Full wwPDB EM Validation Report ⓘ

Nov 2, 2022 – 09:16 PM EDT

PDB ID	:	5U4W
EMDB ID	:	EMD-8508
Title	:	Cryo-EM Structure of Immature Zika Virus
Authors	:	Mangala Prasad, V.; Miller, A.S.; Klose, T.; Sirohi, D.; Buda, G.; Jiang, W.; Kuhn, R.J.; Rossmann, M.G.
Deposited on	:	2016-12-06
Resolution	:	9.10 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

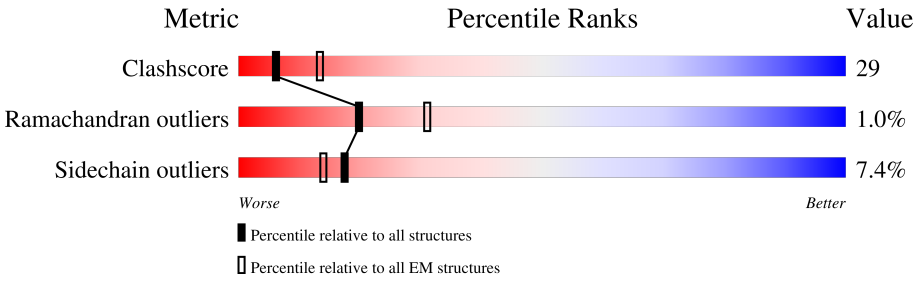
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 9.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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 <=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	A	402	14% 59% 33%
1	C	402	18% 57% 36%
1	E	402	13% 59% 34%
2	B	81	17% 52% 41% 6%
2	D	81	17% 53% 40% 6%
2	F	81	16% 54% 40% 5%
3	G	66	82% 89% 6% 5%
3	I	66	55% 86% 9% 5%

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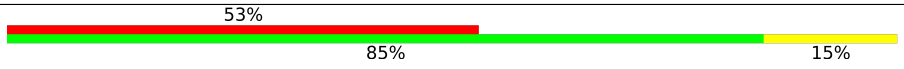
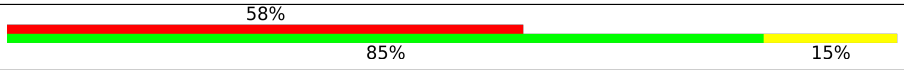
Mol	Chain	Length	Quality of chain
3	K	66	
4	H	53	
4	J	53	
4	L	53	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	A	401	-	-	X	-
5	NAG	B	104	X	-	X	-
5	NAG	D	104	X	-	X	-
5	NAG	F	104	X	-	X	-
6	BMA	B	103	X	-	-	-
6	BMA	D	103	X	-	-	-
6	BMA	F	103	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13368 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 E protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	390	Total	C	N	O	S	0	0
			3046	1926	524	569	27		
1	C	390	Total	C	N	O	S	0	0
			3046	1926	524	569	27		
1	E	390	Total	C	N	O	S	0	0
			3046	1926	524	569	27		

- Molecule 2 is a protein called pr domain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	81	Total	C	N	O	S	0	0
			640	396	106	128	10		
2	D	81	Total	C	N	O	S	0	0
			640	396	106	128	10		
2	F	81	Total	C	N	O	S	0	0
			640	396	106	128	10		

- Molecule 3 is a protein called Protein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	66	Total	C	N	O	0	0
			375	233	71	71		
3	I	66	Total	C	N	O	0	0
			375	233	71	71		
3	K	66	Total	C	N	O	0	0
			375	233	71	71		

- Molecule 4 is a protein called M protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	53	Total	C	N	O	0	0
			315	198	57	60		

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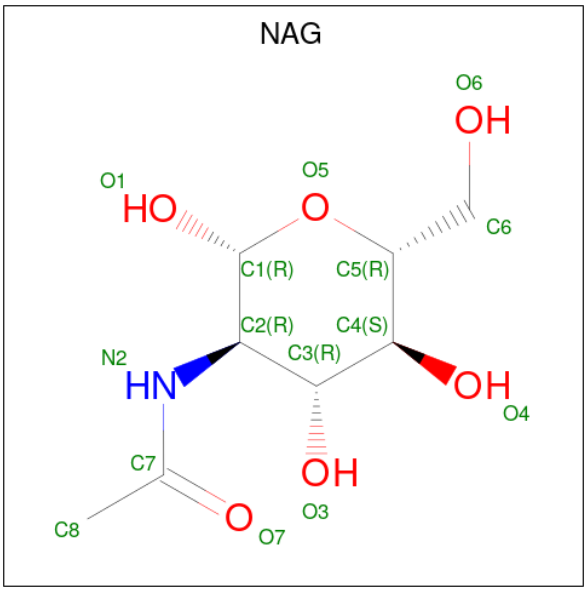
Mol	Chain	Residues	Atoms	AltConf	Trace
4	J	53	Total C N O 315 198 57 60	0	0
4	L	53	Total C N O 315 198 57 60	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C N O 14 8 1 5	0
5	B	1	Total C N O 44 24 3 17	0
5	B	1	Total C N O 44 24 3 17	0
5	B	1	Total C N O 44 24 3 17	0
5	C	1	Total C N O 14 8 1 5	0
5	D	1	Total C N O 44 24 3 17	0
5	D	1	Total C N O 44 24 3 17	0
5	D	1	Total C N O 44 24 3 17	0
5	E	1	Total C N O 14 8 1 5	0

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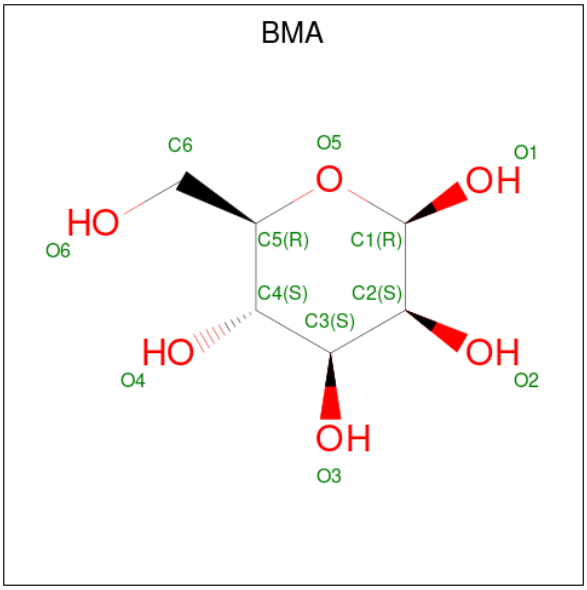
Mol	Chain	Residues	Atoms	AltConf
5	F	1	Total C N O 44 24 3 17	0
5	F	1	Total C N O 44 24 3 17	0
5	F	1	Total C N O 44 24 3 17	0

- Molecule 6 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



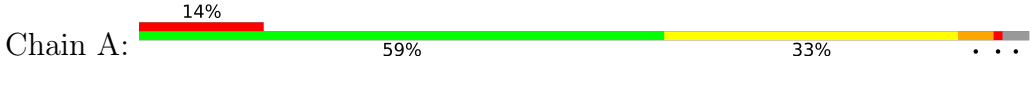
Mol	Chain	Residues	Atoms	AltConf
6	B	1	Total C O 22 12 10	0
6	B	1	Total C O 22 12 10	0
6	D	1	Total C O 22 12 10	0
6	D	1	Total C O 22 12 10	0
6	F	1	Total C O 22 12 10	0
6	F	1	Total C O 22 12 10	0

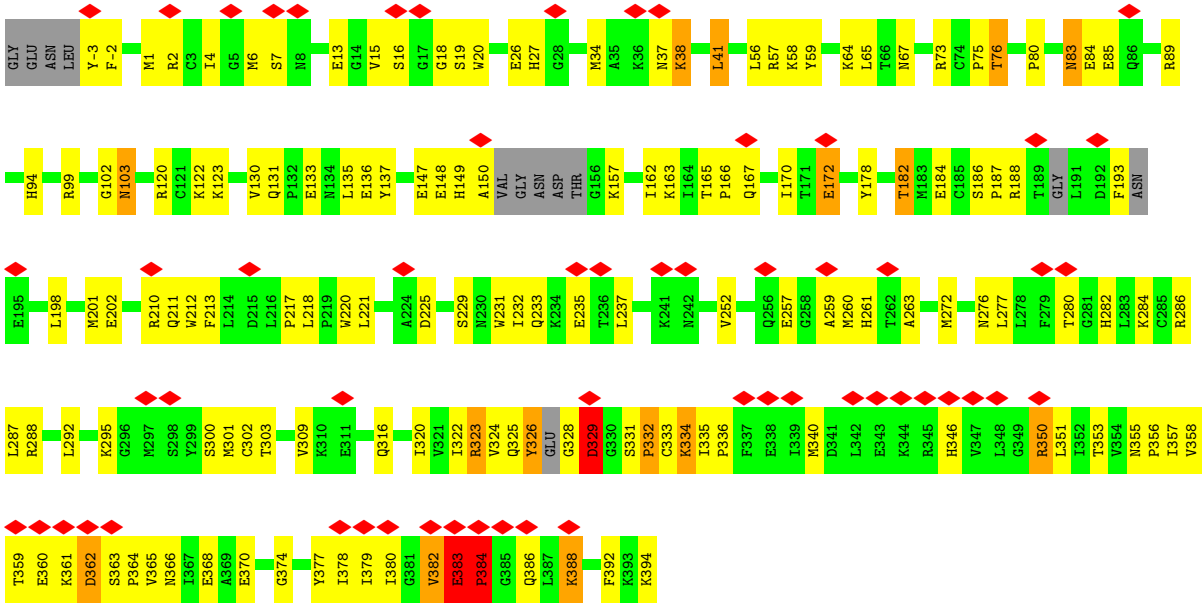
3 Residue-property plots (i)

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

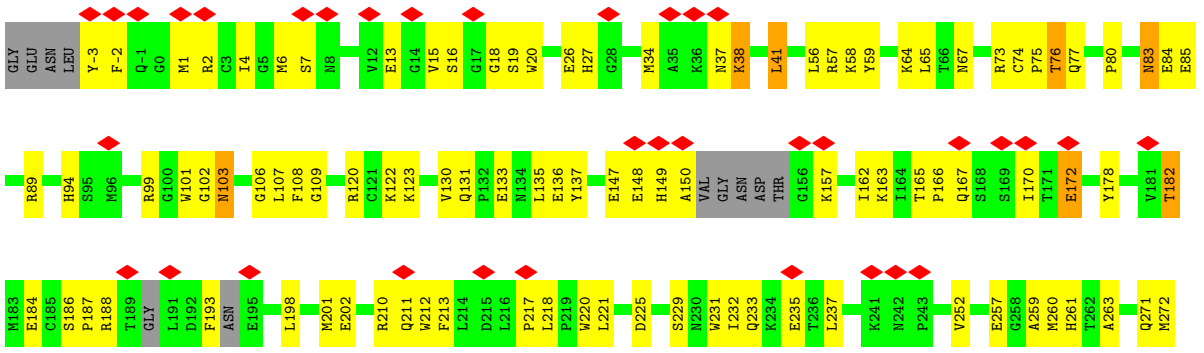
Chain A:

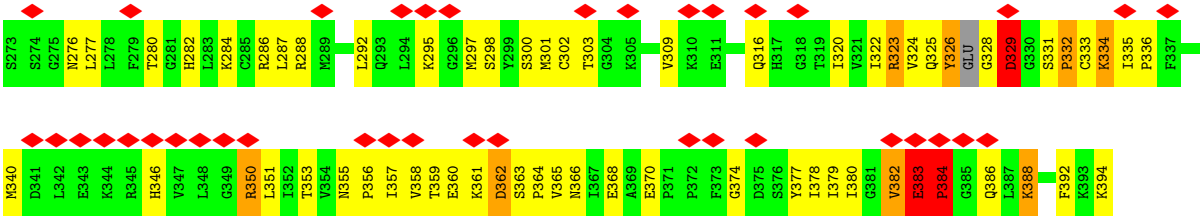




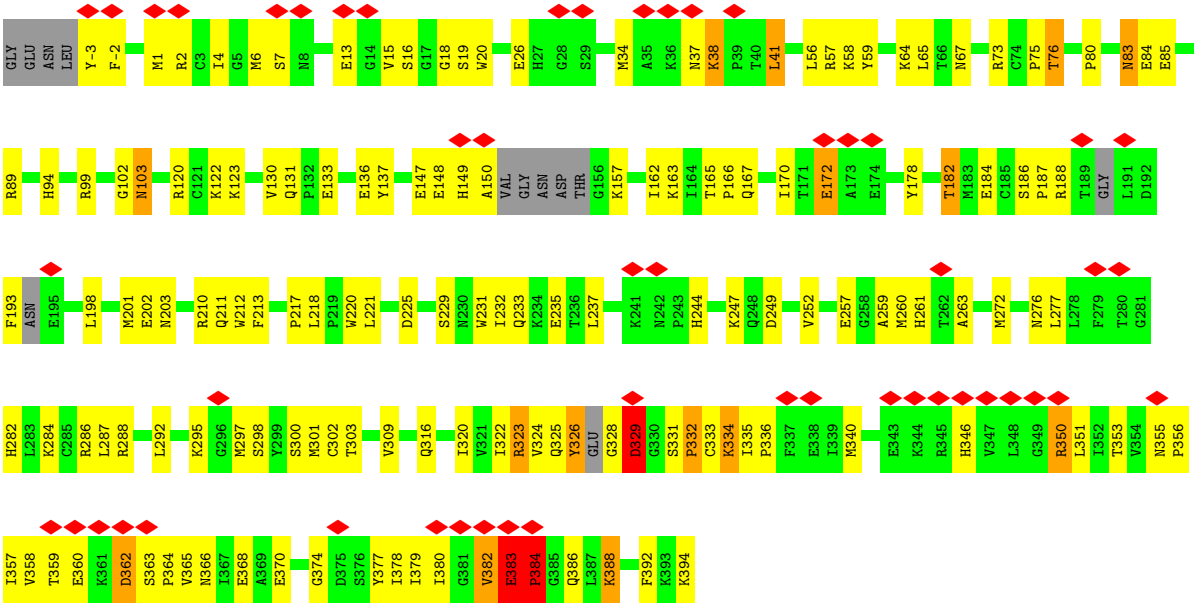
• Molecule 1: E protein

Chain C:

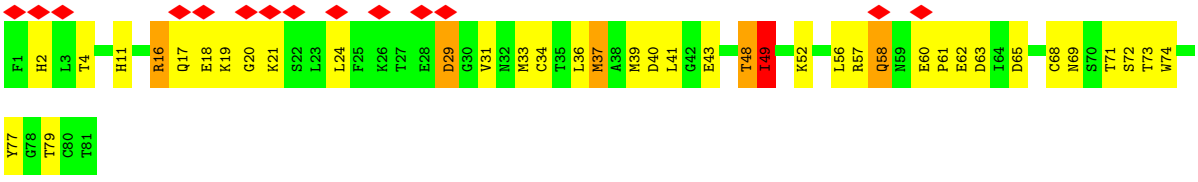




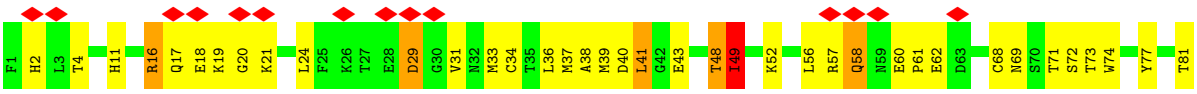
• Molecule 1: E protein



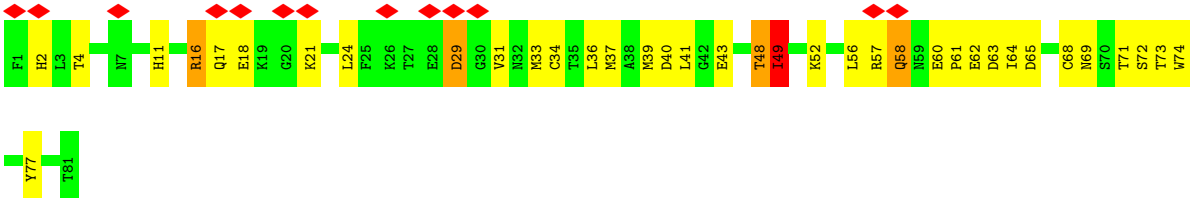
• Molecule 2: pr domain



• Molecule 2: pr domain

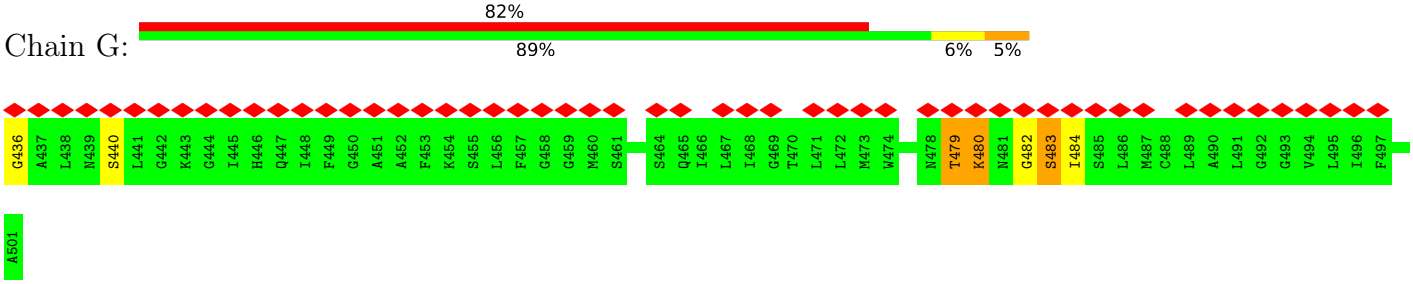


• Molecule 2: pr domain



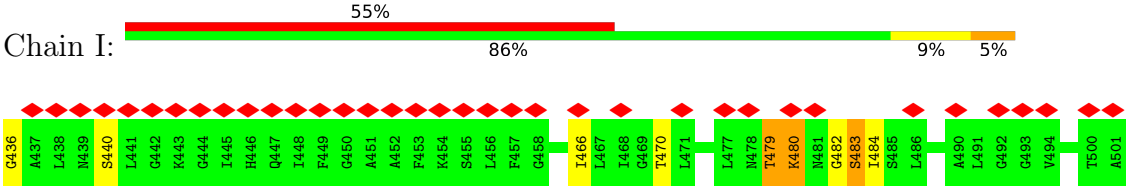
• Molecule 3: Protein E

Chain G:



