



## Full wwPDB EM Validation Report ⓘ

Nov 2, 2022 – 04:08 PM EDT

PDB ID : 5K12  
EMDB ID : EMD-8194  
Title : Cryo-EM structure of glutamate dehydrogenase at 1.8 Å resolution  
Authors : Merk, A.; Bartesaghi, A.; Banerjee, S.; Falconieri, V.; Rao, P.; Earl, L.; Milne, J.; Subramaniam, S.  
Deposited on : 2016-05-17  
Resolution : 1.80 Å (reported)  
Based on initial model : 1NR7

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

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

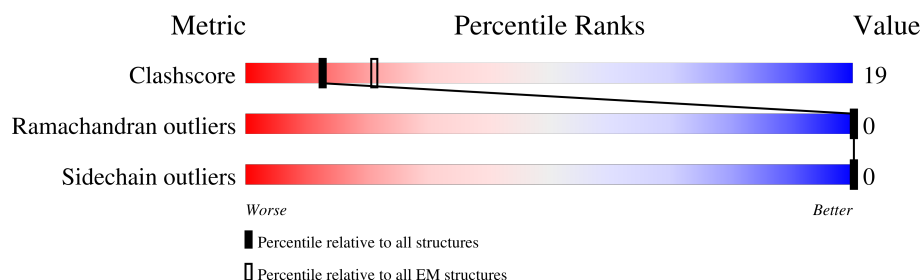
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 1.80 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  $\geq 3$ , 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	558	
1	B	558	
1	C	558	
1	D	558	
1	E	558	
1	F	558	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 14856 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 Glutamate dehydrogenase 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	294	Total	C	N	O	S	0	0
			2295	1445	409	429	12		
1	B	294	Total	C	N	O	S	0	0
			2295	1445	409	429	12		
1	C	294	Total	C	N	O	S	0	0
			2295	1445	409	429	12		
1	D	294	Total	C	N	O	S	0	0
			2295	1445	409	429	12		
1	E	294	Total	C	N	O	S	0	0
			2295	1445	409	429	12		
1	F	294	Total	C	N	O	S	0	0
			2295	1445	409	429	12		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	387	LYS	ASN	conflict	UNP P00366
B	387	LYS	ASN	conflict	UNP P00366
C	387	LYS	ASN	conflict	UNP P00366
D	387	LYS	ASN	conflict	UNP P00366
E	387	LYS	ASN	conflict	UNP P00366
F	387	LYS	ASN	conflict	UNP P00366

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		AltConf
2	A	181	Total	O	0
			181	181	
2	B	182	Total	O	0
			182	182	
2	C	180	Total	O	0
			180	180	
2	D	181	Total	O	0
			181	181	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
2	E	181	Total 181	O 181	0
2	F	181	Total 181	O 181	0

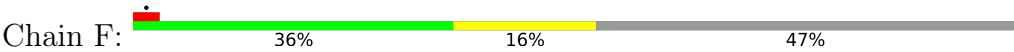






ALA  
GLY  
VAL  
THR  
PHE  
THR

● Molecule 1: Glutamate dehydrogenase 1, mitochondrial



MET TYR ARG ARG LEU GLY GLU ALA LEU LEU LEU LEU LEU SER ARG ARG GLY PRO PRO GLY ALA ALA LEU LEU GLY SER VAL GLY TRP ALA ALA ARG GLN PRO GLN PRO GLY VAL PRO PRO ARG ARG ARG ARG HIS TYR SER GLU ALA ALA ASP ARG

GLU ASP ASP PRO ASN PHE PHE LYS MET VAL VAL GLY PHE PHE ASP ARG GLY ALA ALA SER ILE VAL VAL GLU ASP GLU THR THR GLY GLN GLN LYS ARG ASN ARG VAL ARG SER ILE LEU ARG ILE ILE K53 N56 H57 F63 R66 R67 D68 D69

G70 S71 W72 R79 Q84 H85 H86 T87 C89 K90 G91 G92 I93 S96 T97 D98 V99 S100 E103 V118 D119 V120 A125 K126 A127 D138 N139 E140 L141 E142 K143 R146 R147 M150 A153 K154 D163 V164 P165 D168 M169 D181 T187 G188 H189

Y190 H195 T199 G200 K201 P202 Q205 R211 T212 S213 H221 N225 F226 ILE ASN GLU ALA SER MET THR PRO GLY PHE LEU GLN MET THR PRO GLY PHE LEU GLY ASP THR PHE LEU VAL ILE TYR GLY GLY PHE ASN VAL LEU HIS SER MET ARG LEU HIS ARG PHE GLY

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

GLU LYS GLN THR SER ASN ALA PRO ARG VAL LYS ALA LYS ILE ALA GLY ALA GLY ASP GLY ALA ASN ILE MET VAL ILE PRO D370 L371 Y372 L373 W385 L386 K387 N388 L389 N390 H391 T398 F399 K400 Y401 E402

R403 D404 H408 L409 V413 Q414 E415 S416 L417 E418 K420 K422 G423 H424 G425 G426 T427 P429 I430 F436 I440 A443 S444 E445 K446 D447 S451 A461 R462 M465 R466 T467 A468 M469 K470 Y471 N472 L473 Y482 Y486 Y489 P489 ARG VAL TYR ASN

