1:QX:77:TYR:HA	2:PY:1555:THR:HG23	1.97	0.46
2:DY:1533:ASP:HA	2:EY:1519:VAL:HG21	1.97	0.46
2:LY:1514:ARG:O	2:LY:1518:GLU:HG2	2.16	0.46
2:NY:1487:ASP:OD1	2:NY:1489:THR:OG1	2.32	0.46
1:KX:305:TYR:HB3	1:KX:308:VAL:HG13	1.96	0.46
1:MX:62:ASP:OD1	1:MX:62:ASP:N	2.49	0.46
1:MX:271:PRO:HB3	1:MX:276:TRP:CE2	2.51	0.46
1:NX:289:TYR:HH	1:NX:312:TYR:HH	1.48	0.46
2:LY:1564:ASP:OD1	2:LY:1564:ASP:N	2.42	0.46
2:PY:1503:ASP:OD2	2:PY:1504:SER:N	2.49	0.46
1:AX:73:GLU:HG2	1:AX:286:LYS:HB2	1.96	0.46
1:EX:68:GLN:HB3	1:EX:309:LYS:HA	1.98	0.46
1:FX:59:THR:HG21	1:FX:86:TRP:CZ3	2.50	0.46
1:HX:101:SER:OG	2:FY:1549:ASN:ND2	2.48	0.46
2:NY:1475:LEU:HD22	2:NY:1509:ILE:HD11	1.98	0.46
1:HX:68:GLN:HB3	1:HX:309:LYS:HA	1.97	0.46
1:QX:299:ASP:OD1	1:QX:299:ASP:N	2.33	0.46
2:JY:1534:ASN:OD1	2:JY:1538:LYS:NZ	2.35	0.46
2:NY:1593:LYS:HD2	2:OY:1603:LEU:HD23	1.98	0.46
2:PY:1486:ASP:OD2	2:PY:1487:ASP:N	2.49	0.46
1:BX:283:ARG:HD3	1:CX:94:HIS:NE2	2.31	0.45
1:JX:101:SER:OG	2:HY:1549:ASN:ND2	2.48	0.45
2:KY:1528:ASN:O	2:KY:1531:THR:OG1	2.26	0.45
1:GX:301:PHE:O	2:GY:1476:HIS:HB2	2.16	0.45
1:NX:271:PRO:HA	1:NX:276:TRP:CH2	2.52	0.45
1:PX:121:ASP:O	1:PX:124:GLU:HG3	2.16	0.45
1:PX:289:TYR:OH	1:PX:312:TYR:OH	2.24	0.45
2:AY:1486:ASP:OD1	2:AY:1487:ASP:N	2.49	0.45
1:AX:102:VAL:HG12	1:AX:103:LYS:N	2.31	0.45
1:AX:277:ARG:HH11	1:AX:294:ARG:NH1	2.14	0.45
1:BX:121:ASP:O	1:BX:124:GLU:HG3	2.16	0.45
1:FX:77:TYR:HA	2:EY:1555:THR:HG23	1.96	0.45
1:FX:121:ASP:O	1:FX:124:GLU:HG3	2.15	0.45
1:HX:299:ASP:OD1	1:HX:299:ASP:N	2.31	0.45
1:IX:267:ILE:HG13	1:IX:268:GLU:O	2.17	0.45
1:GX:66:VAL:O	1:GX:307:THR:HA	2.17	0.45
1:IX:88:ILE:HG23	1:IX:97:ILE:HG22	1.99	0.45
1:NX:77:TYR:HA	2:MY:1555:THR:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NX:301:PHE:O	2:NY:1476:HIS:HB2	2.16	0.45
1:OX:277:ARG:HH11	1:OX:294:ARG:NH1	2.14	0.45
2:IY:1486:ASP:OD1	2:IY:1487:ASP:N	2.49	0.45
2:IY:1495:GLU:OE2	2:IY:1506:ARG:NH2	2.49	0.45
1:AX:58:TRP:HH2	1:AX:294:ARG:HH21	1.64	0.45
1:AX:67:ILE:HD11	1:AX:97:ILE:HD13	1.97	0.45
1:FX:57:ILE:HD12	1:FX:308:VAL:HG21	1.98	0.45
1:JX:45:LYS:HE3	1:JX:309:LYS:HD3	1.98	0.45
1:KX:283:ARG:HD3	1:LX:94:HIS:NE2	2.31	0.45
1:QX:57:ILE:HG21	1:QX:97:ILE:HD11	1.98	0.45
1:QX:103:LYS:NZ	1:QX:268:GLU:HB3	2.31	0.45
1:EX:276:TRP:O	1:EX:278:THR:HG22	2.17	0.45
1:EX:278:THR:OG1	1:EX:279:ASN:N	2.48	0.45
1:KX:58:TRP:H	1:KX:305:TYR:HD2	1.63	0.45
1:QX:62:ASP:N	1:QX:62:ASP:OD1	2.50	0.45
2:FY:1543:LEU:HD12	2:GY:1526:LEU:HD11	1.99	0.45
2:PY:1510:LEU:HD23	2:PY:1510:LEU:HA	1.76	0.45
1:AX:288:LEU:HD22	1:BX:68:GLN:HE21	1.82	0.45
1:CX:130:LYS:HA	1:DX:120:ARG:HH22	1.81	0.45
1:EX:280:LEU:N	1:EX:291:PHE:O	2.45	0.45
1:IX:93:ASN:ND2	2:HY:1566:ILE:HD13	2.31	0.45
2:LY:1534:ASN:OD1	2:LY:1538:LYS:NZ	2.34	0.45
1:BX:305:TYR:HB3	1:BX:308:VAL:HG13	1.99	0.45
1:DX:58:TRP:H	1:DX:305:TYR:HD2	1.62	0.45
1:GX:66:VAL:HA	1:GX:95:ILE:O	2.17	0.45
1:NX:271:PRO:HA	1:NX:276:TRP:CZ3	2.52	0.45
1:QX:58:TRP:CZ2	2:QY:1476:HIS:HE1	2.35	0.45
1:QX:59:THR:OG1	1:QX:60:SER:N	2.50	0.45
2:DY:1576:ILE:HG21	2:EY:1584:TYR:CE1	2.42	0.45
1:FX:277:ARG:HD2	1:FX:294:ARG:NH1	2.25	0.45
1:JX:80:THR:HG22	1:JX:280:LEU:HD13	1.99	0.45
1:KX:80:THR:HG23	1:KX:280:LEU:HD13	1.99	0.45
1:MX:66:VAL:HG13	1:MX:307:THR:HA	1.99	0.45
1:NX:105:ASN:OD1	1:NX:266:SER:OG	2.21	0.45
1:QX:284:THR:OG1	1:QX:285:ASN:N	2.50	0.45
2:NY:1514:ARG:O	2:NY:1518:GLU:HG2	2.16	0.45
1:EX:57:ILE:HG21	1:EX:97:ILE:HD11	1.99	0.45
1:IX:121:ASP:O	1:IX:124:GLU:HG3	2.17	0.45
1:NX:88:ILE:HG23	1:NX:97:ILE:HG22	1.98	0.45
1:NX:299:ASP:HB2	2:NY:1512:ILE:HD13	1.98	0.45
1:PX:109:GLU:HG3	2:OY:1543:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:PX:277:ARG:HH11	1:PX:294:ARG:NH1	2.15	0.45
2:NY:1489:THR:O	2:NY:1491:GLN:NE2	2.47	0.45
1:AX:68:GLN:HE22	1:AX:94:HIS:CD2	2.35	0.44
1:GX:68:GLN:HB3	1:GX:309:LYS:HA	1.99	0.44
1:GX:73:GLU:HG2	1:GX:286:LYS:HB2	1.98	0.44
1:KX:280:LEU:N	1:KX:291:PHE:O	2.36	0.44
1:MX:57:ILE:HG21	1:MX:97:ILE:HD11	1.98	0.44
2:AY:1576:ILE:HG21	2:BY:1584:TYR:CE1	2.52	0.44
2:EY:1487:ASP:OD2	2:EY:1489:THR:OG1	2.32	0.44
1:DX:105:ASN:OD1	1:DX:266:SER:OG	2.27	0.44
1:EX:57:ILE:HD12	1:EX:308:VAL:HG21	2.00	0.44
1:JX:121:ASP:HA	1:JX:124:GLU:HG3	1.98	0.44
1:LX:103:LYS:NZ	1:LX:268:GLU:HB3	2.32	0.44
1:NX:121:ASP:O	1:NX:124:GLU:HG3	2.17	0.44
1:CX:106:LEU:HD21	1:CX:267:ILE:HD13	1.99	0.44
1:CX:305:TYR:HB3	1:CX:308:VAL:HG13	2.00	0.44
1:DX:68:GLN:HA	1:DX:94:HIS:HB3	1.98	0.44
1:DX:103:LYS:NZ	1:DX:268:GLU:HB3	2.31	0.44
1:DX:314:GLN:O	1:DX:317:GLU:HG3	2.18	0.44
1:FX:92:SER:O	1:FX:93:ASN:ND2	2.51	0.44
1:IX:36:ARG:NH1	2:HY:1485:LEU:O	2.33	0.44
2:AY:1526:LEU:HD11	2:QY:1543:LEU:HD12	2.00	0.44
2:CY:1489:THR:O	2:CY:1491:GLN:NE2	2.49	0.44
2:LY:1593:LYS:HD2	2:MY:1603:LEU:HD23	1.99	0.44
1:KX:77:TYR:HB2	1:KX:283:ARG:HH21	1.81	0.44
1:LX:67:ILE:HD11	1:LX:97:ILE:HD13	1.99	0.44
1:PX:59:THR:HG21	1:PX:86:TRP:CZ3	2.53	0.44
1:PX:62:ASP:OD1	1:PX:62:ASP:N	2.50	0.44
2:AY:1586:THR:HG22	2:BY:1599:LEU:HB2	1.97	0.44
2:HY:1509:ILE:HD13	2:HY:1509:ILE:HA	1.80	0.44
2:JY:1576:ILE:HG21	2:KY:1584:TYR:CE1	2.47	0.44
1:BX:59:THR:HG21	1:BX:86:TRP:CZ3	2.52	0.44
1:GX:68:GLN:HA	1:GX:94:HIS:HB3	1.99	0.44
1:GX:305:TYR:HB3	1:GX:308:VAL:HG13	1.99	0.44
1:KX:121:ASP:O	1:KX:124:GLU:HG3	2.18	0.44
1:LX:284:THR:HG23	1:LX:286:LYS:H	1.83	0.44
1:NX:71:LYS:HD3	2:MY:1568:SER:HA	1.99	0.44
1:EX:299:ASP:OD1	1:EX:299:ASP:N	2.37	0.44
1:GX:280:LEU:N	1:GX:291:PHE:O	2.36	0.44
1:OX:61:LEU:HD12	2:NY:1527:ARG:HD3	1.98	0.44
1:OX:283:ARG:HD3	1:PX:94:HIS:NE2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EY:1576:ILE:HG21	2:FY:1584:TYR:CE1	2.46	0.44
2:IY:1475:LEU:HD23	2:IY:1475:LEU:HA	1.84	0.44
2:OY:1536:ALA:HB3	2:PY:1519:VAL:HG23	1.99	0.44
1:FX:68:GLN:HB3	1:FX:309:LYS:HA	2.00	0.44
1:FX:305:TYR:HB3	1:FX:308:VAL:HG13	2.00	0.44
1:GX:126:LEU:HD23	1:GX:126:LEU:HA	1.85	0.44
1:OX:59:THR:HG21	1:OX:86:TRP:CZ3	2.52	0.44
1:EX:70:GLU:OE1	1:EX:315:ARG:NH1	2.49	0.44
1:FX:126:LEU:HD23	1:FX:126:LEU:HA	1.77	0.44
1:IX:59:THR:HG21	1:IX:86:TRP:CZ3	2.53	0.44
1:JX:62:ASP:OD1	1:JX:62:ASP:N	2.51	0.44
1:JX:286:LYS:O	1:JX:315:ARG:NH2	2.50	0.44
2:DY:1535:MET:HE2	2:DY:1544:PRO:HD3	2.00	0.44
1:KX:46:ILE:HG21	1:KX:55:ILE:HG21	1.99	0.44
1:KX:277:ARG:HD2	1:KX:294:ARG:NH1	2.30	0.44
1:NX:102:VAL:HG12	1:NX:103:LYS:N	2.33	0.44
1:OX:308:VAL:O	1:OX:308:VAL:HG13	2.18	0.44
2:FY:1486:ASP:OD1	2:FY:1487:ASP:N	2.50	0.44
2:FY:1586:THR:HG22	2:FY:1590:ILE:HD11	1.99	0.44
2:MY:1514:ARG:O	2:MY:1518:GLU:HG2	2.18	0.44
1:AX:82:PHE:CD1	2:QY:1548:LYS:HD3	2.52	0.43
1:BX:130:LYS:HA	1:CX:120:ARG:HH22	1.83	0.43
1:JX:59:THR:HG21	1:JX:86:TRP:CZ3	2.52	0.43
1:JX:276:TRP:O	1:JX:278:THR:HG22	2.18	0.43
1:NX:62:ASP:OD2	1:NX:62:ASP:N	2.50	0.43
1:NX:103:LYS:NZ	1:NX:268:GLU:HB3	2.33	0.43
1:PX:58:TRP:H	1:PX:305:TYR:HD2	1.66	0.43
2:OY:1485:LEU:HD23	2:OY:1485:LEU:HA	1.88	0.43
2:QY:1487:ASP:OD1	2:QY:1489:THR:OG1	2.35	0.43
1:CX:288:LEU:HD21	1:DX:66:VAL:HG11	2.00	0.43
1:DX:77:TYR:HB2	1:DX:283:ARG:HH21	1.82	0.43
1:DX:284:THR:OG1	1:DX:285:ASN:N	2.49	0.43
1:MX:59:THR:HG21	1:MX:86:TRP:HZ3	1.82	0.43
2:EY:1486:ASP:OD2	2:EY:1487:ASP:N	2.51	0.43
1:CX:78:ILE:HD12	1:CX:95:ILE:HD13	1.99	0.43
1:EX:103:LYS:NZ	1:EX:268:GLU:HB3	2.32	0.43
1:GX:67:ILE:HG23	1:GX:308:VAL:HG23	2.01	0.43
1:JX:310:LEU:HD23	1:JX:310:LEU:HA	1.81	0.43
1:LX:106:LEU:HD21	1:LX:267:ILE:HD13	2.01	0.43
2:AY:1514:ARG:O	2:AY:1518:GLU:HG2	2.17	0.43
