



Full wwPDB EM Validation Report ⓘ

Apr 10, 2024 – 04:32 pm BST

PDB ID : 8C8O
EMDB ID : EMD-16489
Title : In situ structure of the Nitrosopumilus maritimus S-layer - Six-fold symmetry (C6)
Authors : von Kuegelgen, A.; Bharat, T.
Deposited on : 2023-01-20
Resolution : 3.40 Å(reported)

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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.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

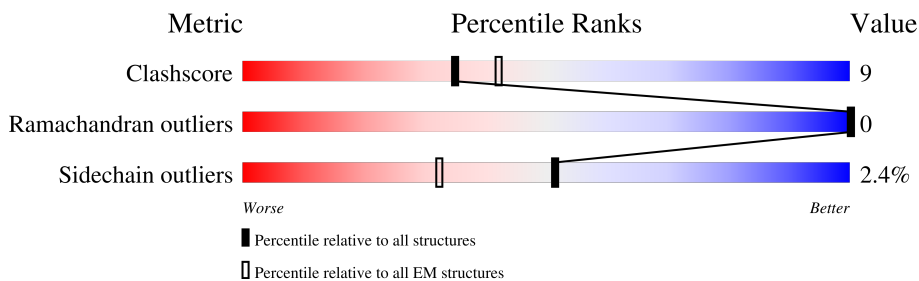
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	A	1734	
1	B	1734	
1	C	1734	
1	D	1734	
1	E	1734	
1	F	1734	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 47220 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.

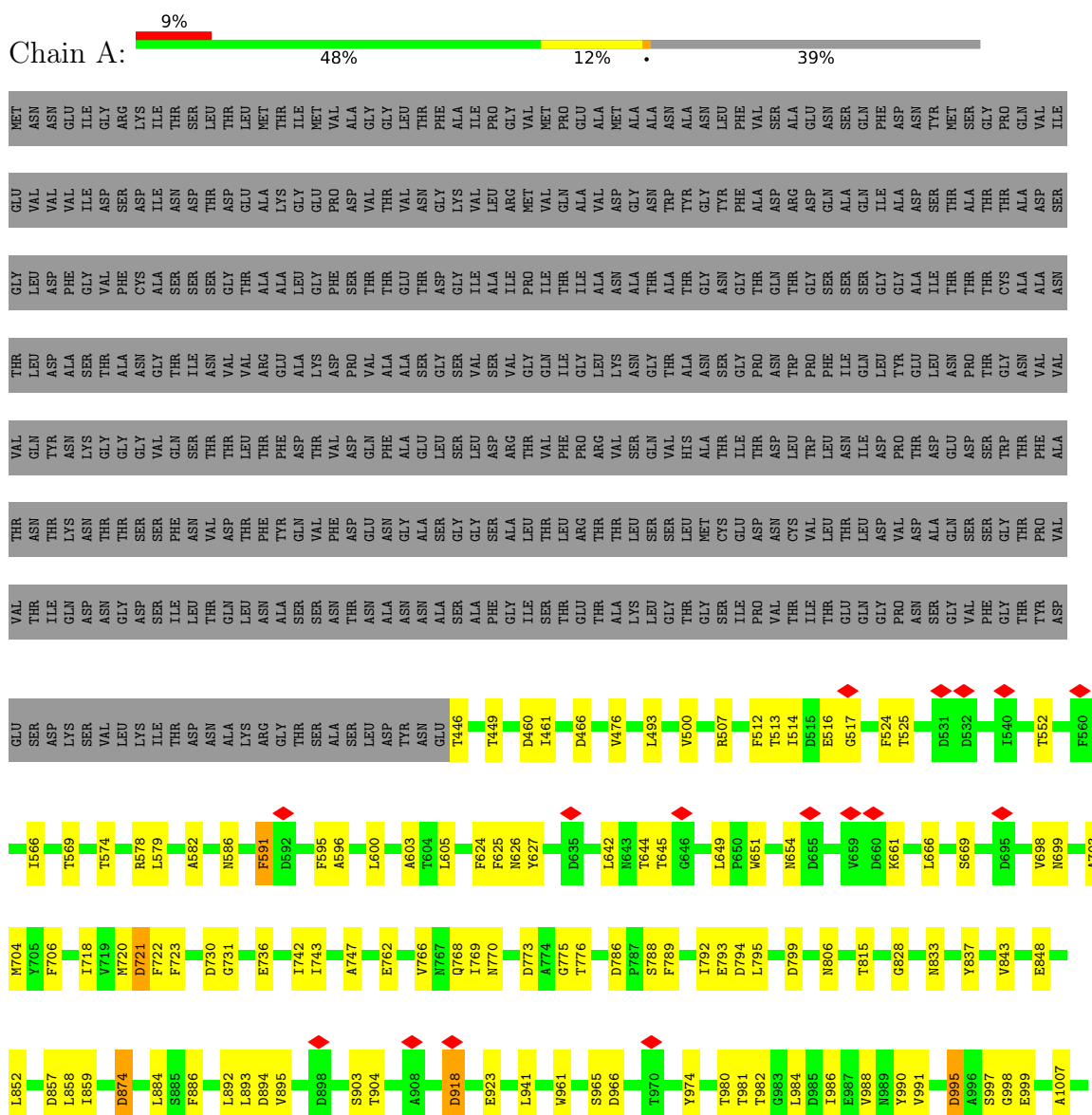
- Molecule 1 is a protein called Cell surface protein.

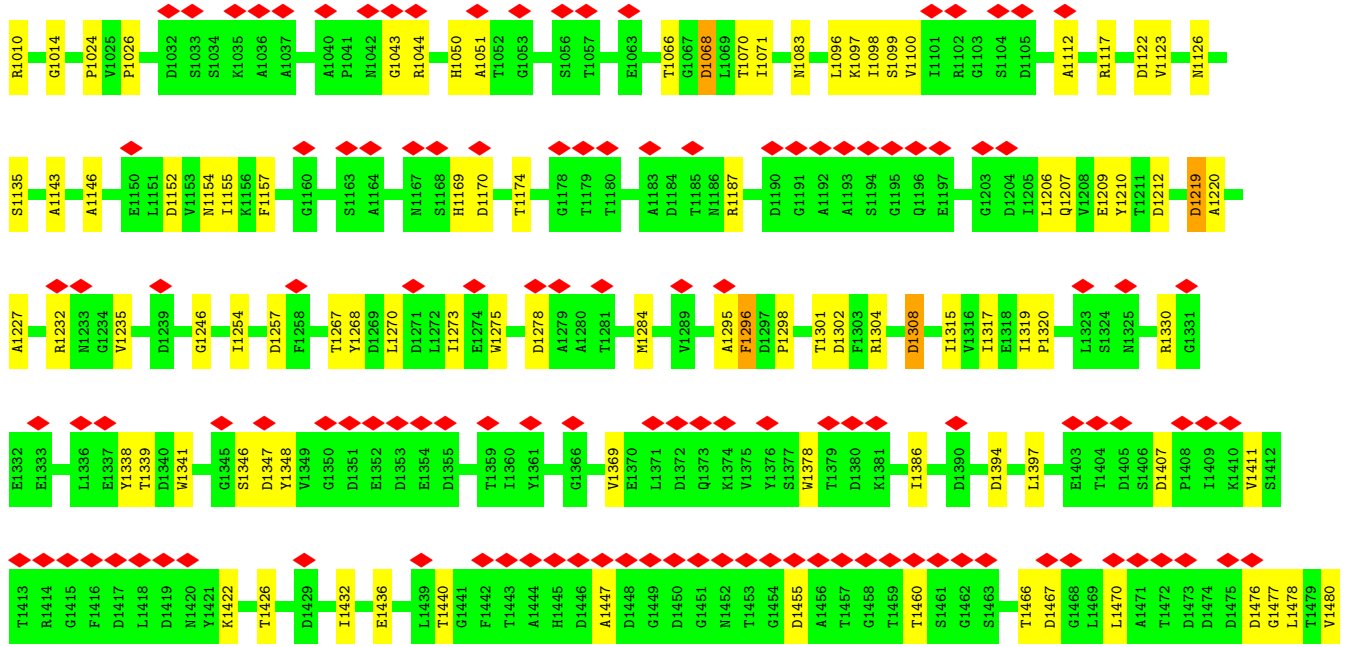
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1053	7870	4853	1255	1751	11	0	0
1	B	1053	7870	4853	1255	1751	11	0	0
1	C	1053	7870	4853	1255	1751	11	0	0
1	D	1053	7870	4853	1255	1751	11	0	0
1	E	1053	7870	4853	1255	1751	11	0	0
1	F	1053	7870	4853	1255	1751	11	0	0

3 Residue-property plots [i](#)

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





S1481	F1482	E1483	F1484	S1485	E1486	D1487	E1488	T1489	I1490	V1491	G1492	S1493	A1494	L1495	I1496	E1497	V1498
ASN	ILE	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
GLN	SER	PHE	TYR	LEU	VAL	GLN	GLN	ASP	ALA	ASN	GLY	VAL	THR	VAL	VAL	SER	LEU
THR	ALA	SER	PRO	PRO	VAL	SER	THR	THR	ASN	VAL	SER	GLY	THR	VAL	VAL	THR	SER
ASP	ASP	ASP	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
SER	SER	SER	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY

• Molecule 1: Cell surface protein



MET	ASN	ASN	TYR	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
GLY	LEU	PHE	GLY	VAL	ASP	SER	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
GLY	LEU	PHE	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
THR	LEU	ASP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
VAL	GLN	TYR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
THR	LEU	ASP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
VAL	GLN	TYR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
THR	LEU	ASP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
VAL	GLN	TYR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY

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SER

• Molecule 1: Cell surface protein



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GLU
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F560
I566
T569
T574
R578
L579
A582
F591
D592
F595
A596
L600
A603
T604
L605
F624
F625
M626
Y627
D635
L642
M643
T644
T645
G646
L649
P650
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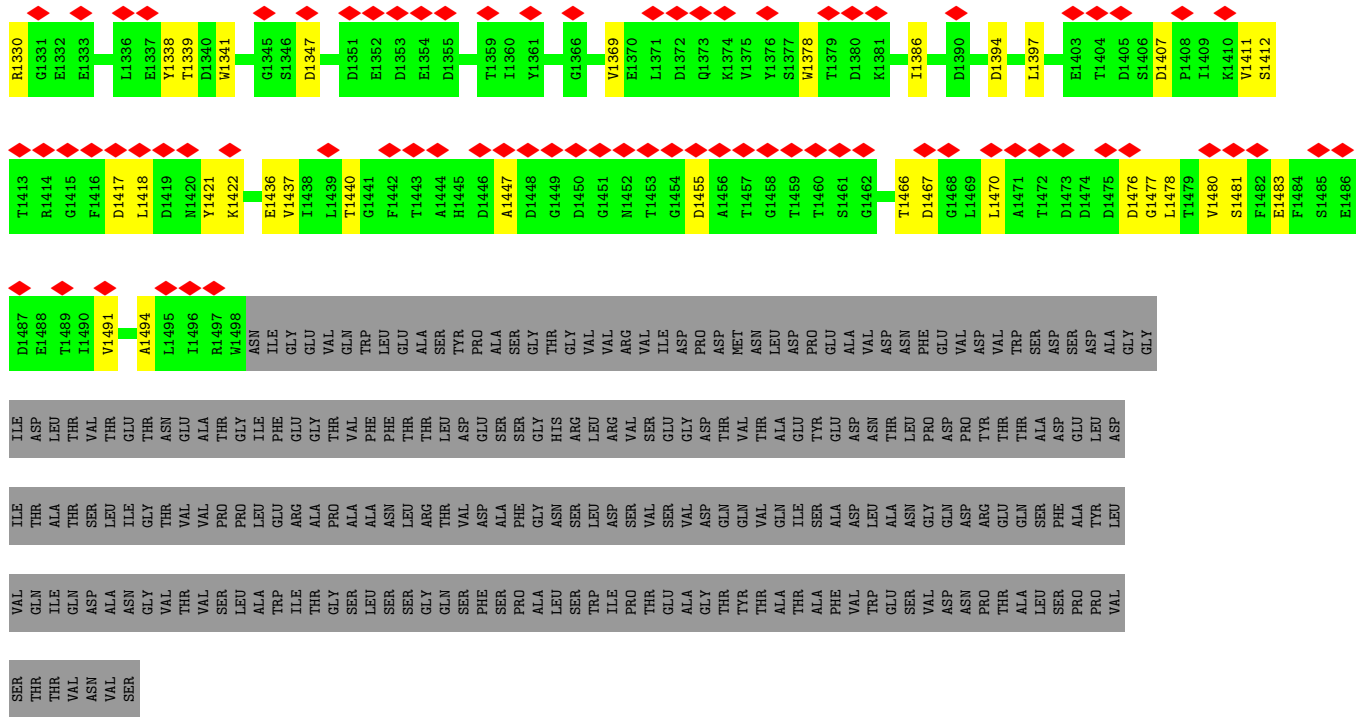
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E736
I742
I743
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V766
Q768
I769
N770
D773
A774
G775
T776
D786
P787
S788
F789
I792
E793
D794
L795
D799
N806
T815
S825
G828
N833
Y837
V843
E848

L852
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D894
V895
D896
S903
T904
A908
D918
E923
L934
L941
W961
S965
D966
Y974
T980
T981
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V991
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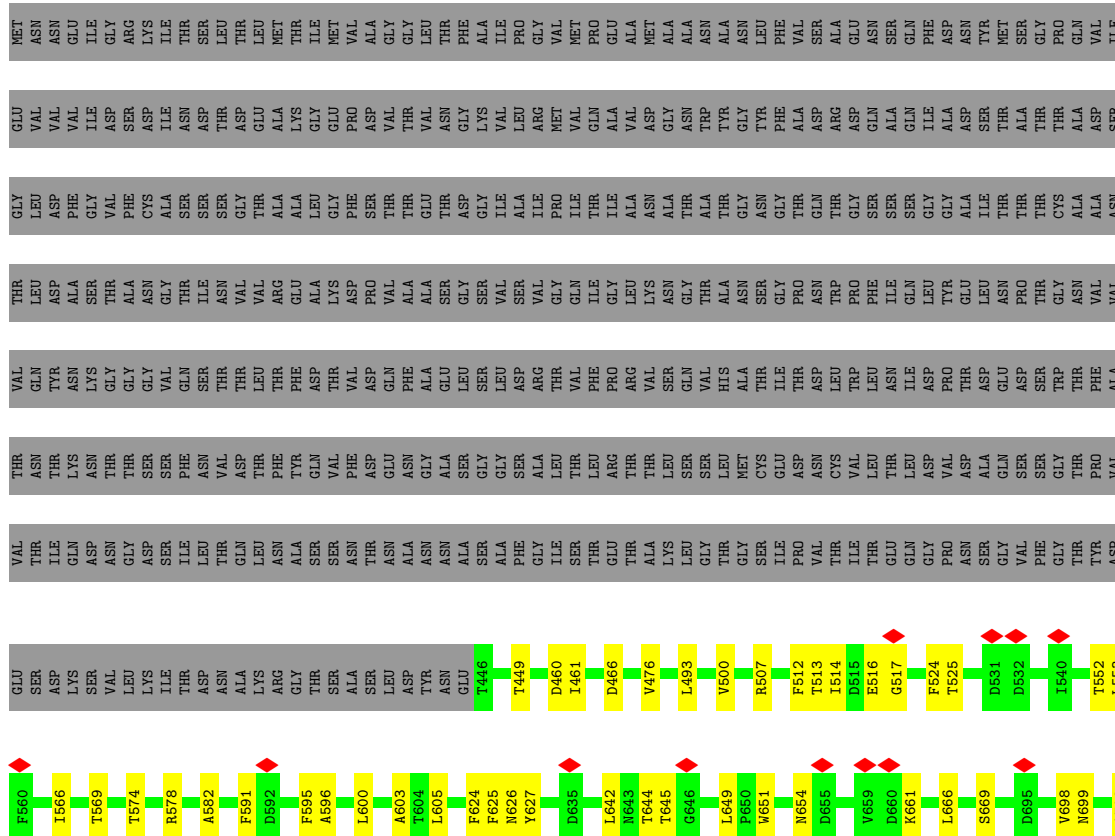
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P1041
M1042
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R1044
H1050
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G1067
L1069
T1070
I1071
D1077
M1083
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G1103
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D1105
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R1117