GLU  
ALA  
GLY  
VAL  
THR  
PHE  
THR



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	21818	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	78000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.034	Depositor
Minimum map value	-0.014	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0085	Depositor
Map size (Å)	149.058, 149.058, 149.058	wwPDB
Map dimensions	234, 234, 234	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.63699996, 0.63699996, 0.63699996	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	0.43	0/2345	0.55	1/3166 (0.0%)
1	B	0.43	0/2345	0.55	1/3166 (0.0%)
1	C	0.43	0/2345	0.55	1/3166 (0.0%)
1	D	0.43	0/2345	0.55	0/3166
1	E	0.43	0/2345	0.55	1/3166 (0.0%)
1	F	0.43	0/2345	0.55	1/3166 (0.0%)
All	All	0.43	0/14070	0.55	5/18996 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	201	LYS	C-N-CD	5.02	138.94	128.40
1	A	201	LYS	C-N-CD	5.01	138.93	128.40
1	F	201	LYS	C-N-CD	5.01	138.92	128.40
1	E	201	LYS	C-N-CD	5.00	138.91	128.40
1	C	201	LYS	C-N-CD	5.00	138.90	128.40

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	2295	0	2261	94	0
1	B	2295	0	2261	93	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2295	0	2261	93	0
1	D	2295	0	2261	92	0
1	E	2295	0	2261	89	0
1	F	2295	0	2261	92	0
2	A	181	0	0	18	0
2	B	182	0	0	20	0
2	C	180	0	0	18	0
2	D	181	0	0	20	0
2	E	181	0	0	16	0
2	F	181	0	0	16	0
All	All	14856	0	13566	512	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 19.