2:CY:1502:SER:N	2:CY:1505:GLU:OE1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:FY:1514:ARG:O	2:FY:1518:GLU:HG2	2.18	0.43
1:KX:73:GLU:O	1:KX:93:ASN:HA	2.18	0.43
1:QX:106:LEU:HD21	1:QX:267:ILE:HD13	2.01	0.43
1:QX:277:ARG:HD2	1:QX:294:ARG:NH1	2.32	0.43
1:BX:276:TRP:O	1:BX:278:THR:HG22	2.18	0.43
2:AY:1586:THR:HG22	2:BY:1599:LEU:HD22	2.00	0.43
1:EX:68:GLN:HG2	1:EX:309:LYS:HG3	2.00	0.43
1:HX:93:ASN:ND2	2:GY:1566:ILE:HD13	2.34	0.43
1:IX:92:SER:O	1:IX:93:ASN:ND2	2.51	0.43
2:CY:1470:SER:OG	2:CY:1471:LYS:N	2.52	0.43
2:IY:1593:LYS:HB2	2:IY:1593:LYS:HE3	1.67	0.43
1:CX:59:THR:HG21	1:CX:86:TRP:CZ3	2.53	0.43
1:FX:102:VAL:HG12	1:FX:103:LYS:N	2.34	0.43
1:NX:37:GLY:HA2	1:NX:298:LYS:HB2	2.01	0.43
1:PX:279:ASN:HA	1:PX:292:ILE:HA	2.01	0.43
2:KY:1514:ARG:O	2:KY:1518:GLU:HG2	2.18	0.43
1:IX:284:THR:HG23	1:IX:286:LYS:H	1.83	0.43
1:JX:271:PRO:HA	1:JX:276:TRP:CH2	2.54	0.43
1:JX:281:VAL:HG12	1:JX:290:GLN:HE22	1.84	0.43
1:KX:126:LEU:HD23	1:KX:126:LEU:HA	1.84	0.43
1:DX:101:SER:OG	2:BY:1549:ASN:ND2	2.52	0.43
1:EX:101:SER:HA	1:EX:271:PRO:HD3	2.01	0.43
1:GX:36:ARG:NH1	2:FY:1485:LEU:O	2.39	0.43
1:JX:82:PHE:CD1	2:IY:1548:LYS:HD3	2.54	0.43
1:KX:73:GLU:HG2	1:KX:286:LYS:HB2	2.00	0.43
1:MX:314:GLN:O	1:MX:317:GLU:HG3	2.19	0.43
2:CY:1486:ASP:OD1	2:CY:1487:ASP:N	2.52	0.43
2:CY:1579:ASP:OD1	2:CY:1580:ILE:N	2.52	0.43
2:DY:1495:GLU:OE2	2:DY:1506:ARG:NH2	2.52	0.43
1:AX:33:ASN:OD1	1:AX:34:PHE:N	2.52	0.43
1:AX:57:ILE:HD12	1:AX:308:VAL:HG21	2.01	0.43
1:QX:67:ILE:HD11	1:QX:97:ILE:HD13	2.00	0.43
2:EY:1501:LEU:HD22	2:EY:1505:GLU:HB3	2.00	0.43
2:JY:1543:LEU:HD12	2:KY:1526:LEU:HD11	2.01	0.43
1:HX:58:TRP:H	1:HX:305:TYR:HD2	1.64	0.42
1:HX:283:ARG:HD3	1:IX:94:HIS:NE2	2.34	0.42
1:IX:314:GLN:O	1:IX:317:GLU:HG3	2.19	0.42
1:NX:283:ARG:NE	1:OX:94:HIS:CE1	2.87	0.42
1:PX:58:TRP:HH2	1:PX:294:ARG:HH21	1.67	0.42
2:DY:1482:LEU:HD23	2:DY:1482:LEU:HA	1.91	0.42
2:IY:1502:SER:O	2:IY:1506:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DX:73:GLU:O	1:DX:93:ASN:HA	2.19	0.42
1:EX:92:SER:HB3	2:DY:1560:ASN:HA	2.01	0.42
1:IX:73:GLU:O	1:IX:93:ASN:HA	2.19	0.42
1:JX:45:LYS:HD3	1:JX:309:LYS:HB3	2.00	0.42
1:JX:103:LYS:NZ	1:JX:268:GLU:HB3	2.33	0.42
2:BY:1568:SER:OG	2:BY:1569:ASP:N	2.51	0.42
2:JY:1568:SER:OG	2:JY:1569:ASP:N	2.51	0.42
2:OY:1543:LEU:HD12	2:PY:1526:LEU:HD11	2.01	0.42
1:DX:305:TYR:HB3	1:DX:308:VAL:HG13	2.00	0.42
1:HX:305:TYR:HB3	1:HX:308:VAL:HG13	2.00	0.42
1:IX:284:THR:OG1	1:IX:285:ASN:N	2.53	0.42
1:MX:271:PRO:HA	1:MX:276:TRP:CZ3	2.53	0.42
2:LY:1593:LYS:HE2	2:MY:1603:LEU:HA	2.02	0.42
1:AX:284:THR:HG23	1:AX:286:LYS:H	1.84	0.42
1:IX:73:GLU:HG2	1:IX:286:LYS:HB2	2.00	0.42
1:LX:271:PRO:HA	1:LX:276:TRP:CZ3	2.55	0.42
1:MX:277:ARG:HD2	1:MX:294:ARG:NH1	2.33	0.42
1:MX:277:ARG:HE	1:MX:292:ILE:HD11	1.84	0.42
1:OX:277:ARG:HD2	1:OX:294:ARG:NH1	2.28	0.42
1:QX:314:GLN:O	1:QX:317:GLU:HG3	2.20	0.42
2:CY:1530:LYS:HD3	2:CY:1530:LYS:HA	1.88	0.42
1:BX:92:SER:HB2	2:AY:1560:ASN:HA	2.02	0.42
1:DX:271:PRO:HA	1:DX:276:TRP:CZ3	2.55	0.42
1:FX:277:ARG:HH11	1:FX:294:ARG:NH1	2.18	0.42
1:HX:272:SER:HB2	1:HX:297:GLN:HE22	1.85	0.42
1:MX:57:ILE:HD13	1:MX:57:ILE:HA	1.89	0.42
1:MX:121:ASP:O	1:MX:124:GLU:HG3	2.19	0.42
1:MX:297:GLN:H	1:MX:300:ASN:HB2	1.85	0.42
1:PX:314:GLN:O	1:PX:317:GLU:HG3	2.19	0.42
2:KY:1486:ASP:OD1	2:KY:1487:ASP:N	2.52	0.42
2:PY:1482:LEU:HD23	2:PY:1482:LEU:HA	1.90	0.42
2:QY:1475:LEU:HD23	2:QY:1475:LEU:HA	1.87	0.42
1:EX:277:ARG:HD2	1:EX:294:ARG:NH1	2.31	0.42
1:HX:265:ASN:OD1	1:HX:265:ASN:N	2.49	0.42
1:OX:299:ASP:OD1	1:OX:299:ASP:N	2.37	0.42
2:EY:1502:SER:O	2:EY:1506:ARG:HG3	2.20	0.42
2:MY:1509:ILE:HD13	2:MY:1509:ILE:HA	1.86	0.42
2:OY:1486:ASP:OD2	2:OY:1487:ASP:N	2.52	0.42
2:PY:1495:GLU:OE2	2:PY:1506:ARG:NH2	2.52	0.42
1:AX:308:VAL:HG23	1:AX:308:VAL:O	2.19	0.42
1:GX:121:ASP:O	1:GX:124:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:PX:305:TYR:HB3	1:PX:308:VAL:HG23	2.02	0.42
2:EY:1586:THR:HG22	2:EY:1590:ILE:HD11	2.01	0.42
1:IX:277:ARG:HD2	1:IX:294:ARG:NH1	2.35	0.42
1:JX:58:TRP:HH2	1:JX:294:ARG:HH21	1.68	0.42
1:LX:70:GLU:OE1	1:LX:315:ARG:NH1	2.51	0.42
1:MX:276:TRP:O	1:MX:278:THR:HG22	2.20	0.42
1:NX:284:THR:HG23	1:NX:287:ALA:H	1.84	0.42
2:GY:1495:GLU:OE2	2:GY:1506:ARG:NH2	2.53	0.42
2:IY:1579:ASP:OD1	2:IY:1580:ILE:N	2.53	0.42
2:NY:1599:LEU:O	2:NY:1603:LEU:HG	2.19	0.42
2:QY:1486:ASP:OD1	2:QY:1487:ASP:N	2.53	0.42
1:BX:102:VAL:HG12	1:BX:103:LYS:N	2.35	0.42
1:LX:62:ASP:OD2	1:LX:62:ASP:N	2.53	0.42
2:GY:1509:ILE:HD13	2:GY:1509:ILE:HA	1.82	0.42
2:IY:1514:ARG:O	2:IY:1518:GLU:HG2	2.20	0.42
2:JY:1586:THR:HG22	2:JY:1590:ILE:HD11	2.02	0.42
2:JY:1599:LEU:O	2:JY:1603:LEU:HG	2.20	0.42
1:AX:284:THR:HG23	1:AX:287:ALA:H	1.85	0.42
1:FX:92:SER:HB2	2:EY:1560:ASN:HA	2.00	0.42
1:IX:77:TYR:CD2	1:JX:96:PHE:HE2	2.38	0.42
1:JX:272:SER:OG	1:JX:297:GLN:NE2	2.50	0.42
1:MX:62:ASP:OD2	2:KY:1548:LYS:NZ	2.53	0.42
1:NX:92:SER:HB3	2:MY:1560:ASN:HA	2.02	0.42
1:NX:278:THR:OG1	1:NX:279:ASN:N	2.52	0.42
2:CY:1535:MET:HE2	2:CY:1544:PRO:HD3	2.02	0.42
2:HY:1514:ARG:O	2:HY:1518:GLU:HG2	2.20	0.42
2:JY:1514:ARG:O	2:JY:1518:GLU:HG2	2.20	0.42
2:QY:1586:THR:HG22	2:QY:1590:ILE:HD11	2.01	0.42
1:AX:70:GLU:OE1	1:AX:315:ARG:NH1	2.53	0.41
1:BX:73:GLU:HG2	1:BX:286:LYS:HB2	2.02	0.41
1:CX:288:LEU:HD22	1:DX:68:GLN:NE2	2.35	0.41
1:EX:121:ASP:O	1:EX:124:GLU:HG3	2.20	0.41
1:HX:77:TYR:HB2	1:HX:283:ARG:HH21	1.85	0.41
1:KX:88:ILE:HG12	1:KX:97:ILE:HG22	2.01	0.41
1:LX:280:LEU:N	1:LX:291:PHE:O	2.39	0.41
1:MX:46:ILE:HG13	1:MX:308:VAL:HG23	2.01	0.41
2:AY:1603:LEU:HA	2:QY:1593:LYS:HE2	2.01	0.41
2:BY:1586:THR:HG22	2:BY:1590:ILE:HD11	2.02	0.41
2:FY:1482:LEU:HD23	2:FY:1482:LEU:HA	1.90	0.41
2:MY:1586:THR:HG22	2:MY:1590:ILE:HD11	2.02	0.41
1:EX:88:ILE:HG22	1:EX:90:PRO:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EX:273:ASP:H	1:EX:297:GLN:NE2	2.18	0.41
1:IX:285:ASN:N	1:IX:285:ASN:OD1	2.53	0.41
1:OX:66:VAL:HG13	1:OX:307:THR:HA	2.02	0.41
1:PX:89:VAL:HG13	1:PX:96:PHE:HB2	2.01	0.41
2:HY:1498:LEU:HD23	2:HY:1498:LEU:HA	1.89	0.41
2:JY:1593:LYS:HD2	2:KY:1603:LEU:HD23	2.02	0.41
2:MY:1502:SER:O	2:MY:1506:ARG:HG3	2.20	0.41
1:HX:103:LYS:NZ	1:HX:268:GLU:HB3	2.35	0.41
1:NX:61:LEU:HD21	1:NX:295:ILE:HD13	2.02	0.41
1:NX:310:LEU:HD23	1:NX:310:LEU:HA	1.77	0.41
2:BY:1486:ASP:OD2	2:BY:1487:ASP:N	2.53	0.41
1:GX:273:ASP:H	1:GX:297:GLN:NE2	2.18	0.41
1:JX:88:ILE:HG12	1:JX:97:ILE:HG22	2.01	0.41
1:KX:36:ARG:NH1	2:JY:1485:LEU:O	2.44	0.41
2:FY:1599:LEU:O	2:FY:1603:LEU:HG	2.20	0.41
2:JY:1510:LEU:HD23	2:JY:1510:LEU:HA	1.84	0.41
1:AX:57:ILE:HG21	1:AX:97:ILE:HD11	2.03	0.41
1:FX:301:PHE:O	2:FY:1476:HIS:HB2	2.21	0.41
1:PX:276:TRP:O	1:PX:278:THR:HG22	2.20	0.41
1:PX:284:THR:OG1	1:PX:285:ASN:N	2.53	0.41
2:DY:1510:LEU:HD23	2:DY:1510:LEU:HA	1.79	0.41
2:KY:1587:GLU:HA	2:KY:1590:ILE:HD12	2.02	0.41
1:CX:66:VAL:HG13	1:CX:307:THR:HA	2.02	0.41
1:CX:284:THR:OG1	1:CX:285:ASN:N	2.52	0.41
1:DX:58:TRP:HH2	1:DX:294:ARG:HH21	1.69	0.41
1:HX:283:ARG:HH11	2:HY:1566:ILE:HG12	1.85	0.41
1:HX:314:GLN:O	1:HX:317:GLU:HG3	2.21	0.41
1:JX:73:GLU:O	1:JX:93:ASN:HA	2.20	0.41
1:KX:87:SER:O	2:IY:1553:ILE:HD11	2.20	0.41
1:LX:284:THR:OG1	1:LX:285:ASN:N	2.53	0.41
1:LX:314:GLN:O	1:LX:317:GLU:HG3	2.21	0.41
2:FY:1576:ILE:HG21	2:GY:1584:TYR:CE1	2.56	0.41
2:IY:1498:LEU:HD11	2:IY:1510:LEU:HD21	2.03	0.41
1:AX:73:GLU:O	1:AX:93:ASN:HA	2.21	0.41
1:AX:277:ARG:HD2	1:AX:294:ARG:NH1	2.31	0.41
1:DX:283:ARG:HB2	1:DX:288:LEU:HD12	2.03	0.41