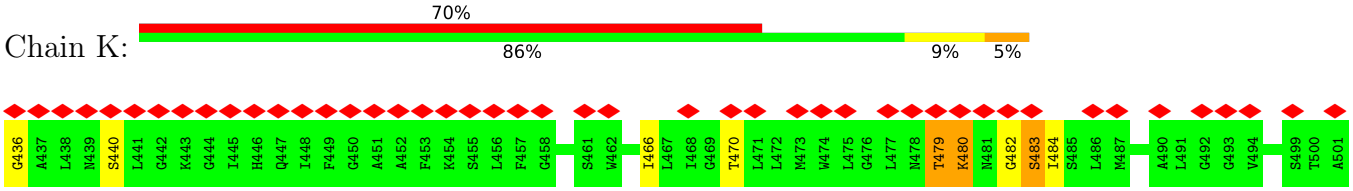
• Molecule 3: Protein E

Chain I:



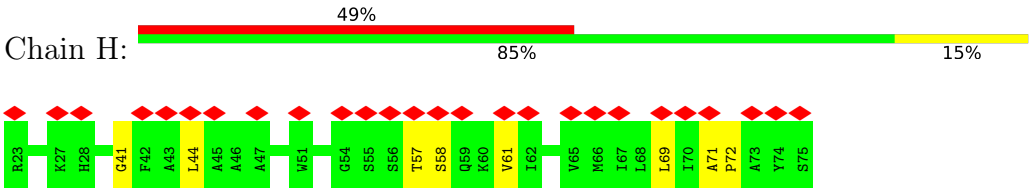
• Molecule 3: Protein E

Chain K:



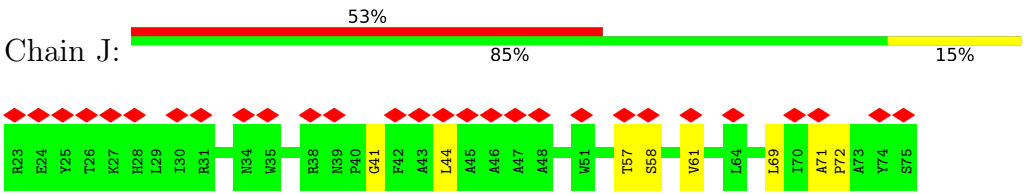
• Molecule 4: M protein

Chain H:



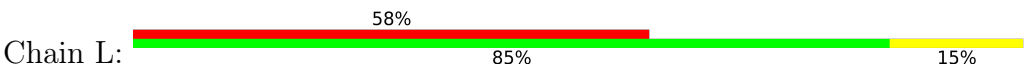
• Molecule 4: M protein

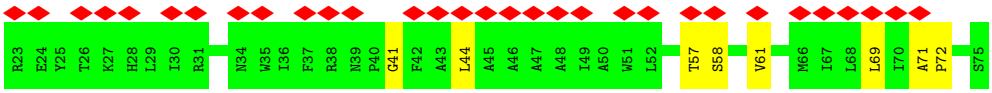
Chain J:



• Molecule 4: M protein

Chain L:




R23
E24
Y25
T26
K27
H28
L29
I30
R31
N34
W35
I36
F37
R38
N39
P40
G41
F42
A43
L44
A45
A46
A47
A48
I49
A50
W51
L52
T57
S58
V61
M66
I67
L68
L69
I70
A71
P72
S75

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	9315	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 ($e^-/Å^2$)	4.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	22.248	Depositor
Minimum map value	-32.937	Depositor
Average map value	0.055	Depositor
Map value standard deviation	1.586	Depositor
Recommended contour level	4.5	Depositor
Map size (Å)	873.6, 873.6, 873.6	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.6, 2.6, 2.6	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA

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	A	0.54	2/3106 (0.1%)	0.78	7/4186 (0.2%)
1	C	0.54	2/3106 (0.1%)	0.78	7/4186 (0.2%)
1	E	0.54	2/3106 (0.1%)	0.78	7/4186 (0.2%)
2	B	0.61	2/652 (0.3%)	0.69	1/883 (0.1%)
2	D	0.61	2/652 (0.3%)	0.69	1/883 (0.1%)
2	F	0.61	2/652 (0.3%)	0.69	1/883 (0.1%)
3	G	0.37	0/379	0.48	0/518
3	I	0.37	0/379	0.48	0/518
3	K	0.37	0/379	0.48	0/518
4	H	0.40	0/321	0.46	0/448
4	J	0.40	0/321	0.46	0/448
4	L	0.40	0/321	0.46	0/448
All	All	0.53	12/13374 (0.1%)	0.73	24/18105 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	D	0	1
2	F	0	1
All	All	0	3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	ILE	C-N	-15.26	1.05	1.34
1	E	335	ILE	C-N	-15.24	1.05	1.34
1	C	335	ILE	C-N	-15.24	1.05	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	334	LYS	C-N	-13.75	1.02	1.34
1	C	334	LYS	C-N	-13.75	1.02	1.34
1	E	334	LYS	C-N	-13.71	1.02	1.34
2	D	48	THR	C-N	-9.52	1.12	1.34
2	B	48	THR	C-N	-9.50	1.12	1.34
2	F	48	THR	C-N	-9.50	1.12	1.34
2	F	49	ILE	C-N	-7.06	1.17	1.34
2	D	49	ILE	C-N	-7.05	1.17	1.34
2	B	49	ILE	C-N	-7.03	1.17	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	334	LYS	O-C-N	-9.86	106.93	122.70
1	C	334	LYS	O-C-N	-9.84	106.96	122.70
1	A	334	LYS	O-C-N	-9.83	106.97	122.70
1	A	384	PRO	N-CA-C	-8.40	90.27	112.10
1	C	384	PRO	N-CA-C	-8.39	90.30	112.10
1	E	384	PRO	N-CA-C	-8.39	90.30	112.10
1	C	383	GLU	N-CA-C	8.20	133.14	111.00
1	A	383	GLU	N-CA-C	8.19	133.11	111.00
1	E	383	GLU	N-CA-C	8.18	133.08	111.00
1	A	332	PRO	N-CA-C	-8.06	91.13	112.10
1	C	332	PRO	N-CA-C	-8.06	91.14	112.10
1	E	332	PRO	N-CA-C	-8.05	91.17	112.10
1	A	334	LYS	C-N-CA	7.29	139.93	121.70
1	C	334	LYS	C-N-CA	7.27	139.88	121.70
1	E	334	LYS	C-N-CA	7.26	139.84	121.70
1	C	334	LYS	CA-C-N	6.81	132.19	117.20
1	A	334	LYS	CA-C-N	6.80	132.16	117.20
1	E	334	LYS	CA-C-N	6.78	132.12	117.20
1	A	329	ASP	N-CA-C	5.36	125.47	111.00
1	C	329	ASP	N-CA-C	5.33	125.39	111.00
1	E	329	ASP	N-CA-C	5.33	125.39	111.00
2	B	48	THR	O-C-N	-5.32	114.19	122.70
2	D	48	THR	O-C-N	-5.29	114.23	122.70
2	F	48	THR	O-C-N	-5.27	114.26	122.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	49	ILE	Mainchain
2	D	49	ILE	Mainchain
2	F	49	ILE	Mainchain

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	A	3046	0	3045	145	0
1	C	3046	0	3044	228	0
1	E	3046	0	3045	167	0
2	B	640	0	607	119	0
2	D	640	0	603	118	0
2	F	640	0	608	86	0
3	G	375	0	264	5	0
3	I	375	0	264	6	0
3	K	375	0	264	6	0
4	H	315	0	225	6	0
4	J	315	0	225	6	0
4	L	315	0	225	6	0
5	A	14	0	11	7	0
5	B	44	0	42	18	0
5	C	14	0	11	6	0
5	D	44	0	42	17	0
5	E	14	0	11	6	0
5	F	44	0	42	17	0
6	B	22	0	17	5	0
6	D	22	0	17	6	0
6	F	22	0	17	6	0
All	All	13368	0	12629	756	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 29.