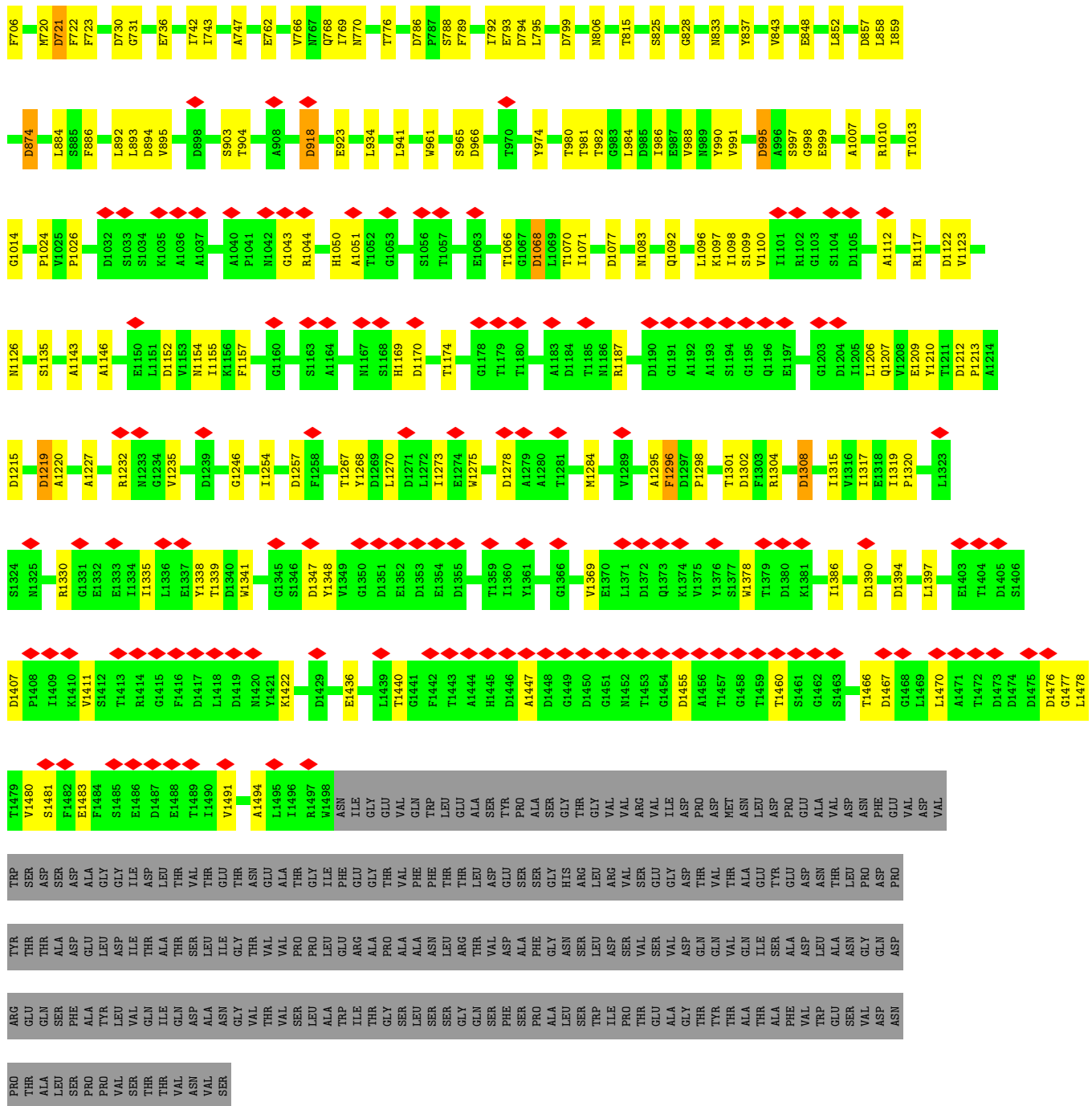
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A1164
N1167
S1168
H1169
D1170
T1174
G1178
T1179
T1180
A1183
D1184
T1185
N1186
R1187
D1190
G1191
A1192
A1193
S1194
G1195
Q1196
E1197
G1203
D1204
I1205
L1206
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D1215

D1219
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V1235
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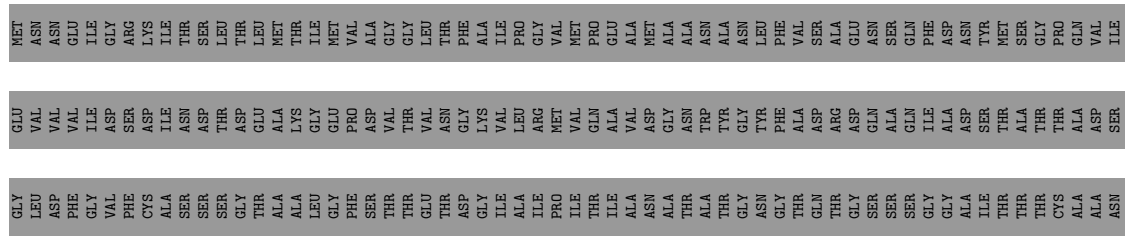


● Molecule 1: Cell surface protein





- Molecule 1: Cell surface protein



GLU ASP
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ALA THR
ASP ASP
GLU GLU

ALA ASP
LEU THR
ALA THR
ASN SER
GLY VAL
GLN ASP
ASP ASP
TYR THR
ASP THR
PRO THR
ALA THR
GLU THR

PHE VAL
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PHE THR
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● Molecule 1: Cell surface protein



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V477
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I514
E516
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F524
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D531
D532

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F722
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S788
F789
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T815
S825

G528
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Y837
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V895
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S903
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Y974
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N989

Y990
V991
D995
A996
G998
E999
A1007
R1010
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V1123
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V1153
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A1192
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S1194
G1195
Q1196
E1197
G1203
D1204
L1205
L1206
Q1207

4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of subtomograms used	108621	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; PseudoSubtomograms as described in Zivanov 2022 (https://elifesciences.org/articles/83724)	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	121	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.489	Depositor
Minimum map value	-0.285	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.08214	Depositor
Map size (\AA)	265.4, 265.4, 265.4	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.327, 1.327, 1.327	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	A	0.24	0/7998	0.49	0/10938
1	B	0.24	0/7998	0.49	0/10938
1	C	0.25	0/7998	0.49	0/10938
1	D	0.24	0/7998	0.49	0/10938
1	E	0.25	0/7998	0.49	0/10938
1	F	0.25	0/7998	0.49	0/10938
All	All	0.25	0/47988	0.49	0/65628