1:DX:310:LEU:HD23	1:DX:310:LEU:HA	1.91	0.41
1:HX:310:LEU:HD23	1:HX:310:LEU:HA	1.82	0.41
1:IX:271:PRO:HA	1:IX:276:TRP:CZ3	2.56	0.41
1:OX:280:LEU:N	1:OX:291:PHE:O	2.39	0.41
2:DY:1486:ASP:OD2	2:DY:1487:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:IY:1562:ASP:N	2:IY:1562:ASP:OD1	2.54	0.41
2:IY:1586:THR:HG22	2:IY:1590:ILE:HD11	2.03	0.41
1:CX:57:ILE:HD13	1:CX:57:ILE:HA	1.93	0.41
1:CX:92:SER:HB3	2:BY:1561:VAL:HG12	2.03	0.41
1:FX:310:LEU:HA	1:FX:310:LEU:HD23	1.79	0.41
1:GX:314:GLN:O	1:GX:317:GLU:HG3	2.21	0.41
1:MX:48:TYR:HB2	1:MX:310:LEU:HD22	2.01	0.41
1:NX:102:VAL:HG23	1:NX:276:TRP:HZ2	1.86	0.41
2:CY:1475:LEU:HD21	2:CY:1505:GLU:HB3	2.02	0.41
2:DY:1548:LYS:HG3	2:EY:1527:ARG:HH22	1.86	0.41
2:HY:1586:THR:HG22	2:HY:1590:ILE:HD11	2.01	0.41
2:LY:1599:LEU:O	2:LY:1603:LEU:HG	2.21	0.41
2:QY:1530:LYS:HD3	2:QY:1530:LYS:HA	1.90	0.41
1:BX:301:PHE:O	2:BY:1476:HIS:HB2	2.21	0.41
1:DX:73:GLU:CD	1:DX:289:TYR:HH	2.23	0.41
1:JX:102:VAL:HG12	1:JX:103:LYS:N	2.36	0.41
2:AY:1530:LYS:HD3	2:AY:1530:LYS:HA	1.94	0.41
2:AY:1543:LEU:HD12	2:BY:1526:LEU:HD11	2.02	0.41
2:FY:1586:THR:HG23	2:GY:1599:LEU:HB2	2.03	0.41
2:HY:1502:SER:O	2:HY:1506:ARG:HG3	2.20	0.41
2:JY:1530:LYS:HD3	2:JY:1530:LYS:HA	1.83	0.41
2:MY:1593:LYS:HB2	2:MY:1593:LYS:HE3	1.74	0.41
2:OY:1579:ASP:OD1	2:OY:1580:ILE:N	2.54	0.41
1:CX:73:GLU:O	1:CX:93:ASN:HA	2.21	0.41
1:DX:276:TRP:O	1:DX:278:THR:HG22	2.21	0.41
1:IX:62:ASP:OD1	1:IX:62:ASP:N	2.54	0.41
1:JX:271:PRO:HA	1:JX:276:TRP:CE3	2.56	0.41
1:JX:278:THR:OG1	1:JX:279:ASN:N	2.54	0.41
1:PX:56:THR:HA	1:PX:292:ILE:HG23	2.03	0.41
1:PX:271:PRO:HA	1:PX:276:TRP:CZ3	2.56	0.41
2:CY:1536:ALA:HB3	2:DY:1519:VAL:HG23	2.03	0.41
2:EY:1523:TYR:OH	2:EY:1527:ARG:NH2	2.35	0.41
2:GY:1514:ARG:O	2:GY:1518:GLU:HG2	2.20	0.41
2:IY:1530:LYS:HD3	2:IY:1530:LYS:HA	1.92	0.41
2:LY:1482:LEU:HD13	2:LY:1513:LYS:HD2	2.03	0.41
2:LY:1586:THR:HG22	2:LY:1590:ILE:HD11	2.03	0.41
2:OY:1495:GLU:OE2	2:OY:1506:ARG:NH2	2.54	0.41
1:AX:88:ILE:HG12	1:AX:97:ILE:HG22	2.04	0.40
1:KX:288:LEU:HD22	1:LX:68:GLN:NE2	2.36	0.40
1:NX:57:ILE:HD12	1:NX:308:VAL:HG21	2.03	0.40
1:OX:59:THR:HG21	1:OX:86:TRP:CH2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:PX:299:ASP:HB2	2:PY:1512:ILE:HD13	2.03	0.40
2:BY:1579:ASP:HB3	2:BY:1582:LYS:HD3	2.03	0.40
2:DY:1530:LYS:HD3	2:DY:1530:LYS:HA	1.91	0.40
2:IY:1489:THR:O	2:IY:1491:GLN:NE2	2.49	0.40
1:CX:70:GLU:OE1	1:CX:315:ARG:NH1	2.54	0.40
1:EX:58:TRP:CZ2	2:EY:1476:HIS:HE1	2.39	0.40
1:GX:61:LEU:HD12	2:FY:1527:ARG:HD3	2.03	0.40
1:LX:73:GLU:O	1:LX:93:ASN:HA	2.22	0.40
1:LX:276:TRP:O	1:LX:278:THR:HG22	2.21	0.40
1:NX:306:LEU:HD23	1:NX:306:LEU:HA	1.86	0.40
1:OX:280:LEU:HB2	1:OX:293:LEU:HD11	2.03	0.40
2:AY:1576:ILE:HG21	2:BY:1584:TYR:HE1	1.84	0.40
2:AY:1584:TYR:CE1	2:QY:1576:ILE:HG21	2.45	0.40
2:QY:1510:LEU:HD23	2:QY:1510:LEU:HA	1.82	0.40
1:AX:306:LEU:HD22	1:QX:279:ASN:ND2	2.37	0.40
1:AX:317:GLU:O	1:AX:321:VAL:HG13	2.22	0.40
1:BX:77:TYR:HA	2:AY:1555:THR:HG23	2.03	0.40
1:BX:102:VAL:HG23	1:BX:276:TRP:HZ2	1.86	0.40
1:FX:68:GLN:HE22	1:FX:94:HIS:CD2	2.40	0.40
1:FX:93:ASN:ND2	2:EY:1566:ILE:HD13	2.37	0.40
1:GX:58:TRP:H	1:GX:305:TYR:HD2	1.68	0.40
1:KX:53:LYS:HD2	1:KX:53:LYS:HA	1.94	0.40
1:MX:57:ILE:HD12	1:MX:308:VAL:HG11	2.03	0.40
1:NX:71:LYS:HE2	2:MY:1566:ILE:HB	2.02	0.40
1:OX:66:VAL:HA	1:OX:95:ILE:O	2.22	0.40
1:OX:312:TYR:HB3	1:OX:315:ARG:HB2	2.04	0.40
1:AX:102:VAL:HG23	1:AX:276:TRP:HZ2	1.85	0.40
1:FX:265:ASN:OD1	1:FX:265:ASN:N	2.53	0.40
1:IX:106:LEU:HD21	1:IX:267:ILE:HD13	2.03	0.40
1:MX:68:GLN:HB3	1:MX:309:LYS:HA	2.04	0.40
1:QX:68:GLN:HA	1:QX:94:HIS:HB3	2.02	0.40
2:AY:1502:SER:O	2:AY:1506:ARG:HG3	2.22	0.40
1:HX:271:PRO:HA	1:HX:276:TRP:CZ3	2.56	0.40
1:IX:107:MET:N	2:HY:1543:LEU:O	2.51	0.40
1:JX:73:GLU:HG2	1:JX:286:LYS:HB2	2.03	0.40
1:NX:284:THR:OG1	1:NX:285:ASN:N	2.54	0.40
1:PX:310:LEU:HD23	1:PX:310:LEU:HA	1.82	0.40
2:AY:1509:ILE:HD13	2:AY:1509:ILE:HA	1.92	0.40
2:CY:1593:LYS:HD2	2:DY:1603:LEU:HD23	2.03	0.40
2:NY:1482:LEU:HD23	2:NY:1482:LEU:HA	1.92	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	AX	160/521 (31%)	154 (96%)	6 (4%)	0	100	100
1	BX	160/521 (31%)	151 (94%)	9 (6%)	0	100	100
1	CX	160/521 (31%)	154 (96%)	6 (4%)	0	100	100
1	DX	160/521 (31%)	156 (98%)	4 (2%)	0	100	100
1	EX	160/521 (31%)	153 (96%)	7 (4%)	0	100	100
1	FX	160/521 (31%)	152 (95%)	8 (5%)	0	100	100
1	GX	160/521 (31%)	153 (96%)	7 (4%)	0	100	100
1	HX	160/521 (31%)	155 (97%)	5 (3%)	0	100	100
1	IX	160/521 (31%)	154 (96%)	6 (4%)	0	100	100
1	JX	160/521 (31%)	151 (94%)	9 (6%)	0	100	100
1	KX	160/521 (31%)	157 (98%)	3 (2%)	0	100	100
1	LX	160/521 (31%)	154 (96%)	6 (4%)	0	100	100
1	MX	160/521 (31%)	155 (97%)	5 (3%)	0	100	100
1	NX	160/521 (31%)	156 (98%)	4 (2%)	0	100	100
1	OX	160/521 (31%)	152 (95%)	8 (5%)	0	100	100
1	PX	160/521 (31%)	154 (96%)	6 (4%)	0	100	100
1	QX	160/521 (31%)	154 (96%)	6 (4%)	0	100	100
2	AY	133/1927 (7%)	127 (96%)	6 (4%)	0	100	100
2	BY	133/1927 (7%)	128 (96%)	5 (4%)	0	100	100
2	CY	133/1927 (7%)	129 (97%)	4 (3%)	0	100	100
2	DY	133/1927 (7%)	126 (95%)	7 (5%)	0	100	100
2	EY	133/1927 (7%)	127 (96%)	6 (4%)	0	100	100
2	FY	133/1927 (7%)	123 (92%)	10 (8%)	0	100	100
2	GY	133/1927 (7%)	129 (97%)	4 (3%)	0	100	100
2	HY	133/1927 (7%)	126 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	IY	133/1927 (7%)	128 (96%)	5 (4%)	0	100	100
2	JY	133/1927 (7%)	127 (96%)	6 (4%)	0	100	100
2	KY	133/1927 (7%)	126 (95%)	7 (5%)	0	100	100
2	LY	133/1927 (7%)	127 (96%)	6 (4%)	0	100	100
2	MY	133/1927 (7%)	126 (95%)	7 (5%)	0	100	100
2	NY	133/1927 (7%)	127 (96%)	6 (4%)	0	100	100
2	OY	133/1927 (7%)	129 (97%)	4 (3%)	0	100	100
2	PY	133/1927 (7%)	127 (96%)	6 (4%)	0	100	100
2	QY	133/1927 (7%)	128 (96%)	5 (4%)	0	100	100
All	All	4981/41616 (12%)	4775 (96%)	206 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AX	152/469 (32%)	143 (94%)	9 (6%)	19	53
1	BX	152/469 (32%)	142 (93%)	10 (7%)	16	49
1	CX	152/469 (32%)	143 (94%)	9 (6%)	19	53
1	DX	152/469 (32%)	145 (95%)	7 (5%)	27	61
1	EX	152/469 (32%)	140 (92%)	12 (8%)	12	41
1	FX	152/469 (32%)	146 (96%)	6 (4%)	32	64
1	GX	152/469 (32%)	142 (93%)	10 (7%)	16	49
1	HX	152/469 (32%)	143 (94%)	9 (6%)	19	53
1	IX	152/469 (32%)	142 (93%)	10 (7%)	16	49
1	JX	152/469 (32%)	143 (94%)	9 (6%)	19	53
1	KX	152/469 (32%)	142 (93%)	10 (7%)	16	49
1	LX	152/469 (32%)	140 (92%)	12 (8%)	12	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	MX	152/469 (32%)	143 (94%)	9 (6%)	19	53
1	NX	152/469 (32%)	147 (97%)	5 (3%)	38	68
1	OX	152/469 (32%)	141 (93%)	11 (7%)	14	45
1	PX	152/469 (32%)	146 (96%)	6 (4%)	32	64
1	QX	152/469 (32%)	142 (93%)	10 (7%)	16	49
2	AY	115/1724 (7%)	112 (97%)	3 (3%)	46	74
2	BY	115/1724 (7%)	111 (96%)	4 (4%)	36	67
2	CY	115/1724 (7%)	111 (96%)	4 (4%)	36	67
2	DY	115/1724 (7%)	110 (96%)	5 (4%)	29	62
2	EY	115/1724 (7%)	114 (99%)	1 (1%)	78	90
2	FY	115/1724 (7%)	112 (97%)	3 (3%)	46	74
2	GY	115/1724 (7%)	112 (97%)	3 (3%)	46	74
2	HY	115/1724 (7%)	111 (96%)	4 (4%)	36	67
2	IY	115/1724 (7%)	111 (96%)	4 (4%)	36	67
2	JY	115/1724 (7%)	113 (98%)	2 (2%)	60	82
2	KY	115/1724 (7%)	112 (97%)	3 (3%)	46	74
2	LY	115/1724 (7%)	111 (96%)	4 (4%)	36	67
2	MY	115/1724 (7%)	111 (96%)	4 (4%)	36	67
2	NY	115/1724 (7%)	111 (96%)	4 (4%)	36	67
2	OY	115/1724 (7%)	112 (97%)	3 (3%)	46	74
2	PY	115/1724 (7%)	111 (96%)	4 (4%)	36	67
2	QY	115/1724 (7%)	110 (96%)	5 (4%)	29	62
All	All	4539/37281 (12%)	4325 (95%)	214 (5%)	30	60