All (756) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:ASP:CB	2:D:39:MET:HB3	1.29	1.56
1:C:108:PHE:CD1	2:F:63:ASP:HA	1.43	1.52
2:B:40:ASP:HA	2:D:39:MET:CB	1.46	1.46
5:F:101:NAG:O4	6:F:102:BMA:C1	1.66	1.42
1:C:108:PHE:HD1	2:F:63:ASP:CA	1.32	1.42
2:B:39:MET:CB	2:D:39:MET:O	1.68	1.40
5:B:101:NAG:O4	6:B:102:BMA:C1	1.66	1.40
5:D:101:NAG:O4	6:D:102:BMA:C1	1.66	1.40
2:B:40:ASP:CA	2:D:39:MET:HB3	1.51	1.39
1:C:101:TRP:CZ2	2:F:64:ILE:HG12	1.57	1.38
2:B:39:MET:C	2:D:39:MET:HA	1.42	1.37
1:C:108:PHE:CD1	2:F:63:ASP:CA	2.05	1.37
2:B:40:ASP:CA	2:D:39:MET:CB	2.05	1.32
2:B:19:LYS:HG2	2:D:20:GLY:CA	1.58	1.32
1:C:74:CYS:SG	2:F:39:MET:CE	2.23	1.26
2:B:39:MET:O	2:D:39:MET:HA	1.22	1.25
2:B:39:MET:HB2	2:D:39:MET:O	1.09	1.24
2:B:39:MET:CB	2:D:41:LEU:N	1.98	1.23
1:C:108:PHE:CB	2:F:63:ASP:OD1	1.86	1.23
2:B:40:ASP:HB2	2:D:39:MET:CE	1.69	1.22
1:C:107:LEU:CD1	1:E:247:LYS:HD3	1.68	1.22
1:C:107:LEU:HD11	1:E:247:LYS:CD	1.71	1.20
2:B:39:MET:C	2:D:39:MET:CA	2.11	1.19
1:A:188:ARG:HD3	1:A:284:LYS:HD2	1.24	1.16
1:C:108:PHE:CD1	2:F:63:ASP:N	2.11	1.16
2:B:39:MET:CB	2:D:39:MET:C	2.15	1.15
2:B:39:MET:CA	2:D:39:MET:O	1.95	1.15
1:C:108:PHE:CE1	2:F:63:ASP:N	2.11	1.15
1:C:188:ARG:HD3	1:C:284:LYS:HD2	1.24	1.14
1:E:188:ARG:HD3	1:E:284:LYS:HD2	1.24	1.14
2:B:79:THR:HG22	2:D:39:MET:HE1	1.20	1.14
2:B:40:ASP:CB	2:D:39:MET:CB	2.24	1.12
2:B:40:ASP:HA	2:D:39:MET:CA	1.78	1.12
1:C:76:THR:HG21	2:F:40:ASP:CG	1.69	1.12
2:B:39:MET:HB2	2:D:39:MET:C	1.68	1.11
1:C:107:LEU:CG	1:E:247:LYS:HD3	1.80	1.11
1:C:101:TRP:CZ2	2:F:64:ILE:CG1	2.33	1.10
2:B:19:LYS:CG	2:D:20:GLY:CA	2.29	1.09
1:C:74:CYS:SG	2:F:39:MET:HE3	1.90	1.09
1:C:108:PHE:HB2	2:F:63:ASP:OD1	0.93	1.09
2:B:39:MET:HB3	2:D:41:LEU:N	1.59	1.08
2:B:40:ASP:HA	2:D:39:MET:CG	1.78	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:TRP:HZ2	2:F:64:ILE:CG1	1.66	1.08
1:C:107:LEU:HD21	1:E:247:LYS:HG2	1.35	1.08
2:B:19:LYS:HG2	2:D:20:GLY:HA3	1.23	1.07
1:C:107:LEU:HD11	1:E:247:LYS:HD3	1.22	1.07
1:C:106:GLY:CA	2:F:65:ASP:HB3	1.85	1.06
2:B:39:MET:CB	2:D:41:LEU:H	1.65	1.05
2:B:39:MET:C	2:D:39:MET:O	1.94	1.05
1:C:74:CYS:SG	2:F:39:MET:HE2	1.91	1.05
1:C:106:GLY:C	2:F:65:ASP:HB3	1.77	1.05
2:B:39:MET:HB3	2:D:41:LEU:H	0.91	1.03
2:B:40:ASP:N	2:D:39:MET:O	1.90	1.03
2:B:39:MET:O	2:D:39:MET:CA	2.06	1.02
2:B:40:ASP:HB2	2:D:39:MET:HE3	1.04	1.00
2:B:40:ASP:CA	2:D:39:MET:CA	2.37	0.99
2:B:40:ASP:N	2:D:39:MET:CA	2.24	0.99
2:B:40:ASP:HB3	2:D:39:MET:CB	1.87	0.99
2:B:39:MET:HG3	2:D:40:ASP:C	1.80	0.99
2:F:2:HIS:NE2	6:F:103:BMA:O2	1.96	0.99
2:B:40:ASP:HB3	2:D:39:MET:HB3	1.01	0.98
2:B:2:HIS:NE2	6:B:103:BMA:O2	1.96	0.98
2:F:2:HIS:HE2	6:F:103:BMA:HO2	1.12	0.98
1:C:108:PHE:HE1	2:F:63:ASP:H	1.01	0.98
2:B:39:MET:C	2:D:39:MET:C	2.22	0.98
1:E:198:LEU:HD22	1:E:277:LEU:HD13	1.46	0.98
1:C:198:LEU:HD22	1:C:277:LEU:HD13	1.45	0.97
1:A:198:LEU:HD22	1:A:277:LEU:HD13	1.46	0.97
2:D:2:HIS:NE2	6:D:103:BMA:O2	1.96	0.97
2:B:40:ASP:N	2:D:39:MET:HA	1.77	0.96
1:C:76:THR:CG2	2:F:40:ASP:CG	2.34	0.96
2:B:37:MET:HE3	2:D:16:ARG:HH11	1.32	0.95
2:B:19:LYS:CG	2:D:20:GLY:HA3	1.94	0.95
1:C:106:GLY:HA3	2:F:65:ASP:HB3	1.44	0.95
1:C:101:TRP:CZ2	2:F:62:GLU:C	2.34	0.95
1:C:101:TRP:HZ2	2:F:64:ILE:HG12	0.88	0.94
2:B:2:HIS:HE2	6:B:103:BMA:HO2	1.12	0.94
2:D:2:HIS:HE2	6:D:103:BMA:HO2	1.13	0.92
2:B:37:MET:CE	2:D:16:ARG:HH11	1.83	0.92
2:B:19:LYS:HD3	2:D:20:GLY:HA2	1.52	0.92
2:B:19:LYS:CG	2:D:20:GLY:HA2	2.01	0.91
1:C:101:TRP:NE1	2:F:64:ILE:O	2.04	0.90
2:B:40:ASP:CA	2:D:39:MET:HA	2.00	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:GLY:HA3	2:F:65:ASP:CB	2.02	0.89
1:A:75:PRO:O	1:A:76:THR:HB	1.72	0.89
1:E:75:PRO:O	1:E:76:THR:HB	1.72	0.88
2:B:20:GLY:CA	2:D:19:LYS:O	2.23	0.87
2:B:39:MET:CG	2:D:40:ASP:C	2.32	0.87
2:B:19:LYS:CD	2:D:20:GLY:HA2	2.03	0.87
1:C:75:PRO:O	1:C:76:THR:HB	1.72	0.86
1:C:106:GLY:O	2:F:64:ILE:C	2.13	0.86
1:C:107:LEU:HD21	1:E:247:LYS:CG	2.05	0.86
5:B:104:NAG:O3	5:B:105:NAG:H1	1.76	0.86
5:F:104:NAG:O3	5:F:105:NAG:H1	1.76	0.86
2:B:19:LYS:HG2	2:D:20:GLY:N	1.89	0.86
5:D:104:NAG:O3	5:D:105:NAG:H1	1.76	0.86
2:B:37:MET:HE3	2:D:16:ARG:NH1	1.90	0.86
1:E:147:GLU:HB3	1:E:157:LYS:HE3	1.58	0.86
1:A:147:GLU:HB3	1:A:157:LYS:HE3	1.58	0.86
2:B:79:THR:CG2	2:D:39:MET:HE1	2.05	0.85
1:C:108:PHE:HB2	2:F:63:ASP:CG	1.96	0.85
1:C:76:THR:HG22	2:F:40:ASP:HB3	1.59	0.85
2:B:40:ASP:CB	2:D:39:MET:HE3	1.99	0.85
1:C:107:LEU:HG	1:E:247:LYS:HD3	1.58	0.84
1:C:109:GLY:CA	1:E:244:HIS:HE1	1.81	0.84
2:B:40:ASP:HA	2:D:39:MET:HA	1.51	0.83
1:C:106:GLY:O	2:F:64:ILE:O	1.97	0.83
1:C:109:GLY:CA	1:E:244:HIS:CE1	2.58	0.83
1:C:147:GLU:HB3	1:C:157:LYS:HE3	1.58	0.83
1:E:188:ARG:CD	1:E:284:LYS:HD2	2.08	0.82
2:B:40:ASP:N	2:D:39:MET:C	2.33	0.81
1:A:170:ILE:HG12	1:A:184:GLU:HB2	1.63	0.81
1:C:109:GLY:HA3	1:E:244:HIS:CE1	2.14	0.81
2:B:79:THR:HG22	2:D:39:MET:CE	2.06	0.80
1:E:170:ILE:HG12	1:E:184:GLU:HB2	1.63	0.80
2:B:19:LYS:C	2:D:20:GLY:HA3	2.03	0.79
1:C:77:GLN:NE2	2:F:40:ASP:N	2.24	0.79
1:C:77:GLN:HG2	2:F:40:ASP:HB3	1.62	0.79
1:C:188:ARG:CD	1:C:284:LYS:HD2	2.08	0.79
1:C:83:ASN:N	1:C:83:ASN:HD22	1.82	0.78
1:E:73:ARG:HG3	1:E:80:PRO:HB3	1.66	0.78
1:C:170:ILE:HG12	1:C:184:GLU:HB2	1.63	0.77
1:A:73:ARG:HG3	1:A:80:PRO:HB3	1.66	0.77
2:B:39:MET:HB3	2:D:39:MET:C	2.04	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LEU:HD22	1:A:213:PHE:HE2	1.49	0.77
1:C:73:ARG:HG3	1:C:80:PRO:HB3	1.66	0.77
1:A:303:THR:HA	1:A:382:VAL:HG21	1.67	0.77
1:A:188:ARG:CD	1:A:284:LYS:HD2	2.08	0.76
1:C:56:LEU:HD22	1:C:213:PHE:HE2	1.49	0.76
1:C:303:THR:HA	1:C:382:VAL:HG21	1.67	0.76
1:E:303:THR:HA	1:E:382:VAL:HG21	1.67	0.76
1:C:107:LEU:HD11	1:E:247:LYS:CG	2.15	0.76
1:A:83:ASN:N	1:A:83:ASN:HD22	1.82	0.76
1:E:56:LEU:HD22	1:E:213:PHE:HE2	1.49	0.76
1:C:76:THR:CG2	2:F:40:ASP:CB	2.65	0.75
1:C:108:PHE:HD1	2:F:63:ASP:HA	0.60	0.75
3:K:479:THR:O	3:K:480:LYS:CB	2.35	0.75
1:C:106:GLY:CA	2:F:65:ASP:CB	2.63	0.74
1:E:388:LYS:H	1:E:388:LYS:HD2	1.51	0.74
2:B:39:MET:CB	2:D:40:ASP:C	2.52	0.74
2:B:40:ASP:CB	2:D:39:MET:CE	2.59	0.74
1:E:83:ASN:N	1:E:83:ASN:HD22	1.82	0.74
1:A:388:LYS:H	1:A:388:LYS:HD2	1.51	0.74
1:A:351:LEU:HB3	1:A:353:THR:O	1.88	0.74
2:B:39:MET:HB2	2:D:40:ASP:CA	2.17	0.74
1:C:351:LEU:HB3	1:C:353:THR:O	1.88	0.74
1:A:309:VAL:HG11	1:A:323:ARG:HH21	1.52	0.74
1:C:99:ARG:HE	1:C:103:ASN:ND2	1.86	0.74
1:C:74:CYS:SG	2:F:39:MET:HG3	2.28	0.74
1:C:388:LYS:H	1:C:388:LYS:HD2	1.51	0.74
1:E:351:LEU:HB3	1:E:353:THR:O	1.88	0.74
3:G:479:THR:O	3:G:480:LYS:CB	2.35	0.74
1:A:99:ARG:HE	1:A:103:ASN:ND2	1.86	0.73
1:E:41:LEU:HD21	1:E:292:LEU:HD11	1.71	0.73
1:C:41:LEU:HD21	1:C:292:LEU:HD11	1.71	0.73
1:E:309:VAL:HG11	1:E:323:ARG:HH21	1.52	0.73
1:C:309:VAL:HG11	1:C:323:ARG:HH21	1.52	0.73
1:E:99:ARG:HE	1:E:103:ASN:ND2	1.86	0.73
3:I:479:THR:O	3:I:480:LYS:CB	2.35	0.72
1:A:41:LEU:HD21	1:A:292:LEU:HD11	1.70	0.72
1:C:148:GLU:OE2	1:C:364:PRO:HB2	1.90	0.71
1:A:148:GLU:OE2	1:A:364:PRO:HB2	1.90	0.71
1:C:77:GLN:HE21	2:F:40:ASP:N	1.85	0.71
1:E:148:GLU:OE2	1:E:364:PRO:HB2	1.90	0.71
1:A:83:ASN:ND2	1:A:83:ASN:H	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:LYS:CB	2:D:20:GLY:HA3	2.21	0.70
1:C:101:TRP:HE1	2:F:64:ILE:H	1.36	0.70
1:C:83:ASN:H	1:C:83:ASN:ND2	1.89	0.70
2:B:20:GLY:HA2	2:D:19:LYS:O	1.92	0.69
1:E:201:MET:HE2	1:E:257:GLU:HG3	1.74	0.69
1:C:76:THR:HG21	2:F:40:ASP:OD2	1.91	0.69
1:E:83:ASN:H	1:E:83:ASN:ND2	1.89	0.69
1:C:101:TRP:CH2	2:F:64:ILE:HG12	2.24	0.69
1:C:101:TRP:CZ2	2:F:64:ILE:N	2.61	0.69
1:C:166:PRO:HB3	1:C:187:PRO:HG2	1.75	0.69
1:E:166:PRO:HB3	1:E:187:PRO:HG2	1.75	0.69
1:C:76:THR:CG2	2:F:40:ASP:HB3	2.22	0.69
1:A:149:HIS:O	1:A:150:ALA:CB	2.41	0.68
1:C:149:HIS:O	1:C:150:ALA:CB	2.41	0.68
1:E:149:HIS:O	1:E:150:ALA:CB	2.41	0.68
1:A:166:PRO:HB3	1:A:187:PRO:HG2	1.75	0.68
1:A:201:MET:HE2	1:A:257:GLU:HG3	1.74	0.68
1:A:83:ASN:N	1:A:83:ASN:ND2	2.42	0.68
1:C:201:MET:HE2	1:C:257:GLU:HG3	1.74	0.68
1:E:83:ASN:N	1:E:83:ASN:ND2	2.42	0.67
2:B:79:THR:HB	2:D:39:MET:HE2	1.77	0.67
1:A:178:TYR:CE1	1:A:295:LYS:HB3	2.30	0.66
1:E:178:TYR:CE1	1:E:295:LYS:HB3	2.30	0.66
1:C:178:TYR:CE1	1:C:295:LYS:HB3	2.30	0.66
1:E:59:TYR:CD1	1:E:220:TRP:HB3	2.30	0.66
1:A:59:TYR:CD1	1:A:220:TRP:HB3	2.30	0.66
2:B:39:MET:HB2	2:D:40:ASP:N	2.10	0.66
1:C:59:TYR:CD1	1:C:220:TRP:HB3	2.30	0.66
1:A:67:ASN:OD1	5:A:401:NAG:O5	2.10	0.66
1:C:83:ASN:N	1:C:83:ASN:ND2	2.42	0.66
2:B:39:MET:CB	2:D:40:ASP:N	2.60	0.64
1:C:107:LEU:HD11	1:E:247:LYS:CE	2.27	0.64
1:A:165:THR:HG23	1:A:166:PRO:HD2	1.80	0.64
1:C:38:LYS:HE2	1:C:292:LEU:O	1.98	0.64
2:F:69:ASN:OD1	5:F:104:NAG:O1	2.15	0.64
1:A:333:CYS:O	1:A:357:ILE:HG23	1.98	0.64
2:D:69:ASN:OD1	5:D:104:NAG:O1	2.15	0.64
2:B:69:ASN:OD1	5:B:104:NAG:O1	2.15	0.63
1:C:56:LEU:HD23	1:C:57:ARG:HB2	1.79	0.63
3:I:436:GLY:O	3:I:440:SER:N	2.29	0.63
1:E:165:THR:HG23	1:E:166:PRO:HD2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:333:CYS:O	1:E:357:ILE:HG23	1.98	0.63
1:E:56:LEU:HD23	1:E:57:ARG:HB2	1.79	0.63
1:A:38:LYS:HE2	1:A:292:LEU:O	1.98	0.63
1:E:38:LYS:HE2	1:E:292:LEU:O	1.98	0.63
1:A:56:LEU:HD23	1:A:57:ARG:HB2	1.79	0.63
1:C:67:ASN:OD1	5:C:401:NAG:O5	2.10	0.63
2:B:57:ARG:HG3	2:B:57:ARG:HH11	1.64	0.62
2:B:63:ASP:HA	2:D:81:THR:OG1	1.99	0.62
1:C:333:CYS:O	1:C:357:ILE:HG23	1.98	0.62
2:B:39:MET:CB	2:D:40:ASP:CA	2.77	0.62
1:A:-2:PHE:CD2	1:A:1:MET:HE2	2.34	0.62
2:F:57:ARG:HH11	2:F:57:ARG:HG3	1.64	0.62
1:C:107:LEU:HD22	1:E:244:HIS:CG	2.34	0.62
2:D:57:ARG:HG3	2:D:57:ARG:HH11	1.64	0.62
1:C:108:PHE:CG	2:F:63:ASP:HA	2.26	0.62
1:E:67:ASN:OD1	5:E:401:NAG:O5	2.10	0.62
5:F:104:NAG:H4	5:F:105:NAG:H5	1.81	0.62
3:K:436:GLY:O	3:K:440:SER:N	2.29	0.62
1:A:360:GLU:HB2	1:A:363:SER:HB3	1.82	0.62
1:C:165:THR:HG23	1:C:166:PRO:HD2	1.80	0.62
5:B:104:NAG:H4	5:B:105:NAG:H5	1.81	0.62
1:C:388:LYS:H	1:C:388:LYS:CD	2.12	0.62
1:E:148:GLU:CD	1:E:364:PRO:HB2	2.20	0.62
1:E:360:GLU:HB2	1:E:363:SER:HB3	1.82	0.62
1:E:388:LYS:H	1:E:388:LYS:CD	2.12	0.62
1:C:101:TRP:HE1	2:F:64:ILE:N	1.97	0.61
1:E:182:THR:HG23	1:E:288:ARG:HB3	1.82	0.61
1:C:148:GLU:CD	1:C:364:PRO:O	2.39	0.61
5:D:104:NAG:H4	5:D:105:NAG:H5	1.81	0.61
1:A:148:GLU:CD	1:A:364:PRO:O	2.39	0.61
1:C:182:THR:HG23	1:C:288:ARG:HB3	1.83	0.61
1:C:360:GLU:HB2	1:C:363:SER:HB3	1.82	0.61
1:A:388:LYS:H	1:A:388:LYS:CD	2.12	0.61
1:E:123:LYS:HE3	1:E:202:GLU:OE1	2.01	0.61
1:E:148:GLU:CD	1:E:364:PRO:O	2.39	0.61
1:E:218:LEU:HD11	1:E:260:MET:HE1	1.83	0.61
2:B:39:MET:O	2:D:38:ALA:O	2.18	0.61
1:A:147:GLU:CB	1:A:157:LYS:HE3	2.30	0.60
1:A:302:CYS:SG	1:A:334:LYS:O	2.58	0.60
1:A:334:LYS:HA	1:A:357:ILE:HG12	1.83	0.60
2:B:37:MET:CE	2:D:16:ARG:NH1	2.52	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:LEU:HD11	1:C:260:MET:HE1	1.83	0.60
1:A:123:LYS:HE3	1:A:202:GLU:OE1	2.01	0.60
1:C:334:LYS:HA	1:C:357:ILE:HG12	1.83	0.60
1:C:302:CYS:SG	1:C:334:LYS:O	2.58	0.60
2:D:2:HIS:CE1	6:D:103:BMA:HO2	2.19	0.60
5:F:104:NAG:C4	5:F:105:NAG:H5	2.32	0.60
3:G:482:GLY:O	3:G:484:ILE:N	2.35	0.60
1:C:101:TRP:CZ2	2:F:64:ILE:HG13	2.32	0.60
1:E:302:CYS:SG	1:E:334:LYS:O	2.59	0.60
3:G:436:GLY:O	3:G:440:SER:N	2.29	0.60
3:I:482:GLY:O	3:I:484:ILE:N	2.35	0.60
1:A:182:THR:HG23	1:A:288:ARG:HB3	1.82	0.60
2:B:19:LYS:CB	2:D:20:GLY:CA	2.79	0.60
5:B:104:NAG:C4	5:B:105:NAG:H5	2.32	0.60
1:C:123:LYS:HE3	1:C:202:GLU:OE1	2.00	0.60
1:A:148:GLU:CD	1:A:364:PRO:HB2	2.21	0.60
1:C:83:ASN:HD22	1:C:83:ASN:H	1.49	0.60
3:K:482:GLY:O	3:K:484:ILE:N	2.35	0.60
1:C:148:GLU:CD	1:C:364:PRO:HB2	2.21	0.59
2:B:79:THR:CG2	2:D:39:MET:CE	2.74	0.59
2:B:69:ASN:HD21	5:B:104:NAG:C1	2.15	0.59
1:E:-3:TYR:CE2	1:E:1:MET:HE1	2.38	0.59
1:A:309:VAL:HB	1:A:323:ARG:HB3	1.85	0.59
1:E:309:VAL:HB	1:E:323:ARG:HB3	1.85	0.59
2:D:69:ASN:HD21	5:D:104:NAG:C1	2.15	0.59
1:E:334:LYS:HA	1:E:357:ILE:HG12	1.83	0.59
1:C:56:LEU:HD23	1:C:56:LEU:C	2.23	0.59
1:C:64:LYS:HB2	1:C:122:LYS:HE3	1.84	0.59
1:C:309:VAL:HB	1:C:323:ARG:HB3	1.85	0.59
5:D:104:NAG:C4	5:D:105:NAG:H5	2.32	0.59
1:A:-2:PHE:CE2	1:A:1:MET:HE2	2.38	0.59
1:C:107:LEU:CG	1:E:247:LYS:CD	2.71	0.59
1:C:188:ARG:HD3	1:C:284:LYS:CD	2.17	0.59
2:B:69:ASN:ND2	5:B:104:NAG:C1	2.66	0.59
2:F:69:ASN:ND2	5:F:104:NAG:C1	2.66	0.59
2:F:69:ASN:HD21	5:F:104:NAG:C1	2.15	0.59
1:A:64:LYS:HB2	1:A:122:LYS:HE3	1.84	0.58
1:E:147:GLU:CB	1:E:157:LYS:HE3	2.30	0.58
2:D:69:ASN:ND2	5:D:104:NAG:C1	2.66	0.58
1:E:56:LEU:HD23	1:E:56:LEU:C	2.23	0.58
1:C:147:GLU:CB	1:C:157:LYS:HE3	2.30	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:LYS:HB2	1:E:122:LYS:HE3	1.84	0.58
2:B:40:ASP:HB2	2:D:39:MET:SD	2.43	0.58
3:I:482:GLY:O	3:I:483:SER:C	2.41	0.58
3:K:482:GLY:O	3:K:483:SER:C	2.41	0.58
1:A:56:LEU:HD23	1:A:56:LEU:C	2.23	0.57
1:A:131:GLN:O	1:A:133:GLU:O	2.23	0.57
1:A:303:THR:HG23	1:A:303:THR:O	2.05	0.57
1:E:303:THR:O	1:E:303:THR:HG23	2.05	0.57
1:E:131:GLN:O	1:E:133:GLU:O	2.23	0.57
1:A:165:THR:CG2	1:A:166:PRO:HD2	2.35	0.57
1:C:76:THR:HG21	2:F:40:ASP:OD1	2.05	0.57
1:C:-2:PHE:CD2	1:C:1:MET:HE2	2.40	0.57
1:C:334:LYS:HE2	1:C:355:ASN:OD1	2.05	0.57
2:B:65:ASP:HB2	2:D:16:ARG:NH2	2.19	0.56
1:C:-2:PHE:CE2	1:C:1:MET:HE2	2.40	0.56
1:C:131:GLN:O	1:C:133:GLU:O	2.23	0.56
1:C:165:THR:CG2	1:C:166:PRO:HD2	2.35	0.56
1:C:303:THR:HG23	1:C:303:THR:O	2.05	0.56
1:A:334:LYS:HE2	1:A:355:ASN:OD1	2.05	0.56
1:E:13:GLU:HG3	1:E:34:MET:O	2.06	0.56
1:E:383:GLU:HG2	1:E:383:GLU:O	2.06	0.56
1:C:13:GLU:HG3	1:C:34:MET:O	2.06	0.56
3:G:482:GLY:O	3:G:483:SER:C	2.41	0.56
2:F:4:THR:HG23	2:F:11:HIS:HB3	1.87	0.55
2:F:52:LYS:HD3	2:F:72:SER:OG	2.06	0.55
1:A:383:GLU:O	1:A:383:GLU:HG2	2.06	0.55
2:B:4:THR:HG23	2:B:11:HIS:HB3	1.87	0.55
1:E:334:LYS:HE2	1:E:355:ASN:OD1	2.05	0.55
1:C:166:PRO:HB3	1:C:187:PRO:CG	2.36	0.55
2:D:52:LYS:HD3	2:D:72:SER:OG	2.07	0.55
1:A:218:LEU:HD11	1:A:260:MET:HE1	1.89	0.55
1:C:-3:TYR:CE2	1:C:1:MET:HE1	2.41	0.55
2:D:4:THR:HG23	2:D:11:HIS:HB3	1.88	0.55
1:C:326:TYR:C	1:C:328:GLY:N	2.60	0.55
1:C:383:GLU:O	1:C:383:GLU:HG2	2.06	0.55
1:E:326:TYR:C	1:E:328:GLY:N	2.60	0.55
1:C:107:LEU:HD21	1:E:247:LYS:CD	2.36	0.55
1:E:165:THR:CG2	1:E:166:PRO:HD2	2.35	0.55
1:A:167:GLN:HG2	1:A:167:GLN:O	2.07	0.55
2:F:16:ARG:O	2:F:16:ARG:HD3	2.07	0.55
1:A:13:GLU:HG3	1:A:34:MET:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LEU:HD22	1:A:213:PHE:CE2	2.37	0.55
1:A:166:PRO:HB3	1:A:187:PRO:CG	2.36	0.55
1:C:101:TRP:HZ2	2:F:64:ILE:N	2.05	0.55
1:E:-2:PHE:CE2	1:E:1:MET:HE2	2.42	0.55
2:B:20:GLY:HA3	2:D:19:LYS:O	2.04	0.55
1:E:166:PRO:HB3	1:E:187:PRO:CG	2.36	0.55
2:B:52:LYS:HD3	2:B:72:SER:OG	2.06	0.54
2:B:19:LYS:O	2:D:20:GLY:O	2.25	0.54
1:E:201:MET:CE	1:E:257:GLU:HG3	2.37	0.54
1:A:326:TYR:C	1:A:328:GLY:N	2.60	0.54
2:B:16:ARG:O	2:B:16:ARG:HD3	2.06	0.54
1:C:201:MET:CE	1:C:257:GLU:HG3	2.37	0.54
1:C:76:THR:HG22	2:F:40:ASP:CB	2.29	0.54
1:E:325:GLN:OE1	1:E:362:ASP:HA	2.08	0.54
2:F:2:HIS:CE1	6:F:103:BMA:O2	2.58	0.54
2:B:2:HIS:CE1	6:B:103:BMA:HO2	2.23	0.54
1:E:7:SER:HB3	1:E:316:GLN:HE22	1.73	0.54
1:E:56:LEU:HD22	1:E:213:PHE:CE2	2.37	0.54
1:A:325:GLN:OE1	1:A:362:ASP:HA	2.08	0.54
1:E:-2:PHE:CD2	1:E:1:MET:HE2	2.43	0.54
1:A:201:MET:CE	1:A:257:GLU:HG3	2.37	0.54
2:B:2:HIS:CE1	6:B:103:BMA:O2	2.58	0.54
2:B:39:MET:HG3	2:D:40:ASP:O	2.06	0.54
2:D:16:ARG:O	2:D:16:ARG:HD3	2.06	0.54
1:A:7:SER:HB3	1:A:316:GLN:HE22	1.73	0.54
1:C:326:TYR:O	1:C:328:GLY:N	2.41	0.53
5:D:104:NAG:O7	5:D:104:NAG:H1	2.07	0.53
5:F:104:NAG:O7	5:F:104:NAG:H1	2.07	0.53
1:A:326:TYR:O	1:A:328:GLY:N	2.41	0.53
1:C:37:ASN:O	1:C:38:LYS:HD2	2.09	0.53
1:E:167:GLN:O	1:E:167:GLN:HG2	2.07	0.53
1:A:37:ASN:O	1:A:38:LYS:HD2	2.09	0.53
1:C:167:GLN:O	1:C:167:GLN:HG2	2.07	0.53
1:C:7:SER:HB3	1:C:316:GLN:HE22	1.73	0.53
1:C:147:GLU:OE1	1:C:157:LYS:NZ	2.42	0.53
5:B:104:NAG:O7	5:B:104:NAG:H1	2.07	0.53
1:C:56:LEU:HD22	1:C:213:PHE:CE2	2.37	0.53
1:E:326:TYR:O	1:E:328:GLY:N	2.41	0.53
1:C:325:GLN:OE1	1:C:362:ASP:HA	2.08	0.53
2:D:2:HIS:CE1	6:D:103:BMA:O2	2.58	0.53
1:A:301:MET:O	1:A:302:CYS:C	2.47	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:GLY:HA3	2:F:65:ASP:HB2	1.86	0.53
1:A:386:GLN:O	1:A:388:LYS:HD2	2.09	0.52
1:C:108:PHE:CD1	2:F:63:ASP:CB	2.91	0.52
1:E:37:ASN:O	1:E:38:LYS:HD2	2.09	0.52
2:B:31:VAL:O	5:B:104:NAG:H3	2.10	0.52
1:C:109:GLY:HA3	1:E:244:HIS:NE2	2.23	0.52
2:D:31:VAL:O	5:D:104:NAG:H3	2.10	0.52
2:D:60:GLU:HG3	2:D:61:PRO:HD2	1.92	0.52
1:C:301:MET:O	1:C:302:CYS:C	2.47	0.52
2:D:31:VAL:HG21	5:D:105:NAG:O3	2.10	0.52
1:E:148:GLU:OE2	1:E:323:ARG:NH1	2.43	0.52
1:E:386:GLN:O	1:E:388:LYS:HD2	2.09	0.52
2:F:31:VAL:O	5:F:104:NAG:H3	2.10	0.52
2:B:31:VAL:HG21	5:B:105:NAG:O3	2.10	0.52
2:B:60:GLU:HG3	2:B:61:PRO:HD2	1.91	0.52
1:C:323:ARG:HG3	1:C:366:ASN:OD1	2.10	0.52