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	A	7870	0	7314	138	0
1	B	7870	0	7314	138	0
1	C	7870	0	7314	139	0
1	D	7870	0	7314	139	0
1	E	7870	0	7314	144	0
1	F	7870	0	7314	142	0
All	All	47220	0	43884	792	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (792) 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:D:999:GLU:OE1	1:E:1304:ARG:NH1	2.15	0.80
1:A:999:GLU:OE1	1:B:1304:ARG:NH1	2.16	0.78
1:B:999:GLU:OE1	1:C:1304:ARG:NH1	2.17	0.78
1:C:999:GLU:OE1	1:D:1304:ARG:NH1	2.17	0.78
1:A:1304:ARG:NH1	1:F:999:GLU:OE1	2.17	0.78
1:E:999:GLU:OE1	1:F:1304:ARG:NH1	2.17	0.78
1:B:768:GLN:HE21	1:B:991:VAL:HG12	1.53	0.74
1:A:768:GLN:HE21	1:A:991:VAL:HG12	1.53	0.73
1:E:768:GLN:HE21	1:E:991:VAL:HG12	1.53	0.73
1:C:768:GLN:HE21	1:C:991:VAL:HG12	1.53	0.73
1:D:768:GLN:HE21	1:D:991:VAL:HG12	1.53	0.73
1:F:768:GLN:HE21	1:F:991:VAL:HG12	1.53	0.72
1:E:743:ILE:HG13	1:E:789:PHE:HB3	1.77	0.67
1:D:743:ILE:HG13	1:D:789:PHE:HB3	1.77	0.67
1:B:574:THR:OG1	1:B:806:ASN:ND2	2.29	0.66
1:C:574:THR:OG1	1:C:806:ASN:ND2	2.29	0.66
1:D:574:THR:OG1	1:D:806:ASN:ND2	2.29	0.66
1:E:574:THR:OG1	1:E:806:ASN:ND2	2.29	0.66
1:F:574:THR:OG1	1:F:806:ASN:ND2	2.29	0.66
1:F:743:ILE:HG13	1:F:789:PHE:HB3	1.77	0.66
1:C:743:ILE:HG13	1:C:789:PHE:HB3	1.77	0.66
1:D:1220:ALA:O	1:E:1466:THR:OG1	2.13	0.66
1:A:574:THR:OG1	1:A:806:ASN:ND2	2.29	0.66
1:A:1220:ALA:O	1:B:1466:THR:OG1	2.13	0.66
1:A:743:ILE:HG13	1:A:789:PHE:HB3	1.77	0.65
1:B:743:ILE:HG13	1:B:789:PHE:HB3	1.77	0.65
1:B:766:VAL:HG11	1:B:792:ILE:HD12	1.78	0.65
1:A:1097:LYS:HB3	1:A:1209:GLU:HB3	1.79	0.65
1:B:1097:LYS:HB3	1:B:1209:GLU:HB3	1.79	0.65
1:C:766:VAL:HG11	1:C:792:ILE:HD12	1.78	0.65
1:C:1097:LYS:HB3	1:C:1209:GLU:HB3	1.79	0.65
1:F:1097:LYS:HB3	1:F:1209:GLU:HB3	1.79	0.65
1:E:1394:ASP:HB3	1:E:1397:LEU:HB3	1.79	0.64
1:A:1394:ASP:HB3	1:A:1397:LEU:HB3	1.79	0.64
1:E:512:PHE:HB3	1:E:722:PHE:HB2	1.80	0.64
1:F:512:PHE:HB3	1:F:722:PHE:HB2	1.80	0.64
1:A:766:VAL:HG11	1:A:792:ILE:HD12	1.78	0.64
1:B:1394:ASP:HB3	1:B:1397:LEU:HB3	1.79	0.64
1:D:1097:LYS:HB3	1:D:1209:GLU:HB3	1.79	0.64
1:E:1097:LYS:HB3	1:E:1209:GLU:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1394:ASP:HB3	1:F:1397:LEU:HB3	1.79	0.64
1:F:766:VAL:HG11	1:F:792:ILE:HD12	1.78	0.64
1:D:1394:ASP:HB3	1:D:1397:LEU:HB3	1.80	0.64
1:D:512:PHE:HB3	1:D:722:PHE:HB2	1.80	0.64
1:D:766:VAL:HG11	1:D:792:ILE:HD12	1.78	0.64
1:A:512:PHE:HB3	1:A:722:PHE:HB2	1.80	0.63
1:C:1394:ASP:HB3	1:C:1397:LEU:HB3	1.79	0.63
1:E:766:VAL:HG11	1:E:792:ILE:HD12	1.78	0.63
1:E:1220:ALA:O	1:F:1466:THR:OG1	2.16	0.63
1:C:512:PHE:HB3	1:C:722:PHE:HB2	1.80	0.63
1:C:1220:ALA:O	1:D:1466:THR:OG1	2.17	0.63
1:E:1050:HIS:HD2	1:E:1051:ALA:N	1.97	0.63
1:D:1050:HIS:HD2	1:D:1051:ALA:N	1.97	0.62
1:B:1295:ALA:HB1	1:B:1320:PRO:HB3	1.81	0.62
1:C:1050:HIS:HD2	1:C:1051:ALA:N	1.97	0.62
1:F:1050:HIS:HD2	1:F:1051:ALA:N	1.97	0.62
1:A:1050:HIS:HD2	1:A:1051:ALA:N	1.97	0.62
1:B:512:PHE:HB3	1:B:722:PHE:HB2	1.80	0.62
1:B:1050:HIS:HD2	1:B:1051:ALA:N	1.97	0.62
1:C:1295:ALA:HB1	1:C:1320:PRO:HB3	1.81	0.62
1:B:1436:GLU:N	1:B:1436:GLU:OE2	2.33	0.62
1:A:1295:ALA:HB1	1:A:1320:PRO:HB3	1.81	0.62
1:F:1436:GLU:OE2	1:F:1436:GLU:N	2.33	0.62
1:A:1436:GLU:OE2	1:A:1436:GLU:N	2.33	0.62
1:E:1436:GLU:OE2	1:E:1436:GLU:N	2.33	0.62
1:C:1066:THR:OG1	1:C:1068:ASP:OD1	2.17	0.61
1:C:1436:GLU:OE2	1:C:1436:GLU:N	2.33	0.61
1:A:886:PHE:HA	1:B:1301:THR:HG21	1.83	0.61
1:D:1295:ALA:HB1	1:D:1320:PRO:HB3	1.81	0.61
1:E:886:PHE:HA	1:F:1301:THR:HG21	1.82	0.61
1:E:1476:ASP:OD1	1:E:1477:GLY:N	2.31	0.61
1:B:1066:THR:OG1	1:B:1068:ASP:OD1	2.17	0.61
1:C:1476:ASP:OD1	1:C:1477:GLY:N	2.31	0.61
1:D:1122:ASP:OD1	1:D:1126:ASN:ND2	2.34	0.61
1:F:1295:ALA:HB1	1:F:1320:PRO:HB3	1.81	0.61
1:D:1436:GLU:N	1:D:1436:GLU:OE2	2.33	0.60
1:D:1481:SER:HB3	1:D:1491:VAL:HG12	1.83	0.60
1:E:1066:THR:OG1	1:E:1068:ASP:OD1	2.17	0.60
1:E:1122:ASP:OD1	1:E:1126:ASN:ND2	2.34	0.60
1:B:886:PHE:HA	1:C:1301:THR:HG21	1.83	0.60
1:C:1122:ASP:OD1	1:C:1126:ASN:ND2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1295:ALA:HB1	1:E:1320:PRO:HB3	1.81	0.60
1:A:1466:THR:OG1	1:F:1220:ALA:O	2.18	0.60
1:B:1481:SER:HB3	1:B:1491:VAL:HG12	1.83	0.60
1:E:1481:SER:HB3	1:E:1491:VAL:HG12	1.83	0.60
1:A:1122:ASP:OD1	1:A:1126:ASN:ND2	2.34	0.60
1:C:1481:SER:HB3	1:C:1491:VAL:HG12	1.82	0.60
1:D:886:PHE:HA	1:E:1301:THR:HG21	1.83	0.59
1:F:1122:ASP:OD1	1:F:1126:ASN:ND2	2.34	0.59
1:B:1220:ALA:O	1:C:1466:THR:OG1	2.16	0.59
1:C:886:PHE:HA	1:D:1301:THR:HG21	1.84	0.59
1:F:1481:SER:HB3	1:F:1491:VAL:HG12	1.82	0.59
1:B:1122:ASP:OD1	1:B:1126:ASN:ND2	2.34	0.59
1:A:1481:SER:HB3	1:A:1491:VAL:HG12	1.83	0.59
1:F:1476:ASP:OD1	1:F:1477:GLY:N	2.31	0.59
1:C:625:PHE:HE1	1:C:627:TYR:HB3	1.69	0.58
1:B:1476:ASP:OD1	1:B:1477:GLY:N	2.31	0.58
1:D:625:PHE:HE1	1:D:627:TYR:HB3	1.69	0.58
1:F:569:THR:HB	1:F:582:ALA:HB3	1.86	0.58
1:A:569:THR:HB	1:A:582:ALA:HB3	1.85	0.58
1:A:1301:THR:HG21	1:F:886:PHE:HA	1.84	0.58
1:B:625:PHE:HE1	1:B:627:TYR:HB3	1.69	0.58
1:A:1066:THR:OG1	1:A:1068:ASP:OD1	2.17	0.58
1:E:569:THR:HB	1:E:582:ALA:HB3	1.85	0.58
1:A:1308:ASP:OD1	1:A:1308:ASP:N	2.37	0.58
1:A:1476:ASP:OD1	1:A:1477:GLY:N	2.31	0.57
1:D:569:THR:HB	1:D:582:ALA:HB3	1.85	0.57
1:E:625:PHE:HE1	1:E:627:TYR:HB3	1.69	0.57
1:E:1206:LEU:N	1:E:1227:ALA:O	2.32	0.57
1:A:625:PHE:HE1	1:A:627:TYR:HB3	1.68	0.57
1:E:624:PHE:HB2	1:E:723:PHE:HB2	1.87	0.57
1:C:1308:ASP:N	1:C:1308:ASP:OD1	2.37	0.57
1:B:569:THR:HB	1:B:582:ALA:HB3	1.85	0.57
1:D:624:PHE:HB2	1:D:723:PHE:HB2	1.87	0.57
1:D:995:ASP:OD2	1:D:997:SER:N	2.38	0.57
1:C:995:ASP:OD2	1:C:997:SER:N	2.38	0.57
1:F:1308:ASP:OD1	1:F:1308:ASP:N	2.37	0.57
1:C:569:THR:HB	1:C:582:ALA:HB3	1.85	0.56
1:A:524:PHE:HB2	1:A:566:ILE:HB	1.88	0.56
1:E:995:ASP:OD2	1:E:997:SER:N	2.38	0.56
1:C:524:PHE:HB2	1:C:566:ILE:HB	1.88	0.56
1:F:624:PHE:HB2	1:F:723:PHE:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:995:ASP:OD2	1:F:997:SER:N	2.38	0.56
1:B:524:PHE:HB2	1:B:566:ILE:HB	1.88	0.56
1:B:624:PHE:HB2	1:B:723:PHE:HB2	1.87	0.56
1:D:524:PHE:HB2	1:D:566:ILE:HB	1.88	0.56
1:F:524:PHE:HB2	1:F:566:ILE:HB	1.88	0.56
1:B:1206:LEU:N	1:B:1227:ALA:O	2.32	0.56
1:F:625:PHE:HE1	1:F:627:TYR:HB3	1.68	0.56
1:B:995:ASP:OD2	1:B:997:SER:N	2.38	0.56
1:D:1066:THR:OG1	1:D:1068:ASP:OD1	2.17	0.56
1:A:995:ASP:OD2	1:A:997:SER:N	2.38	0.56
1:A:1206:LEU:N	1:A:1227:ALA:O	2.32	0.56
1:D:1206:LEU:N	1:D:1227:ALA:O	2.32	0.56
1:F:837:TYR:O	1:F:1010:ARG:N	2.39	0.56
1:F:1206:LEU:N	1:F:1227:ALA:O	2.32	0.56
1:C:624:PHE:HB2	1:C:723:PHE:HB2	1.87	0.55
1:E:524:PHE:HB2	1:E:566:ILE:HB	1.88	0.55
1:B:837:TYR:O	1:B:1010:ARG:N	2.40	0.55
1:F:1066:THR:OG1	1:F:1068:ASP:OD1	2.17	0.55
1:E:1308:ASP:N	1:E:1308:ASP:OD1	2.37	0.55
1:B:1308:ASP:OD1	1:B:1308:ASP:N	2.37	0.55
1:D:1308:ASP:OD1	1:D:1308:ASP:N	2.37	0.55
1:A:624:PHE:HB2	1:A:723:PHE:HB2	1.87	0.55
1:D:837:TYR:O	1:D:1010:ARG:N	2.39	0.55
1:A:837:TYR:O	1:A:1010:ARG:N	2.40	0.54
1:E:1096:LEU:HB3	1:E:1112:ALA:HB3	1.89	0.54
1:C:1096:LEU:HB3	1:C:1112:ALA:HB3	1.89	0.54
1:C:837:TYR:O	1:C:1010:ARG:N	2.40	0.54
1:D:1476:ASP:OD1	1:D:1477:GLY:N	2.31	0.54
1:C:966:ASP:OD1	1:C:966:ASP:N	2.41	0.54
1:E:965:SER:OG	1:E:966:ASP:OD1	2.26	0.54
1:A:1096:LEU:HB3	1:A:1112:ALA:HB3	1.89	0.53
1:B:1096:LEU:HB3	1:B:1112:ALA:HB3	1.89	0.53
1:A:966:ASP:OD1	1:A:966:ASP:N	2.41	0.53
1:F:966:ASP:OD1	1:F:966:ASP:N	2.41	0.53
1:E:1050:HIS:CD2	1:E:1051:ALA:N	2.77	0.53
1:F:1044:ARG:HA	1:F:1169:HIS:HB3	1.91	0.53
1:A:1044:ARG:HA	1:A:1169:HIS:HB3	1.91	0.53
1:B:500:VAL:O	1:B:578:ARG:NH2	2.40	0.53
1:C:1206:LEU:N	1:C:1227:ALA:O	2.32	0.53
1:D:642:LEU:HD11	1:D:703:ALA:HB2	1.91	0.53
1:F:1096:LEU:HB3	1:F:1112:ALA:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:642:LEU:HD11	1:C:703:ALA:HB2	1.91	0.53
1:D:966:ASP:OD1	1:D:966:ASP:N	2.41	0.53
1:E:837:TYR:O	1:E:1010:ARG:N	2.39	0.53
1:E:1296:PHE:HB3	1:E:1317:ILE:HG23	1.91	0.53
1:A:1098:ILE:HD11	1:A:1206:LEU:HD11	1.91	0.53
1:B:642:LEU:HD11	1:B:703:ALA:HB2	1.91	0.53
1:C:1098:ILE:HD11	1:C:1206:LEU:HD11	1.91	0.53
1:D:769:ILE:HD11	1:D:892:LEU:HB2	1.91	0.53
1:D:1050:HIS:CD2	1:D:1051:ALA:N	2.77	0.53
1:D:1096:LEU:HB3	1:D:1112:ALA:HB3	1.89	0.53
1:A:769:ILE:HD11	1:A:892:LEU:HB2	1.91	0.53
1:C:1478:LEU:HB3	1:C:1494:ALA:HB3	1.91	0.53
1:A:642:LEU:HD11	1:A:703:ALA:HB2	1.91	0.53
1:B:596:ALA:HB3	1:B:704:MET:HB2	1.91	0.53
1:D:815:THR:OG1	1:E:1083:ASN:OD1	2.27	0.53
1:E:1044:ARG:HA	1:E:1169:HIS:HB3	1.91	0.53
1:E:500:VAL:O	1:E:578:ARG:NH2	2.40	0.53
1:F:666:LEU:HD21	1:F:669:SER:HB2	1.91	0.53
1:F:1050:HIS:CD2	1:F:1051:ALA:N	2.77	0.53
1:A:645:THR:HA	1:A:698:VAL:HA	1.91	0.52
1:A:768:GLN:NE2	1:A:991:VAL:HG12	2.23	0.52
1:A:1296:PHE:HB3	1:A:1317:ILE:HG23	1.91	0.52
1:B:1044:ARG:HA	1:B:1169:HIS:HB3	1.91	0.52
1:C:645:THR:HA	1:C:698:VAL:HA	1.92	0.52
1:E:596:ALA:HB3	1:E:704:MET:HB2	1.91	0.52
1:F:596:ALA:HB3	1:F:704:MET:HB2	1.91	0.52
1:B:1478:LEU:HB3	1:B:1494:ALA:HB3	1.91	0.52
1:C:1050:HIS:CD2	1:C:1051:ALA:N	2.77	0.52
1:E:642:LEU:HD11	1:E:703:ALA:HB2	1.91	0.52
1:E:966:ASP:OD1	1:E:966:ASP:N	2.41	0.52
1:B:769:ILE:HD11	1:B:892:LEU:HB2	1.91	0.52
1:B:1296:PHE:HB3	1:B:1317:ILE:HG23	1.91	0.52
1:C:1296:PHE:HB3	1:C:1317:ILE:HG23	1.91	0.52
1:D:965:SER:OG	1:D:966:ASP:OD1	2.26	0.52
1:D:1478:LEU:HB3	1:D:1494:ALA:HB3	1.91	0.52
1:F:1296:PHE:HB3	1:F:1317:ILE:HG23	1.91	0.52
1:B:645:THR:HA	1:B:698:VAL:HA	1.92	0.52
1:E:769:ILE:HD11	1:E:892:LEU:HB2	1.91	0.52
1:A:1440:THR:N	1:A:1470:LEU:O	2.40	0.52
1:C:769:ILE:HD11	1:C:892:LEU:HB2	1.91	0.52
1:F:642:LEU:HD11	1:F:703:ALA:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1050:HIS:CD2	1:A:1051:ALA:N	2.77	0.52
1:B:966:ASP:N	1:B:966:ASP:OD1	2.41	0.52
1:F:1478:LEU:HB3	1:F:1494:ALA:HB3	1.91	0.52
1:A:965:SER:OG	1:A:966:ASP:OD1	2.26	0.52
1:B:768:GLN:NE2	1:B:991:VAL:HG12	2.23	0.52
1:B:1050:HIS:CD2	1:B:1051:ALA:N	2.77	0.52
1:E:961:TRP:CD1	1:E:981:THR:HG22	2.45	0.52
1:E:1478:LEU:HB3	1:E:1494:ALA:HB3	1.91	0.52
1:F:1098:ILE:HD11	1:F:1206:LEU:HD11	1.91	0.52
1:A:596:ALA:HB3	1:A:704:MET:HB2	1.91	0.52
1:B:1098:ILE:HD11	1:B:1206:LEU:HD11	1.91	0.52
1:C:596:ALA:HB3	1:C:704:MET:HB2	1.91	0.52
1:C:961:TRP:CD1	1:C:981:THR:HG22	2.45	0.52
1:C:1044:ARG:HA	1:C:1169:HIS:HB3	1.91	0.52
1:D:645:THR:HA	1:D:698:VAL:HA	1.92	0.52
1:D:1044:ARG:HA	1:D:1169:HIS:HB3	1.91	0.52
1:F:768:GLN:NE2	1:F:991:VAL:HG12	2.23	0.52
1:A:1467:ASP:OD1	1:A:1467:ASP:N	2.43	0.52
1:B:815:THR:OG1	1:C:1083:ASN:OD1	2.28	0.52
1:B:1050:HIS:HD2	1:B:1051:ALA:H	1.58	0.52
1:B:1235:VAL:HG13	1:B:1254:ILE:HG23	1.92	0.52
1:D:596:ALA:HB3	1:D:704:MET:HB2	1.91	0.52
1:D:1050:HIS:HD2	1:D:1051:ALA:H	1.58	0.52
1:D:1296:PHE:HB3	1:D:1317:ILE:HG23	1.91	0.52
1:E:1174:THR:OG1	1:E:1187:ARG:NH1	2.43	0.52
1:F:769:ILE:HD11	1:F:892:LEU:HB2	1.91	0.52
1:C:815:THR:OG1	1:D:1083:ASN:OD1	2.28	0.52
1:D:666:LEU:HD21	1:D:669:SER:HB2	1.91	0.52
1:F:645:THR:HA	1:F:698:VAL:HA	1.91	0.52
1:F:961:TRP:CD1	1:F:981:THR:HG22	2.45	0.52
1:A:666:LEU:HD21	1:A:669:SER:HB2	1.91	0.51
1:B:1174:THR:OG1	1:B:1187:ARG:NH1	2.43	0.51
1:F:466:ASP:OD2	1:F:466:ASP:N	2.43	0.51
1:A:961:TRP:CD1	1:A:981:THR:HG22	2.45	0.51
1:B:517:GLY:HA3	1:B:603:ALA:HB2	1.93	0.51
1:D:961:TRP:CD1	1:D:981:THR:HG22	2.45	0.51
1:D:1098:ILE:HD11	1:D:1206:LEU:HD11	1.91	0.51
1:E:645:THR:HA	1:E:698:VAL:HA	1.91	0.51
1:E:666:LEU:HD21	1:E:669:SER:HB2	1.91	0.51
1:A:1174:THR:OG1	1:A:1187:ARG:NH1	2.43	0.51
1:C:1174:THR:OG1	1:C:1187:ARG:NH1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:517:GLY:HA3	1:F:603:ALA:HB2	1.93	0.51
1:F:1467:ASP:OD1	1:F:1467:ASP:N	2.43	0.51
1:A:517:GLY:HA3	1:A:603:ALA:HB2	1.93	0.51
1:B:1467:ASP:OD1	1:B:1467:ASP:N	2.43	0.51
1:F:1235:VAL:HG13	1:F:1254:ILE:HG23	1.92	0.51
1:B:961:TRP:CD1	1:B:981:THR:HG22	2.45	0.51
1:C:768:GLN:NE2	1:C:991:VAL:HG12	2.23	0.51
1:D:500:VAL:O	1:D:578:ARG:NH2	2.40	0.51
1:E:815:THR:OG1	1:F:1083:ASN:OD1	2.27	0.51
1:A:1478:LEU:HB3	1:A:1494:ALA:HB3	1.91	0.51
1:F:1174:THR:OG1	1:F:1187:ARG:NH1	2.43	0.51
1:C:666:LEU:HD21	1:C:669:SER:HB2	1.91	0.51
1:E:1071:ILE:HG12	1:E:1155:ILE:HD11	1.93	0.51
1:E:1098:ILE:HD11	1:E:1206:LEU:HD11	1.91	0.51
1:B:1071:ILE:HG12	1:B:1155:ILE:HD11	1.93	0.51
1:D:1219:ASP:OD2	1:E:1422:LYS:NZ	2.34	0.51
1:B:965:SER:OG	1:B:966:ASP:OD1	2.26	0.51
1:D:903:SER:HG	1:D:974:TYR:HH	1.56	0.51
1:E:768:GLN:NE2	1:E:991:VAL:HG12	2.23	0.51
1:F:1050:HIS:HD2	1:F:1051:ALA:H	1.58	0.51
1:B:666:LEU:HD21	1:B:669:SER:HB2	1.91	0.50
1:C:517:GLY:HA3	1:C:603:ALA:HB2	1.93	0.50
1:C:965:SER:OG	1:C:966:ASP:OD1	2.26	0.50
1:C:1467:ASP:N	1:C:1467:ASP:OD1	2.43	0.50
1:D:768:GLN:NE2	1:D:991:VAL:HG12	2.23	0.50
1:F:1071:ILE:HG12	1:F:1155:ILE:HD11	1.93	0.50
1:A:1235:VAL:HG13	1:A:1254:ILE:HG23	1.92	0.50
1:E:517:GLY:HA3	1:E:603:ALA:HB2	1.93	0.50
1:E:1235:VAL:HG13	1:E:1254:ILE:HG23	1.92	0.50
1:E:1467:ASP:N	1:E:1467:ASP:OD1	2.43	0.50
1:C:1235:VAL:HG13	1:C:1254:ILE:HG23	1.92	0.50
1:D:1235:VAL:HG13	1:D:1254:ILE:HG23	1.92	0.50
1:D:1467:ASP:OD1	1:D:1467:ASP:N	2.43	0.50
1:D:1174:THR:OG1	1:D:1187:ARG:NH1	2.43	0.50
1:A:1050:HIS:HD2	1:A:1051:ALA:H	1.58	0.50
1:C:918:ASP:HB3	1:C:923:GLU:HG3	1.94	0.50
1:C:1050:HIS:HD2	1:C:1051:ALA:H	1.58	0.50
1:C:1071:ILE:HG12	1:C:1155:ILE:HD11	1.93	0.50
1:D:517:GLY:HA3	1:D:603:ALA:HB2	1.93	0.50
1:A:500:VAL:O	1:A:578:ARG:NH2	2.40	0.50
1:E:1050:HIS:HD2	1:E:1051:ALA:H	1.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1071:ILE:HG12	1:D:1155:ILE:HD11	1.93	0.50
1:D:1440:THR:N	1:D:1470:LEU:O	2.40	0.50
1:E:1440:THR:N	1:E:1470:LEU:O	2.40	0.50
1:C:1298:PRO:HB2	1:C:1301:THR:HA	1.94	0.49
1:D:513:THR:OG1	1:D:514:ILE:N	2.45	0.49
1:F:918:ASP:HB3	1:F:923:GLU:HG3	1.94	0.49
1:A:642:LEU:HD22	1:A:651:TRP:CZ2	2.47	0.49
1:A:1071:ILE:HG12	1:A:1155:ILE:HD11	1.93	0.49
1:B:642:LEU:HD22	1:B:651:TRP:CZ2	2.47	0.49
1:C:1440:THR:N	1:C:1470:LEU:O	2.40	0.49
1:D:642:LEU:HD22	1:D:651:TRP:CZ2	2.47	0.49
1:D:1339:THR:OG1	1:D:1341:TRP:NE1	2.46	0.49
1:E:513:THR:OG1	1:E:514:ILE:N	2.45	0.49
1:E:918:ASP:HB3	1:E:923:GLU:HG3	1.94	0.49
1:F:513:THR:OG1	1:F:514:ILE:N	2.45	0.49
1:A:1298:PRO:HB2	1:A:1301:THR:HA	1.94	0.49
1:A:1339:THR:OG1	1:A:1341:TRP:NE1	2.46	0.49
1:D:466:ASP:OD2	1:D:466:ASP:N	2.44	0.49
1:E:466:ASP:OD2	1:E:466:ASP:N	2.44	0.49
1:B:1298:PRO:HB2	1:B:1301:THR:HA	1.94	0.49
1:C:513:THR:OG1	1:C:514:ILE:N	2.45	0.49
1:D:1298:PRO:HB2	1:D:1301:THR:HA	1.94	0.49
1:F:642:LEU:HD22	1:F:651:TRP:CZ2	2.47	0.49
1:F:1339:THR:OG1	1:F:1341:TRP:NE1	2.46	0.49
1:C:1270:LEU:HD12	1:C:1315:ILE:HD13	1.95	0.49
1:D:918:ASP:HB3	1:D:923:GLU:HG3	1.94	0.49
1:F:1270:LEU:HD12	1:F:1315:ILE:HD13	1.95	0.49
1:A:980:THR:HG22	1:A:982:THR:H	1.78	0.49
1:A:995:ASP:N	1:A:999:GLU:O	2.45	0.49
1:C:893:LEU:HD23	1:C:941:LEU:HD21	1.95	0.49
1:A:513:THR:OG1	1:A:514:ILE:N	2.45	0.49
1:A:815:THR:OG1	1:B:1083:ASN:OD1	2.28	0.49
1:A:984:LEU:HA	1:B:1397:LEU:HD13	1.94	0.49
1:B:980:THR:HG22	1:B:982:THR:H	1.78	0.49
1:B:1339:THR:OG1	1:B:1341:TRP:NE1	2.46	0.49
1:C:1339:THR:OG1	1:C:1341:TRP:NE1	2.46	0.49
1:E:642:LEU:HD22	1:E:651:TRP:CZ2	2.47	0.49
1:E:893:LEU:HD23	1:E:941:LEU:HD21	1.95	0.49
1:F:980:THR:HG22	1:F:982:THR:H	1.78	0.49
1:A:837:TYR:CZ	1:A:843:VAL:HG23	2.48	0.49
1:A:1270:LEU:HD12	1:A:1315:ILE:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:918:ASP:HB3	1:B:923:GLU:HG3	1.94	0.49
1:F:965:SER:OG	1:F:966:ASP:OD1	2.26	0.49
1:A:1083:ASN:OD1	1:F:815:THR:OG1	2.28	0.48
1:D:893:LEU:HD23	1:D:941:LEU:HD21	1.95	0.48
1:D:1270:LEU:HD12	1:D:1315:ILE:HD13	1.95	0.48
1:E:1339:THR:OG1	1:E:1341:TRP:NE1	2.46	0.48
1:A:918:ASP:HB3	1:A:923:GLU:HG3	1.94	0.48
1:C:642:LEU:HD22	1:C:651:TRP:CZ2	2.47	0.48
1:C:980:THR:HG22	1:C:982:THR:H	1.78	0.48
1:B:513:THR:OG1	1:B:514:ILE:N	2.45	0.48
1:B:837:TYR:CZ	1:B:843:VAL:HG23	2.48	0.48
1:B:893:LEU:HD23	1:B:941:LEU:HD21	1.95	0.48
1:B:1270:LEU:HD12	1:B:1315:ILE:HD13	1.95	0.48
1:C:1117:ARG:HG2	1:C:1135:SER:HB3	1.95	0.48
1:E:1117:ARG:HG2	1:E:1135:SER:HB3	1.95	0.48
1:E:1270:LEU:HD12	1:E:1315:ILE:HD13	1.95	0.48
1:E:1298:PRO:HB2	1:E:1301:THR:HA	1.94	0.48
1:F:903:SER:HG	1:F:974:TYR:HH	1.60	0.48
1:F:1298:PRO:HB2	1:F:1301:THR:HA	1.94	0.48
1:A:893:LEU:HD23	1:A:941:LEU:HD21	1.95	0.48
1:E:837:TYR:CZ	1:E:843:VAL:HG23	2.48	0.48
1:B:833:ASN:OD1	1:B:833:ASN:N	2.46	0.48
1:B:1275:TRP:HB2	1:B:1284:MET:HG2	1.96	0.48
1:C:837:TYR:CZ	1:C:843:VAL:HG23	2.48	0.48
1:D:1407:ASP:HA	1:D:1483:GLU:OE2	2.14	0.48
1:F:837:TYR:CZ	1:F:843:VAL:HG23	2.48	0.48
1:F:893:LEU:HD23	1:F:941:LEU:HD21	1.95	0.48
1:C:1275:TRP:HB2	1:C:1284:MET:HG2	1.96	0.48
1:D:837:TYR:CZ	1:D:843:VAL:HG23	2.48	0.48
1:E:1407:ASP:HA	1:E:1483:GLU:OE2	2.14	0.48
1:F:1407:ASP:HA	1:F:1483:GLU:OE2	2.14	0.48
1:A:512:PHE:HA	1:A:516:GLU:HG3	1.96	0.48
1:C:1407:ASP:HA	1:C:1483:GLU:OE2	2.14	0.48
1:D:980:THR:HG22	1:D:982:THR:H	1.78	0.48
1:D:1117:ARG:HG2	1:D:1135:SER:HB3	1.95	0.48
1:E:980:THR:HG22	1:E:982:THR:H	1.78	0.48
1:F:1275:TRP:HB2	1:F:1284:MET:HG2	1.96	0.48
1:A:1407:ASP:HA	1:A:1483:GLU:OE2	2.14	0.48
1:B:1440:THR:N	1:B:1470:LEU:O	2.40	0.48
1:C:449:THR:HG21	1:D:859:ILE:H	1.79	0.48
1:C:512:PHE:HA	1:C:516:GLU:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1275:TRP:HB2	1:A:1284:MET:HG2	1.96	0.47
1:B:512:PHE:HA	1:B:516:GLU:HG3	1.96	0.47
1:B:1407:ASP:HA	1:B:1483:GLU:OE2	2.14	0.47
1:C:466:ASP:N	1:C:466:ASP:OD2	2.43	0.47
1:C:500:VAL:O	1:C:578:ARG:NH2	2.40	0.47
1:D:984:LEU:HA	1:E:1397:LEU:HD13	1.94	0.47
1:D:995:ASP:N	1:D:999:GLU:O	2.45	0.47
1:F:552:THR:HG22	1:F:654:ASN:H	1.79	0.47
1:A:644:THR:O	1:A:699:ASN:N	2.45	0.47
1:F:1440:THR:N	1:F:1470:LEU:O	2.40	0.47
1:A:552:THR:HG22	1:A:654:ASN:H	1.79	0.47
1:A:859:ILE:H	1:F:449:THR:HG21	1.79	0.47
1:B:1117:ARG:HG2	1:B:1135:SER:HB3	1.95	0.47
1:C:833:ASN:OD1	1:C:833:ASN:N	2.46	0.47
1:E:984:LEU:HA	1:F:1397:LEU:HD13	1.96	0.47
1:F:512:PHE:HA	1:F:516:GLU:HG3	1.96	0.47
1:B:644:THR:O	1:B:699:ASN:N	2.45	0.47
1:A:833:ASN:OD1	1:A:833:ASN:N	2.46	0.47
1:D:512:PHE:HA	1:D:516:GLU:HG3	1.96	0.47
1:A:449:THR:HG21	1:B:859:ILE:H	1.80	0.47
1:F:704:MET:HB3	1:F:706:PHE:CE2	2.50	0.47
1:A:1117:ARG:HG2	1:A:1135:SER:HB3	1.95	0.47
1:B:1447:ALA:N	1:B:1455:ASP:OD2	2.48	0.47
1:E:449:THR:HG21	1:F:859:ILE:H	1.80	0.47
1:E:1099:SER:OG	1:E:1207:GLN:NE2	2.46	0.47
1:F:1044:ARG:HG2	1:F:1169:HIS:HB3	1.97	0.47
1:B:1043:GLY:O	1:B:1348:TYR:OH	2.31	0.47
1:D:1447:ALA:N	1:D:1455:ASP:OD2	2.48	0.47
1:E:1044:ARG:HG2	1:E:1169:HIS:HB3	1.97	0.47
1:E:1447:ALA:N	1:E:1455:ASP:OD2	2.48	0.47
1:F:1099:SER:OG	1:F:1207:GLN:NE2	2.46	0.47