All (214) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AX	59	THR
1	AX	62	ASP
1	AX	63	ASN
1	AX	104	SER
1	AX	113	VAL
1	AX	118	MET
1	AX	264	ASP

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Mol	Chain	Res	Type
1	AX	270	SER
1	AX	317	GLU
1	BX	41	VAL
1	BX	59	THR
1	BX	63	ASN
1	BX	93	ASN
1	BX	113	VAL
1	BX	114	ASN
1	BX	124	GLU
1	BX	126	LEU
1	BX	264	ASP
1	BX	317	GLU
1	CX	43	ASN
1	CX	63	ASN
1	CX	93	ASN
1	CX	113	VAL
1	CX	114	ASN
1	CX	124	GLU
1	CX	126	LEU
1	CX	267	ILE
1	CX	317	GLU
1	DX	41	VAL
1	DX	63	ASN
1	DX	93	ASN
1	DX	102	VAL
1	DX	113	VAL
1	DX	114	ASN
1	DX	317	GLU
1	EX	59	THR
1	EX	63	ASN
1	EX	93	ASN
1	EX	113	VAL
1	EX	114	ASN
1	EX	121	ASP
1	EX	124	GLU
1	EX	270	SER
1	EX	278	THR
1	EX	299	ASP
1	EX	317	GLU
1	EX	321	VAL
1	FX	41	VAL
1	FX	63	ASN