All (512) 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:B:142:GLU:O	1:B:146:ARG:HG3	1.62	0.99
1:D:142:GLU:O	1:D:146:ARG:HG3	1.62	0.99
1:A:142:GLU:O	1:A:146:ARG:HG3	1.62	0.99
1:C:142:GLU:O	1:C:146:ARG:HG3	1.62	0.99
1:E:142:GLU:O	1:E:146:ARG:HG3	1.62	0.98
1:F:142:GLU:O	1:F:146:ARG:HG3	1.62	0.98
1:E:90:LYS:HE3	2:E:721:HOH:O	1.76	0.85
1:F:90:LYS:HE3	2:F:721:HOH:O	1.76	0.85
1:B:90:LYS:HE3	2:B:722:HOH:O	1.76	0.85
1:D:90:LYS:HE3	2:D:721:HOH:O	1.76	0.85
1:E:201:LYS:HZ1	1:E:388:ASN:HD21	1.23	0.85
1:C:90:LYS:HE3	2:C:720:HOH:O	1.76	0.84
1:F:201:LYS:HZ1	1:F:388:ASN:HD21	1.23	0.84
1:A:90:LYS:HE3	2:A:722:HOH:O	1.76	0.84
1:C:201:LYS:HZ3	1:C:388:ASN:HD21	1.24	0.83
1:A:201:LYS:HZ3	1:A:388:ASN:HD21	1.24	0.83
1:F:211:ARG:NH2	2:F:603:HOH:O	2.13	0.82
1:E:211:ARG:NH2	2:E:603:HOH:O	2.13	0.82
1:B:211:ARG:NH2	2:B:603:HOH:O	2.13	0.81
1:D:211:ARG:NH2	2:D:603:HOH:O	2.13	0.81
1:A:211:ARG:NH2	2:A:603:HOH:O	2.13	0.80
1:C:211:ARG:NH2	2:C:603:HOH:O	2.13	0.80
1:E:201:LYS:NZ	1:E:388:ASN:HD21	1.81	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:201:LYS:NZ	1:F:388:ASN:HD21	1.81	0.78
1:A:201:LYS:NZ	1:A:388:ASN:HD21	1.81	0.78
1:C:201:LYS:NZ	1:C:388:ASN:HD21	1.81	0.78
1:B:201:LYS:HZ3	1:B:388:ASN:HD21	1.29	0.77
1:D:201:LYS:HZ3	1:D:388:ASN:HD21	1.29	0.77
1:A:201:LYS:NZ	1:A:388:ASN:ND2	2.33	0.76
1:C:201:LYS:NZ	1:C:388:ASN:ND2	2.33	0.76
1:B:201:LYS:NZ	1:B:388:ASN:HD21	1.81	0.76
1:D:201:LYS:NZ	1:D:388:ASN:HD21	1.81	0.76
1:B:201:LYS:NZ	1:B:388:ASN:ND2	2.33	0.76
1:D:201:LYS:NZ	1:D:388:ASN:ND2	2.33	0.76
1:E:201:LYS:NZ	1:E:388:ASN:ND2	2.33	0.75
1:F:150:MET:HE3	2:F:775:HOH:O	1.86	0.75
1:F:201:LYS:NZ	1:F:388:ASN:ND2	2.33	0.75
1:E:150:MET:HE3	2:E:775:HOH:O	1.86	0.75
1:A:414:GLN:HG2	1:A:429:PRO:HD2	1.69	0.75
1:C:414:GLN:HG2	1:C:429:PRO:HD2	1.69	0.75
1:F:79:ARG:NE	1:F:163:ASP:OD2	2.20	0.75
1:E:79:ARG:NE	1:E:163:ASP:OD2	2.20	0.74
1:A:211:ARG:O	2:A:601:HOH:O	2.05	0.74
1:B:211:ARG:O	2:B:601:HOH:O	2.05	0.74
1:A:150:MET:CE	2:A:775:HOH:O	2.35	0.74
1:D:211:ARG:O	2:D:601:HOH:O	2.05	0.74
1:B:142:GLU:OE1	2:B:602:HOH:O	2.06	0.74
1:C:211:ARG:O	2:C:601:HOH:O	2.05	0.74
1:D:142:GLU:OE1	2:D:602:HOH:O	2.06	0.74
1:C:150:MET:CE	2:C:774:HOH:O	2.35	0.74
1:C:79:ARG:NE	1:C:163:ASP:OD2	2.20	0.74
1:F:150:MET:CE	2:F:775:HOH:O	2.35	0.73
1:E:150:MET:CE	2:E:775:HOH:O	2.35	0.73
1:F:211:ARG:O	2:F:601:HOH:O	2.05	0.73
1:A:142:GLU:OE1	2:A:602:HOH:O	2.06	0.73
1:C:142:GLU:OE1	2:C:602:HOH:O	2.06	0.73
1:E:211:ARG:O	2:E:601:HOH:O	2.05	0.73
1:B:150:MET:CE	2:B:776:HOH:O	2.35	0.73
1:D:150:MET:CE	2:D:775:HOH:O	2.35	0.73
1:E:414:GLN:HG2	1:E:429:PRO:HD2	1.69	0.73
1:B:414:GLN:HG2	1:B:429:PRO:HD2	1.69	0.72
1:F:126:LYS:NZ	1:F:168:ASP:OD2	2.22	0.72
1:F:142:GLU:OE1	2:F:602:HOH:O	2.06	0.72
1:E:126:LYS:NZ	1:E:168:ASP:OD2	2.22	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:GLU:OE1	2:E:602:HOH:O	2.06	0.72
1:F:414:GLN:HG2	1:F:429:PRO:HD2	1.69	0.72
1:F:423:LYS:HD3	1:F:426:GLY:HA3	1.71	0.72
1:A:423:LYS:HD3	1:A:426:GLY:HA3	1.71	0.72
1:B:423:LYS:HD3	1:B:426:GLY:HA3	1.71	0.72
1:D:414:GLN:HG2	1:D:429:PRO:HD2	1.69	0.72
1:E:423:LYS:HD3	1:E:426:GLY:HA3	1.72	0.72
1:D:423:LYS:HD3	1:D:426:GLY:HA3	1.72	0.72
1:C:423:LYS:HD3	1:C:426:GLY:HA3	1.72	0.72
1:A:126:LYS:NZ	1:A:168:ASP:OD2	2.22	0.71
1:A:79:ARG:NE	1:A:163:ASP:OD2	2.20	0.71