1:A:130:VAL:O	1:A:193:PHE:HB3	2.10	0.52
1:A:148:GLU:OE2	1:A:323:ARG:NH1	2.43	0.52
1:C:18:GLY:O	1:C:288:ARG:NH2	2.43	0.52
1:E:188:ARG:HD3	1:E:284:LYS:CD	2.17	0.52
1:E:272:MET:HB2	1:E:276:ASN:O	2.10	0.52
5:D:104:NAG:O4	5:D:105:NAG:H5	2.10	0.52
1:A:272:MET:HB2	1:A:276:ASN:O	2.10	0.51
2:F:34:CYS:HA	2:F:68:CYS:HA	1.92	0.51
1:A:-3:TYR:HE1	1:A:366:ASN:HD21	1.59	0.51
1:C:107:LEU:HD11	1:E:247:LYS:HG3	1.88	0.51
1:C:357:ILE:HG22	1:C:358:VAL:N	2.25	0.51
2:D:49:ILE:HG13	2:D:49:ILE:O	2.10	0.51
2:F:31:VAL:HG21	5:F:105:NAG:O3	2.10	0.51
1:C:130:VAL:O	1:C:193:PHE:HB3	2.10	0.51
1:E:301:MET:O	1:E:302:CYS:C	2.47	0.51
1:E:357:ILE:HG22	1:E:358:VAL:N	2.25	0.51
1:A:67:ASN:HD22	5:A:401:NAG:C7	2.24	0.51
1:C:67:ASN:HD22	5:C:401:NAG:C7	2.24	0.51
2:D:49:ILE:HD11	2:D:77:TYR:CZ	2.46	0.51
1:E:340:MET:CE	1:E:379:ILE:HG13	2.41	0.51
5:E:401:NAG:O3	5:F:101:NAG:C1	2.59	0.51
1:A:340:MET:CE	1:A:379:ILE:HG13	2.41	0.51
2:B:49:ILE:HG13	2:B:49:ILE:O	2.10	0.51
5:F:104:NAG:O4	5:F:105:NAG:H5	2.10	0.51
1:A:18:GLY:O	1:A:288:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:401:NAG:H62	5:B:101:NAG:C7	2.41	0.51
1:C:148:GLU:OE2	1:C:323:ARG:NH1	2.43	0.51
1:C:340:MET:CE	1:C:379:ILE:HG13	2.41	0.51
1:C:382:VAL:O	1:C:384:PRO:HD2	2.11	0.51
1:C:386:GLN:O	1:C:388:LYS:HD2	2.10	0.51
2:F:2:HIS:CE1	6:F:103:BMA:HO2	2.29	0.51
2:F:49:ILE:O	2:F:49:ILE:HG13	2.10	0.51
2:F:49:ILE:HD11	2:F:77:TYR:CZ	2.46	0.51
2:F:60:GLU:HG3	2:F:61:PRO:HD2	1.92	0.51
5:A:401:NAG:O3	5:B:101:NAG:C1	2.59	0.51
5:B:104:NAG:O4	5:B:105:NAG:H5	2.10	0.51
1:E:130:VAL:O	1:E:193:PHE:HB3	2.10	0.51
1:A:186:SER:C	1:A:188:ARG:H	2.14	0.51
1:C:201:MET:HE1	1:C:257:GLU:HA	1.93	0.51
1:E:67:ASN:HD22	5:E:401:NAG:C7	2.24	0.51
1:A:323:ARG:HG3	1:A:366:ASN:OD1	2.10	0.51
1:A:357:ILE:HG22	1:A:358:VAL:N	2.25	0.51
2:B:34:CYS:HA	2:B:68:CYS:HA	1.92	0.51
2:D:34:CYS:HA	2:D:68:CYS:HA	1.92	0.51
2:F:18:GLU:O	2:F:21:LYS:HG2	2.11	0.51
4:J:71:ALA:N	4:J:72:PRO:HD2	2.26	0.51
1:A:2:ARG:HG3	1:A:2:ARG:HH11	1.76	0.50
1:C:2:ARG:HH11	1:C:2:ARG:HG3	1.76	0.50
1:E:323:ARG:HG3	1:E:366:ASN:OD1	2.10	0.50
2:B:18:GLU:O	2:B:21:LYS:HG2	2.11	0.50
2:B:37:MET:O	2:D:19:LYS:HD2	2.11	0.50
1:C:-3:TYR:HE1	1:C:366:ASN:HD21	1.59	0.50
1:C:272:MET:HB2	1:C:276:ASN:O	2.10	0.50
1:E:186:SER:C	1:E:188:ARG:H	2.14	0.50
1:C:186:SER:C	1:C:188:ARG:H	2.14	0.50
1:E:382:VAL:O	1:E:384:PRO:HD2	2.11	0.50
1:A:89:ARG:HG2	1:A:229:SER:HB3	1.94	0.50
5:C:401:NAG:H62	5:D:101:NAG:C7	2.41	0.50
2:D:18:GLU:O	2:D:21:LYS:HG2	2.11	0.50
5:E:401:NAG:H62	5:F:101:NAG:C7	2.41	0.50
4:L:71:ALA:N	4:L:72:PRO:HD2	2.26	0.50
1:A:382:VAL:O	1:A:384:PRO:HD2	2.11	0.50
2:B:49:ILE:HD11	2:B:77:TYR:CZ	2.46	0.50
1:E:201:MET:HE1	1:E:257:GLU:HA	1.93	0.50
4:H:71:ALA:N	4:H:72:PRO:HD2	2.26	0.50
5:C:401:NAG:O3	5:D:101:NAG:C1	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:57:ARG:HG3	2:D:57:ARG:NH1	2.26	0.50
1:E:89:ARG:HG2	1:E:229:SER:HB3	1.94	0.50
1:E:147:GLU:OE1	1:E:157:LYS:NZ	2.42	0.50
4:H:41:GLY:O	4:H:44:LEU:N	2.45	0.50
2:B:39:MET:HB2	2:D:40:ASP:HA	1.92	0.49
2:B:39:MET:HB3	2:D:40:ASP:N	2.24	0.49
1:A:201:MET:HE1	1:A:257:GLU:HA	1.93	0.49
1:E:-3:TYR:HE1	1:E:366:ASN:HD21	1.59	0.49
2:F:57:ARG:HG3	2:F:57:ARG:NH1	2.26	0.49
1:C:237:LEU:O	1:C:252:VAL:HG23	2.13	0.49
1:E:237:LEU:O	1:E:252:VAL:HG23	2.13	0.49
1:E:26:GLU:OE2	1:E:282:HIS:CD2	2.66	0.49
2:F:69:ASN:CG	5:F:104:NAG:HO1	2.14	0.49
4:J:41:GLY:O	4:J:44:LEU:N	2.45	0.49
1:A:147:GLU:OE1	1:A:157:LYS:NZ	2.42	0.49
1:E:2:ARG:HG3	1:E:2:ARG:HH11	1.76	0.49
4:L:41:GLY:O	4:L:44:LEU:N	2.45	0.49
1:A:382:VAL:O	1:A:384:PRO:CD	2.61	0.49
1:C:149:HIS:O	1:C:150:ALA:HB2	2.13	0.49
1:E:18:GLY:O	1:E:288:ARG:NH2	2.43	0.49
1:E:382:VAL:O	1:E:384:PRO:CD	2.61	0.49
1:A:26:GLU:OE2	1:A:282:HIS:CD2	2.66	0.49
1:C:26:GLU:OE2	1:C:282:HIS:CD2	2.66	0.49
2:D:69:ASN:CG	5:D:104:NAG:HO1	2.16	0.49
1:C:89:ARG:HG2	1:C:229:SER:HB3	1.94	0.49
1:C:101:TRP:CZ2	2:F:63:ASP:N	2.80	0.49
1:C:324:VAL:HG11	1:C:380:ILE:HD13	1.95	0.49
1:A:172:GLU:OE2	1:A:182:THR:HB	2.13	0.49
2:B:57:ARG:HG3	2:B:57:ARG:NH1	2.26	0.49
1:E:172:GLU:OE2	1:E:182:THR:HB	2.13	0.49
3:I:482:GLY:C	3:I:484:ILE:N	2.66	0.49
1:A:357:ILE:CG2	1:A:358:VAL:N	2.76	0.48
2:B:69:ASN:CG	5:B:104:NAG:HO1	2.14	0.48
1:E:357:ILE:CG2	1:E:358:VAL:N	2.76	0.48
3:G:482:GLY:C	3:G:484:ILE:N	2.66	0.48
1:A:148:GLU:OE1	1:A:364:PRO:HB2	2.14	0.48
1:C:382:VAL:O	1:C:384:PRO:CD	2.61	0.48
1:A:324:VAL:HG11	1:A:380:ILE:HD13	1.95	0.48
1:C:172:GLU:OE2	1:C:182:THR:HB	2.13	0.48
1:E:20:TRP:NE1	1:E:288:ARG:NH1	2.62	0.48
1:A:20:TRP:NE1	1:A:288:ARG:NH1	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:HIS:O	1:A:150:ALA:HB2	2.13	0.48
2:B:20:GLY:N	2:D:19:LYS:O	2.46	0.48
3:K:482:GLY:C	3:K:484:ILE:N	2.66	0.48
1:A:2:ARG:O	1:A:6:MET:HG3	2.14	0.48
1:A:237:LEU:O	1:A:252:VAL:HG23	2.12	0.48
1:C:148:GLU:OE1	1:C:364:PRO:HB2	2.14	0.48
1:C:149:HIS:O	1:C:150:ALA:HB3	2.14	0.48
1:E:165:THR:HG22	1:E:167:GLN:H	1.79	0.48
1:C:107:LEU:CD2	1:E:247:LYS:HD3	2.41	0.48
1:C:2:ARG:O	1:C:6:MET:HG3	2.14	0.48
1:C:301:MET:HG3	1:C:336:PRO:HG3	1.96	0.48
1:A:-3:TYR:CE2	1:A:1:MET:HE1	2.48	0.47
2:B:37:MET:O	2:D:19:LYS:CD	2.62	0.47
1:C:165:THR:HG22	1:C:167:GLN:H	1.79	0.47
1:A:15:VAL:HG22	1:A:15:VAL:O	2.14	0.47
1:C:15:VAL:HG22	1:C:15:VAL:O	2.14	0.47
1:C:357:ILE:CG2	1:C:358:VAL:N	2.76	0.47
1:A:67:ASN:ND2	5:A:401:NAG:C7	2.77	0.47
1:A:165:THR:HG22	1:A:167:GLN:H	1.79	0.47
1:C:76:THR:CG2	2:F:40:ASP:OD2	2.58	0.47
1:E:324:VAL:HG11	1:E:380:ILE:HD13	1.95	0.47
1:C:172:GLU:OE2	1:C:172:GLU:HA	2.14	0.47
1:E:15:VAL:O	1:E:15:VAL:HG22	2.14	0.47
1:C:350:ARG:HD2	1:C:370:GLU:OE1	2.15	0.47
2:D:24:LEU:HD23	2:D:33:MET:HA	1.97	0.47
1:E:2:ARG:O	1:E:6:MET:HG3	2.14	0.47
1:E:149:HIS:O	1:E:150:ALA:HB3	2.14	0.47
1:A:172:GLU:OE2	1:A:172:GLU:HA	2.14	0.47
1:E:67:ASN:ND2	5:E:401:NAG:C7	2.77	0.47
1:E:148:GLU:OE1	1:E:364:PRO:HB2	2.13	0.47
1:E:350:ARG:HD2	1:E:370:GLU:OE1	2.15	0.47
1:A:188:ARG:HD3	1:A:284:LYS:CD	2.17	0.47
1:A:210:ARG:C	1:A:212:TRP:H	2.18	0.47
1:A:301:MET:HG3	1:A:336:PRO:HG3	1.96	0.47
2:B:19:LYS:CD	2:D:20:GLY:CA	2.77	0.47
1:C:20:TRP:NE1	1:C:288:ARG:NH1	2.62	0.47
1:E:379:ILE:HG21	1:E:386:GLN:NE2	2.30	0.47
2:B:24:LEU:HD23	2:B:33:MET:HA	1.97	0.47
1:C:74:CYS:SG	2:F:39:MET:SD	3.12	0.47
1:C:218:LEU:HD11	1:C:260:MET:CE	2.45	0.47
1:E:172:GLU:OE2	1:E:172:GLU:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:301:MET:HG3	1:E:336:PRO:HG3	1.96	0.47
1:A:379:ILE:HG21	1:A:386:GLN:NE2	2.30	0.46
1:C:74:CYS:SG	2:F:39:MET:CG	3.01	0.46
1:C:379:ILE:HG21	1:C:386:GLN:NE2	2.30	0.46
1:A:350:ARG:HD2	1:A:370:GLU:OE1	2.15	0.46
1:C:67:ASN:ND2	5:C:401:NAG:C7	2.77	0.46
1:E:41:LEU:CD2	1:E:292:LEU:HD11	2.43	0.46
1:E:210:ARG:C	1:E:212:TRP:H	2.18	0.46
1:A:218:LEU:HD11	1:A:260:MET:CE	2.45	0.46
1:A:59:TYR:CE1	1:A:220:TRP:HB3	2.50	0.46
1:E:59:TYR:CE1	1:E:220:TRP:HB3	2.50	0.46
1:E:149:HIS:O	1:E:150:ALA:HB2	2.13	0.46
1:E:67:ASN:HD22	5:E:401:NAG:C8	2.29	0.46
1:A:133:GLU:HA	1:A:166:PRO:HG2	1.98	0.46
1:A:261:HIS:C	1:A:263:ALA:H	2.19	0.46
1:C:374:GLY:O	1:C:392:PHE:HA	2.16	0.46
1:E:232:ILE:O	1:E:233:GLN:HG2	2.16	0.46
1:A:232:ILE:O	1:A:233:GLN:HG2	2.16	0.46
1:A:374:GLY:O	1:A:392:PHE:HA	2.16	0.46
1:C:133:GLU:HA	1:C:166:PRO:HG2	1.98	0.46
1:C:67:ASN:HD22	5:C:401:NAG:C8	2.29	0.46
1:C:210:ARG:C	1:C:212:TRP:H	2.18	0.45
1:E:-2:PHE:HZ	1:E:4:ILE:HD12	1.82	0.45
2:F:24:LEU:HD23	2:F:33:MET:HA	1.97	0.45
1:C:41:LEU:CD2	1:C:292:LEU:HD11	2.43	0.45
1:C:106:GLY:O	2:F:65:ASP:N	2.49	0.45
1:C:261:HIS:C	1:C:263:ALA:H	2.19	0.45
1:A:359:THR:HG22	1:A:360:GLU:HG3	1.99	0.45
1:C:-2:PHE:CD2	1:C:1:MET:CE	2.99	0.45
1:E:374:GLY:O	1:E:392:PHE:HA	2.16	0.45
1:C:259:ALA:O	1:C:263:ALA:HB2	2.17	0.45
1:E:218:LEU:HD11	1:E:260:MET:CE	2.45	0.45
5:F:105:NAG:H83	5:F:105:NAG:O1	2.17	0.45
1:C:210:ARG:O	1:C:211:GLN:HB2	2.17	0.45
1:C:359:THR:HG22	1:C:360:GLU:HG3	1.99	0.45
1:E:259:ALA:O	1:E:263:ALA:HB2	2.17	0.45
1:A:-2:PHE:CD2	1:A:1:MET:CE	2.99	0.45
2:B:40:ASP:CB	2:D:39:MET:CG	2.92	0.45
5:B:105:NAG:H83	5:B:105:NAG:O1	2.17	0.45
1:C:232:ILE:O	1:C:233:GLN:HG2	2.16	0.45
5:D:105:NAG:H83	5:D:105:NAG:O1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:-2:PHE:CD2	1:E:1:MET:CE	2.99	0.45
1:E:83:ASN:HD22	1:E:83:ASN:H	1.49	0.45
1:E:210:ARG:O	1:E:211:GLN:HB2	2.17	0.45
1:A:67:ASN:HD22	5:A:401:NAG:C8	2.29	0.45
1:A:259:ALA:O	1:A:263:ALA:HB2	2.17	0.45
1:C:235:GLU:H	1:C:235:GLU:CD	2.19	0.45
1:E:133:GLU:HA	1:E:166:PRO:HG2	1.98	0.45
1:E:261:HIS:C	1:E:263:ALA:H	2.19	0.45
2:B:79:THR:CB	2:D:39:MET:HE2	2.47	0.44
1:C:-2:PHE:HZ	1:C:4:ILE:HD12	1.82	0.44
1:A:-2:PHE:HZ	1:A:4:ILE:HD12	1.82	0.44
1:A:149:HIS:O	1:A:150:ALA:HB3	2.14	0.44
1:C:107:LEU:HD22	1:E:244:HIS:CB	2.48	0.44
1:A:99:ARG:HE	1:A:103:ASN:HD22	1.62	0.44
1:C:59:TYR:CE1	1:C:220:TRP:HB3	2.50	0.44
1:E:235:GLU:CD	1:E:235:GLU:H	2.19	0.44
2:F:69:ASN:ND2	5:F:104:NAG:O1	2.51	0.44
1:A:235:GLU:H	1:A:235:GLU:CD	2.19	0.44
1:E:359:THR:HG22	1:E:360:GLU:HG3	1.99	0.44
1:C:218:LEU:CD1	1:C:260:MET:HE1	2.48	0.44
2:D:69:ASN:ND2	5:D:104:NAG:O1	2.51	0.44
2:B:69:ASN:ND2	5:B:104:NAG:O1	2.51	0.44
1:E:323:ARG:HD3	1:E:364:PRO:HB3	1.99	0.44
2:B:40:ASP:CB	2:D:39:MET:SD	2.88	0.44
1:C:76:THR:HG1	1:E:249:ASP:CG	2.20	0.44
1:C:101:TRP:CZ2	2:F:62:GLU:O	2.70	0.44
1:C:101:TRP:CE2	2:F:63:ASP:N	2.86	0.44
1:A:210:ARG:O	1:A:211:GLN:HB2	2.17	0.44
1:A:260:MET:O	1:A:263:ALA:HB3	2.18	0.44
2:B:37:MET:C	2:D:19:LYS:CD	2.86	0.44
1:C:323:ARG:HD3	1:C:364:PRO:HB3	1.99	0.44
1:E:260:MET:O	1:E:263:ALA:HB3	2.18	0.44
1:A:232:ILE:O	1:A:233:GLN:CG	2.66	0.43
1:C:85:GLU:OE1	1:C:94:HIS:NE2	2.47	0.43
2:D:57:ARG:C	2:D:58:GLN:HG2	2.38	0.43
1:E:99:ARG:HE	1:E:103:ASN:HD22	1.62	0.43
1:E:363:SER:O	1:E:365:VAL:HG23	2.18	0.43
1:A:64:LYS:HG2	1:A:65:LEU:N	2.34	0.43
1:A:363:SER:O	1:A:365:VAL:HG23	2.19	0.43
1:C:133:GLU:HA	1:C:166:PRO:CG	2.48	0.43
1:C:232:ILE:O	1:C:233:GLN:CG	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:MET:O	1:C:263:ALA:HB3	2.18	0.43
1:E:64:LYS:HG2	1:E:65:LEU:N	2.33	0.43
1:E:162:ILE:O	1:E:162:ILE:HG13	2.18	0.43
2:F:29:ASP:OD1	2:F:29:ASP:N	2.51	0.43
1:A:102:GLY:HA3	2:B:62:GLU:HB3	2.01	0.43
1:A:392:PHE:CE2	1:A:394:LYS:HB2	2.54	0.43
1:C:64:LYS:HG2	1:C:65:LEU:N	2.33	0.43
1:C:392:PHE:CE2	1:C:394:LYS:HB2	2.54	0.43
1:E:187:PRO:O	1:E:188:ARG:C	2.56	0.43
1:E:392:PHE:CE2	1:E:394:LYS:HB2	2.54	0.43
1:A:162:ILE:O	1:A:162:ILE:HG13	2.18	0.43
1:C:363:SER:O	1:C:365:VAL:HG23	2.18	0.43
2:D:73:THR:HG22	2:D:74:TRP:O	2.18	0.43
1:E:56:LEU:CD2	1:E:57:ARG:HB2	2.47	0.43
1:C:187:PRO:O	1:C:188:ARG:C	2.56	0.43
1:E:133:GLU:HA	1:E:166:PRO:CG	2.48	0.43
1:A:323:ARG:HD3	1:A:364:PRO:HB3	1.99	0.43
1:C:56:LEU:CD2	1:C:57:ARG:HB2	2.47	0.43
2:B:29:ASP:OD1	2:B:29:ASP:N	2.51	0.43
2:F:57:ARG:C	2:F:58:GLN:HG2	2.38	0.43
1:A:133:GLU:HA	1:A:166:PRO:CG	2.48	0.43
1:A:303:THR:O	1:A:329:ASP:HB3	2.19	0.43
2:B:79:THR:CB	2:D:39:MET:CE	2.97	0.43
1:C:162:ILE:O	1:C:162:ILE:HG13	2.18	0.43
1:E:16:SER:HB3	1:E:19:SER:HB3	2.01	0.43
2:F:73:THR:HG22	2:F:74:TRP:O	2.18	0.43
1:A:85:GLU:OE1	1:A:94:HIS:NE2	2.47	0.43
1:C:107:LEU:CD1	1:E:247:LYS:CD	2.48	0.43
2:B:57:ARG:C	2:B:58:GLN:HG2	2.38	0.42
2:B:73:THR:HG22	2:B:74:TRP:O	2.18	0.42
1:E:85:GLU:OE1	1:E:94:HIS:NE2	2.47	0.42
1:A:41:LEU:CD2	1:A:292:LEU:HD11	2.43	0.42
1:C:137:TYR:N	1:C:137:TYR:CD1	2.87	0.42
2:D:29:ASP:OD1	2:D:29:ASP:N	2.51	0.42
1:E:16:SER:HB3	1:E:19:SER:CB	2.49	0.42
1:E:137:TYR:N	1:E:137:TYR:CD1	2.87	0.42
1:A:355:ASN:N	1:A:356:PRO:CD	2.82	0.42
3:I:466:ILE:O	3:I:470:THR:N	2.37	0.42
4:L:58:SER:O	4:L:61:VAL:N	2.52	0.42
1:A:187:PRO:O	1:A:188:ARG:C	2.56	0.42
1:E:73:ARG:NE	1:E:80:PRO:HA	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:GLY:HA3	2:F:62:GLU:HB3	2.01	0.42
1:E:232:ILE:O	1:E:233:GLN:CG	2.66	0.42
4:H:57:THR:O	4:H:61:VAL:HG23	2.20	0.42
4:J:57:THR:O	4:J:61:VAL:HG23	2.19	0.42
3:K:466:ILE:O	3:K:470:THR:N	2.37	0.42
1:A:58:LYS:O	1:A:220:TRP:HA	2.19	0.42
1:C:16:SER:HB3	1:C:19:SER:CB	2.49	0.42
1:C:355:ASN:N	1:C:356:PRO:CD	2.82	0.42
1:E:355:ASN:N	1:E:356:PRO:CD	2.82	0.42
1:A:137:TYR:CD1	1:A:137:TYR:N	2.87	0.42
2:B:16:ARG:HG3	2:B:43:GLU:OE2	2.20	0.42
4:H:71:ALA:HB3	4:H:72:PRO:HD3	2.02	0.42
1:A:135:LEU:HD23	1:A:135:LEU:HA	1.84	0.42
1:C:58:LYS:O	1:C:220:TRP:HA	2.19	0.42
1:E:58:LYS:O	1:E:220:TRP:HA	2.19	0.42
1:E:203:ASN:HD22	1:E:203:ASN:HA	1.65	0.42
4:L:71:ALA:HB3	4:L:72:PRO:HD3	2.02	0.42
1:A:218:LEU:CD1	1:A:260:MET:HE1	2.50	0.42
1:C:303:THR:O	1:C:329:ASP:HB3	2.19	0.42
2:D:16:ARG:HG3	2:D:43:GLU:OE2	2.20	0.42
1:E:75:PRO:O	1:E:76:THR:CB	2.52	0.42
1:A:16:SER:HB3	1:A:19:SER:CB	2.49	0.42
1:A:64:LYS:CB	1:A:122:LYS:HE3	2.49	0.42
1:A:102:GLY:HA2	2:B:60:GLU:O	2.20	0.42
1:A:221:LEU:HG	1:A:231:TRP:CE3	2.55	0.42
1:C:99:ARG:HE	1:C:103:ASN:HD22	1.62	0.42
1:C:102:GLY:HA2	2:D:60:GLU:O	2.20	0.42
5:F:101:NAG:C4	6:F:102:BMA:C1	2.86	0.42
1:A:322:ILE:HD11	1:A:378:ILE:HD13	2.02	0.42
2:B:49:ILE:HD11	2:B:77:TYR:OH	2.20	0.42
1:C:101:TRP:NE1	2:F:64:ILE:N	2.49	0.42
1:C:135:LEU:HD23	1:C:135:LEU:HA	1.84	0.42
1:C:221:LEU:HG	1:C:231:TRP:CE3	2.55	0.42
1:E:76:THR:O	1:E:76:THR:HG23	2.20	0.42
1:E:303:THR:O	1:E:329:ASP:HB3	2.19	0.42
2:B:20:GLY:O	2:D:21:LYS:HE3	2.20	0.41
1:C:76:THR:O	1:C:76:THR:HG23	2.20	0.41
1:C:102:GLY:HA3	2:D:62:GLU:HB3	2.01	0.41
1:C:217:PRO:O	1:C:218:LEU:HD23	2.20	0.41
1:A:16:SER:HB3	1:A:19:SER:HB3	2.01	0.41
5:A:401:NAG:O3	5:B:101:NAG:O5	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:ASN:OD1	2:B:69:ASN:C	2.59	0.41
1:C:221:LEU:HD13	1:C:225:ASP:OD2	2.20	0.41
2:D:49:ILE:HD11	2:D:77:TYR:OH	2.20	0.41
1:E:221:LEU:HG	1:E:231:TRP:CE3	2.55	0.41
4:L:57:THR:O	4:L:61:VAL:HG23	2.20	0.41
1:A:27:HIS:HB2	1:A:280:THR:HG23	2.02	0.41
1:A:136:GLU:OE2	1:A:163:LYS:HD3	2.20	0.41
1:A:221:LEU:HD13	1:A:225:ASP:OD2	2.20	0.41
1:A:320:ILE:O	1:A:368:GLU:HA	2.20	0.41
1:C:16:SER:HB3	1:C:19:SER:HB3	2.01	0.41
1:C:320:ILE:O	1:C:368:GLU:HA	2.20	0.41
1:E:320:ILE:O	1:E:368:GLU:HA	2.20	0.41
4:H:69:LEU:O	4:H:72:PRO:HD2	2.21	0.41
1:A:73:ARG:NE	1:A:80:PRO:HA	2.35	0.41
1:A:217:PRO:O	1:A:218:LEU:HD23	2.20	0.41
1:A:257:GLU:HG2	1:A:261:HIS:CD2	2.56	0.41
2:B:19:LYS:HB3	2:D:20:GLY:CA	2.51	0.41
1:C:73:ARG:NE	1:C:80:PRO:HA	2.34	0.41
1:E:257:GLU:HG2	1:E:261:HIS:CD2	2.56	0.41
1:E:297:MET:O	1:E:298:SER:HB2	2.21	0.41
2:F:69:ASN:OD1	2:F:69:ASN:C	2.59	0.41
4:J:58:SER:O	4:J:61:VAL:N	2.52	0.41
1:C:64:LYS:CB	1:C:122:LYS:HE3	2.49	0.41
1:C:361:LYS:O	1:C:362:ASP:HB2	2.21	0.41
5:D:101:NAG:C4	6:D:102:BMA:C1	2.86	0.41
2:F:16:ARG:HG3	2:F:43:GLU:OE2	2.20	0.41
4:H:58:SER:O	4:H:61:VAL:N	2.52	0.41
4:J:69:LEU:O	4:J:72:PRO:HD2	2.21	0.41
1:A:361:LYS:O	1:A:362:ASP:HB2	2.21	0.41
1:C:257:GLU:HG2	1:C:261:HIS:CD2	2.56	0.41
1:C:322:ILE:HD11	1:C:378:ILE:HD13	2.02	0.41
1:E:322:ILE:HD11	1:E:378:ILE:HD13	2.02	0.41
2:B:69:ASN:CG	5:B:104:NAG:O1	2.59	0.41
1:E:217:PRO:O	1:E:218:LEU:HD23	2.20	0.41
1:E:221:LEU:HD13	1:E:225:ASP:OD2	2.21	0.41
1:A:148:GLU:OE1	1:A:364:PRO:O	2.39	0.41
2:B:19:LYS:CB	2:D:20:GLY:HA2	2.49	0.41
1:C:107:LEU:CD2	1:E:247:LYS:CG	2.89	0.41
1:C:136:GLU:OE2	1:C:163:LYS:HD3	2.20	0.41
2:D:69:ASN:OD1	2:D:69:ASN:C	2.59	0.41
1:E:102:GLY:HA2	2:F:60:GLU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:GLU:OE2	1:E:163:LYS:HD3	2.20	0.41
1:E:148:GLU:OE1	1:E:364:PRO:O	2.39	0.41
1:C:233:GLN:HA	1:C:235:GLU:OE2	2.21	0.40
1:E:233:GLN:HA	1:E:235:GLU:OE2	2.21	0.40
2:F:49:ILE:HD11	2:F:77:TYR:OH	2.20	0.40
4:J:71:ALA:HB3	4:J:72:PRO:HD3	2.02	0.40
4:L:69:LEU:O	4:L:72:PRO:HD2	2.21	0.40
1:C:148:GLU:OE1	1:C:364:PRO:O	2.39	0.40
1:C:271:GLN:HG2	1:C:272:MET:N	2.37	0.40
1:A:233:GLN:HA	1:A:235:GLU:OE2	2.21	0.40
1:C:27:HIS:HB2	1:C:280:THR:HG23	2.03	0.40
1:C:297:MET:O	1:C:298:SER:HB2	2.21	0.40
1:A:76:THR:O	1:A:76:THR:HG23	2.20	0.40
2:B:37:MET:C	2:D:19:LYS:HD3	2.41	0.40
1:C:75:PRO:O	1:C:76:THR:CB	2.52	0.40
2:B:19:LYS:O	2:D:20:GLY:HA3	2.21	0.40
1:C:101:TRP:HE1	2:F:64:ILE:C	2.18	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	A	380/402 (94%)	344 (90%)	33 (9%)	3 (1%)	19	60
1	C	380/402 (94%)	345 (91%)	32 (8%)	3 (1%)	19	60
1	E	380/402 (94%)	345 (91%)	32 (8%)	3 (1%)	19	60
2	B	79/81 (98%)	70 (89%)	9 (11%)	0	100	100
2	D	79/81 (98%)	70 (89%)	9 (11%)	0	100	100
2	F	79/81 (98%)	70 (89%)	9 (11%)	0	100	100
3	G	64/66 (97%)	50 (78%)	11 (17%)	3 (5%)	2	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	I	64/66 (97%)	50 (78%)	11 (17%)	3 (5%)	2 21
3	K	64/66 (97%)	50 (78%)	11 (17%)	3 (5%)	2 21
4	H	51/53 (96%)	47 (92%)	4 (8%)	0	100 100
4	J	51/53 (96%)	47 (92%)	4 (8%)	0	100 100
4	L	51/53 (96%)	47 (92%)	4 (8%)	0	100 100
All	All	1722/1806 (95%)	1535 (89%)	169 (10%)	18 (1%)	20 55