1:A:704:MET:HB3	1:A:706:PHE:CE2	2.50	0.47
1:A:1447:ALA:N	1:A:1455:ASP:OD2	2.48	0.47
1:B:704:MET:HB3	1:B:706:PHE:CE2	2.50	0.47
1:C:1044:ARG:HG2	1:C:1169:HIS:HB3	1.97	0.47
1:F:1447:ALA:N	1:F:1455:ASP:OD2	2.48	0.47
1:C:1447:ALA:N	1:C:1455:ASP:OD2	2.48	0.47
1:E:552:THR:HG22	1:E:654:ASN:H	1.79	0.47
1:E:1275:TRP:HB2	1:E:1284:MET:HG2	1.96	0.47
1:B:552:THR:HG22	1:B:654:ASN:H	1.79	0.46
1:F:1117:ARG:HG2	1:F:1135:SER:HB3	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1044:ARG:HG2	1:B:1169:HIS:HB3	1.97	0.46
1:D:1099:SER:OG	1:D:1207:GLN:NE2	2.46	0.46
1:E:512:PHE:HA	1:E:516:GLU:HG3	1.96	0.46
1:A:1099:SER:OG	1:A:1207:GLN:NE2	2.46	0.46
1:C:786:ASP:OD1	1:C:786:ASP:N	2.49	0.46
1:E:625:PHE:CE1	1:E:627:TYR:HB3	2.50	0.46
1:B:995:ASP:N	1:B:999:GLU:O	2.45	0.46
1:D:704:MET:HB3	1:D:706:PHE:CE2	2.50	0.46
1:D:1044:ARG:HG2	1:D:1169:HIS:HB3	1.97	0.46
1:D:1275:TRP:HB2	1:D:1284:MET:HG2	1.96	0.46
1:E:786:ASP:N	1:E:786:ASP:OD1	2.49	0.46
1:E:794:ASP:OD1	1:E:998:GLY:HA3	2.16	0.46
1:F:1270:LEU:HD21	1:F:1284:MET:HB2	1.98	0.46
1:B:626:ASN:O	1:B:720:MET:HA	2.16	0.46
1:C:773:ASP:OD2	1:C:775:GLY:N	2.43	0.46
1:E:995:ASP:N	1:E:999:GLU:O	2.45	0.46
1:E:1050:HIS:CD2	1:E:1051:ALA:H	2.33	0.46
1:E:1238:SER:HG	1:E:1243:TYR:HH	1.60	0.46
1:F:500:VAL:O	1:F:578:ARG:NH2	2.40	0.46
1:F:605:LEU:HD13	1:F:698:VAL:HG13	1.98	0.46
1:A:1397:LEU:HD13	1:F:984:LEU:HA	1.98	0.46
1:B:625:PHE:CE1	1:B:627:TYR:HB3	2.50	0.46
1:C:704:MET:HB3	1:C:706:PHE:CE2	2.50	0.46
1:D:1050:HIS:CD2	1:D:1051:ALA:H	2.34	0.46
1:E:1270:LEU:HD21	1:E:1284:MET:HB2	1.98	0.46
1:A:770:ASN:HB2	1:A:776:THR:HG21	1.98	0.46
1:C:552:THR:HG22	1:C:654:ASN:H	1.79	0.46
1:C:644:THR:O	1:C:699:ASN:N	2.45	0.46
1:D:552:THR:HG22	1:D:654:ASN:H	1.79	0.46
1:F:1050:HIS:CD2	1:F:1051:ALA:H	2.33	0.46
1:A:1050:HIS:CD2	1:A:1051:ALA:H	2.33	0.46
1:B:730:ASP:HA	1:B:884:LEU:HD23	1.98	0.46
1:C:626:ASN:O	1:C:720:MET:HA	2.16	0.46
1:E:704:MET:HB3	1:E:706:PHE:CE2	2.50	0.46
1:F:644:THR:O	1:F:699:ASN:N	2.45	0.46
1:A:1044:ARG:HG2	1:A:1169:HIS:HB3	1.97	0.46
1:B:984:LEU:HA	1:C:1397:LEU:HD13	1.97	0.46
1:C:730:ASP:HA	1:C:884:LEU:HD23	1.98	0.46
1:C:1050:HIS:CD2	1:C:1051:ALA:H	2.33	0.46
1:E:605:LEU:HD13	1:E:698:VAL:HG13	1.98	0.46
1:A:626:ASN:O	1:A:720:MET:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:786:ASP:OD1	1:B:786:ASP:N	2.49	0.45
1:C:1369:VAL:HG22	1:C:1386:ILE:HG12	1.98	0.45
1:D:895:VAL:HG12	1:D:988:VAL:HG12	1.98	0.45
1:F:794:ASP:OD1	1:F:998:GLY:HA3	2.16	0.45
1:A:1206:LEU:O	1:A:1227:ALA:N	2.40	0.45
1:D:794:ASP:OD1	1:D:998:GLY:HA3	2.16	0.45
1:E:626:ASN:O	1:E:720:MET:HA	2.16	0.45
1:C:794:ASP:OD1	1:C:998:GLY:HA3	2.16	0.45
1:C:984:LEU:HA	1:D:1397:LEU:HD13	1.97	0.45
1:D:1043:GLY:O	1:D:1348:TYR:OH	2.31	0.45
1:A:794:ASP:OD1	1:A:998:GLY:HA3	2.16	0.45
1:B:794:ASP:OD1	1:B:998:GLY:HA3	2.16	0.45
1:B:795:LEU:HB3	1:B:799:ASP:O	2.17	0.45
1:B:1270:LEU:HD21	1:B:1284:MET:HB2	1.98	0.45
1:C:1270:LEU:HD21	1:C:1284:MET:HB2	1.98	0.45
1:D:449:THR:HG21	1:E:859:ILE:H	1.81	0.45
1:F:833:ASN:OD1	1:F:833:ASN:N	2.46	0.45
1:A:605:LEU:HD13	1:A:698:VAL:HG13	1.98	0.45
1:B:723:PHE:HE1	1:B:742:ILE:HG22	1.82	0.45
1:B:770:ASN:HB2	1:B:776:THR:HG21	1.98	0.45
1:B:1050:HIS:CD2	1:B:1051:ALA:H	2.33	0.45
1:C:770:ASN:HB2	1:C:776:THR:HG21	1.98	0.45
1:E:723:PHE:HE1	1:E:742:ILE:HG22	1.82	0.45
1:E:773:ASP:OD2	1:E:775:GLY:N	2.43	0.45
1:F:625:PHE:CE1	1:F:627:TYR:HB3	2.50	0.45
1:B:1014:GLY:N	1:B:1212:ASP:OD2	2.50	0.45
1:C:848:GLU:O	1:C:848:GLU:HG3	2.17	0.45
1:D:605:LEU:HD13	1:D:698:VAL:HG13	1.98	0.45
1:D:770:ASN:HB2	1:D:776:THR:HG21	1.98	0.45
1:D:848:GLU:HG3	1:D:848:GLU:O	2.17	0.45
1:F:461:ILE:HG12	1:F:476:VAL:HG22	1.98	0.45
1:A:1270:LEU:O	1:A:1273:ILE:HG22	2.17	0.45
1:D:1014:GLY:N	1:D:1212:ASP:OD2	2.50	0.45
1:D:1369:VAL:HG22	1:D:1386:ILE:HG12	1.98	0.45
1:E:1369:VAL:HG22	1:E:1386:ILE:HG12	1.98	0.45
1:F:1369:VAL:HG22	1:F:1386:ILE:HG12	1.98	0.45
1:C:895:VAL:HG12	1:C:988:VAL:HG12	1.98	0.45
1:D:1270:LEU:HD21	1:D:1284:MET:HB2	1.98	0.45
1:E:895:VAL:HG12	1:E:988:VAL:HG12	1.98	0.45
1:E:1043:GLY:O	1:E:1348:TYR:OH	2.31	0.45
1:F:1270:LEU:O	1:F:1273:ILE:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:PHE:CE1	1:A:627:TYR:HB3	2.50	0.45
1:A:1369:VAL:HG22	1:A:1386:ILE:HG12	1.98	0.45
1:B:466:ASP:OD2	1:B:466:ASP:N	2.43	0.45
1:B:605:LEU:HD13	1:B:698:VAL:HG13	1.98	0.45
1:C:795:LEU:HB3	1:C:799:ASP:O	2.17	0.45
1:C:1068:ASP:OD2	1:C:1156:LYS:NZ	2.34	0.45
1:D:626:ASN:O	1:D:720:MET:HA	2.16	0.45
1:F:786:ASP:OD1	1:F:786:ASP:N	2.49	0.45
1:A:723:PHE:HE1	1:A:742:ILE:HG22	1.82	0.45
1:A:795:LEU:HB3	1:A:799:ASP:O	2.17	0.45
1:F:626:ASN:O	1:F:720:MET:HA	2.16	0.45
1:A:730:ASP:HA	1:A:884:LEU:HD23	1.98	0.44
1:A:903:SER:OG	1:A:974:TYR:OH	2.29	0.44
1:B:1369:VAL:HG22	1:B:1386:ILE:HG12	1.98	0.44
1:C:723:PHE:HE1	1:C:742:ILE:HG22	1.82	0.44
1:D:1270:LEU:O	1:D:1273:ILE:HG22	2.17	0.44
1:C:460:ASP:OD2	1:C:461:ILE:N	2.50	0.44
1:C:1099:SER:OG	1:C:1207:GLN:NE2	2.46	0.44
1:C:1270:LEU:O	1:C:1273:ILE:HG22	2.17	0.44
1:D:723:PHE:HE1	1:D:742:ILE:HG22	1.82	0.44
1:E:461:ILE:HG12	1:E:476:VAL:HG22	1.99	0.44
1:C:605:LEU:HD13	1:C:698:VAL:HG13	1.98	0.44
1:C:903:SER:OG	1:C:974:TYR:OH	2.29	0.44
1:D:730:ASP:HA	1:D:884:LEU:HD23	1.98	0.44
1:E:848:GLU:O	1:E:848:GLU:HG3	2.17	0.44
1:F:848:GLU:O	1:F:848:GLU:HG3	2.17	0.44
1:A:461:ILE:HG12	1:A:476:VAL:HG22	1.98	0.44
1:A:786:ASP:OD1	1:A:786:ASP:N	2.49	0.44
1:A:1270:LEU:HD21	1:A:1284:MET:HB2	1.98	0.44
1:B:1270:LEU:O	1:B:1273:ILE:HG22	2.17	0.44
1:C:1014:GLY:N	1:C:1212:ASP:OD2	2.50	0.44
1:B:1273:ILE:HD12	1:B:1273:ILE:HA	1.85	0.44
1:D:460:ASP:OD2	1:D:461:ILE:N	2.51	0.44
1:E:770:ASN:HB2	1:E:776:THR:HG21	1.98	0.44
1:E:1270:LEU:O	1:E:1273:ILE:HG22	2.17	0.44
1:F:730:ASP:HA	1:F:884:LEU:HD23	1.98	0.44
1:A:848:GLU:O	1:A:848:GLU:HG3	2.17	0.44
1:D:795:LEU:HB3	1:D:799:ASP:O	2.17	0.44
1:E:730:ASP:HA	1:E:884:LEU:HD23	1.98	0.44
1:A:1026:PRO:HG2	1:A:1157:PHE:HA	2.00	0.44
1:B:848:GLU:HG3	1:B:848:GLU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1143:ALA:HB3	1:C:1146:ALA:HB2	2.00	0.44
1:E:795:LEU:HB3	1:E:799:ASP:O	2.17	0.44
1:E:1096:LEU:HD12	1:E:1210:TYR:HB2	2.00	0.44
1:F:770:ASN:HB2	1:F:776:THR:HG21	1.98	0.44
1:A:1267:THR:HB	1:A:1304:ARG:HH12	1.83	0.44
1:B:1026:PRO:HG2	1:B:1157:PHE:HA	2.00	0.44
1:E:644:THR:O	1:E:699:ASN:N	2.45	0.44
1:E:1014:GLY:N	1:E:1212:ASP:OD2	2.50	0.44
1:B:460:ASP:OD2	1:B:461:ILE:N	2.50	0.44
1:D:644:THR:O	1:D:699:ASN:N	2.45	0.44
1:E:460:ASP:OD2	1:E:461:ILE:N	2.50	0.44
1:F:460:ASP:OD2	1:F:461:ILE:N	2.50	0.44
1:F:1267:THR:HB	1:F:1304:ARG:HH12	1.83	0.44
1:B:449:THR:HG21	1:C:859:ILE:H	1.82	0.43
1:C:461:ILE:HG12	1:C:476:VAL:HG22	1.99	0.43
1:D:1143:ALA:HB3	1:D:1146:ALA:HB2	2.00	0.43
1:E:493:LEU:HD22	1:E:747:ALA:HB3	2.00	0.43
1:F:723:PHE:HE1	1:F:742:ILE:HG22	1.82	0.43
1:F:1026:PRO:HG2	1:F:1157:PHE:HA	2.00	0.43
1:B:895:VAL:HG12	1:B:988:VAL:HG12	1.98	0.43
1:B:1143:ALA:HB3	1:B:1146:ALA:HB2	2.00	0.43
1:D:461:ILE:HG12	1:D:476:VAL:HG22	1.99	0.43
1:D:786:ASP:OD1	1:D:786:ASP:N	2.49	0.43
1:F:493:LEU:HD22	1:F:747:ALA:HB3	2.00	0.43
1:F:795:LEU:HB3	1:F:799:ASP:O	2.17	0.43
1:F:895:VAL:HG12	1:F:988:VAL:HG12	1.98	0.43
1:A:1096:LEU:HD12	1:A:1210:TYR:HB2	2.00	0.43
1:A:1422:LYS:NZ	1:F:1219:ASP:OD2	2.33	0.43
1:E:1267:THR:HB	1:E:1304:ARG:HH12	1.83	0.43
1:F:1143:ALA:HB3	1:F:1146:ALA:HB2	2.00	0.43
1:A:1122:ASP:OD1	1:A:1123:VAL:N	2.52	0.43
1:B:461:ILE:HG12	1:B:476:VAL:HG22	1.99	0.43
1:C:1206:LEU:O	1:C:1227:ALA:N	2.40	0.43
1:F:1014:GLY:N	1:F:1212:ASP:OD2	2.50	0.43
1:A:460:ASP:OD2	1:A:461:ILE:N	2.50	0.43
1:A:858:LEU:HG	1:F:449:THR:HB	2.00	0.43
1:B:493:LEU:HD22	1:B:747:ALA:HB3	2.00	0.43
1:B:1267:THR:HB	1:B:1304:ARG:HH12	1.83	0.43
1:F:1273:ILE:HD12	1:F:1273:ILE:HA	1.85	0.43
1:A:1014:GLY:N	1:A:1212:ASP:OD2	2.50	0.43
1:C:1026:PRO:HG2	1:C:1157:PHE:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1026:PRO:HG2	1:E:1157:PHE:HA	2.00	0.43
1:F:1122:ASP:OD1	1:F:1123:VAL:N	2.52	0.43
1:C:493:LEU:HD22	1:C:747:ALA:HB3	2.00	0.43
1:C:1219:ASP:OD2	1:D:1422:LYS:NZ	2.33	0.43
1:D:1096:LEU:HD12	1:D:1210:TYR:HB2	2.00	0.43
1:A:895:VAL:HG12	1:A:988:VAL:HG12	1.98	0.43
1:B:986:ILE:N	1:B:1007:ALA:O	2.52	0.43
1:B:1096:LEU:HD12	1:B:1210:TYR:HB2	2.00	0.43
1:F:995:ASP:N	1:F:999:GLU:O	2.45	0.43
1:D:986:ILE:N	1:D:1007:ALA:O	2.52	0.43
1:E:833:ASN:OD1	1:E:833:ASN:N	2.46	0.43
1:A:1143:ALA:HB3	1:A:1146:ALA:HB2	2.00	0.43
1:B:985:ASP:OD1	1:B:985:ASP:N	2.49	0.43
1:B:1122:ASP:OD1	1:B:1123:VAL:N	2.52	0.43
1:E:449:THR:HB	1:F:858:LEU:HG	2.00	0.43
1:E:986:ILE:N	1:E:1007:ALA:O	2.52	0.43
1:F:986:ILE:N	1:F:1007:ALA:O	2.52	0.43
1:F:1480:VAL:O	1:F:1492:GLY:N	2.42	0.43
1:C:1024:PRO:HB3	1:C:1257:ASP:HA	2.01	0.42
1:C:1096:LEU:HD12	1:C:1210:TYR:HB2	2.00	0.42
1:D:1122:ASP:OD1	1:D:1123:VAL:N	2.52	0.42
1:E:874:ASP:OD2	1:E:904:THR:HG22	2.20	0.42
1:A:466:ASP:OD2	1:A:466:ASP:N	2.44	0.42
1:A:986:ILE:N	1:A:1007:ALA:O	2.52	0.42
1:B:449:THR:HB	1:C:858:LEU:HG	2.01	0.42
1:C:874:ASP:OD2	1:C:904:THR:HG22	2.19	0.42
1:C:1436:GLU:OE1	1:C:1466:THR:HG22	2.19	0.42
1:F:1096:LEU:HD12	1:F:1210:TYR:HB2	2.00	0.42
1:C:1122:ASP:OD1	1:C:1123:VAL:N	2.52	0.42
1:D:1024:PRO:HB3	1:D:1257:ASP:HA	2.01	0.42
1:D:1267:THR:HB	1:D:1304:ARG:HH12	1.83	0.42
1:E:1143:ALA:HB3	1:E:1146:ALA:HB2	2.00	0.42
1:F:773:ASP:OD2	1:F:775:GLY:N	2.43	0.42
1:A:449:THR:HB	1:B:858:LEU:HG	2.01	0.42
1:A:1024:PRO:HB3	1:A:1257:ASP:HA	2.01	0.42
1:A:1268:TYR:O	1:A:1302:ASP:HB3	2.20	0.42
1:B:1024:PRO:HB3	1:B:1257:ASP:HA	2.01	0.42
1:B:1436:GLU:OE1	1:B:1466:THR:HG22	2.19	0.42
1:F:1024:PRO:HB3	1:F:1257:ASP:HA	2.01	0.42
1:A:493:LEU:HD22	1:A:747:ALA:HB3	2.00	0.42
1:B:874:ASP:OD2	1:B:904:THR:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:449:THR:HB	1:D:858:LEU:HG	2.00	0.42
1:D:1268:TYR:O	1:D:1302:ASP:HB3	2.20	0.42
1:E:1122:ASP:OD1	1:E:1123:VAL:N	2.52	0.42
1:F:1268:TYR:O	1:F:1302:ASP:HB3	2.20	0.42
1:B:721:ASP:N	1:B:721:ASP:OD1	2.53	0.42
1:B:1099:SER:OG	1:B:1207:GLN:NE2	2.46	0.42
1:C:995:ASP:N	1:C:999:GLU:O	2.45	0.42
1:D:493:LEU:HD22	1:D:747:ALA:HB3	2.00	0.42
1:D:514:ILE:O	1:D:600:LEU:HD12	2.20	0.42
1:D:1026:PRO:HG2	1:D:1157:PHE:HA	2.00	0.42
1:E:1268:TYR:O	1:E:1302:ASP:HB3	2.20	0.42
1:F:909:ASN:ND2	1:F:971:PRO:O	2.46	0.42
1:A:446:THR:O	1:A:446:THR:OG1	2.36	0.42
1:A:514:ILE:O	1:A:600:LEU:HD12	2.20	0.42
1:B:579:LEU:HD22	1:B:718:ILE:HB	2.02	0.42
1:B:773:ASP:OD2	1:B:775:GLY:N	2.43	0.42
1:C:579:LEU:HD22	1:C:718:ILE:HB	2.02	0.42
1:D:833:ASN:OD1	1:D:833:ASN:N	2.46	0.42
1:F:514:ILE:O	1:F:600:LEU:HD12	2.20	0.42
1:F:721:ASP:OD1	1:F:721:ASP:N	2.53	0.42
1:A:874:ASP:OD2	1:A:904:THR:HG22	2.20	0.42
1:C:514:ILE:O	1:C:600:LEU:HD12	2.20	0.42
1:C:595:PHE:N	1:C:595:PHE:CD2	2.88	0.42
1:C:1267:THR:HB	1:C:1304:ARG:HH12	1.83	0.42
1:F:762:GLU:O	1:F:788:SER:HA	2.20	0.42
1:F:1255:GLU:HA	1:F:1256:PRO:HD3	1.89	0.42
1:A:852:LEU:HD11	1:A:990:TYR:OH	2.20	0.42
1:A:1273:ILE:HD12	1:A:1273:ILE:HA	1.85	0.42
1:C:986:ILE:N	1:C:1007:ALA:O	2.52	0.42
1:C:1268:TYR:O	1:C:1302:ASP:HB3	2.20	0.42
1:D:721:ASP:OD1	1:D:721:ASP:N	2.53	0.42
1:D:893:LEU:HD12	1:D:894:ASP:N	2.35	0.42
1:E:446:THR:O	1:E:446:THR:OG1	2.36	0.42
1:F:874:ASP:OD2	1:F:904:THR:HG22	2.19	0.42
1:A:595:PHE:N	1:A:595:PHE:CD2	2.88	0.42
1:A:762:GLU:O	1:A:788:SER:HA	2.20	0.42
1:A:828:GLY:HA3	1:A:990:TYR:HE2	1.85	0.42
1:A:1100:VAL:HG22	1:A:1206:LEU:HD13	2.02	0.42
1:B:595:PHE:N	1:B:595:PHE:CD2	2.88	0.42
1:B:893:LEU:HD12	1:B:894:ASP:N	2.35	0.42
1:C:893:LEU:HD12	1:C:894:ASP:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:595:PHE:N	1:E:595:PHE:CD2	2.88	0.42
1:D:1436:GLU:OE1	1:D:1466:THR:HG22	2.19	0.41
1:A:1043:GLY:O	1:A:1348:TYR:OH	2.31	0.41
1:B:1268:TYR:O	1:B:1302:ASP:HB3	2.20	0.41
1:C:1070:THR:HG22	1:C:1154:ASN:HB3	2.02	0.41
1:D:625:PHE:CE1	1:D:627:TYR:HB3	2.51	0.41
1:D:874:ASP:OD2	1:D:904:THR:HG22	2.19	0.41
1:D:1100:VAL:HG22	1:D:1206:LEU:HD13	2.02	0.41
1:E:721:ASP:OD1	1:E:721:ASP:N	2.53	0.41
1:D:595:PHE:CD2	1:D:595:PHE:N	2.88	0.41
1:D:1070:THR:HG22	1:D:1154:ASN:HB3	2.02	0.41
1:E:762:GLU:O	1:E:788:SER:HA	2.20	0.41
1:E:852:LEU:HD11	1:E:990:TYR:OH	2.20	0.41
1:E:893:LEU:HD12	1:E:894:ASP:N	2.35	0.41
1:E:1100:VAL:HG22	1:E:1206:LEU:HD13	2.02	0.41
1:F:852:LEU:HD11	1:F:990:TYR:OH	2.20	0.41
1:B:762:GLU:O	1:B:788:SER:HA	2.20	0.41
1:C:852:LEU:HD11	1:C:990:TYR:OH	2.20	0.41
1:E:1436:GLU:OE1	1:E:1466:THR:HG22	2.20	0.41
1:F:519:THR:HA	1:F:520:PRO:HD3	1.94	0.41
1:A:893:LEU:HD12	1:A:894:ASP:N	2.35	0.41
1:B:514:ILE:O	1:B:600:LEU:HD12	2.20	0.41
1:B:828:GLY:HA3	1:B:990:TYR:HE2	1.85	0.41
1:C:895:VAL:HG22	1:C:934:LEU:HD22	2.03	0.41
1:C:1100:VAL:HG22	1:C:1206:LEU:HD13	2.02	0.41
1:D:449:THR:HB	1:E:858:LEU:HG	2.02	0.41
1:D:852:LEU:HD11	1:D:990:TYR:OH	2.20	0.41
1:D:895:VAL:HG22	1:D:934:LEU:HD22	2.03	0.41
1:F:595:PHE:N	1:F:595:PHE:CD2	2.88	0.41
1:A:525:THR:HB	1:A:595:PHE:HB2	2.03	0.41
1:A:1219:ASP:OD2	1:B:1422:LYS:NZ	2.35	0.41
1:A:1436:GLU:OE1	1:A:1466:THR:HG22	2.20	0.41
1:C:553:LEU:HB2	1:C:595:PHE:HE1	1.85	0.41
1:C:721:ASP:OD1	1:C:721:ASP:N	2.53	0.41
1:D:1077:ASP:OD2	1:D:1210:TYR:OH	2.38	0.41
1:E:514:ILE:O	1:E:600:LEU:HD12	2.20	0.41
1:E:828:GLY:HA3	1:E:990:TYR:HE2	1.85	0.41
1:F:1043:GLY:O	1:F:1348:TYR:OH	2.31	0.41
1:C:525:THR:HB	1:C:595:PHE:HB2	2.03	0.41
1:C:1412:SER:HA	1:C:1417:ASP:HA	2.03	0.41
1:D:825:SER:HB3	1:D:995:ASP:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:828:GLY:HA3	1:D:990:TYR:HE2	1.85	0.41
1:E:845:ILE:N	1:E:953:GLY:O	2.35	0.41
1:E:1068:ASP:OD2	1:E:1156:LYS:NZ	2.34	0.41
1:E:1480:VAL:O	1:E:1492:GLY:N	2.42	0.41
1:F:1460:THR:HG23	1:F:1470:LEU:HD12	2.02	0.41
1:B:1070:THR:HG22	1:B:1154:ASN:HB3	2.02	0.41
1:C:1077:ASP:OD2	1:C:1210:TYR:OH	2.38	0.41
1:D:553:LEU:HB2	1:D:595:PHE:HE1	1.86	0.41
1:D:1092:GLN:NE2	1:D:1213:PRO:HB3	2.36	0.41
1:F:478:ILE:O	1:F:757:PHE:N	2.44	0.41
1:F:828:GLY:HA3	1:F:990:TYR:HE2	1.85	0.41
1:F:1100:VAL:HG22	1:F:1206:LEU:HD13	2.02	0.41
1:F:1436:GLU:OE1	1:F:1466:THR:HG22	2.20	0.41
1:A:586:ASN:HB3	1:A:591:PHE:CE1	2.56	0.41
1:A:721:ASP:OD1	1:A:721:ASP:N	2.53	0.41
1:A:773:ASP:OD2	1:A:775:GLY:N	2.43	0.41
1:A:793:GLU:O	1:A:795:LEU:N	2.54	0.41
1:A:1480:VAL:O	1:A:1492:GLY:N	2.43	0.41
1:B:525:THR:HB	1:B:595:PHE:HB2	2.03	0.41
1:B:793:GLU:O	1:B:795:LEU:N	2.54	0.41
1:B:852:LEU:HD11	1:B:990:TYR:OH	2.20	0.41
1:B:1412:SER:HA	1:B:1417:ASP:HA	2.03	0.41
1:B:1460:THR:HG23	1:B:1470:LEU:HD12	2.02	0.41
1:C:1013:THR:HG22	1:C:1215:ASP:HB2	2.03	0.41
1:D:525:THR:HB	1:D:595:PHE:HB2	2.03	0.41
1:D:762:GLU:O	1:D:788:SER:HA	2.20	0.41
1:D:1013:THR:HG22	1:D:1215:ASP:HB2	2.03	0.41
1:D:1460:THR:HG23	1:D:1470:LEU:HD12	2.02	0.41
1:E:586:ASN:HB3	1:E:591:PHE:CE1	2.56	0.41
1:E:825:SER:HB3	1:E:995:ASP:O	2.21	0.41
1:E:903:SER:OG	1:E:974:TYR:OH	2.29	0.41
1:E:1024:PRO:HB3	1:E:1257:ASP:HA	2.01	0.41
1:E:1092:GLN:NE2	1:E:1213:PRO:HB3	2.36	0.41
1:E:1255:GLU:HA	1:E:1256:PRO:HD3	1.89	0.41
1:F:579:LEU:HD22	1:F:718:ILE:HB	2.02	0.41
1:F:586:ASN:HB3	1:F:591:PHE:CE1	2.56	0.41
1:F:793:GLU:O	1:F:795:LEU:N	2.54	0.41
1:F:893:LEU:HD12	1:F:894:ASP:N	2.35	0.41
1:F:1070:THR:HG22	1:F:1154:ASN:HB3	2.02	0.41
1:B:1100:VAL:HG22	1:B:1206:LEU:HD13	2.02	0.41
1:B:1219:ASP:OD2	1:C:1422:LYS:NZ	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1411:VAL:HG23	1:B:1480:VAL:HG22	2.03	0.41
1:C:762:GLU:O	1:C:788:SER:HA	2.20	0.41
1:C:828:GLY:HA3	1:C:990:TYR:HE2	1.85	0.41
1:D:793:GLU:O	1:D:795:LEU:N	2.54	0.41
1:D:1335:ILE:HD13	1:D:1335:ILE:HA	1.93	0.41
1:D:1411:VAL:HG23	1:D:1480:VAL:HG22	2.03	0.41
1:F:525:THR:HB	1:F:595:PHE:HB2	2.03	0.41
1:F:553:LEU:HB2	1:F:595:PHE:HE1	1.85	0.41
1:A:1426:THR:HG22	1:A:1432:ILE:O	2.22	0.40
1:C:793:GLU:O	1:C:795:LEU:N	2.54	0.40
1:D:1246:GLY:H	1:D:1319:ILE:HB	1.86	0.40
1:E:540:ILE:HD13	1:E:540:ILE:HA	1.84	0.40
1:E:1070:THR:HG22	1:E:1154:ASN:HB3	2.02	0.40
1:E:1246:GLY:H	1:E:1319:ILE:HB	1.86	0.40
1:E:1412:SER:HA	1:E:1417:ASP:HA	2.03	0.40
1:E:1460:THR:HG23	1:E:1470:LEU:HD12	2.02	0.40
1:F:731:GLY:HA2	1:F:736:GLU:HG3	2.03	0.40
1:A:579:LEU:HD22	1:A:718:ILE:HB	2.02	0.40
1:A:1246:GLY:H	1:A:1319:ILE:HB	1.86	0.40
1:A:1460:THR:HG23	1:A:1470:LEU:HD12	2.02	0.40
1:B:553:LEU:HB2	1:B:595:PHE:HE1	1.86	0.40
1:B:1013:THR:HG22	1:B:1215:ASP:HB2	2.03	0.40
1:B:1202:GLN:NE2	1:B:1346:SER:O	2.54	0.40
1:C:731:GLY:HA2	1:C:736:GLU:HG3	2.03	0.40
1:D:731:GLY:HA2	1:D:736:GLU:HG3	2.03	0.40
1:D:1390:ASP:N	1:D:1390:ASP:OD1	2.54	0.40
1:E:579:LEU:HD22	1:E:718:ILE:HB	2.02	0.40
1:E:895:VAL:HG22	1:E:934:LEU:HD22	2.03	0.40
1:E:1219:ASP:OD2	1:F:1422:LYS:NZ	2.34	0.40
1:F:1092:GLN:NE2	1:F:1213:PRO:HB3	2.36	0.40
1:B:895:VAL:HG22	1:B:934:LEU:HD22	2.03	0.40
1:B:1246:GLY:H	1:B:1319:ILE:HB	1.86	0.40
1:B:1346:SER:OG	1:B:1348:TYR:O	2.38	0.40
1:C:825:SER:HB3	1:C:995:ASP:O	2.21	0.40
1:C:1411:VAL:HG23	1:C:1480:VAL:HG22	2.03	0.40
1:F:1412:SER:HA	1:F:1417:ASP:HA	2.03	0.40
1:A:731:GLY:HA2	1:A:736:GLU:HG3	2.03	0.40
1:A:1070:THR:HG22	1:A:1154:ASN:HB3	2.02	0.40
1:B:1426:THR:HG22	1:B:1432:ILE:O	2.22	0.40
1:C:1092:GLN:NE2	1:C:1213:PRO:HB3	2.36	0.40
1:D:736:GLU:H	1:D:736:GLU:HG2	1.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:478:ILE:O	1:E:757:PHE:N	2.44	0.40
1:E:1273:ILE:HD12	1:E:1273:ILE:HA	1.85	0.40
1:F:702:PHE:CZ	1:F:722:PHE:HE2	2.40	0.40
1:A:1346:SER:OG	1:A:1348:TYR:O	2.38	0.40
1:A:1411:VAL:HG23	1:A:1480:VAL:HG22	2.03	0.40
1:C:625:PHE:CE1	1:C:627:TYR:HB3	2.50	0.40
1:C:1411:VAL:CG1	1:C:1418:LEU:HB2	2.52	0.40
1:C:1421:TYR:CZ	1:C:1437:VAL:HG22	2.57	0.40
1:D:934:LEU:HD12	1:D:934:LEU:HA	1.92	0.40
1:E:525:THR:HB	1:E:595:PHE:HB2	2.03	0.40
1:E:793:GLU:O	1:E:795:LEU:N	2.54	0.40
1:E:995:ASP:OD2	1:E:995:ASP:C	2.60	0.40
1:F:825:SER:HB3	1:F:995:ASP:O	2.21	0.40
1:F:995:ASP:OD2	1:F:995:ASP:C	2.60	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	1051/1734 (61%)	1024 (97%)	27 (3%)	0	100	100
1	B	1051/1734 (61%)	1024 (97%)	27 (3%)	0	100	100
1	C	1051/1734 (61%)	1025 (98%)	26 (2%)	0	100	100
1	D	1051/1734 (61%)	1025 (98%)	26 (2%)	0	100	100
1	E	1051/1734 (61%)	1024 (97%)	27 (3%)	0	100	100
1	F	1051/1734 (61%)	1025 (98%)	26 (2%)	0	100	100
All	All	6306/10404 (61%)	6147 (98%)	159 (2%)	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	A	879/1438 (61%)	858 (98%)	21 (2%)	49	74
1	B	879/1438 (61%)	858 (98%)	21 (2%)	49	74
1	C	879/1438 (61%)	858 (98%)	21 (2%)	49	74
1	D	879/1438 (61%)	858 (98%)	21 (2%)	49	74
1	E	879/1438 (61%)	858 (98%)	21 (2%)	49	74
1	F	879/1438 (61%)	858 (98%)	21 (2%)	49	74
All	All	5274/8628 (61%)	5148 (98%)	126 (2%)	51	74