1:C:126:LYS:NZ	1:C:168:ASP:OD2	2.22	0.71
1:C:90:LYS:NZ	1:C:199:THR:OG1	2.22	0.71
1:A:90:LYS:NZ	1:A:199:THR:OG1	2.22	0.71
1:B:201:LYS:HZ1	1:B:388:ASN:ND2	1.88	0.71
1:D:201:LYS:HZ1	1:D:388:ASN:ND2	1.88	0.70
1:D:126:LYS:NZ	1:D:168:ASP:OD2	2.22	0.70
1:D:79:ARG:NE	1:D:163:ASP:OD2	2.20	0.70
1:B:79:ARG:NE	1:B:163:ASP:OD2	2.20	0.70
1:B:126:LYS:NZ	1:B:168:ASP:OD2	2.22	0.70
1:E:90:LYS:NZ	1:E:199:THR:OG1	2.22	0.70
1:A:150:MET:HE3	2:A:775:HOH:O	1.90	0.69
1:F:90:LYS:NZ	1:F:199:THR:OG1	2.22	0.69
1:B:90:LYS:NZ	1:B:199:THR:OG1	2.22	0.69
1:D:90:LYS:NZ	1:D:199:THR:OG1	2.22	0.69
1:F:415:GLU:O	1:F:419:ARG:HG2	1.93	0.68
1:E:415:GLU:O	1:E:419:ARG:HG2	1.93	0.68
1:C:150:MET:HE3	2:C:774:HOH:O	1.92	0.68
1:D:415:GLU:O	1:D:419:ARG:HG2	1.93	0.68
1:B:415:GLU:O	1:B:419:ARG:HG2	1.93	0.68
1:A:415:GLU:O	1:A:419:ARG:HG2	1.93	0.67
1:C:415:GLU:O	1:C:419:ARG:HG2	1.93	0.67
1:E:221:HIS:O	1:E:225:ASN:ND2	2.29	0.66
1:F:221:HIS:O	1:F:225:ASN:ND2	2.29	0.66
1:C:63:PHE:HB2	1:C:147:ARG:HE	1.61	0.66
1:A:63:PHE:HB2	1:A:147:ARG:HE	1.61	0.66
1:B:63:PHE:HB2	1:B:147:ARG:HE	1.61	0.66
1:D:63:PHE:HB2	1:D:147:ARG:HE	1.61	0.65
1:A:221:HIS:O	1:A:225:ASN:ND2	2.29	0.65
1:E:63:PHE:HB2	1:E:147:ARG:HE	1.61	0.65
1:F:63:PHE:HB2	1:F:147:ARG:HE	1.61	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:HIS:O	1:C:225:ASN:ND2	2.29	0.65
1:D:221:HIS:O	1:D:225:ASN:ND2	2.29	0.65
1:B:221:HIS:O	1:B:225:ASN:ND2	2.29	0.65
1:C:201:LYS:HZ1	1:C:388:ASN:ND2	1.94	0.64
1:A:201:LYS:HZ1	1:A:388:ASN:ND2	1.94	0.64
1:D:100:SER:OG	1:D:103:GLU:HG2	1.98	0.64
1:A:100:SER:OG	1:A:103:GLU:HG2	1.98	0.64
1:B:100:SER:OG	1:B:103:GLU:HG2	1.98	0.64
1:C:100:SER:OG	1:C:103:GLU:HG2	1.97	0.64
1:F:146:ARG:NH1	1:F:181:ASP:OD2	2.32	0.63
1:E:146:ARG:NH1	1:E:181:ASP:OD2	2.32	0.63
1:D:150:MET:HE3	2:D:775:HOH:O	1.98	0.63
1:B:146:ARG:NH1	1:B:181:ASP:OD2	2.32	0.63
1:B:150:MET:HE3	2:B:776:HOH:O	1.98	0.63
1:D:146:ARG:NH1	1:D:181:ASP:OD2	2.32	0.63
1:E:100:SER:OG	1:E:103:GLU:HG2	1.98	0.62
1:B:414:GLN:HE21	1:B:428:ILE:HA	1.64	0.62
1:F:100:SER:OG	1:F:103:GLU:HG2	1.98	0.62
1:A:146:ARG:NH1	1:A:181:ASP:OD2	2.32	0.62
1:C:146:ARG:NH1	1:C:181:ASP:OD2	2.32	0.62
1:D:414:GLN:HE21	1:D:428:ILE:HA	1.64	0.62
1:A:414:GLN:HE21	1:A:428:ILE:HA	1.64	0.62
1:B:189:HIS:HB3	2:B:761:HOH:O	2.00	0.62
1:C:414:GLN:HE21	1:C:428:ILE:HA	1.64	0.62
1:D:189:HIS:HB3	2:D:760:HOH:O	1.99	0.62
1:A:189:HIS:HB3	2:A:760:HOH:O	1.99	0.62
1:C:189:HIS:HB3	2:C:759:HOH:O	1.99	0.62
1:E:201:LYS:HZ2	1:E:388:ASN:ND2	1.96	0.62
1:F:201:LYS:HZ2	1:F:388:ASN:ND2	1.96	0.61
1:E:90:LYS:HD2	1:E:164:VAL:O	2.00	0.61
1:F:90:LYS:HD2	1:F:164:VAL:O	2.01	0.61
1:A:90:LYS:HD2	1:A:164:VAL:O	2.00	0.61
1:E:414:GLN:HE21	1:E:428:ILE:HA	1.64	0.61
1:F:189:HIS:HB3	2:F:760:HOH:O	1.99	0.61
1:C:90:LYS:HD2	1:C:164:VAL:O	2.00	0.61
1:E:189:HIS:HB3	2:E:760:HOH:O	1.99	0.61
1:F:414:GLN:HE21	1:F:428:ILE:HA	1.64	0.61
1:D:90:LYS:HD2	1:D:164:VAL:O	2.00	0.60
1:B:90:LYS:HD2	1:B:164:VAL:O	2.01	0.60
1:E:202:PRO:HD2	1:E:205:GLN:HB2	1.83	0.60
1:F:202:PRO:HD2	1:F:205:GLN:HB2	1.83	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:PRO:HD2	1:A:205:GLN:HB2	1.83	0.60
1:C:202:PRO:HD2	1:C:205:GLN:HB2	1.83	0.60
1:A:195:HIS:HE1	1:A:391:HIS:CD2	2.21	0.59
1:C:195:HIS:HE1	1:C:391:HIS:CD2	2.21	0.59
1:B:91:GLY:O	1:B:165:PRO:HA	2.03	0.58
1:B:195:HIS:HE1	1:B:391:HIS:CD2	2.21	0.58