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Mol	Chain	Res	Type
1	FX	93	ASN
1	FX	104	SER
1	FX	113	VAL
1	FX	284	THR
1	GX	49	LEU
1	GX	59	THR
1	GX	62	ASP
1	GX	63	ASN
1	GX	93	ASN
1	GX	113	VAL
1	GX	124	GLU
1	GX	278	THR
1	GX	284	THR
1	GX	317	GLU
1	HX	49	LEU
1	HX	62	ASP
1	HX	63	ASN
1	HX	80	THR
1	HX	93	ASN
1	HX	113	VAL
1	HX	267	ILE
1	HX	278	THR
1	HX	317	GLU
1	IX	43	ASN
1	IX	62	ASP
1	IX	63	ASN
1	IX	77	TYR
1	IX	93	ASN
1	IX	113	VAL
1	IX	114	ASN
1	IX	124	GLU
1	IX	278	THR
1	IX	317	GLU
1	JX	59	THR
1	JX	62	ASP
1	JX	63	ASN
1	JX	93	ASN
1	JX	104	SER
1	JX	113	VAL
1	JX	114	ASN
1	JX	264	ASP
1	JX	284	THR

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Mol	Chain	Res	Type
1	KX	63	ASN
1	KX	93	ASN
1	KX	113	VAL
1	KX	120	ARG
1	KX	264	ASP
1	KX	270	SER
1	KX	284	THR
1	KX	299	ASP
1	KX	308	VAL
1	KX	317	GLU
1	LX	43	ASN
1	LX	62	ASP
1	LX	63	ASN
1	LX	80	THR
1	LX	93	ASN
1	LX	104	SER
1	LX	113	VAL
1	LX	114	ASN
1	LX	124	GLU
1	LX	267	ILE
1	LX	278	THR
1	LX	317	GLU
1	MX	62	ASP
1	MX	63	ASN
1	MX	78	ILE
1	MX	113	VAL
1	MX	114	ASN
1	MX	124	GLU
1	MX	270	SER
1	MX	278	THR
1	MX	317	GLU
1	NX	59	THR
1	NX	62	ASP
1	NX	80	THR
1	NX	93	ASN
1	NX	113	VAL
1	OX	43	ASN
1	OX	63	ASN
1	OX	82	PHE
1	OX	93	ASN
1	OX	94	HIS
1	OX	113	VAL

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Mol	Chain	Res	Type
1	OX	114	ASN
1	OX	120	ARG
1	OX	264	ASP
1	OX	299	ASP
1	OX	317	GLU
1	PX	62	ASP
1	PX	63	ASN
1	PX	93	ASN
1	PX	113	VAL
1	PX	267	ILE
1	PX	317	GLU
1	QX	62	ASP
1	QX	63	ASN
1	QX	93	ASN
1	QX	102	VAL
1	QX	113	VAL
1	QX	264	ASP
1	QX	267	ILE
1	QX	278	THR
1	QX	308	VAL
1	QX	317	GLU
2	AY	1497	CYS
2	AY	1514	ARG
2	AY	1520	ASP
2	BY	1479	SER
2	BY	1497	CYS
2	BY	1514	ARG
2	BY	1520	ASP
2	CY	1481	CYS
2	CY	1509	ILE
2	CY	1520	ASP
2	CY	1599	LEU
2	DY	1470	SER
2	DY	1479	SER
2	DY	1497	CYS
2	DY	1514	ARG
2	DY	1520	ASP
2	EY	1497	CYS
2	FY	1497	CYS
2	FY	1514	ARG
2	FY	1520	ASP
2	GY	1497	CYS

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Mol	Chain	Res	Type
2	GY	1520	ASP
2	GY	1579	ASP
2	HY	1479	SER
2	HY	1481	CYS
2	HY	1497	CYS
2	HY	1514	ARG
2	IY	1479	SER
2	IY	1497	CYS
2	IY	1514	ARG
2	IY	1520	ASP
2	JY	1481	CYS
2	JY	1499	GLU
2	KY	1497	CYS
2	KY	1514	ARG
2	KY	1520	ASP
2	LY	1497	CYS
2	LY	1509	ILE
2	LY	1514	ARG
2	LY	1520	ASP
2	MY	1497	CYS
2	MY	1514	ARG
2	MY	1520	ASP
2	MY	1577	GLU
2	NY	1497	CYS
2	NY	1499	GLU
2	NY	1514	ARG
2	NY	1594	ASN
2	OY	1479	SER
2	OY	1509	ILE
2	OY	1520	ASP
2	PY	1479	SER
2	PY	1497	CYS
2	PY	1514	ARG
2	PY	1520	ASP
2	QY	1479	SER
2	QY	1497	CYS
2	QY	1520	ASP
2	QY	1555	THR
2	QY	1577	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
1	AX	43	ASN
1	AX	68	GLN
1	AX	93	ASN
1	BX	93	ASN
1	BX	94	HIS
1	CX	68	GLN
1	CX	290	GLN
1	DX	68	GLN
1	DX	93	ASN
1	DX	94	HIS
1	DX	297	GLN
1	EX	68	GLN
1	EX	297	GLN
1	FX	93	ASN
1	FX	297	GLN
1	GX	68	GLN
1	GX	297	GLN
1	HX	68	GLN
1	HX	93	ASN
1	HX	297	GLN
1	IX	93	ASN
1	IX	94	HIS
1	JX	68	GLN
1	JX	93	ASN
1	JX	94	HIS
1	JX	297	GLN
1	KX	93	ASN
1	LX	68	GLN
1	LX	94	HIS
1	LX	297	GLN
1	MX	68	GLN
1	MX	93	ASN
1	MX	297	GLN
1	NX	63	ASN
1	NX	68	GLN
1	NX	93	ASN
1	OX	68	GLN
1	OX	93	ASN
1	OX	265	ASN
1	PX	68	GLN
1	PX	93	ASN
1	PX	297	GLN
1	QX	68	GLN

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Mol	Chain	Res	Type
1	QX	93	ASN
2	AY	1549	ASN
2	AY	1557	ASN
2	AY	1583	GLN
2	AY	1594	ASN
2	BY	1476	HIS
2	BY	1549	ASN
2	BY	1557	ASN
2	BY	1583	GLN
2	CY	1476	HIS
2	CY	1528	ASN
2	CY	1557	ASN
2	CY	1583	GLN
2	CY	1594	ASN
2	DY	1549	ASN
2	DY	1557	ASN
2	DY	1583	GLN
2	EY	1476	HIS
2	EY	1557	ASN
2	EY	1583	GLN
2	FY	1476	HIS
2	FY	1528	ASN
2	FY	1549	ASN
2	FY	1583	GLN
2	FY	1594	ASN
2	GY	1476	HIS
2	GY	1549	ASN
2	GY	1557	ASN
2	GY	1583	GLN
2	HY	1549	ASN
2	HY	1583	GLN
2	HY	1594	ASN
2	IY	1476	HIS
2	IY	1549	ASN
2	IY	1583	GLN
2	IY	1594	ASN
2	JY	1476	HIS
2	JY	1549	ASN
2	JY	1557	ASN
2	JY	1583	GLN
2	JY	1594	ASN
2	KY	1476	HIS

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Mol	Chain	Res	Type
2	KY	1549	ASN
2	KY	1557	ASN
2	KY	1583	GLN
2	LY	1476	HIS
2	LY	1549	ASN
2	LY	1557	ASN
2	LY	1583	GLN
2	LY	1594	ASN
2	MY	1476	HIS
2	MY	1549	ASN
2	MY	1557	ASN
2	MY	1583	GLN
2	MY	1594	ASN
2	NY	1476	HIS
2	NY	1549	ASN
2	NY	1583	GLN
2	NY	1594	ASN
2	OY	1476	HIS
2	OY	1557	ASN
2	OY	1583	GLN
2	OY	1594	ASN
2	PY	1549	ASN
2	PY	1557	ASN
2	PY	1583	GLN
2	PY	1594	ASN
2	QY	1476	HIS
2	QY	1528	ASN
2	QY	1549	ASN
2	QY	1557	ASN
2	QY	1583	GLN
2	QY	1594	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 monosaccharides 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.