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	507	ARG
1	A	591	PHE
1	A	649	LEU
1	A	661	LYS
1	A	721	ASP
1	A	857	ASP
1	A	874	ASP
1	A	918	ASP
1	A	995	ASP
1	A	1068	ASP
1	A	1152	ASP
1	A	1170	ASP
1	A	1219	ASP
1	A	1232	ARG
1	A	1278	ASP
1	A	1296	PHE
1	A	1308	ASP
1	A	1330	ARG
1	A	1338	TYR
1	A	1347	ASP
1	A	1378	TRP
1	B	507	ARG

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Mol	Chain	Res	Type
1	B	591	PHE
1	B	649	LEU
1	B	661	LYS
1	B	721	ASP
1	B	857	ASP
1	B	874	ASP
1	B	918	ASP
1	B	995	ASP
1	B	1068	ASP
1	B	1152	ASP
1	B	1170	ASP
1	B	1219	ASP
1	B	1232	ARG
1	B	1278	ASP
1	B	1296	PHE
1	B	1308	ASP
1	B	1330	ARG
1	B	1338	TYR
1	B	1347	ASP
1	B	1378	TRP
1	C	507	ARG
1	C	591	PHE
1	C	649	LEU
1	C	661	LYS
1	C	721	ASP
1	C	857	ASP
1	C	874	ASP
1	C	918	ASP
1	C	995	ASP
1	C	1068	ASP
1	C	1152	ASP
1	C	1170	ASP
1	C	1219	ASP
1	C	1232	ARG
1	C	1278	ASP
1	C	1296	PHE
1	C	1308	ASP
1	C	1330	ARG
1	C	1338	TYR
1	C	1347	ASP
1	C	1378	TRP
1	D	507	ARG