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	ASP
1	A	383	GLU
1	A	384	PRO
1	C	329	ASP
1	C	383	GLU
1	C	384	PRO
1	E	329	ASP
1	E	383	GLU
1	E	384	PRO
3	G	480	LYS
3	I	480	LYS
3	K	480	LYS
3	G	479	THR
3	I	479	THR
3	K	479	THR
3	G	483	SER
3	I	483	SER
3	K	483	SER

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	A	339/348 (97%)	316 (93%)	23 (7%)	16 41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	339/348 (97%)	316 (93%)	23 (7%)	16 41
1	E	339/348 (97%)	316 (93%)	23 (7%)	16 41
2	B	75/75 (100%)	65 (87%)	10 (13%)	4 18
2	D	75/75 (100%)	65 (87%)	10 (13%)	4 18
2	F	75/75 (100%)	65 (87%)	10 (13%)	4 18
3	G	16/50 (32%)	16 (100%)	0	100 100
3	I	16/50 (32%)	16 (100%)	0	100 100
3	K	16/50 (32%)	16 (100%)	0	100 100
4	H	16/43 (37%)	16 (100%)	0	100 100
4	J	16/43 (37%)	16 (100%)	0	100 100
4	L	16/43 (37%)	16 (100%)	0	100 100
All	All	1338/1548 (86%)	1239 (93%)	99 (7%)	17 38