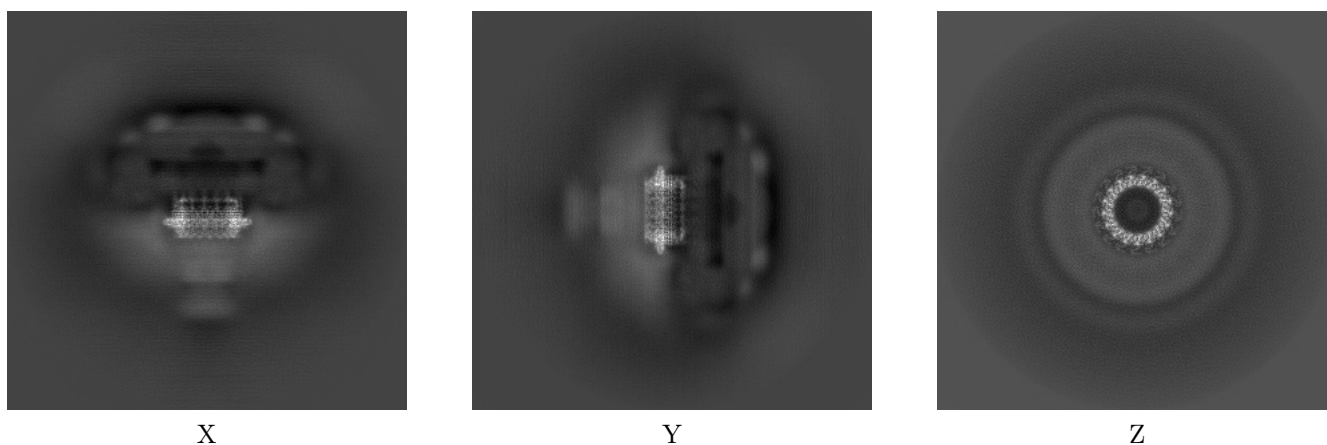
6 Map visualisation [i](#)

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

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

6.1 Orthogonal projections [i](#)

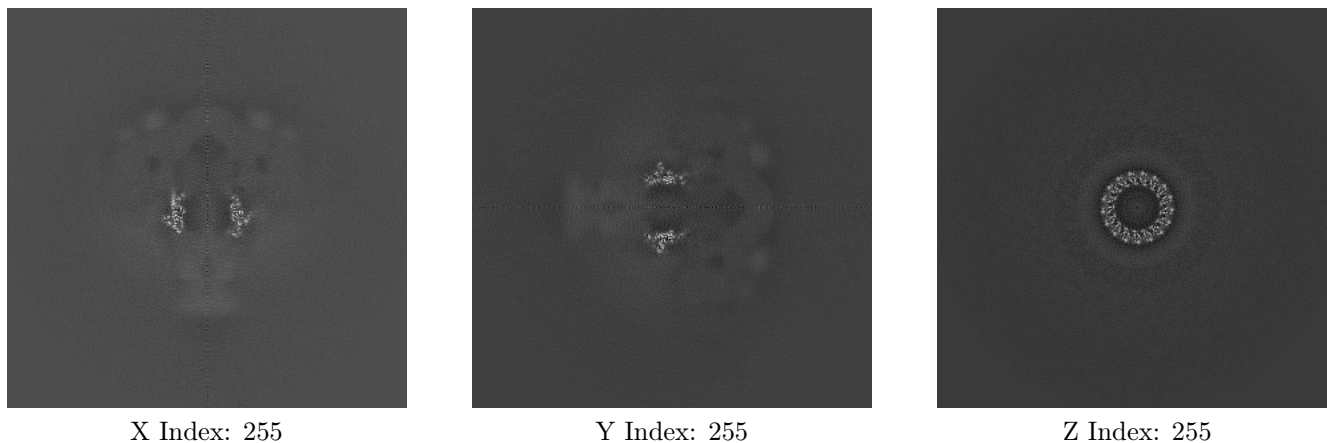
6.1.1 Primary map



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

6.2 Central slices [i](#)

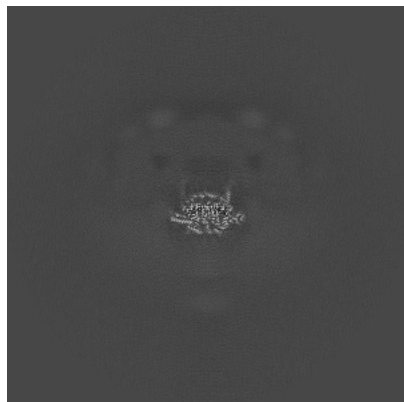
6.2.1 Primary map



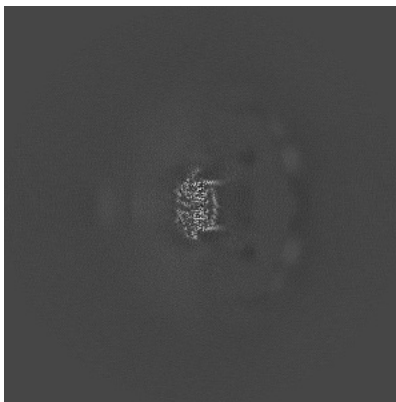
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

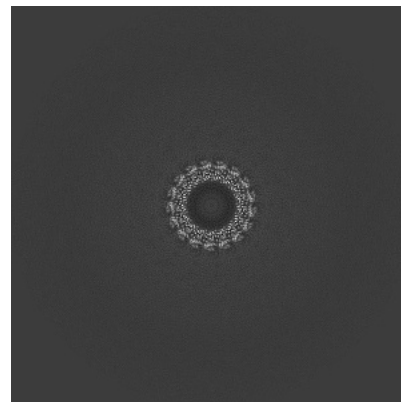
6.3.1 Primary map



X Index: 288



Y Index: 223



Z Index: 243

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

6.4 Orthogonal surface views [i](#)

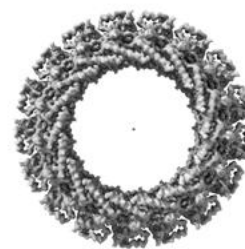
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