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Mol	Chain	Res	Type
1	D	591	PHE
1	D	649	LEU
1	D	661	LYS
1	D	721	ASP
1	D	857	ASP
1	D	874	ASP
1	D	918	ASP
1	D	995	ASP
1	D	1068	ASP
1	D	1152	ASP
1	D	1170	ASP
1	D	1219	ASP
1	D	1232	ARG
1	D	1278	ASP
1	D	1296	PHE
1	D	1308	ASP
1	D	1330	ARG
1	D	1338	TYR
1	D	1347	ASP
1	D	1378	TRP
1	E	507	ARG
1	E	591	PHE
1	E	649	LEU
1	E	661	LYS
1	E	721	ASP
1	E	857	ASP
1	E	874	ASP
1	E	918	ASP
1	E	995	ASP
1	E	1068	ASP
1	E	1152	ASP
1	E	1170	ASP
1	E	1219	ASP
1	E	1232	ARG
1	E	1278	ASP
1	E	1296	PHE
1	E	1308	ASP
1	E	1330	ARG
1	E	1338	TYR
1	E	1347	ASP
1	E	1378	TRP
1	F	507	ARG

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Mol	Chain	Res	Type
1	F	591	PHE
1	F	649	LEU
1	F	661	LYS
1	F	721	ASP
1	F	857	ASP
1	F	874	ASP
1	F	918	ASP
1	F	995	ASP
1	F	1068	ASP
1	F	1152	ASP
1	F	1170	ASP
1	F	1219	ASP
1	F	1232	ARG
1	F	1278	ASP
1	F	1296	PHE
1	F	1308	ASP
1	F	1330	ARG
1	F	1338	TYR
1	F	1347	ASP
1	F	1378	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	806	ASN
1	A	1050	HIS
1	B	806	ASN
1	B	1050	HIS
1	C	806	ASN
1	C	1050	HIS
1	D	806	ASN
1	D	1050	HIS
1	E	806	ASN
1	E	1050	HIS
1	F	806	ASN
1	F	1050	HIS

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.

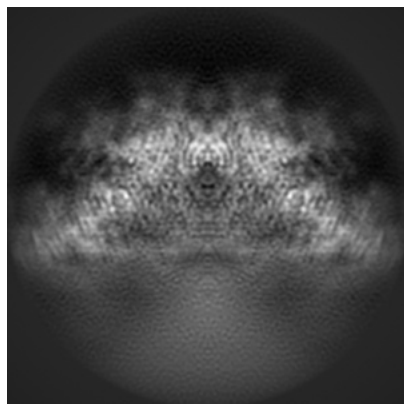
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16489. These allow visual inspection of the internal detail of the map and identification of artifacts.

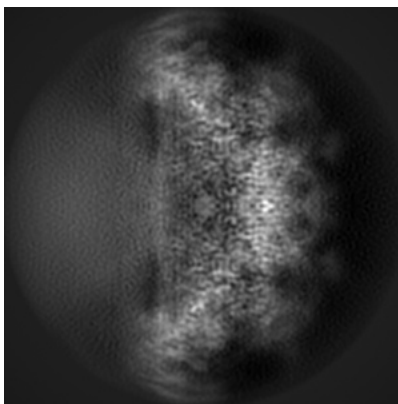
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

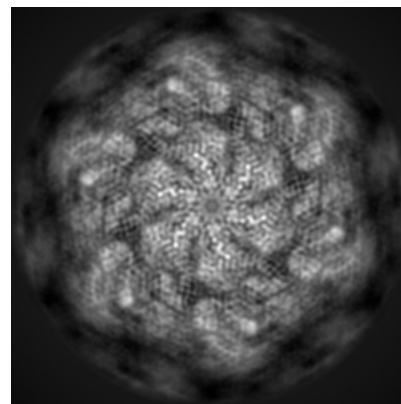
6.1.1 Primary map



X

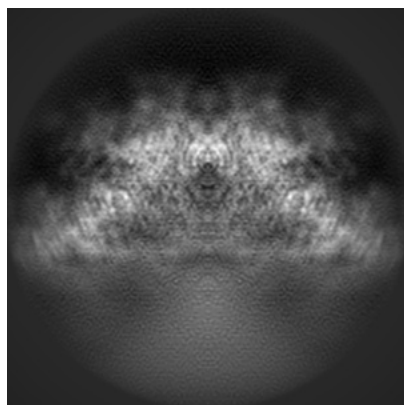


Y

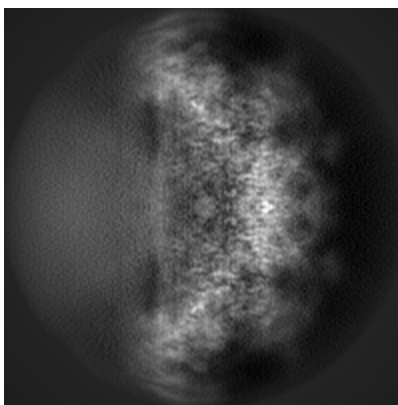


Z

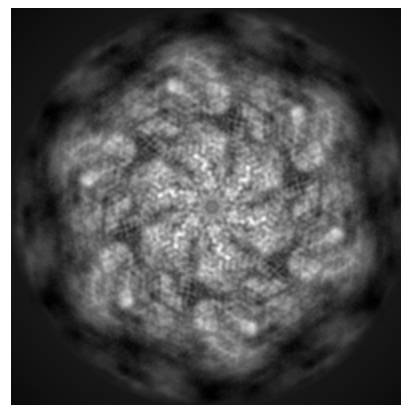
6.1.2 Raw map



X



Y

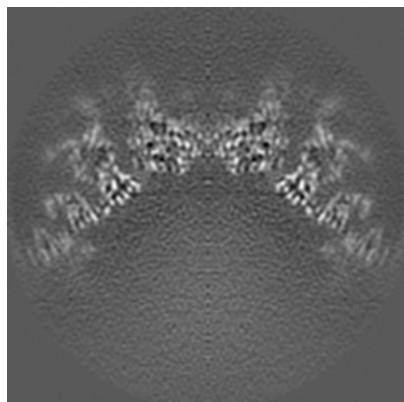


Z

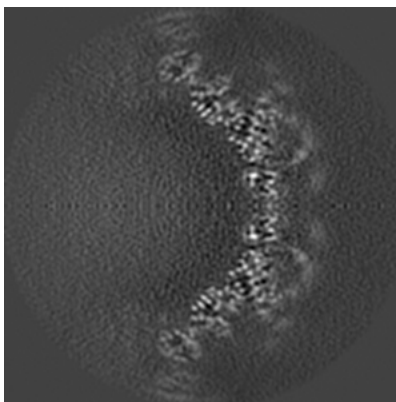
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

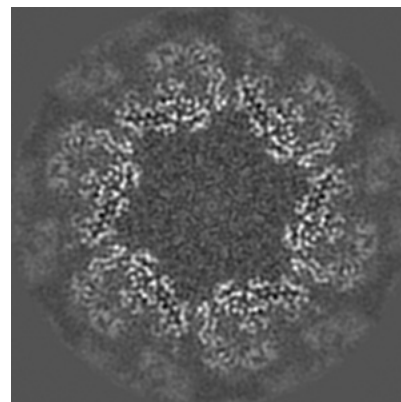
6.2.1 Primary map



X Index: 100

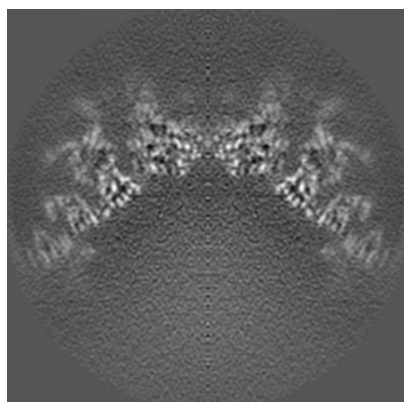


Y Index: 100

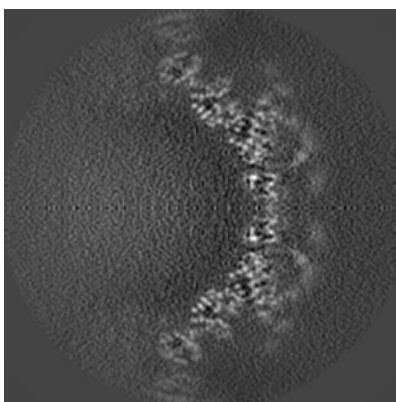


Z Index: 100

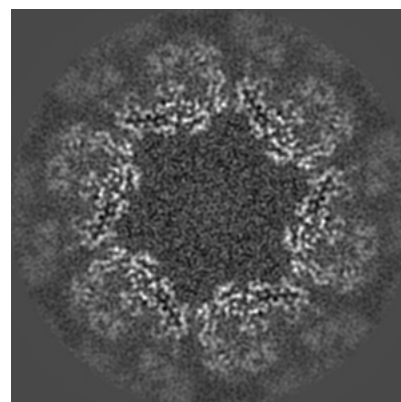
6.2.2 Raw map



X Index: 100



Y Index: 100

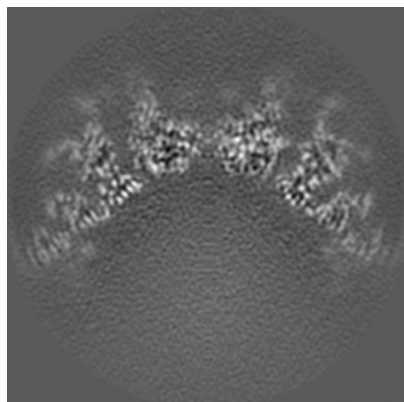


Z Index: 100

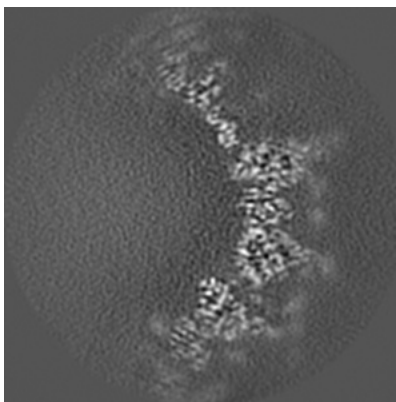
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

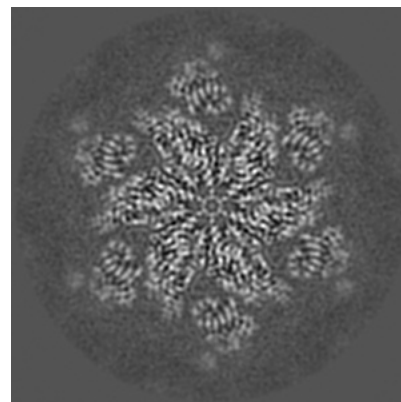
6.3.1 Primary map



X Index: 99

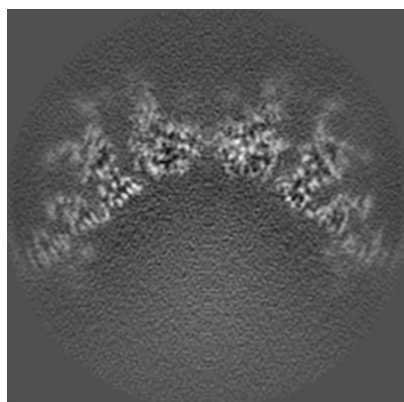


Y Index: 114

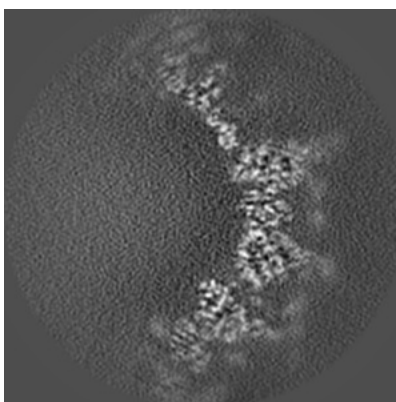


Z Index: 126

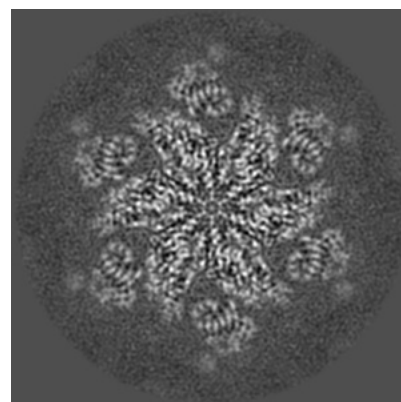
6.3.2 Raw map



X Index: 99



Y Index: 114

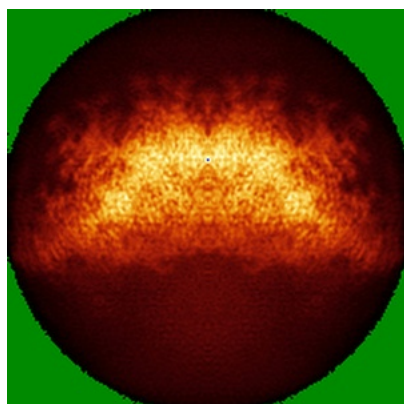


Z Index: 126

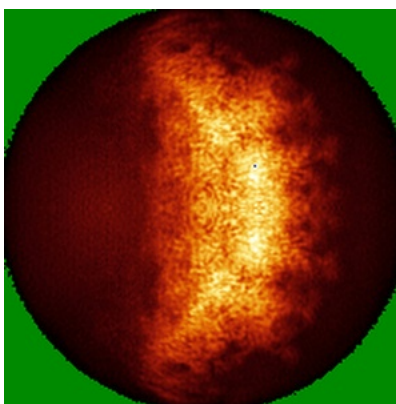
The images above show the largest variance slices of the map in three orthogonal directions.