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LYS
1	A	41	LEU
1	A	76	THR
1	A	83	ASN
1	A	84	GLU
1	A	103	ASN
1	A	120	ARG
1	A	172	GLU
1	A	182	THR
1	A	286	ARG
1	A	287	LEU
1	A	300	SER
1	A	323	ARG
1	A	326	TYR
1	A	329	ASP
1	A	331	SER
1	A	332	PRO
1	A	346	HIS
1	A	350	ARG
1	A	362	ASP
1	A	377	TYR
1	A	382	VAL

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Mol	Chain	Res	Type
1	A	388	LYS
2	B	16	ARG
2	B	17	GLN
2	B	29	ASP
2	B	36	LEU
2	B	37	MET
2	B	41	LEU
2	B	48	THR
2	B	56	LEU
2	B	58	GLN
2	B	71	THR
1	C	38	LYS
1	C	41	LEU
1	C	76	THR
1	C	83	ASN
1	C	84	GLU
1	C	103	ASN
1	C	120	ARG
1	C	172	GLU
1	C	182	THR
1	C	286	ARG
1	C	287	LEU
1	C	300	SER
1	C	323	ARG
1	C	326	TYR
1	C	329	ASP
1	C	331	SER
1	C	332	PRO
1	C	346	HIS
1	C	350	ARG
1	C	362	ASP
1	C	377	TYR
1	C	382	VAL
1	C	388	LYS
2	D	16	ARG
2	D	17	GLN
2	D	29	ASP
2	D	36	LEU
2	D	37	MET
2	D	41	LEU
2	D	48	THR
2	D	56	LEU

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Mol	Chain	Res	Type
2	D	58	GLN
2	D	71	THR
1	E	38	LYS
1	E	41	LEU
1	E	76	THR
1	E	83	ASN
1	E	84	GLU
1	E	103	ASN
1	E	120	ARG
1	E	172	GLU
1	E	182	THR
1	E	286	ARG
1	E	287	LEU
1	E	300	SER
1	E	323	ARG
1	E	326	TYR
1	E	329	ASP
1	E	331	SER
1	E	332	PRO
1	E	346	HIS
1	E	350	ARG
1	E	362	ASP
1	E	377	TYR
1	E	382	VAL
1	E	388	LYS
2	F	16	ARG
2	F	17	GLN
2	F	29	ASP
2	F	36	LEU
2	F	37	MET
2	F	41	LEU
2	F	48	THR
2	F	56	LEU
2	F	58	GLN
2	F	71	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-1	GLN
1	A	37	ASN
1	A	83	ASN

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Mol	Chain	Res	Type
1	A	103	ASN
1	A	200	GLN
1	A	203	ASN
1	A	248	GLN
1	A	261	HIS
1	A	316	GLN
1	A	366	ASN
2	B	7	ASN
2	B	17	GLN
1	C	-1	GLN
1	C	37	ASN
1	C	83	ASN
1	C	103	ASN
1	C	200	GLN
1	C	203	ASN
1	C	248	GLN
1	C	261	HIS
1	C	316	GLN
2	D	7	ASN
2	D	17	GLN
1	E	-1	GLN
1	E	37	ASN
1	E	83	ASN
1	E	103	ASN
1	E	200	GLN
1	E	203	ASN
1	E	244	HIS
1	E	248	GLN
1	E	261	HIS
1	E	316	GLN
1	E	366	ASN
2	F	7	ASN
2	F	17	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	E	401	-	14,14,15	0.53	0	17,19,21	4.73	2 (11%)
5	NAG	F	101	-	14,14,15	1.86	1 (7%)	17,19,21	1.69	4 (23%)
5	NAG	D	105	-	15,15,15	0.47	0	21,21,21	0.64	0
6	BMA	B	102	-	11,11,12	0.89	1 (9%)	15,15,17	0.89	1 (6%)
5	NAG	F	105	-	15,15,15	0.47	0	21,21,21	0.64	0
5	NAG	B	101	-	14,14,15	1.88	1 (7%)	17,19,21	1.69	4 (23%)
5	NAG	A	401	-	14,14,15	0.53	0	17,19,21	4.73	2 (11%)
5	NAG	B	104	-	15,15,15	0.40	0	21,21,21	0.78	0
5	NAG	F	104	-	15,15,15	0.41	0	21,21,21	0.78	0
6	BMA	D	103	-	11,11,12	1.10	1 (9%)	15,15,17	2.91	4 (26%)
5	NAG	D	104	-	15,15,15	0.41	0	21,21,21	0.77	0
6	BMA	F	103	-	11,11,12	1.10	1 (9%)	15,15,17	2.91	4 (26%)
6	BMA	B	103	-	11,11,12	1.10	1 (9%)	15,15,17	2.91	4 (26%)
6	BMA	F	102	-	11,11,12	0.88	1 (9%)	15,15,17	0.89	1 (6%)
6	BMA	D	102	-	11,11,12	0.87	1 (9%)	15,15,17	0.89	1 (6%)
5	NAG	C	401	-	14,14,15	0.52	0	17,19,21	4.72	2 (11%)
5	NAG	D	101	-	14,14,15	1.85	1 (7%)	17,19,21	1.69	4 (23%)
5	NAG	B	105	-	15,15,15	0.47	0	21,21,21	0.64	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	401	-	-	5/6/23/26	0/1/1/1
5	NAG	F	101	-	-	4/6/23/26	0/1/1/1
5	NAG	D	105	-	-	5/6/26/26	0/1/1/1
6	BMA	B	102	-	-	2/2/19/22	0/1/1/1
5	NAG	F	105	-	-	5/6/26/26	0/1/1/1
5	NAG	B	101	-	-	4/6/23/26	0/1/1/1
5	NAG	F	104	-	1/1/6/7	3/6/26/26	0/1/1/1
5	NAG	B	104	-	1/1/6/7	3/6/26/26	0/1/1/1
6	BMA	F	103	-	1/1/4/5	1/2/19/22	0/1/1/1
6	BMA	D	103	-	1/1/4/5	1/2/19/22	0/1/1/1
5	NAG	D	104	-	1/1/6/7	3/6/26/26	0/1/1/1
5	NAG	A	401	-	-	5/6/23/26	0/1/1/1
6	BMA	B	103	-	1/1/4/5	1/2/19/22	0/1/1/1
6	BMA	F	102	-	-	2/2/19/22	0/1/1/1
6	BMA	D	102	-	-	2/2/19/22	0/1/1/1
5	NAG	C	401	-	-	5/6/23/26	0/1/1/1
5	NAG	D	101	-	-	4/6/23/26	0/1/1/1
5	NAG	B	105	-	-	5/6/26/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	101	NAG	C2-N2	-6.58	1.35	1.46
5	F	101	NAG	C2-N2	-6.51	1.35	1.46
5	D	101	NAG	C2-N2	-6.50	1.35	1.46
6	B	103	BMA	C6-C5	-2.49	1.43	1.51
6	F	103	BMA	C6-C5	-2.49	1.43	1.51
6	D	103	BMA	C6-C5	-2.48	1.43	1.51
6	B	102	BMA	O3-C3	2.28	1.48	1.43
6	F	102	BMA	O3-C3	2.28	1.48	1.43
6	D	102	BMA	O3-C3	2.27	1.48	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	401	NAG	O4-C4-C5	17.46	152.65	109.30
5	E	401	NAG	O4-C4-C5	17.45	152.62	109.30
5	C	401	NAG	O4-C4-C5	17.43	152.57	109.30
6	F	103	BMA	C6-C5-C4	8.47	132.84	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	103	BMA	C6-C5-C4	8.46	132.81	113.00
6	B	103	BMA	C6-C5-C4	8.45	132.79	113.00
5	E	401	NAG	O4-C4-C3	-8.32	91.11	110.35
5	A	401	NAG	O4-C4-C3	-8.32	91.12	110.35
5	C	401	NAG	O4-C4-C3	-8.32	91.12	110.35
6	F	103	BMA	O5-C5-C6	5.43	115.71	107.20
6	B	103	BMA	O5-C5-C6	5.42	115.70	107.20
6	D	103	BMA	O5-C5-C6	5.40	115.67	107.20
5	F	101	NAG	C2-N2-C7	4.67	129.55	122.90
5	D	101	NAG	C2-N2-C7	4.64	129.51	122.90
5	B	101	NAG	C2-N2-C7	4.64	129.51	122.90
6	D	103	BMA	O6-C6-C5	3.74	124.13	111.29
6	F	103	BMA	O6-C6-C5	3.74	124.11	111.29
6	B	103	BMA	O6-C6-C5	3.74	124.11	111.29
5	B	101	NAG	C1-C2-N2	3.41	116.31	110.49
5	D	101	NAG	C1-C2-N2	3.41	116.31	110.49
5	F	101	NAG	C1-C2-N2	3.38	116.26	110.49
6	F	103	BMA	C1-O5-C5	2.96	116.21	112.19
6	D	103	BMA	C1-O5-C5	2.95	116.19	112.19
6	B	103	BMA	C1-O5-C5	2.93	116.16	112.19
6	D	102	BMA	O3-C3-C4	2.80	116.81	110.35
6	F	102	BMA	O3-C3-C4	2.79	116.81	110.35
6	B	102	BMA	O3-C3-C4	2.78	116.79	110.35
5	F	101	NAG	O7-C7-N2	2.70	126.92	121.95
5	B	101	NAG	O7-C7-N2	2.70	126.91	121.95
5	D	101	NAG	O7-C7-N2	2.70	126.91	121.95
5	B	101	NAG	C8-C7-N2	-2.06	112.60	116.10
5	D	101	NAG	C8-C7-N2	-2.06	112.61	116.10
5	F	101	NAG	C8-C7-N2	-2.04	112.64	116.10

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	104	NAG	C1
5	D	104	NAG	C1
5	F	104	NAG	C1
6	B	103	BMA	C5
6	D	103	BMA	C5
6	F	103	BMA	C5

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	401	NAG	C8-C7-N2-C2
5	A	401	NAG	O7-C7-N2-C2
5	B	101	NAG	C8-C7-N2-C2
5	B	101	NAG	O7-C7-N2-C2
5	B	104	NAG	C1-C2-N2-C7
5	B	105	NAG	C1-C2-N2-C7
5	B	105	NAG	C8-C7-N2-C2
5	B	105	NAG	O7-C7-N2-C2
5	C	401	NAG	C8-C7-N2-C2
5	C	401	NAG	O7-C7-N2-C2
5	D	101	NAG	C8-C7-N2-C2
5	D	101	NAG	O7-C7-N2-C2
5	D	104	NAG	C1-C2-N2-C7
5	D	105	NAG	C1-C2-N2-C7
5	D	105	NAG	C8-C7-N2-C2
5	D	105	NAG	O7-C7-N2-C2
5	E	401	NAG	C8-C7-N2-C2
5	E	401	NAG	O7-C7-N2-C2
5	F	101	NAG	C8-C7-N2-C2
5	F	101	NAG	O7-C7-N2-C2
5	F	104	NAG	C1-C2-N2-C7
5	F	105	NAG	C1-C2-N2-C7
5	F	105	NAG	C8-C7-N2-C2
5	F	105	NAG	O7-C7-N2-C2
5	B	104	NAG	C4-C5-C6-O6
5	D	104	NAG	C4-C5-C6-O6
5	F	104	NAG	C4-C5-C6-O6
5	B	104	NAG	O5-C5-C6-O6
5	D	104	NAG	O5-C5-C6-O6
5	F	104	NAG	O5-C5-C6-O6
6	B	103	BMA	O5-C5-C6-O6
6	D	103	BMA	O5-C5-C6-O6
6	F	103	BMA	O5-C5-C6-O6
5	B	105	NAG	C4-C5-C6-O6
5	D	105	NAG	C4-C5-C6-O6
5	F	105	NAG	C4-C5-C6-O6
5	B	105	NAG	O5-C5-C6-O6
5	D	105	NAG	O5-C5-C6-O6
5	F	105	NAG	O5-C5-C6-O6
5	A	401	NAG	C1-C2-N2-C7
5	C	401	NAG	C1-C2-N2-C7
5	E	401	NAG	C1-C2-N2-C7
6	B	102	BMA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	D	102	BMA	O5-C5-C6-O6
6	F	102	BMA	O5-C5-C6-O6
6	B	102	BMA	C4-C5-C6-O6
6	D	102	BMA	C4-C5-C6-O6
6	F	102	BMA	C4-C5-C6-O6
5	A	401	NAG	C4-C5-C6-O6
5	C	401	NAG	C4-C5-C6-O6
5	E	401	NAG	C4-C5-C6-O6
5	B	101	NAG	O5-C5-C6-O6
5	D	101	NAG	O5-C5-C6-O6
5	F	101	NAG	O5-C5-C6-O6
5	A	401	NAG	O5-C5-C6-O6
5	C	401	NAG	O5-C5-C6-O6
5	E	401	NAG	O5-C5-C6-O6
5	B	101	NAG	C4-C5-C6-O6
5	D	101	NAG	C4-C5-C6-O6
5	F	101	NAG	C4-C5-C6-O6

There are no ring outliers.