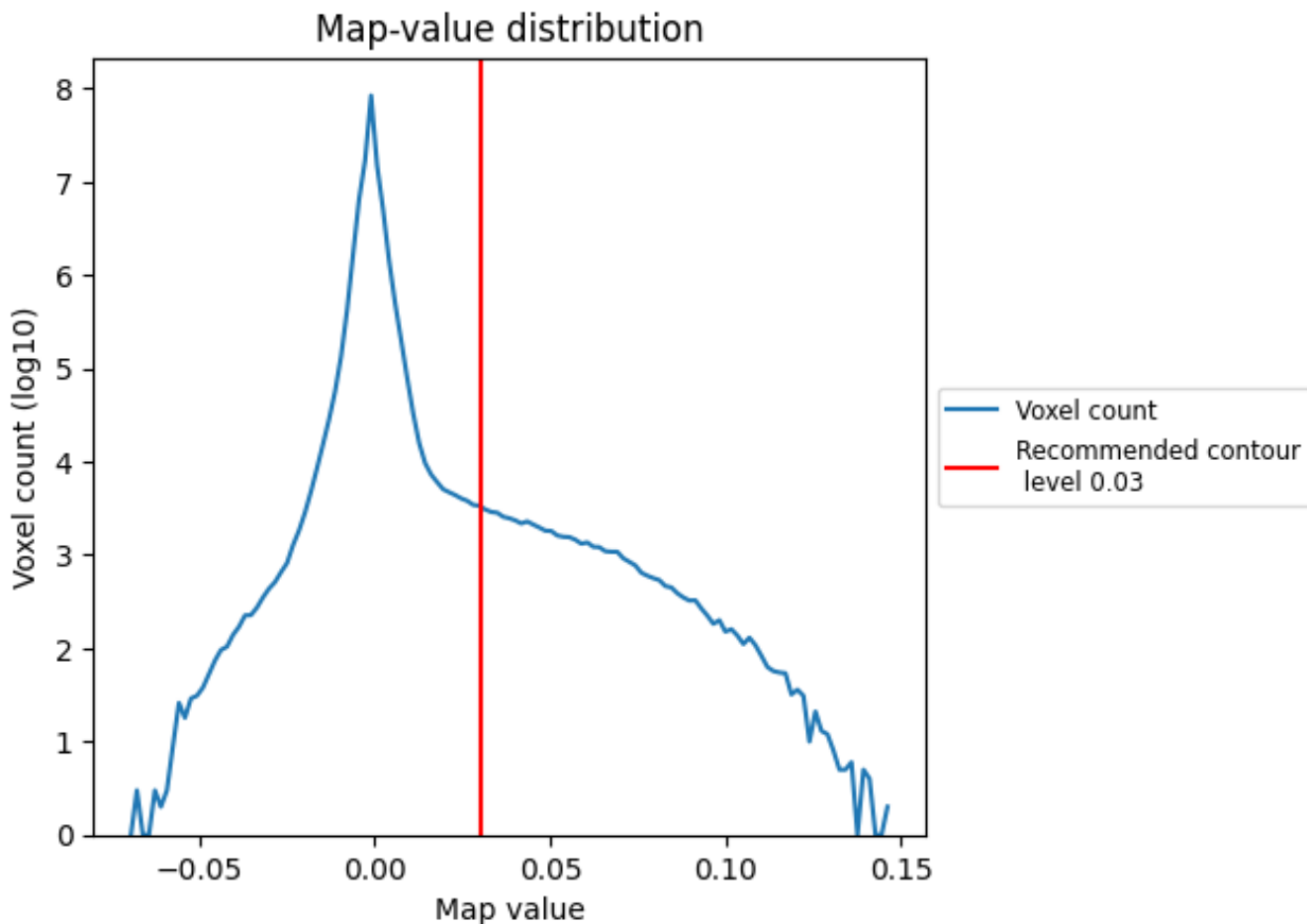
6.5 Mask visualisation

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

7 Map analysis [i](#)

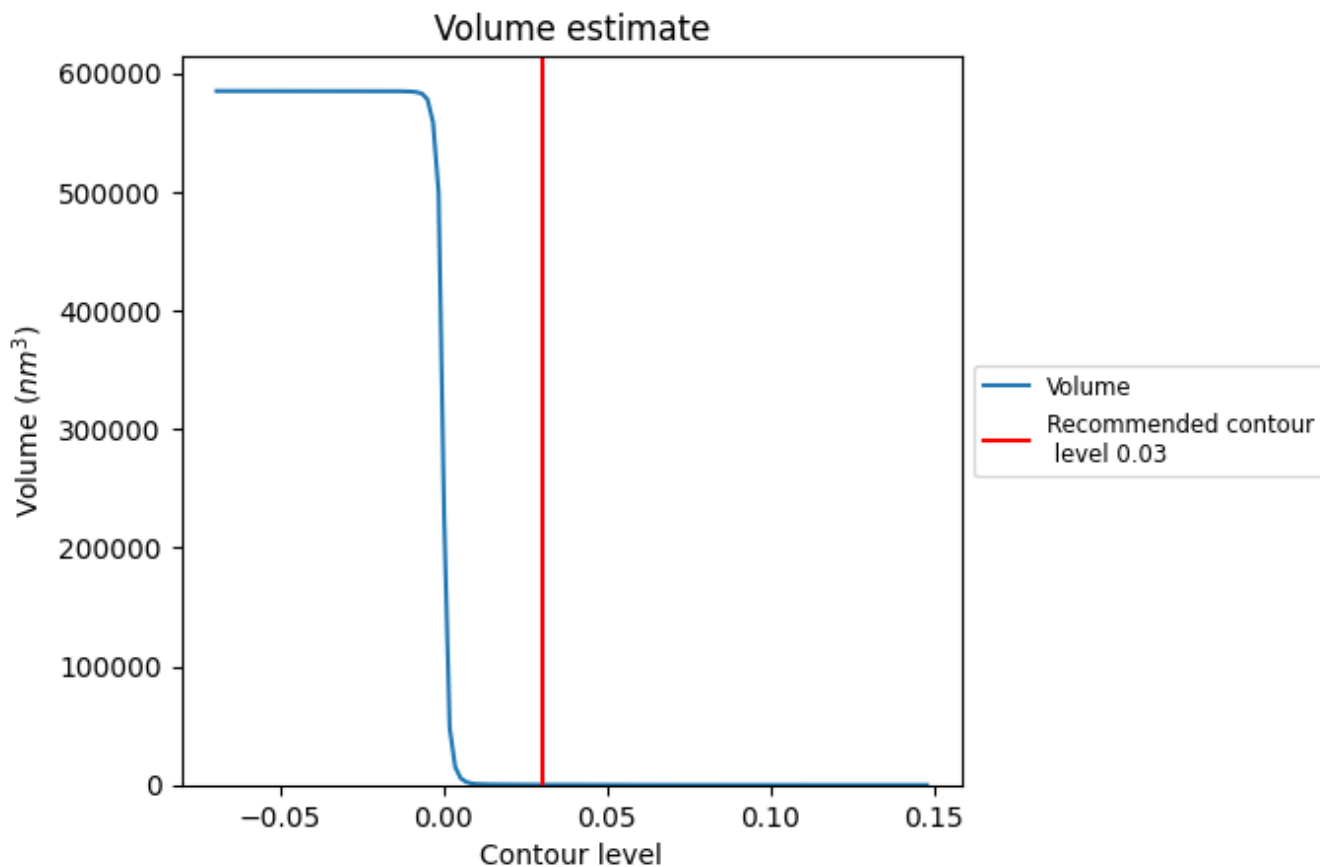
This section contains the results of statistical analysis of the map.

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.

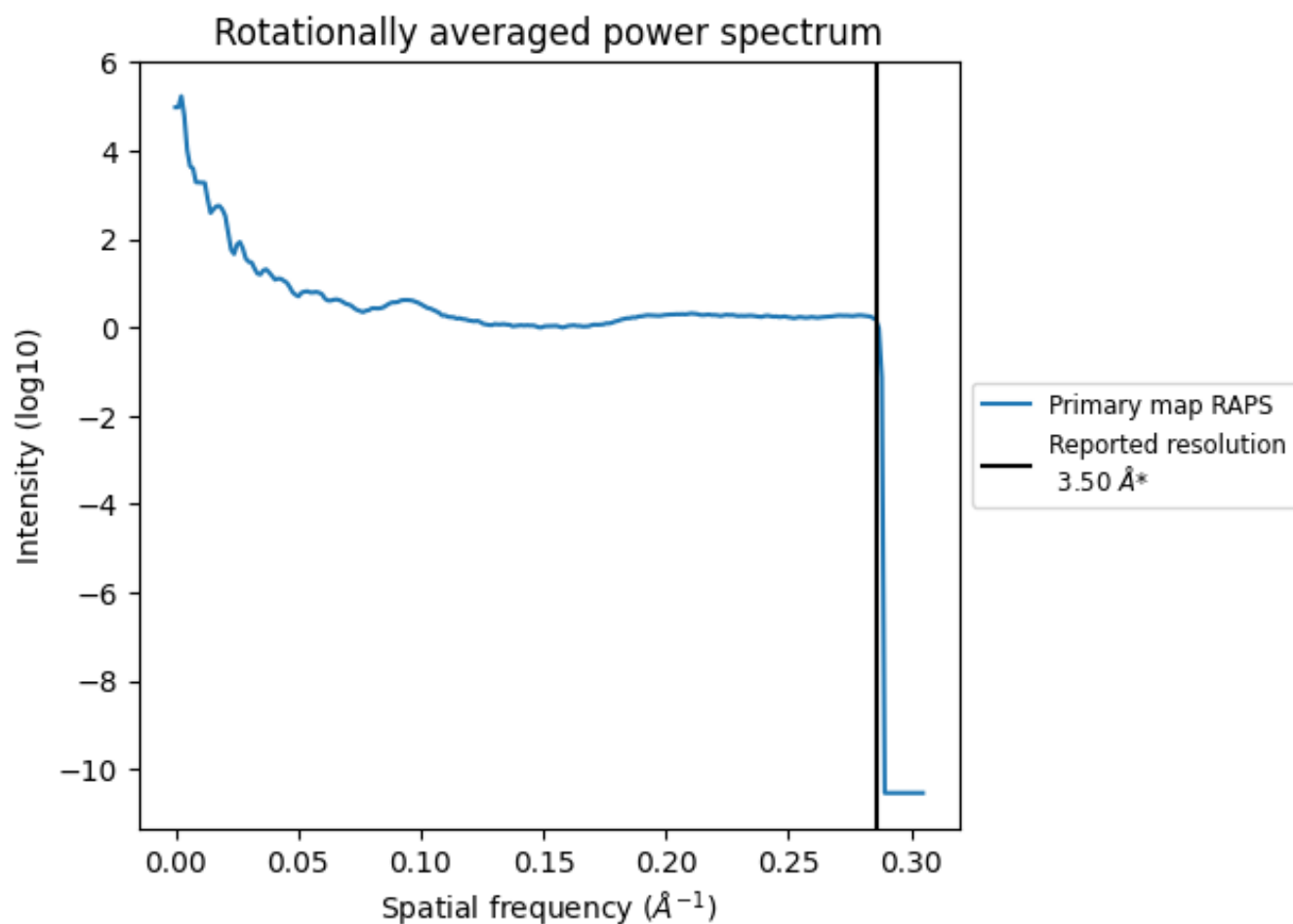
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 244 nm^3 ; this corresponds to an approximate mass of 220 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 [\(i\)](#)