1:D:91:GLY:O	1:D:165:PRO:HA	2.03	0.58
1:D:195:HIS:HE1	1:D:391:HIS:CD2	2.21	0.58
1:F:91:GLY:O	1:F:165:PRO:HA	2.03	0.58
1:E:91:GLY:O	1:E:165:PRO:HA	2.03	0.58
1:E:195:HIS:HE1	1:E:391:HIS:CD2	2.21	0.58
1:F:195:HIS:HE1	1:F:391:HIS:CD2	2.21	0.58
1:B:202:PRO:HD2	1:B:205:GLN:HB2	1.83	0.58
1:D:202:PRO:HD2	1:D:205:GLN:HB2	1.83	0.58
1:C:91:GLY:O	1:C:165:PRO:HA	2.03	0.58
1:E:56:ASN:OD1	1:E:57:HIS:N	2.37	0.58
1:B:56:ASN:OD1	1:B:57:HIS:N	2.37	0.58
1:D:56:ASN:OD1	1:D:57:HIS:N	2.37	0.58
1:F:56:ASN:OD1	1:F:57:HIS:N	2.37	0.58
1:A:91:GLY:O	1:A:165:PRO:HA	2.03	0.58
1:A:372:TYR:HD2	1:A:373:LEU:HD12	1.69	0.58
1:C:372:TYR:HD2	1:C:373:LEU:HD12	1.69	0.58
1:B:372:TYR:HD2	1:B:373:LEU:HD12	1.69	0.57
1:C:56:ASN:OD1	1:C:57:HIS:N	2.37	0.57
1:E:372:TYR:HD2	1:E:373:LEU:HD12	1.69	0.57
1:F:372:TYR:HD2	1:F:373:LEU:HD12	1.69	0.57
1:A:56:ASN:OD1	1:A:57:HIS:N	2.37	0.57
1:D:372:TYR:HD2	1:D:373:LEU:HD12	1.69	0.57
1:D:387:LYS:HD2	1:D:445:GLU:OE2	2.04	0.57
1:B:387:LYS:HD2	1:B:445:GLU:OE2	2.04	0.57
1:A:471:TYR:HB3	1:A:473:LEU:HD12	1.87	0.57
1:C:471:TYR:HB3	1:C:473:LEU:HD12	1.87	0.57
1:D:471:TYR:HB3	1:D:473:LEU:HD12	1.87	0.57
1:B:471:TYR:HB3	1:B:473:LEU:HD12	1.87	0.57
1:C:387:LYS:HD2	1:C:445:GLU:OE2	2.04	0.57
1:E:471:TYR:HB3	1:E:473:LEU:HD12	1.87	0.57
1:F:471:TYR:HB3	1:F:473:LEU:HD12	1.87	0.57
1:E:387:LYS:HD2	1:E:445:GLU:OE2	2.04	0.56
1:F:387:LYS:HD2	1:F:445:GLU:OE2	2.04	0.56
1:A:387:LYS:HD2	1:A:445:GLU:OE2	2.04	0.56
1:A:79:ARG:HH11	1:A:127:ALA:HB2	1.70	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:ARG:HH11	1:C:127:ALA:HB2	1.70	0.56
1:D:79:ARG:HH11	1:D:127:ALA:HB2	1.70	0.55
1:F:79:ARG:HH11	1:F:127:ALA:HB2	1.70	0.55
1:B:79:ARG:HH11	1:B:127:ALA:HB2	1.70	0.55
1:E:79:ARG:HH11	1:E:127:ALA:HB2	1.70	0.55
1:A:451:SER:HB2	1:B:400:LYS:HB3	1.89	0.54
1:B:190:TYR:OH	1:E:154:LYS:O	2.15	0.54
1:B:87:THR:HG22	2:B:658:HOH:O	2.07	0.54
1:C:87:THR:HG22	2:C:658:HOH:O	2.07	0.54
1:D:87:THR:HG22	2:D:658:HOH:O	2.07	0.54
1:A:87:THR:HG22	2:A:657:HOH:O	2.07	0.54
1:E:403:ARG:NE	2:E:616:HOH:O	2.41	0.54
1:F:87:THR:HG22	2:F:657:HOH:O	2.07	0.54
1:F:403:ARG:NE	2:F:616:HOH:O	2.41	0.54
1:C:403:ARG:NE	2:C:616:HOH:O	2.41	0.53
1:D:403:ARG:NE	2:D:616:HOH:O	2.41	0.53
1:E:87:THR:HG22	2:E:658:HOH:O	2.07	0.53
1:A:403:ARG:NE	2:A:616:HOH:O	2.41	0.53
1:B:403:ARG:NE	2:B:616:HOH:O	2.41	0.53
1:C:153:ALA:HB1	1:C:187:ILE:HG13	1.90	0.53
1:A:153:ALA:HB1	1:A:187:ILE:HG13	1.90	0.53
1:B:451:SER:HB2	1:F:400:LYS:HB3	1.89	0.53
1:E:153:ALA:HB1	1:E:187:ILE:HG13	1.90	0.53
1:F:153:ALA:HB1	1:F:187:ILE:HG13	1.90	0.52
1:D:140:GLU:OE1	1:D:143:LYS:HD2	2.10	0.52
1:B:140:GLU:OE1	1:B:143:LYS:HD2	2.10	0.52
1:A:140:GLU:OE1	1:A:143:LYS:HD2	2.10	0.52
1:B:153:ALA:HB1	1:B:187:ILE:HG13	1.90	0.52
1:C:140:GLU:OE1	1:C:143:LYS:HD2	2.10	0.52
1:E:140:GLU:OE1	1:E:143:LYS:HD2	2.10	0.52
1:C:451:SER:HB2	1:D:400:LYS:HB3	1.92	0.51
1:D:153:ALA:HB1	1:D:187:ILE:HG13	1.90	0.51
1:F:140:GLU:OE1	1:F:143:LYS:HD2	2.10	0.51
1:E:398:THR:HG22	1:E:402:GLU:HG2	1.92	0.51
1:F:90:LYS:HZ3	1:F:164:VAL:HG12	1.74	0.51
1:B:398:THR:HG22	1:B:402:GLU:HG2	1.92	0.51
1:C:400:LYS:HB3	1:E:451:SER:HB2	1.92	0.51
1:F:398:THR:HG22	1:F:402:GLU:HG2	1.92	0.51
1:A:429:PRO:HA	1:B:416:SER:HB3	1.92	0.51
1:D:190:TYR:OH	1:F:154:LYS:O	2.18	0.51