18 monomers are involved in 76 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	401	NAG	6	0
5	F	101	NAG	4	0
5	D	105	NAG	6	0
6	B	102	BMA	1	0
5	F	105	NAG	6	0
5	B	101	NAG	4	0
5	A	401	NAG	7	0
5	B	104	NAG	12	0
5	F	104	NAG	11	0
6	D	103	BMA	4	0
5	D	104	NAG	11	0
6	F	103	BMA	4	0
6	B	103	BMA	4	0
6	F	102	BMA	2	0
6	D	102	BMA	2	0
5	C	401	NAG	6	0
5	D	101	NAG	4	0
5	B	105	NAG	6	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2
2	D	2
2	F	2
1	A	2
1	C	2
1	E	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	49:ILE	C	50:THR	N	1.17
1	D	49:ILE	C	50:THR	N	1.17
1	F	49:ILE	C	50:THR	N	1.17
1	B	48:THR	C	49:ILE	N	1.12
1	D	48:THR	C	49:ILE	N	1.12
1	F	48:THR	C	49:ILE	N	1.12
1	A	335:ILE	C	336:PRO	N	1.05
1	C	335:ILE	C	336:PRO	N	1.05
1	E	335:ILE	C	336:PRO	N	1.05
1	A	334:LYS	C	335:ILE	N	1.02
1	C	334:LYS	C	335:ILE	N	1.02
1	E	334:LYS	C	335:ILE	N	1.02

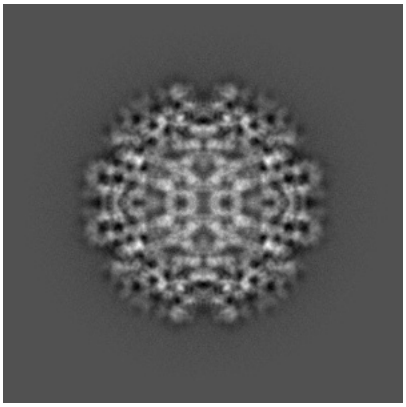
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8508. These allow visual inspection of the internal detail of the map and identification of artifacts.

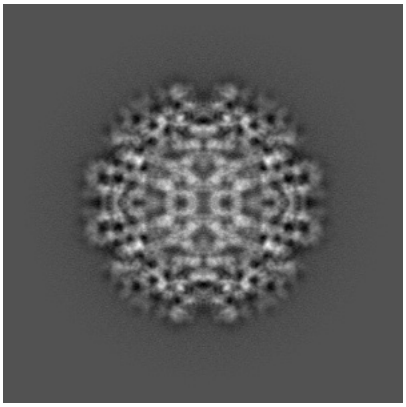
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

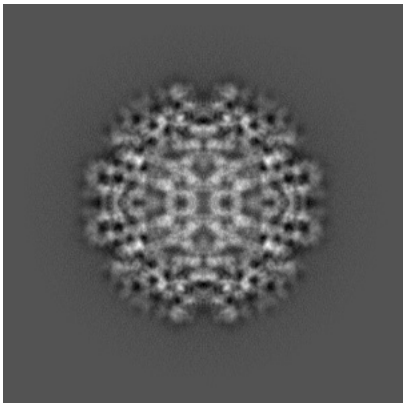
6.1.1 Primary map



X



Y

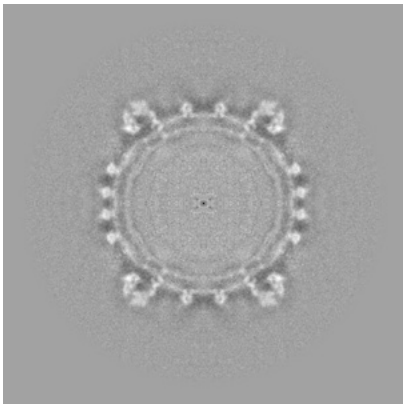


Z

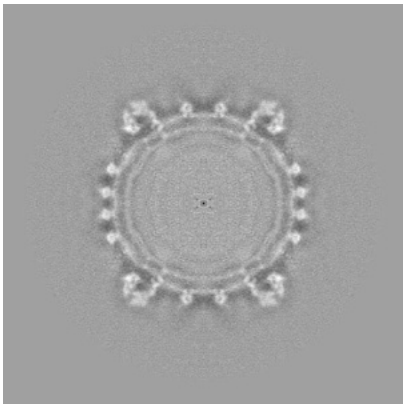
The images above show the map projected in three orthogonal directions.

6.2 Central slices

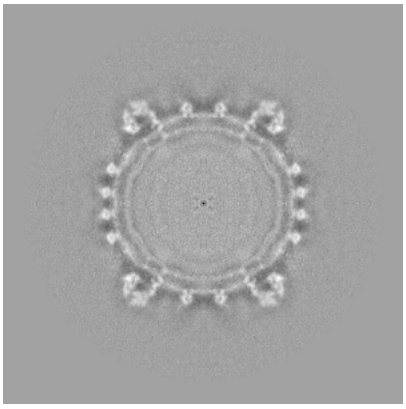
6.2.1 Primary map



X Index: 168



Y Index: 168

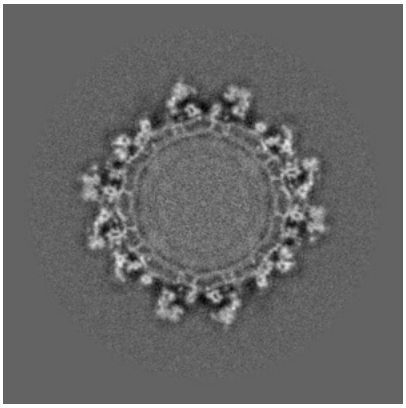


Z Index: 168

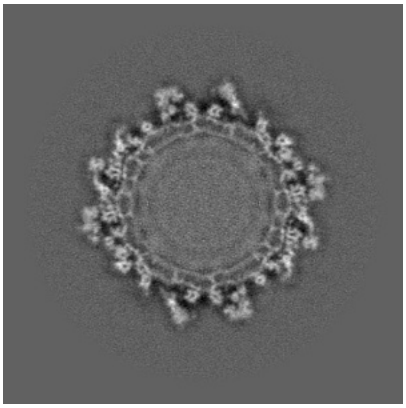
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

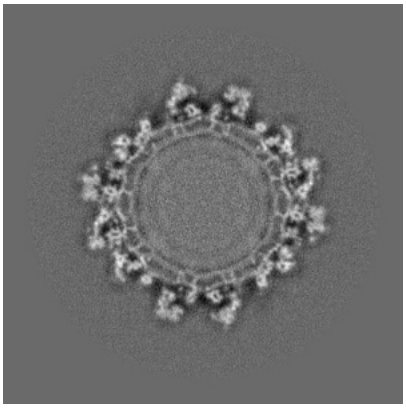
6.3.1 Primary map



X Index: 188



Y Index: 149

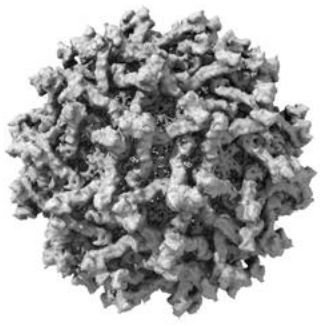


Z Index: 188

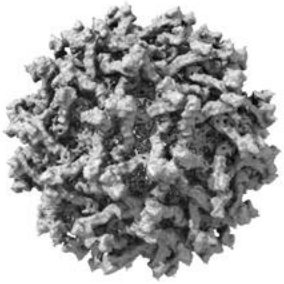
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

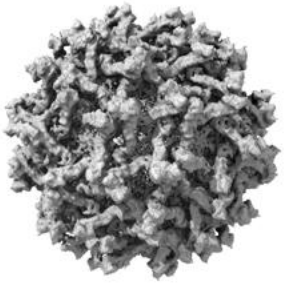
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

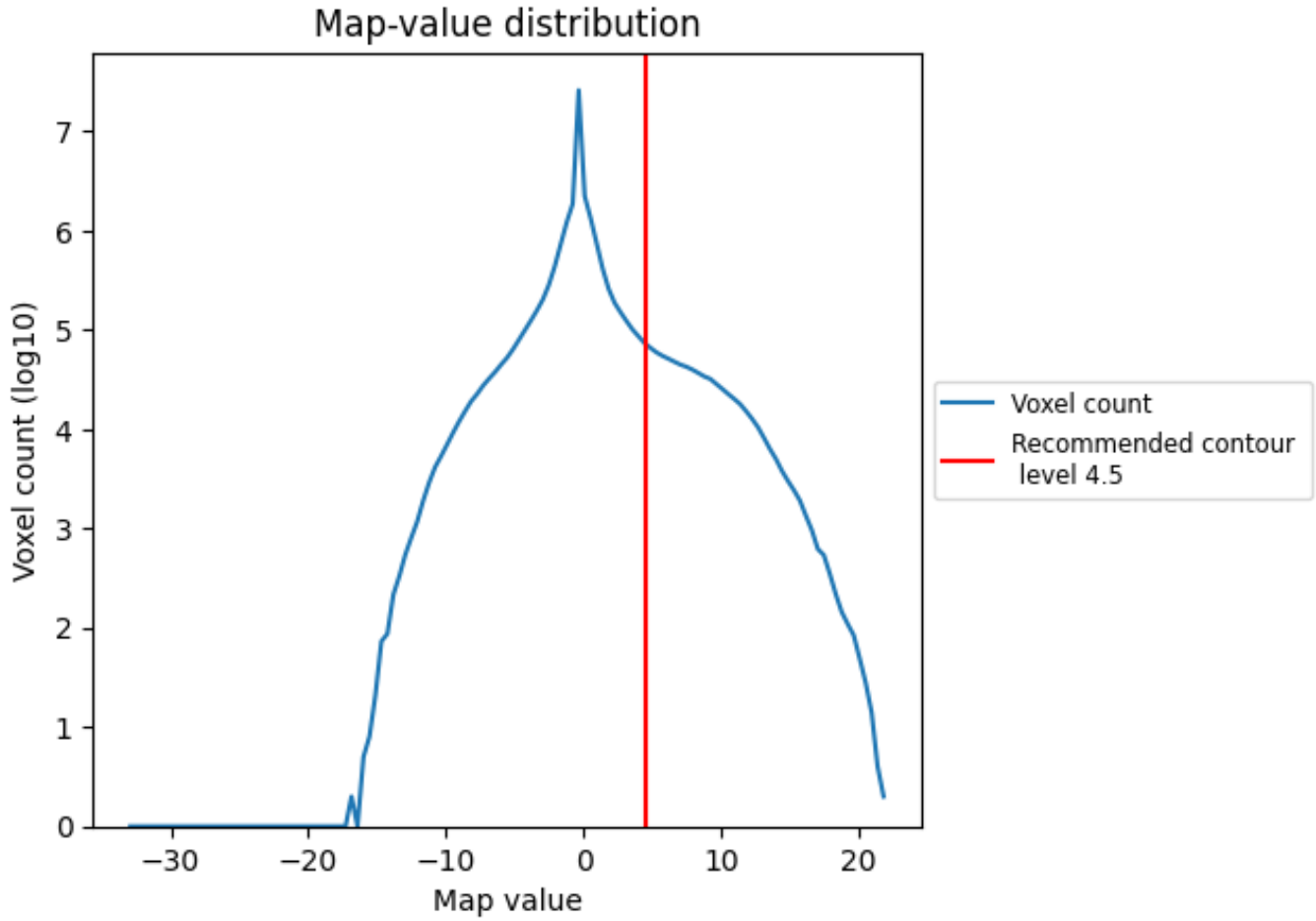
6.5 Mask visualisation (i)

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

7 Map analysis

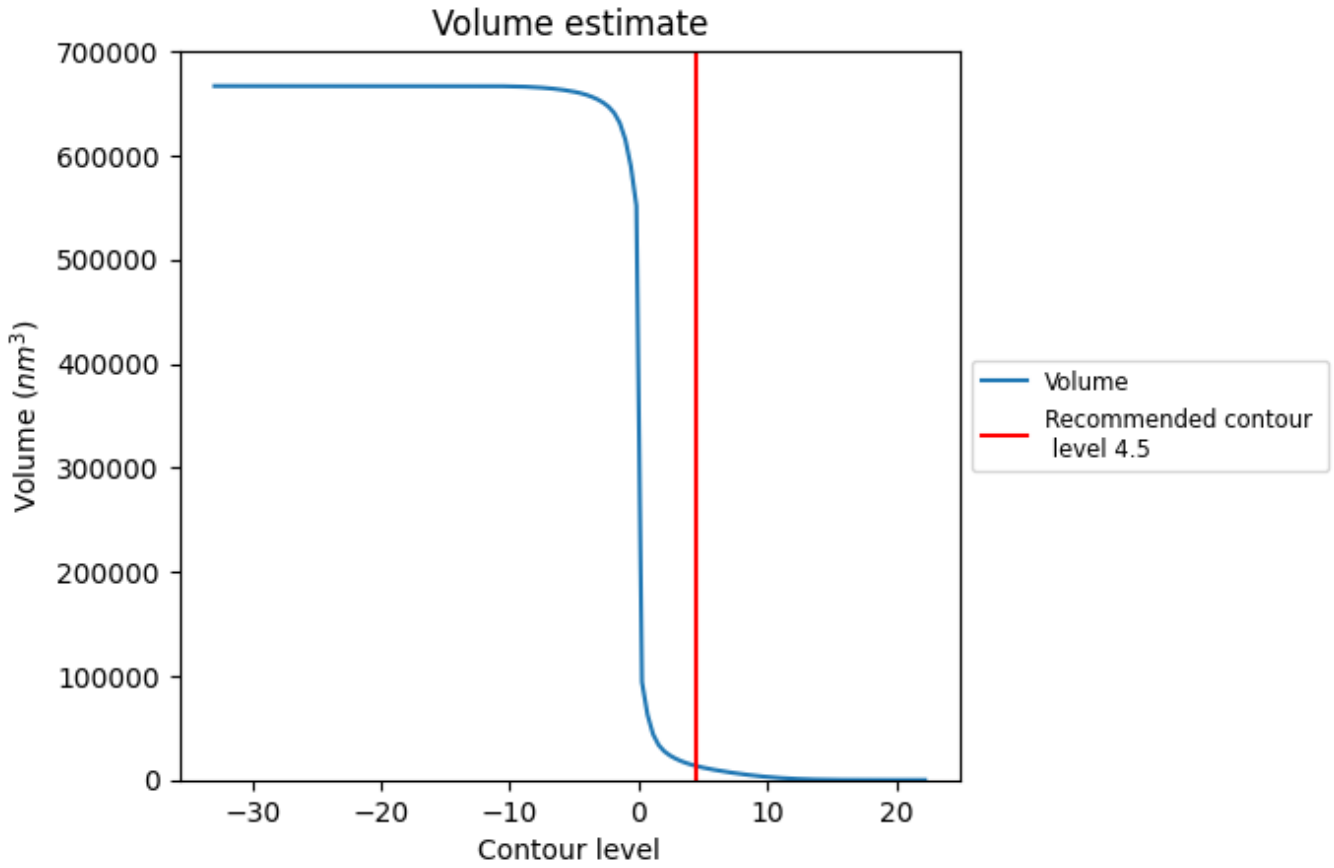
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