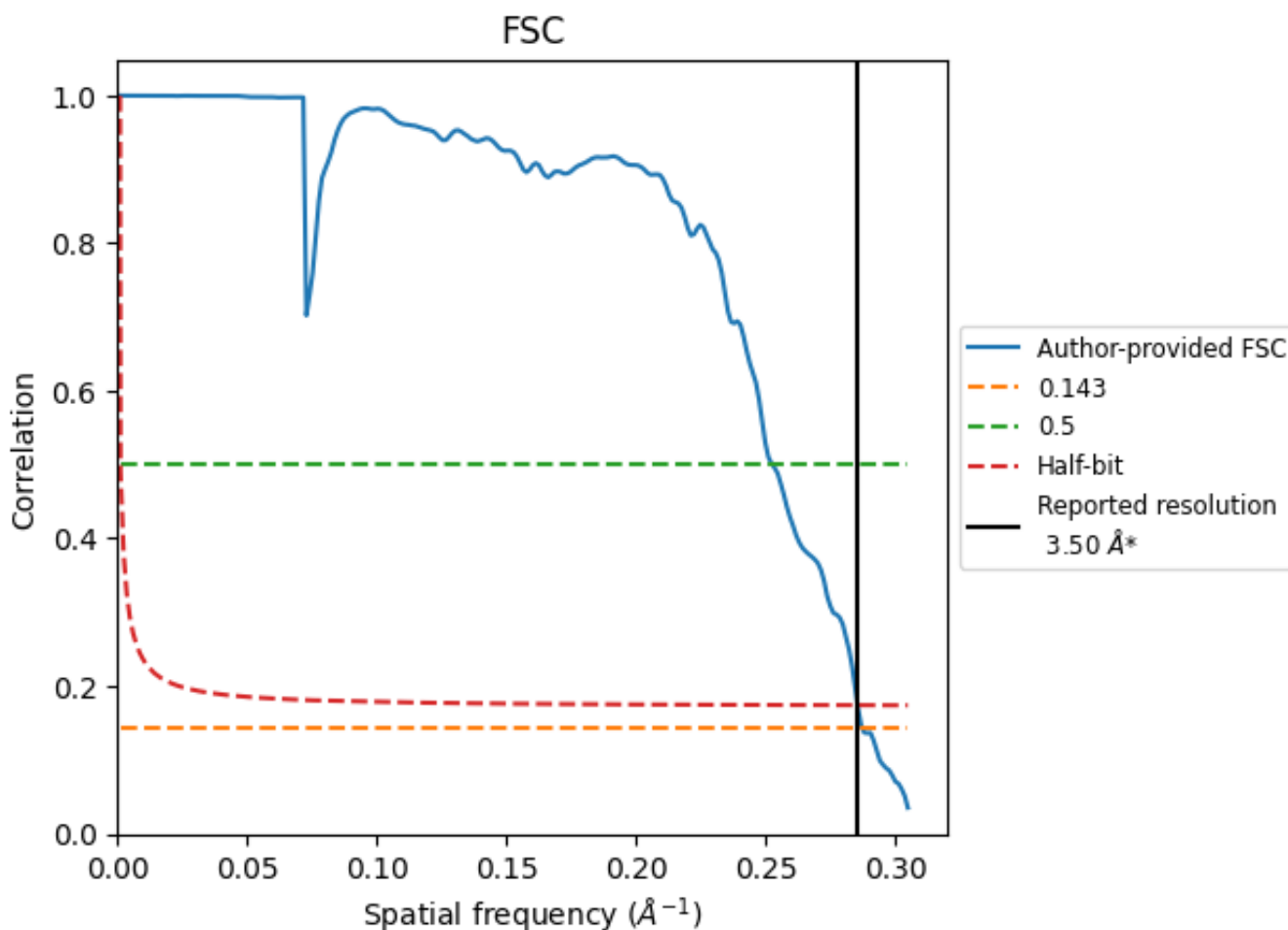


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

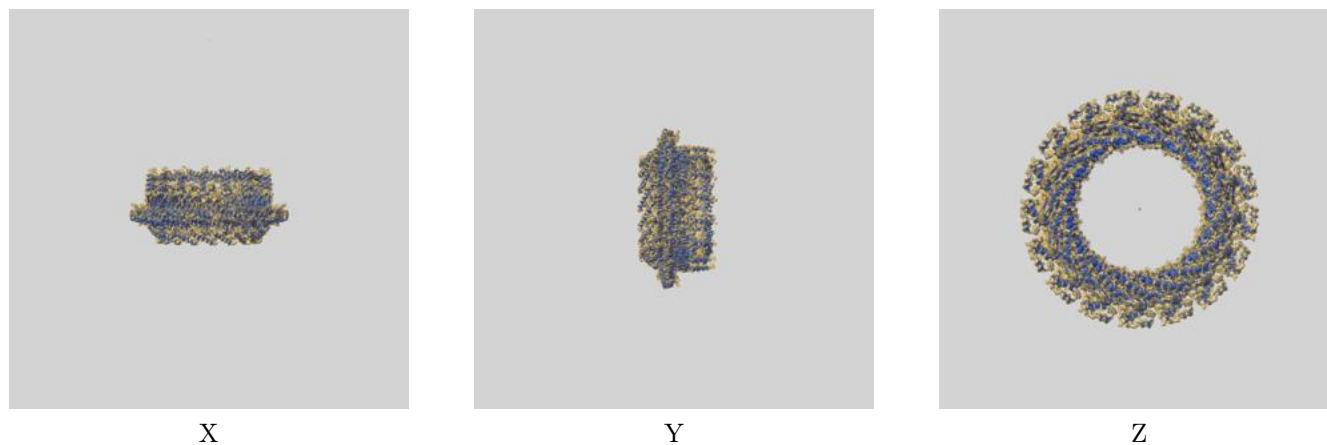
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.48	3.96	3.50
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

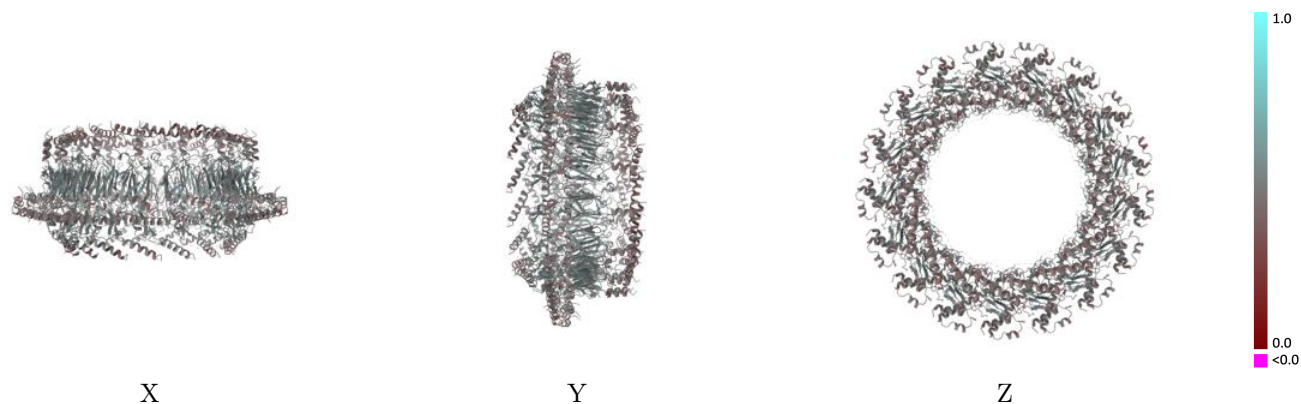
This section contains information regarding the fit between EMDB map EMD-20021 and PDB model 6X6J. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



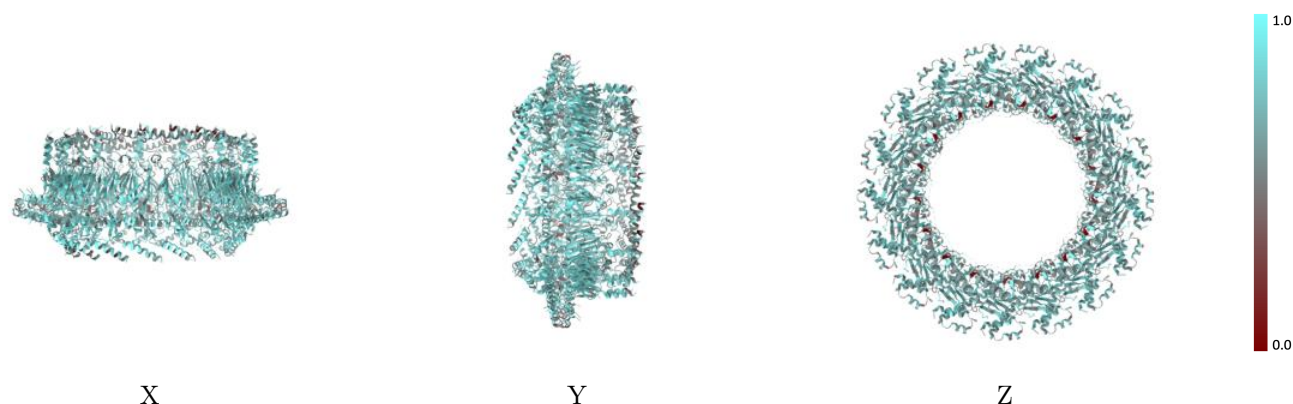
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



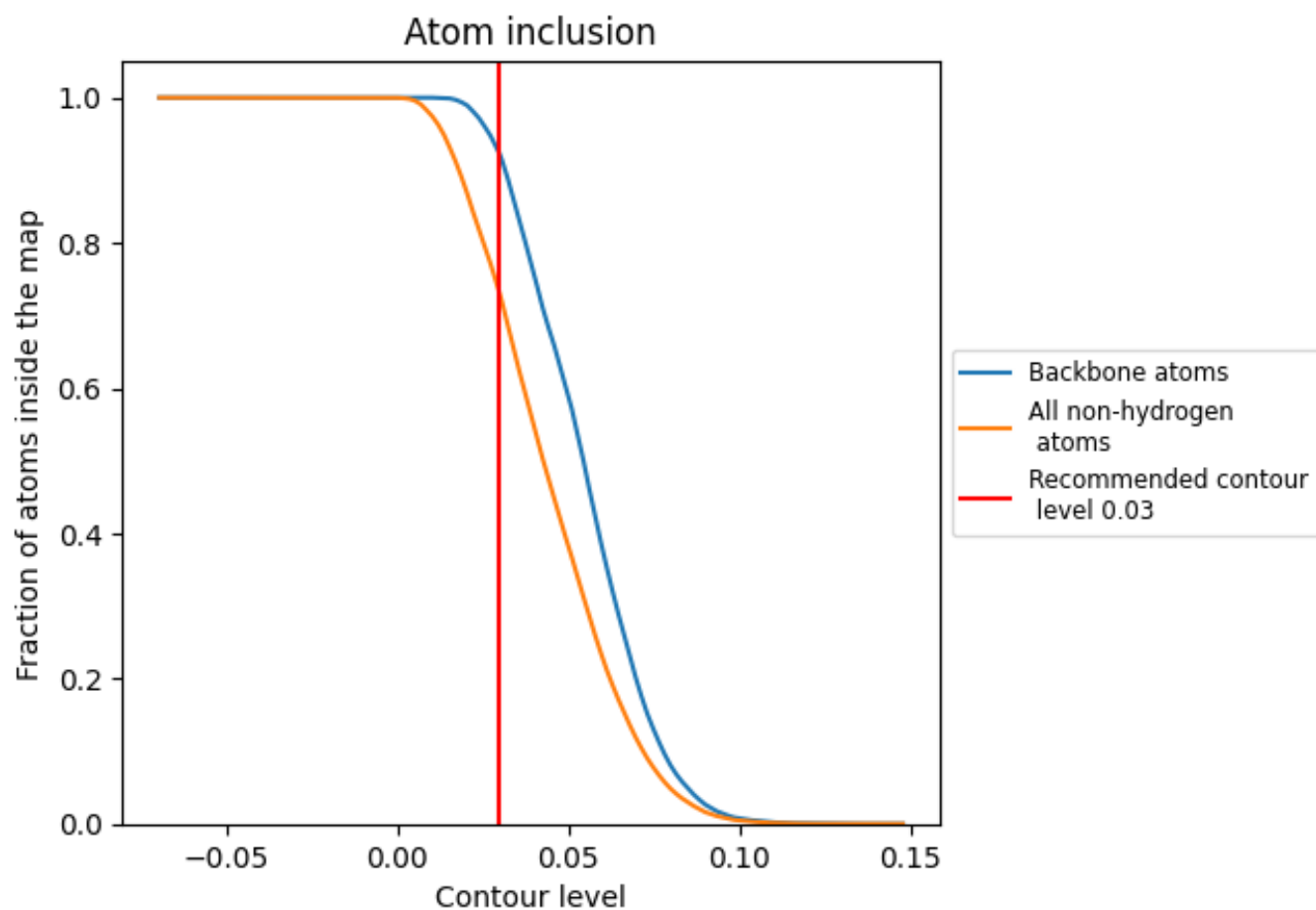
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 73% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7301	 0.4730
AX	 0.7667	 0.4910
AY	 0.6670	 0.4470
BX	 0.7720	 0.4910
BY	 0.6815	 0.4480
CX	 0.7720	 0.4910
CY	 0.6718	 0.4460
DX	 0.7736	 0.4930
DY	 0.6728	 0.4530
EX	 0.7796	 0.4950
EY	 0.6737	 0.4500
FX	 0.7789	 0.4930
FY	 0.6737	 0.4470
GX	 0.7804	 0.4950
GY	 0.6776	 0.4480
HX	 0.7743	 0.4920
HY	 0.6757	 0.4460
IX	 0.7720	 0.4950
IY	 0.6795	 0.4450
JX	 0.7698	 0.4880
JY	 0.6602	 0.4430
KX	 0.7804	 0.4920
KY	 0.6699	 0.4480
LX	 0.7743	 0.4920
LY	 0.6834	 0.4470
MX	 0.7690	 0.4930
MY	 0.6728	 0.4470
NX	 0.7667	 0.4920
NY	 0.6757	 0.4470
OX	 0.7758	 0.4930
OY	 0.6680	 0.4470
PX	 0.7736	 0.4910
PY	 0.6786	 0.4490
QX	 0.7774	 0.4960
QY	 0.6824	 0.4500