1:D:398:THR:HG22	1:D:402:GLU:HG2	1.92	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:LYS:HB3	1:F:451:SER:HB2	1.92	0.51
1:D:187:ILE:HG23	2:D:766:HOH:O	2.11	0.51
1:B:187:ILE:HG23	2:B:767:HOH:O	2.11	0.51
1:F:187:ILE:HG23	2:F:766:HOH:O	2.11	0.50
1:E:90:LYS:HZ3	1:E:164:VAL:HG12	1.75	0.50
1:E:187:ILE:HG23	2:E:767:HOH:O	2.11	0.50
1:A:398:THR:HG22	1:A:402:GLU:HG2	1.92	0.50
1:C:398:THR:HG22	1:C:402:GLU:HG2	1.92	0.50
1:C:187:ILE:HG23	2:C:765:HOH:O	2.11	0.50
1:D:154:LYS:O	1:F:190:TYR:OH	2.18	0.50
1:F:436:PHE:CZ	1:F:440:ILE:HD11	2.47	0.50
1:A:187:ILE:HG23	2:A:766:HOH:O	2.11	0.50
1:B:142:GLU:O	1:B:146:ARG:CG	2.50	0.50
1:E:436:PHE:CZ	1:E:440:ILE:HD11	2.47	0.50
1:A:436:PHE:CG	1:B:408:HIS:HB3	2.47	0.50
1:C:142:GLU:O	1:C:146:ARG:CG	2.50	0.50
1:D:436:PHE:CZ	1:D:440:ILE:HD11	2.47	0.50
1:A:429:PRO:HA	1:B:416:SER:CB	2.42	0.50
1:B:436:PHE:CZ	1:B:440:ILE:HD11	2.47	0.50
1:D:451:SER:HB2	1:E:400:LYS:HB3	1.93	0.50
1:D:142:GLU:O	1:D:146:ARG:CG	2.50	0.49
1:E:430:ILE:HD12	2:E:710:HOH:O	2.13	0.49
1:B:482:TYR:O	1:B:486:ILE:HD12	2.12	0.49
1:F:430:ILE:HD12	2:F:710:HOH:O	2.13	0.49
1:A:90:LYS:HZ3	1:A:164:VAL:HG12	1.76	0.49
1:C:372:TYR:CD2	1:C:373:LEU:HD12	2.48	0.49
1:C:482:TYR:O	1:C:486:ILE:HD12	2.12	0.49
1:D:482:TYR:O	1:D:486:ILE:HD12	2.12	0.49
1:B:150:MET:HE2	2:B:776:HOH:O	2.08	0.49
1:C:436:PHE:CZ	1:C:440:ILE:HD11	2.47	0.49
1:E:482:TYR:O	1:E:486:ILE:HD12	2.12	0.49
1:A:372:TYR:CD2	1:A:373:LEU:HD12	2.48	0.48
1:A:436:PHE:CZ	1:A:440:ILE:HD11	2.47	0.48
1:A:436:PHE:HB2	1:B:408:HIS:CD2	2.48	0.48
1:A:482:TYR:O	1:A:486:ILE:HD12	2.12	0.48
1:C:90:LYS:HZ3	1:C:164:VAL:HG12	1.76	0.48
1:A:416:SER:HB3	1:F:429:PRO:HA	1.95	0.48
1:E:372:TYR:CD2	1:E:373:LEU:HD12	2.48	0.48
1:F:372:TYR:CD2	1:F:373:LEU:HD12	2.48	0.48
1:F:482:TYR:O	1:F:486:ILE:HD12	2.12	0.48
1:A:66:ARG:HD3	1:A:72:TRP:CZ2	2.48	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:ILE:HD12	2:B:711:HOH:O	2.13	0.48
1:C:66:ARG:HD3	1:C:72:TRP:CZ2	2.48	0.48
1:D:150:MET:HE2	2:D:775:HOH:O	2.08	0.48
1:D:430:ILE:HD12	2:D:710:HOH:O	2.13	0.48
1:A:430:ILE:HD12	2:A:710:HOH:O	2.13	0.48
1:D:404:ASP:O	1:D:408:HIS:ND1	2.32	0.48
1:B:436:PHE:CG	1:F:408:HIS:HB3	2.49	0.48
1:C:430:ILE:HD12	2:C:709:HOH:O	2.13	0.48
1:C:404:ASP:O	1:C:408:HIS:ND1	2.32	0.48
1:E:66:ARG:HD3	1:E:72:TRP:CZ2	2.48	0.48
1:B:404:ASP:O	1:B:408:HIS:ND1	2.32	0.48
1:F:66:ARG:HD3	1:F:72:TRP:CZ2	2.48	0.48
1:A:404:ASP:O	1:A:408:HIS:ND1	2.32	0.48
1:A:190:TYR:OH	1:C:154:LYS:O	2.18	0.47
1:D:66:ARG:HD3	1:D:72:TRP:CZ2	2.48	0.47
1:B:56:ASN:HD22	1:B:84:GLN:H	1.63	0.47
1:B:66:ARG:HD3	1:B:72:TRP:CZ2	2.48	0.47
1:C:416:SER:HB3	1:E:429:PRO:HA	1.97	0.47
1:D:56:ASN:HD22	1:D:84:GLN:N	2.12	0.47
1:D:372:TYR:CD2	1:D:373:LEU:HD12	2.48	0.47
1:A:56:ASN:HD22	1:A:84:GLN:N	2.12	0.47
1:C:56:ASN:HD22	1:C:84:GLN:N	2.12	0.47
1:D:56:ASN:HD22	1:D:84:GLN:H	1.63	0.47
1:A:56:ASN:HD22	1:A:84:GLN:H	1.63	0.47
1:B:56:ASN:HD22	1:B:84:GLN:N	2.12	0.47
1:B:372:TYR:CD2	1:B:373:LEU:HD12	2.48	0.47
1:F:56:ASN:HD22	1:F:84:GLN:H	1.63	0.47
1:B:56:ASN:CG	1:B:57:HIS:HD1	2.18	0.47
1:C:56:ASN:HD22	1:C:84:GLN:H	1.63	0.47
1:D:56:ASN:CG	1:D:57:HIS:HD1	2.18	0.47
1:E:56:ASN:HD22	1:E:84:GLN:H	1.63	0.47
1:E:56:ASN:HD22	1:E:84:GLN:N	2.12	0.47
1:A:154:LYS:O	1:C:190:TYR:OH	2.20	0.46
1:F:56:ASN:HD22	1:F:84:GLN:N	2.12	0.46
1:A:56:ASN:CG	1:A:57:HIS:HD1	2.18	0.46
1:D:429:PRO:HA	1:E:416:SER:HB3	1.96	0.46