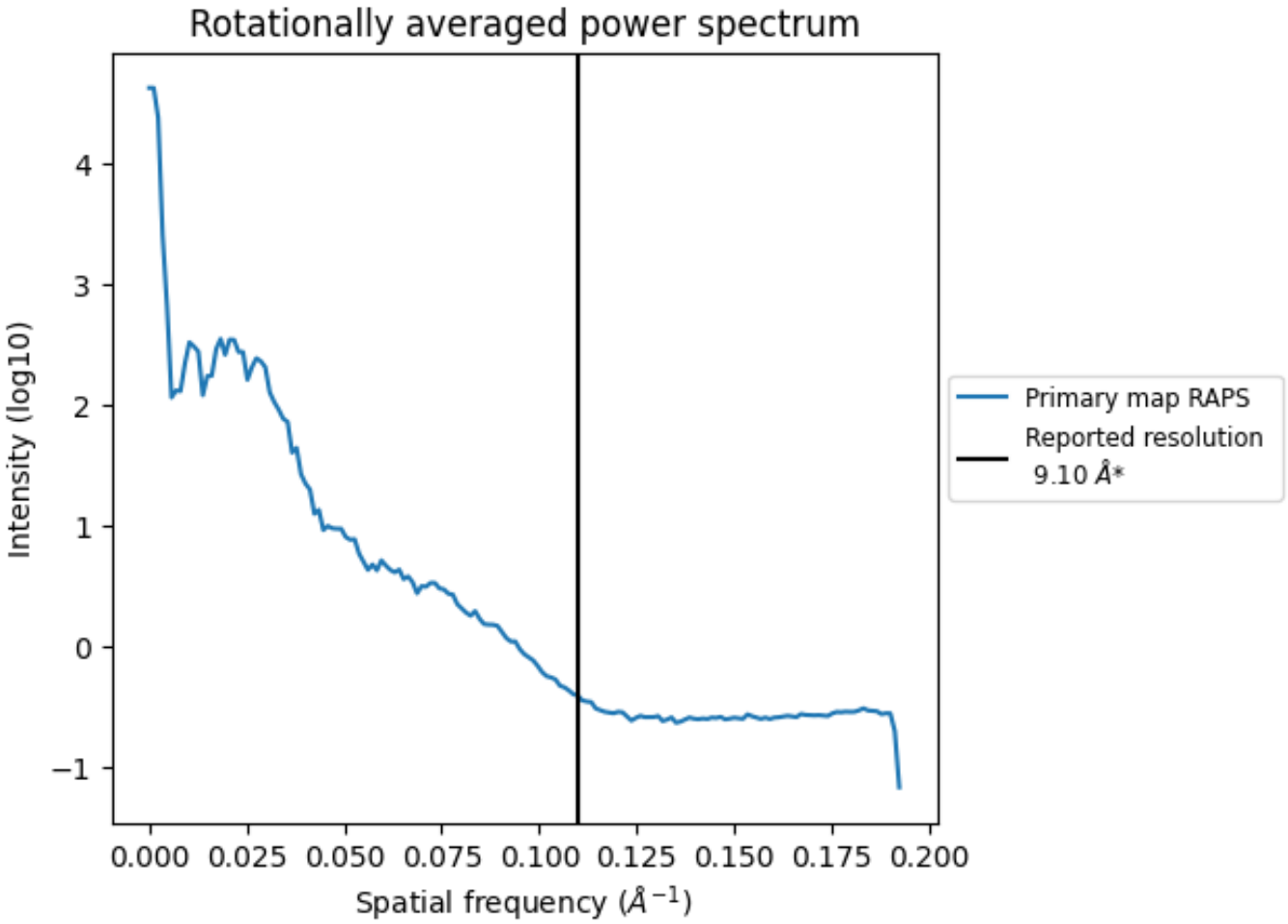
7.2 Volume estimate



The volume at the recommended contour level is 13362 nm^3; this corresponds to an approximate mass of 12070 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)

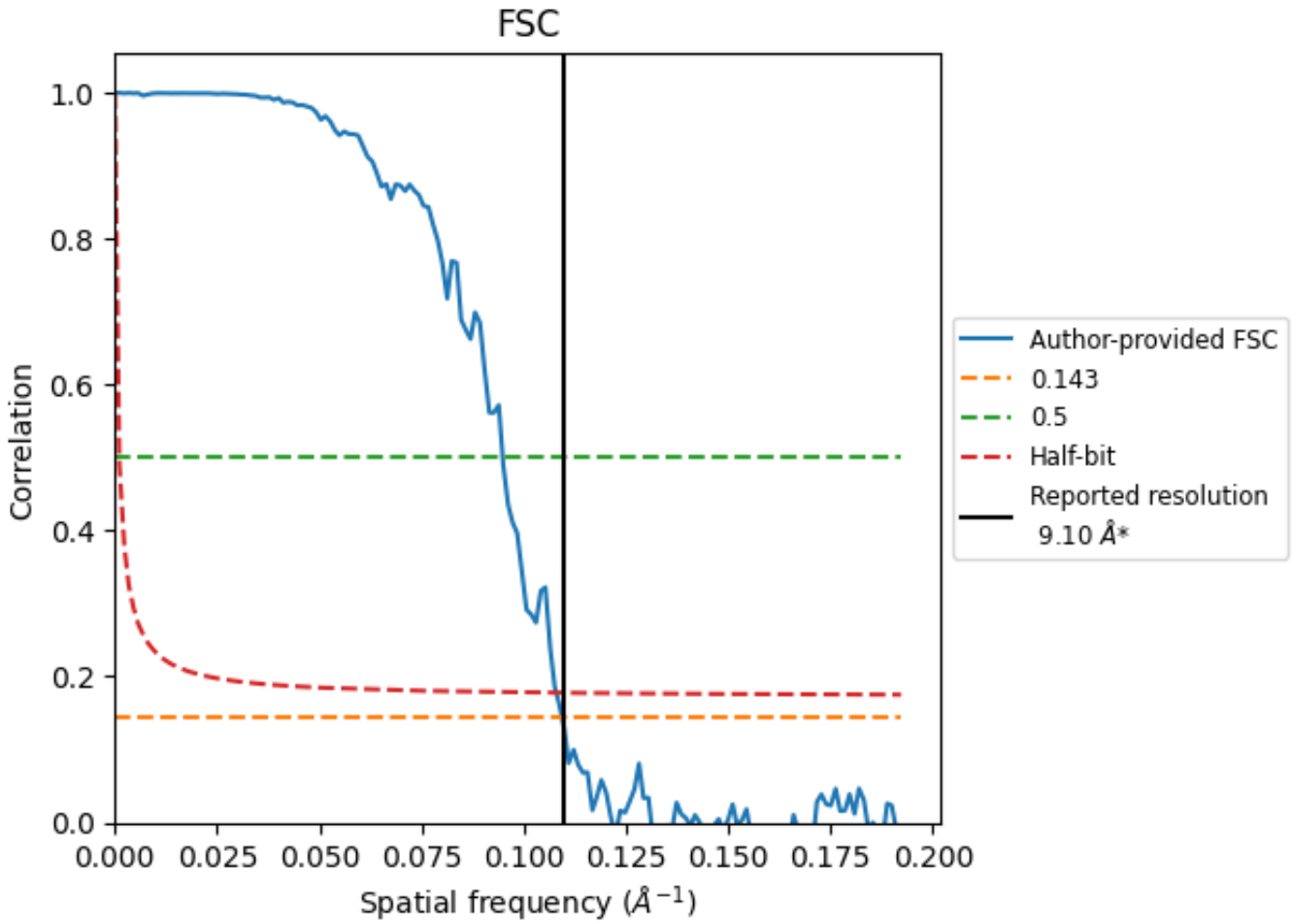


*Reported resolution corresponds to spatial frequency of 0.110 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.110 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.10	-	-
Author-provided FSC curve	9.14	10.54	9.26
Unmasked-calculated*	-	-	-

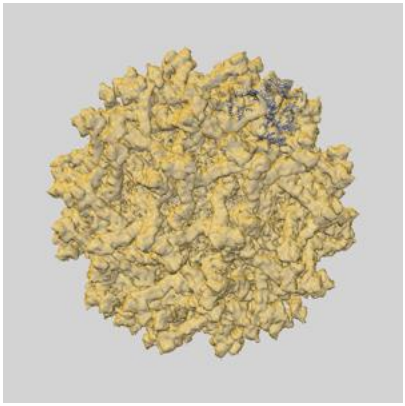
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit

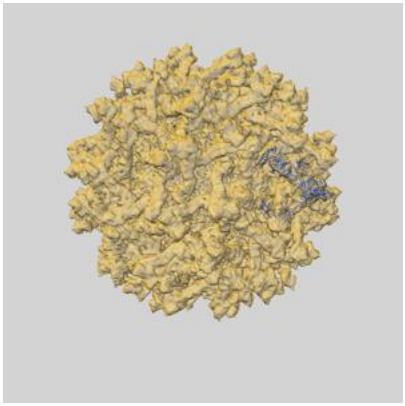
This section contains information regarding the fit between EMDB map EMD-8508 and PDB model 5U4W. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlays

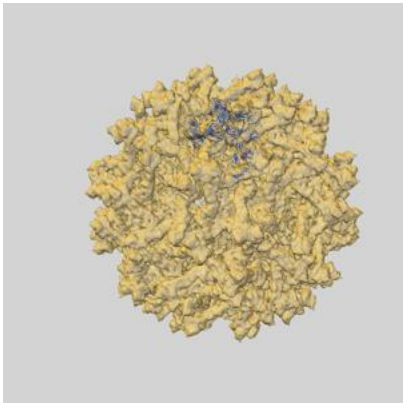
9.1.1 Map-model overlay



X

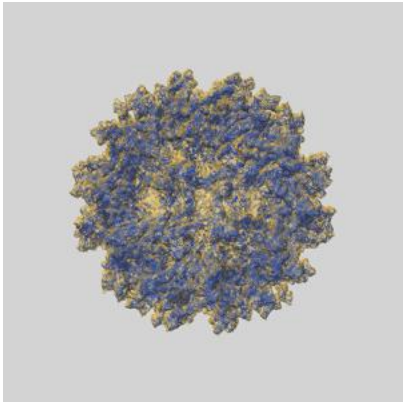


Y

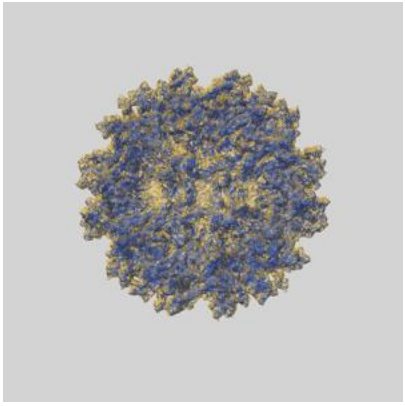


Z

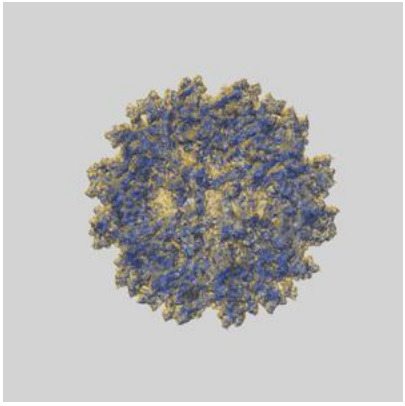
9.1.2 Map-model assembly overlay



X



Y



Z

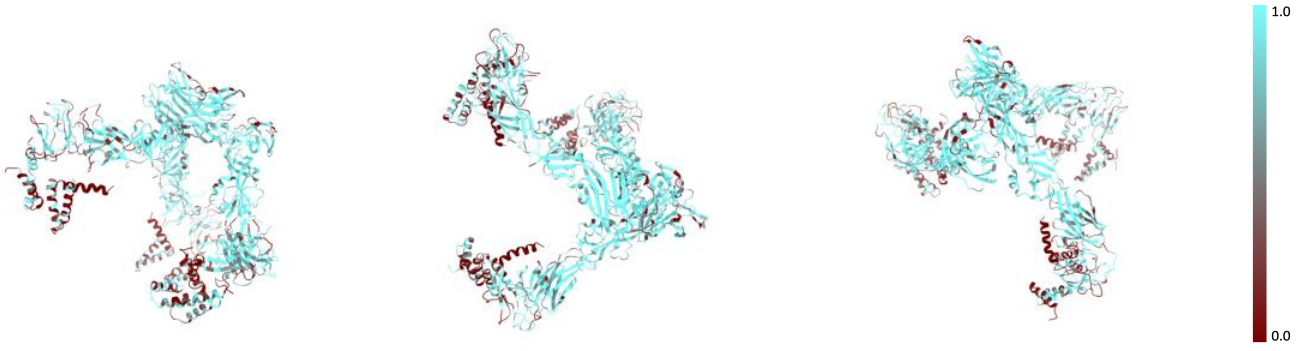
The images above show the 3D surface view of the map at the recommended contour level 4.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

X Y Z

The images above show the model with each residue coloured according 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.

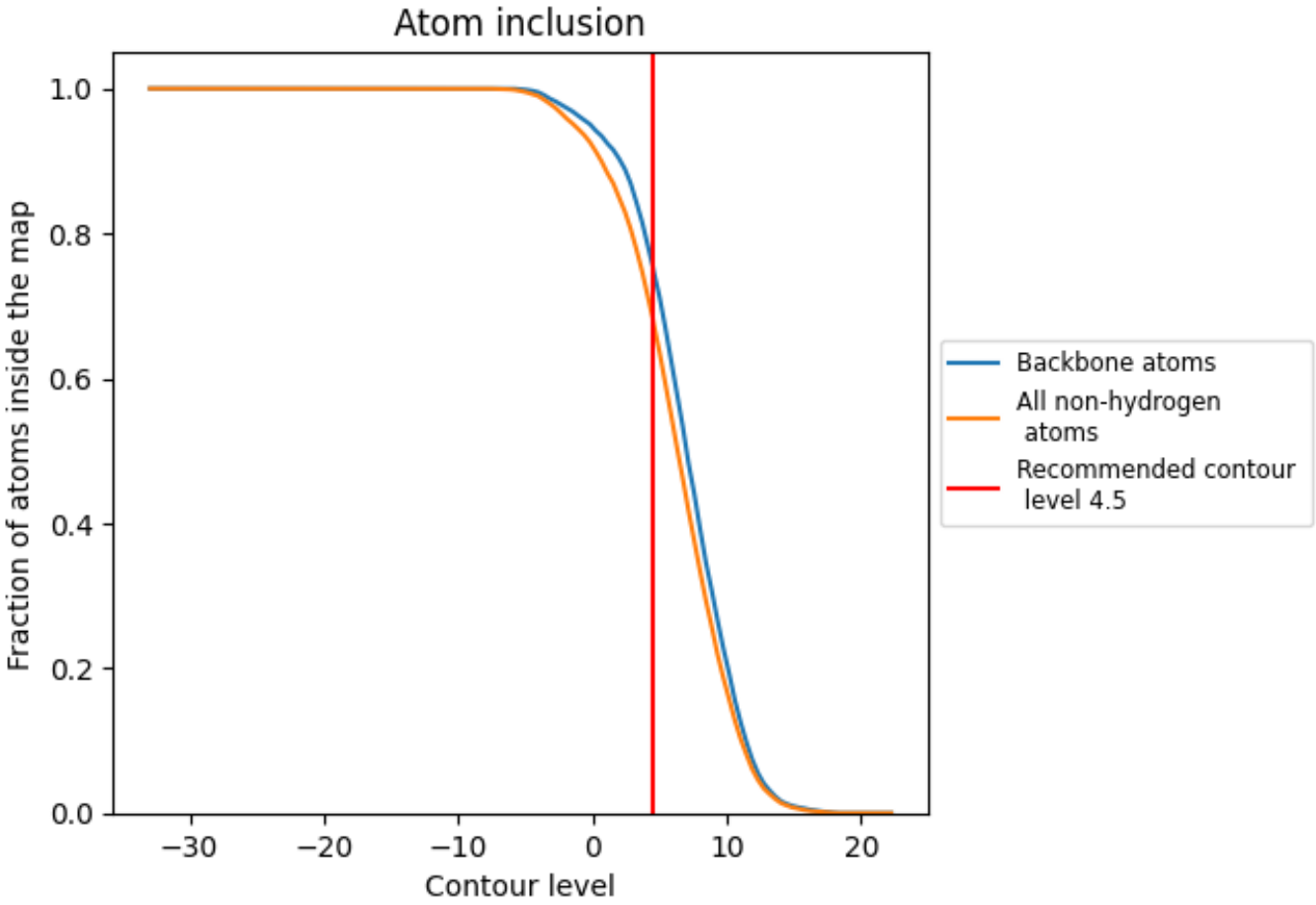
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (4.5).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 68% 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 (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6821	0.0790
A	0.7575	0.0770
B	0.7284	0.0690
C	0.7194	0.0800
D	0.7112	0.0570
E	0.7661	0.0960
F	0.7328	0.0780
G	0.1524	-0.0040
H	0.4679	0.1010
I	0.3717	0.0740
J	0.4583	0.1290
K	0.2968	0.0370
L	0.4071	0.0950