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

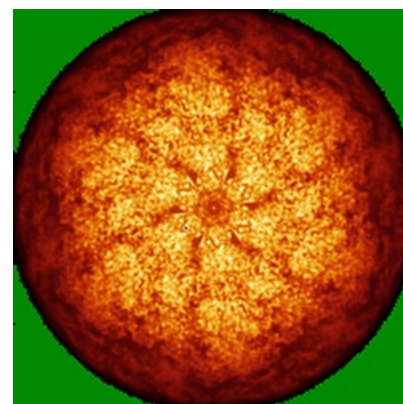
6.4.1 Primary map



X

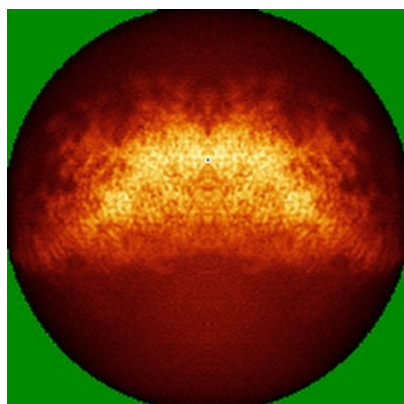


Y

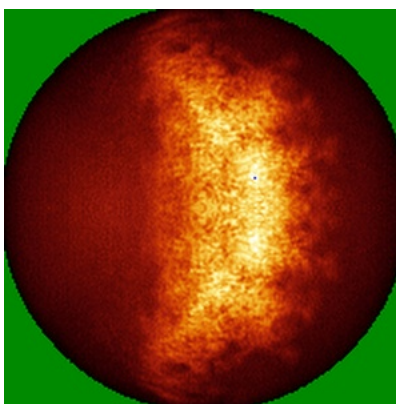


Z

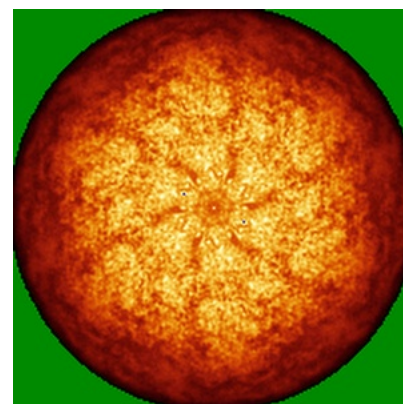
6.4.2 Raw map



X



Y

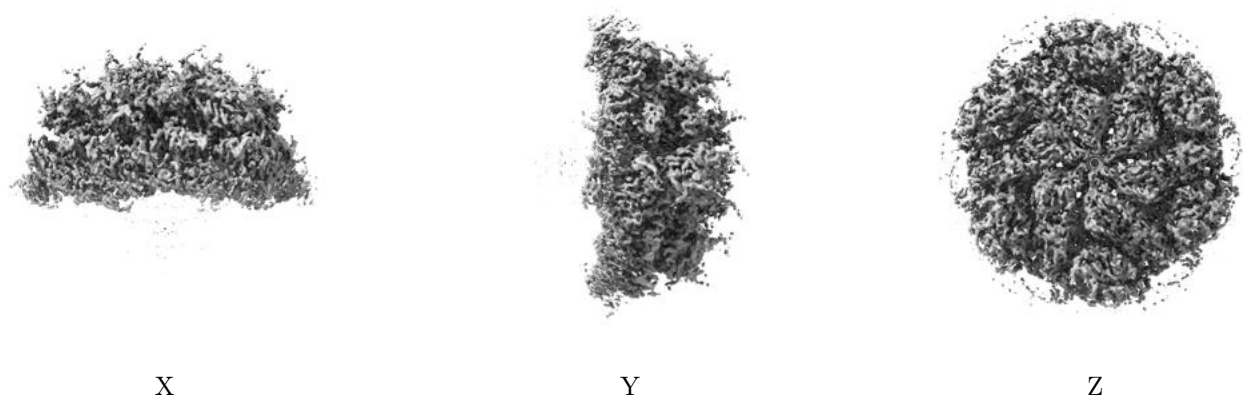


Z

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

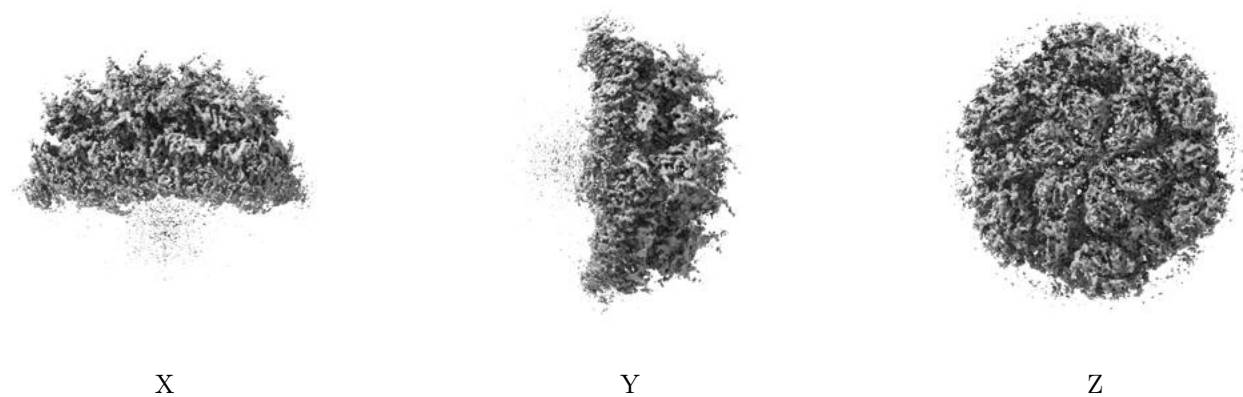
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08214. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

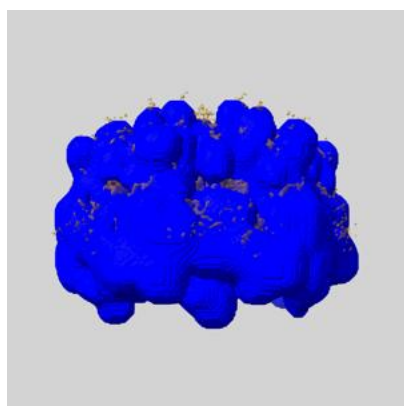
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

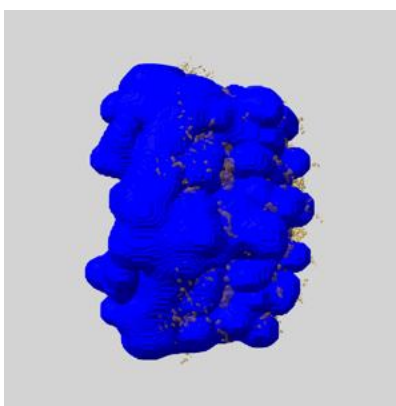
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

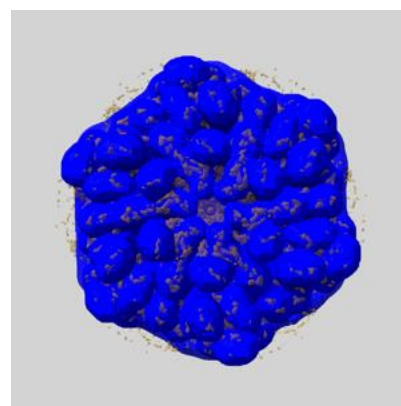
6.6.1 emd_16489_msk_1.map [i](#)



X



Y

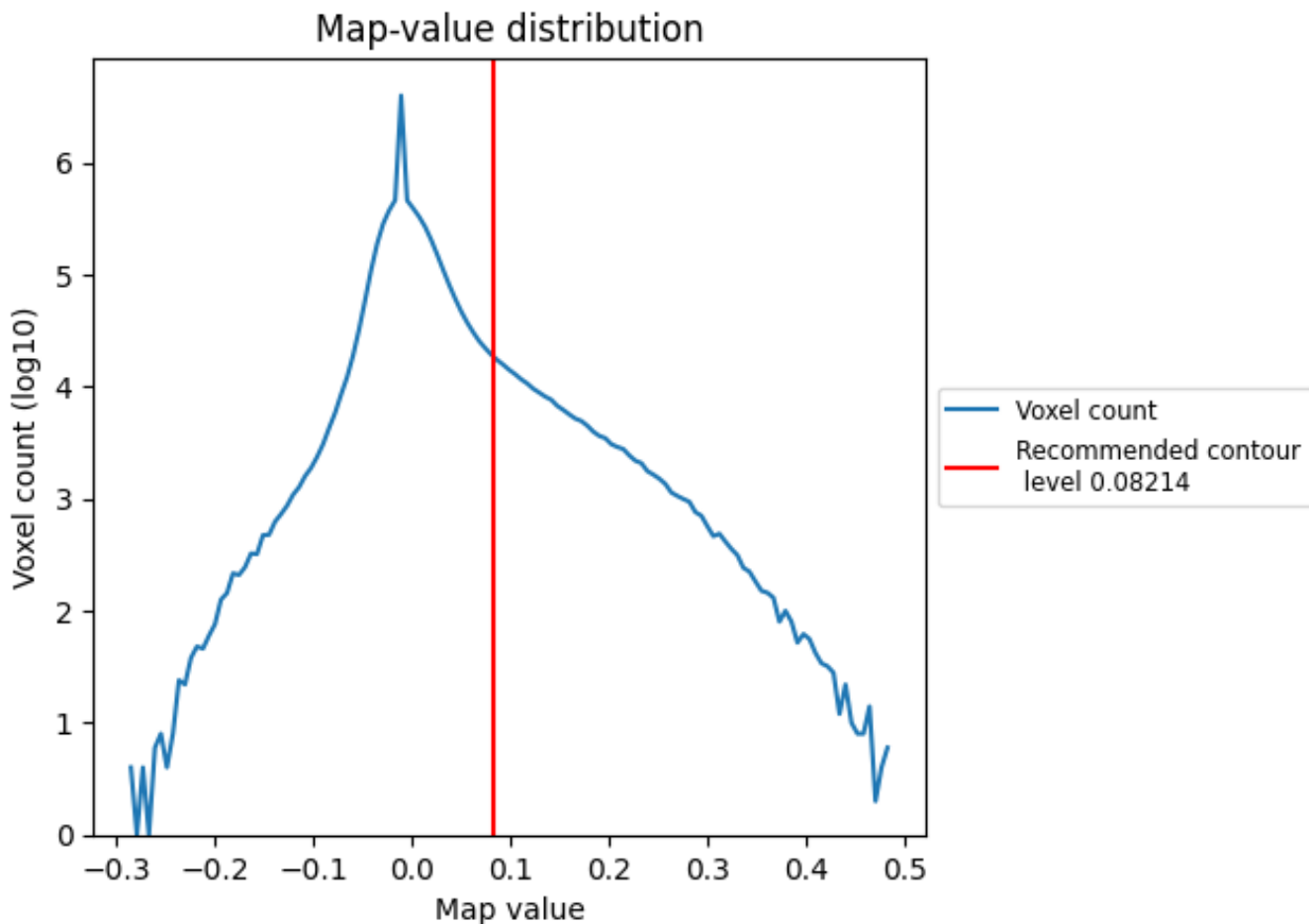


Z

7 Map analysis [i](#)

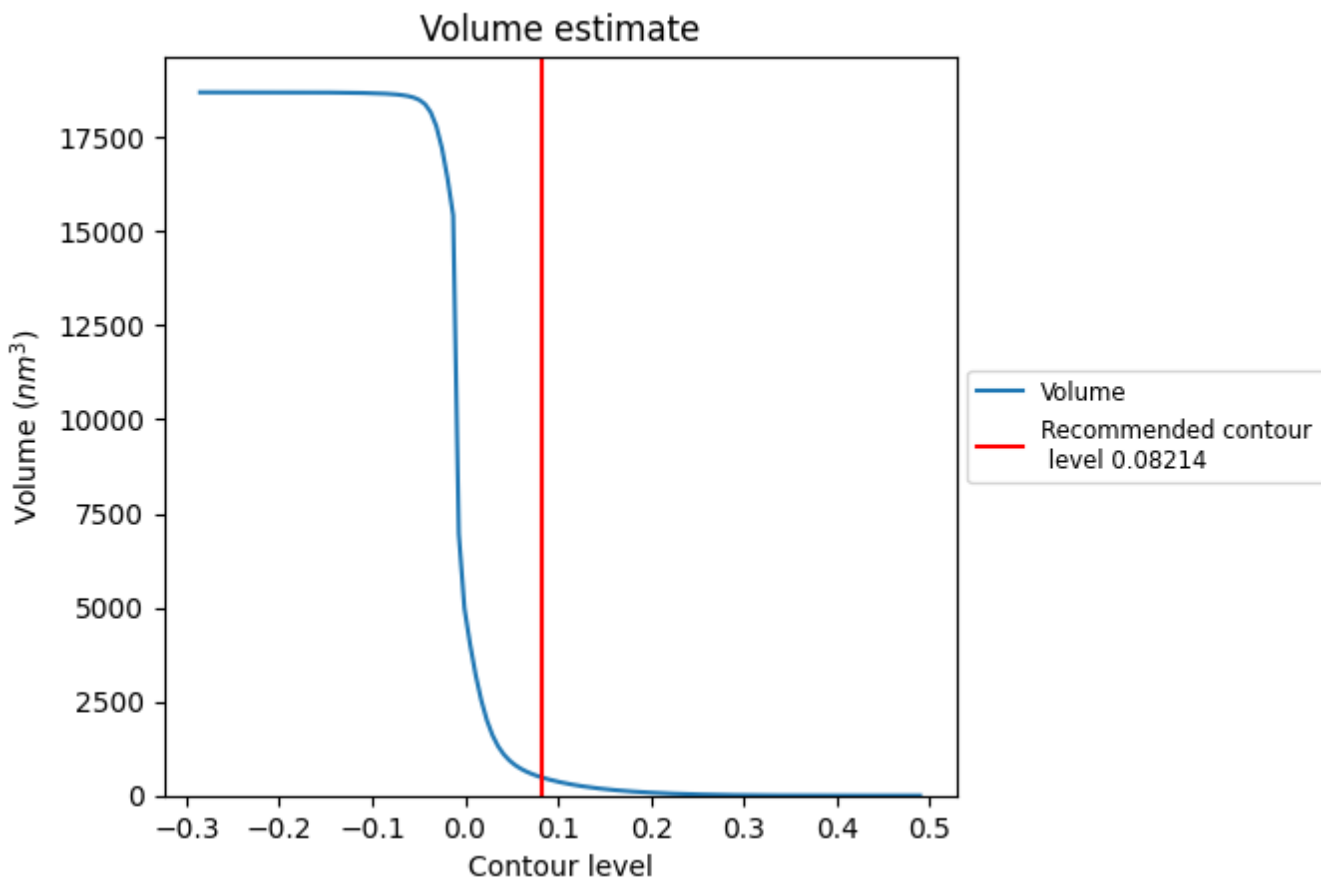
This section contains the results of statistical analysis of the map.