1:C:56:ASN:CG	1:C:57:HIS:HD1	2.18	0.46
1:C:429:PRO:HA	1:D:416:SER:HB3	1.97	0.46
1:E:430:ILE:HG12	2:E:631:HOH:O	2.16	0.46
1:F:430:ILE:HG12	2:F:631:HOH:O	2.16	0.46
1:D:430:ILE:HG12	2:D:631:HOH:O	2.16	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:ILE:HG12	2:B:631:HOH:O	2.16	0.45
1:F:56:ASN:CG	1:F:57:HIS:HD1	2.18	0.45
1:B:436:PHE:HB2	1:F:408:HIS:CD2	2.51	0.45
1:C:430:ILE:HG12	2:C:631:HOH:O	2.16	0.45
1:E:56:ASN:CG	1:E:57:HIS:HD1	2.18	0.45
1:A:430:ILE:HG12	2:A:631:HOH:O	2.16	0.45
1:B:461:ALA:O	1:B:465:MET:HG3	2.17	0.45
1:D:461:ALA:O	1:D:465:MET:HG3	2.17	0.45
1:C:461:ALA:O	1:C:465:MET:HG3	2.17	0.45
1:E:461:ALA:O	1:E:465:MET:HG3	2.17	0.45
1:A:461:ALA:O	1:A:465:MET:HG3	2.17	0.45
1:D:409:LEU:O	1:D:413:VAL:HG23	2.17	0.45
1:D:423:LYS:HD3	1:D:426:GLY:CA	2.44	0.45
1:E:421:PHE:CD2	1:E:423:LYS:HE2	2.52	0.45
1:F:421:PHE:CD2	1:F:423:LYS:HE2	2.52	0.45
1:F:461:ALA:O	1:F:465:MET:HG3	2.17	0.45
1:A:409:LEU:O	1:A:413:VAL:HG23	2.17	0.45
1:B:409:LEU:O	1:B:413:VAL:HG23	2.17	0.45
1:B:423:LYS:HD3	1:B:426:GLY:CA	2.44	0.45
1:C:409:LEU:O	1:C:413:VAL:HG23	2.17	0.45
1:E:91:GLY:HA3	1:E:125:ALA:O	2.17	0.45
1:E:142:GLU:HG2	1:E:146:ARG:HD2	1.99	0.45
1:B:400:LYS:HA	1:B:403:ARG:HG2	1.99	0.44
1:B:414:GLN:NE2	1:B:428:ILE:HA	2.31	0.44
1:D:400:LYS:HA	1:D:403:ARG:HG2	1.99	0.44
1:F:142:GLU:HG2	1:F:146:ARG:HD2	1.99	0.44
1:A:408:HIS:CD2	1:F:436:PHE:HB2	2.53	0.44
1:B:142:GLU:HG2	1:B:146:ARG:HD2	1.99	0.44
1:D:414:GLN:NE2	1:D:428:ILE:HA	2.31	0.44
1:F:91:GLY:HA3	1:F:125:ALA:O	2.18	0.44
1:A:142:GLU:HG2	1:A:146:ARG:HD2	1.99	0.44
1:C:142:GLU:HG2	1:C:146:ARG:HD2	1.99	0.44
1:E:213:SER:HB2	2:E:642:HOH:O	2.17	0.44
1:E:423:LYS:HD3	1:E:426:GLY:CA	2.44	0.44
1:E:414:GLN:NE2	1:E:428:ILE:HA	2.31	0.44
1:F:213:SER:HB2	2:F:642:HOH:O	2.17	0.44
1:A:118:VAL:HG23	1:A:120:VAL:HG23	2.00	0.44
1:A:436:PHE:HB2	1:B:408:HIS:HD2	1.81	0.44
1:B:398:THR:O	1:B:402:GLU:HG2	2.18	0.44
1:B:421:PHE:CD2	1:B:423:LYS:HE2	2.52	0.44
1:C:118:VAL:HG23	1:C:120:VAL:HG23	2.00	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:GLU:HG2	1:D:146:ARG:HD2	1.99	0.44
1:E:417:LEU:HD12	1:E:429:PRO:HG2	1.99	0.44
1:F:417:LEU:HD12	1:F:429:PRO:HG2	1.99	0.44
1:F:423:LYS:HD3	1:F:426:GLY:CA	2.44	0.44
1:C:400:LYS:HA	1:C:403:ARG:HG2	1.99	0.44
1:C:408:HIS:CD2	1:E:436:PHE:HB2	2.53	0.44
1:C:414:GLN:NE2	1:C:428:ILE:HA	2.31	0.44
1:D:421:PHE:CD2	1:D:423:LYS:HE2	2.52	0.44
1:A:400:LYS:HA	1:A:403:ARG:HG2	1.99	0.44
1:A:417:LEU:HD12	1:A:429:PRO:HG2	1.99	0.44
1:C:213:SER:HB2	2:C:642:HOH:O	2.17	0.44
1:D:398:THR:O	1:D:402:GLU:HG2	2.18	0.44
1:F:142:GLU:O	1:F:146:ARG:CG	2.50	0.44
1:F:414:GLN:NE2	1:F:428:ILE:HA	2.31	0.44
1:A:91:GLY:HA3	1:A:125:ALA:O	2.18	0.44
1:A:414:GLN:NE2	1:A:428:ILE:HA	2.31	0.44
1:B:91:GLY:HA3	1:B:125:ALA:O	2.18	0.44
1:C:403:ARG:NH2	2:C:616:HOH:O	2.51	0.44
1:A:213:SER:HB2	2:A:642:HOH:O	2.17	0.44
1:A:398:THR:O	1:A:402:GLU:HG2	2.18	0.44
1:A:403:ARG:NH2	2:A:616:HOH:O	2.51	0.44
1:A:408:HIS:HB3	1:F:436:PHE:CG	2.53	0.44
1:A:416:SER:CB	1:F:429:PRO:HA	2.47	0.44
1:A:421:PHE:CD2	1:A:423:LYS:HE2	2.52	0.44
1:B:213:SER:HB2	2:B:641:HOH:O	2.17	0.44
1:C:398:THR:O	1:C:402:GLU:HG2	2.18	0.44
1:C:423:LYS:HD3	1:C:426:GLY:CA	2.44	0.44
1:D:91:GLY:HA3	1:D:125:ALA:O	2.18	0.44
1:D:213:SER:HB2	2:D:642:HOH:O	2.17	0.44
1:F:409:LEU:O	1:F:413:VAL:HG23	2.17	0.44