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.

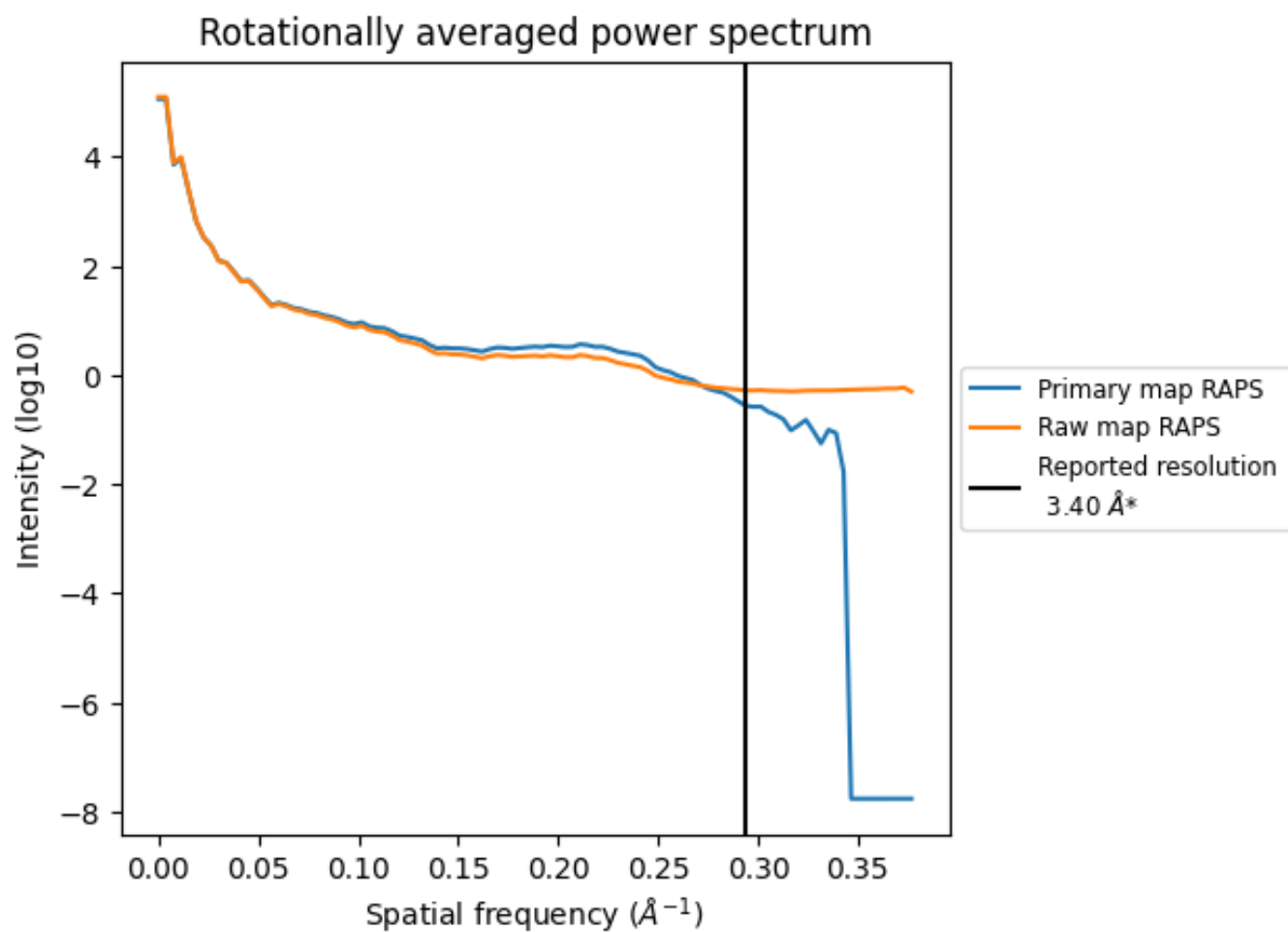
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 486 nm^3 ; this corresponds to an approximate mass of 439 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

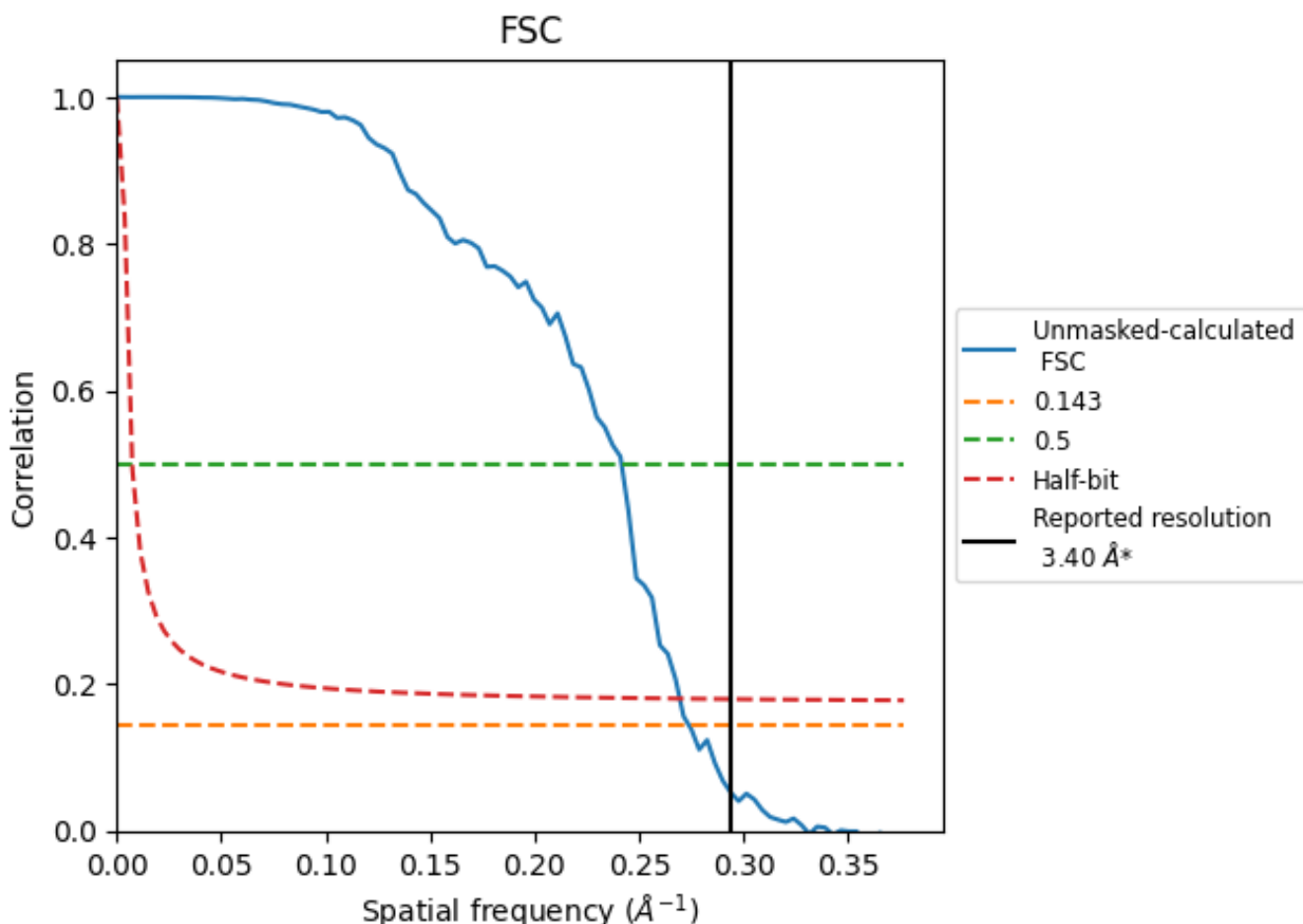


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 \AA^{-1}

8.2 Resolution estimates [i](#)

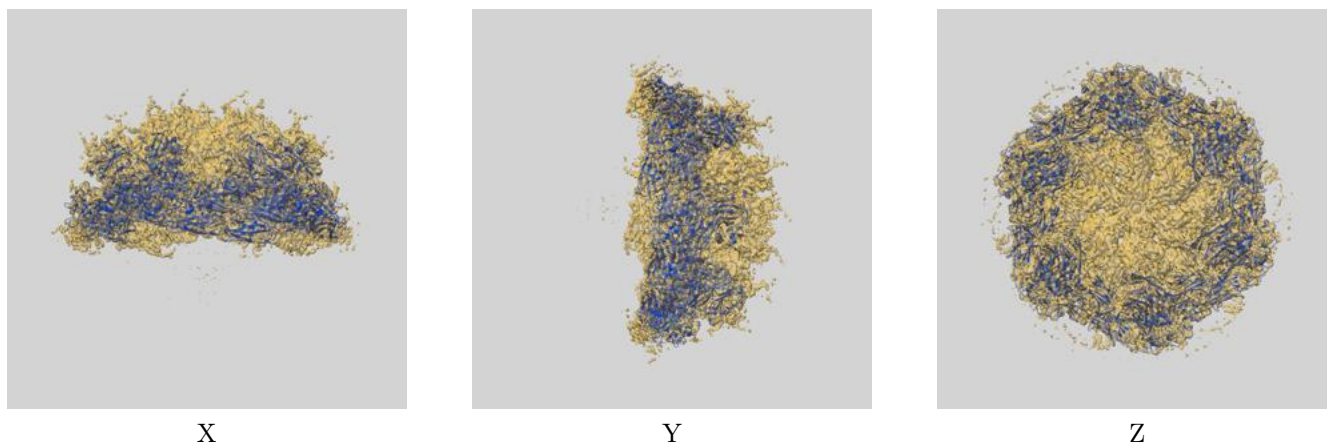
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.65	4.14	3.71

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

9 Map-model fit [i](#)

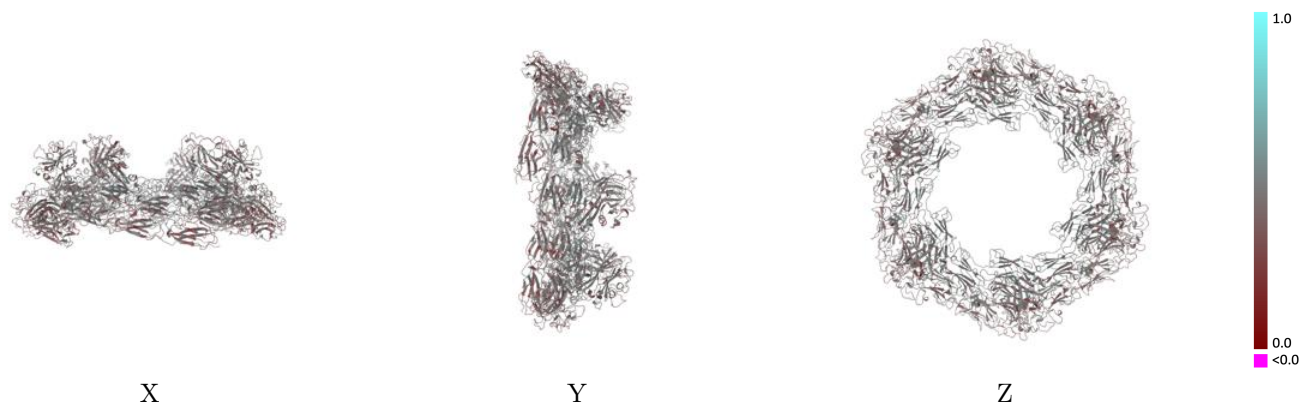
This section contains information regarding the fit between EMDB map EMD-16489 and PDB model 8C8O. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)



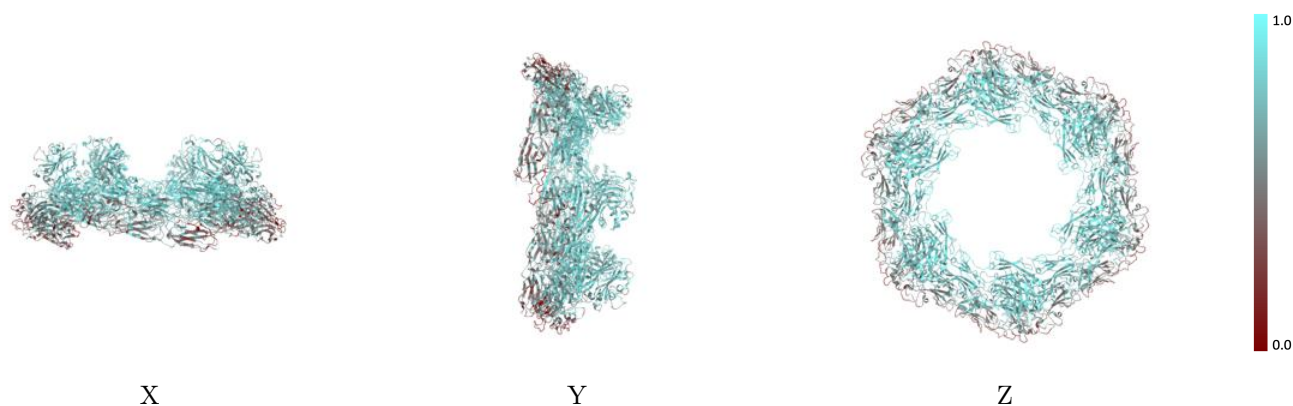
The images above show the 3D surface view of the map at the recommended contour level 0.08214 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



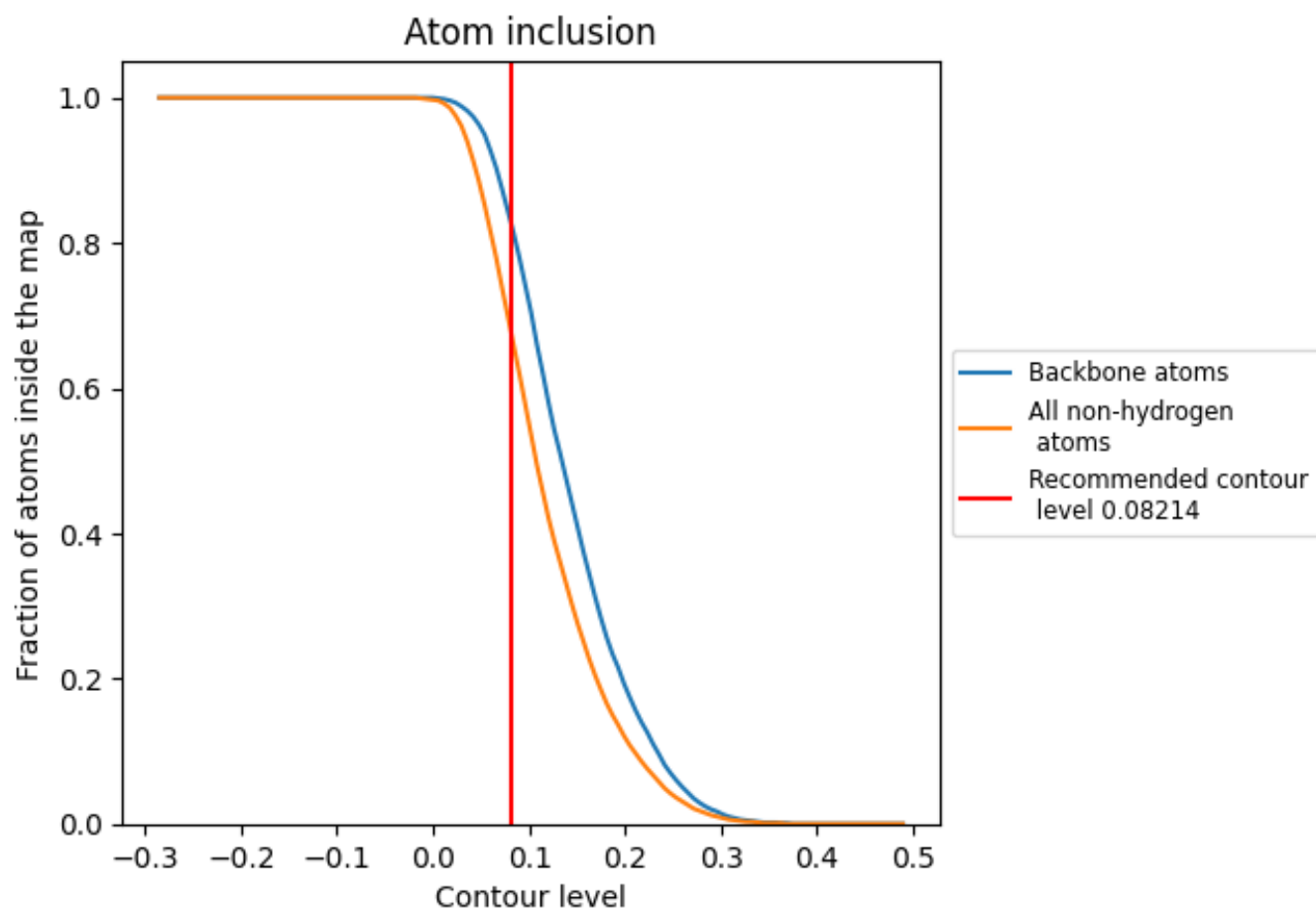
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08214).















9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.08214) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6710	 0.4340
A	 0.6700	 0.4340
B	 0.6710	 0.4330
C	 0.6710	 0.4340
D	 0.6700	 0.4360
E	 0.6720	 0.4340
F	 0.6710	 0.4330