1:A:423:LYS:HD3	1:A:426:GLY:CA	2.44	0.43
1:C:91:GLY:HA3	1:C:125:ALA:O	2.18	0.43
1:C:408:HIS:HB3	1:E:436:PHE:CG	2.53	0.43
1:C:417:LEU:HD12	1:C:429:PRO:HG2	1.99	0.43
1:C:421:PHE:CD2	1:C:423:LYS:HE2	2.52	0.43
1:D:436:PHE:HB2	1:E:408:HIS:CD2	2.53	0.43
1:E:409:LEU:O	1:E:413:VAL:HG23	2.17	0.43
1:B:466:ARG:HG3	2:B:717:HOH:O	2.18	0.43
1:D:466:ARG:HG3	2:D:716:HOH:O	2.18	0.43
1:F:385:TRP:CZ2	1:F:389:LEU:HD11	2.54	0.43
1:F:400:LYS:HA	1:F:403:ARG:HG2	1.99	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:ILE:HD11	2:B:714:HOH:O	2.18	0.43
1:E:118:VAL:HG23	1:E:120:VAL:HG23	2.00	0.43
1:E:142:GLU:O	1:E:146:ARG:CG	2.50	0.43
1:E:385:TRP:CZ2	1:E:389:LEU:HD11	2.54	0.43
1:E:398:THR:O	1:E:402:GLU:HG2	2.18	0.43
1:E:400:LYS:HA	1:E:403:ARG:HG2	1.99	0.43
1:E:466:ARG:HG3	2:E:716:HOH:O	2.19	0.43
1:F:466:ARG:HG3	2:F:716:HOH:O	2.18	0.43
1:D:429:PRO:HA	1:E:416:SER:CB	2.48	0.43
1:F:118:VAL:HG23	1:F:120:VAL:HG23	2.00	0.43
1:C:385:TRP:CZ2	1:C:389:LEU:HD11	2.54	0.43
1:C:436:PHE:CG	1:D:408:HIS:HB3	2.54	0.43
1:D:417:LEU:HD12	1:D:429:PRO:HG2	1.99	0.43
1:E:93:ILE:HD11	2:E:713:HOH:O	2.18	0.43
1:F:398:THR:O	1:F:402:GLU:HG2	2.18	0.43
1:A:67:ARG:HB2	1:A:71:SER:HB3	2.01	0.43
1:A:93:ILE:HG12	1:A:127:ALA:HB3	2.01	0.43
1:A:385:TRP:CZ2	1:A:389:LEU:HD11	2.54	0.43
1:A:436:PHE:CD1	1:B:408:HIS:HB3	2.54	0.43
1:B:403:ARG:NH2	2:B:616:HOH:O	2.51	0.43
1:C:67:ARG:HB2	1:C:71:SER:HB3	2.01	0.43
1:C:93:ILE:HG12	1:C:127:ALA:HB3	2.01	0.43
1:D:93:ILE:HD11	2:D:713:HOH:O	2.18	0.43
1:D:385:TRP:CZ2	1:D:389:LEU:HD11	2.54	0.43
1:E:403:ARG:NH2	2:E:616:HOH:O	2.51	0.43
1:A:93:ILE:HD11	2:A:713:HOH:O	2.18	0.43
1:B:385:TRP:CZ2	1:B:389:LEU:HD11	2.54	0.43
1:B:417:LEU:HD12	1:B:429:PRO:HG2	1.99	0.43
1:C:93:ILE:HD11	2:C:711:HOH:O	2.18	0.43
1:A:66:ARG:NH1	1:A:70:GLY:O	2.52	0.43
1:C:66:ARG:NH1	1:C:70:GLY:O	2.52	0.43
1:F:93:ILE:HD11	2:F:713:HOH:O	2.18	0.43
1:F:403:ARG:NH2	2:F:616:HOH:O	2.51	0.43
1:D:67:ARG:HB2	1:D:71:SER:HB3	2.01	0.43
1:D:118:VAL:HG23	1:D:120:VAL:HG23	2.00	0.43
1:D:403:ARG:NH2	2:D:616:HOH:O	2.51	0.43
1:D:436:PHE:CG	1:E:408:HIS:HB3	2.54	0.43
1:B:66:ARG:NH1	1:B:70:GLY:O	2.52	0.42
1:B:67:ARG:HB2	1:B:71:SER:HB3	2.01	0.42
1:C:416:SER:CB	1:E:429:PRO:HA	2.48	0.42
1:C:429:PRO:HA	1:D:416:SER:CB	2.49	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:ARG:NH1	1:D:70:GLY:O	2.52	0.42
1:B:96:SER:HB3	1:B:99:VAL:HG13	2.02	0.42
1:B:118:VAL:HG23	1:B:120:VAL:HG23	2.00	0.42
1:D:96:SER:HB3	1:D:99:VAL:HG13	2.02	0.42
1:E:66:ARG:NH1	1:E:70:GLY:O	2.52	0.42
1:D:443:ALA:HA	1:D:447:ASP:OD2	2.20	0.42
1:F:66:ARG:NH1	1:F:70:GLY:O	2.52	0.42
1:B:443:ALA:HA	1:B:447:ASP:OD2	2.20	0.42
1:C:436:PHE:HB2	1:D:408:HIS:CD2	2.53	0.42
1:E:443:ALA:HA	1:E:447:ASP:OD2	2.20	0.42
1:D:374:ASN:O	2:D:604:HOH:O	2.22	0.42
1:F:443:ALA:HA	1:F:447:ASP:OD2	2.20	0.42
1:A:96:SER:HB3	1:A:99:VAL:HG13	2.02	0.42
1:A:96:SER:O	1:A:99:VAL:HG22	2.20	0.42
1:C:96:SER:HB3	1:C:99:VAL:HG13	2.02	0.42
1:D:150:MET:HG2	1:D:154:LYS:NZ	2.35	0.42
1:B:150:MET:HG2	1:B:154:LYS:NZ	2.35	0.42
1:B:429:PRO:HA	1:F:416:SER:HB3	2.01	0.42
1:C:96:SER:O	1:C:99:VAL:HG22	2.20	0.42
1:A:466:ARG:HG3	2:A:716:HOH:O	2.19	0.42
1:A:468:ALA:O	1:A:472:ASN:HA	2.20	0.42
1:C:466:ARG:HG3	2:C:715:HOH:O	2.19	0.42
1:C:468:ALA:O	1:C:472:ASN:HA	2.20	0.42
1:E:150:MET:HG2	1:E:154:LYS:NZ	2.35	0.42
1:A:414:GLN:O	1:A:417:LEU:N	2.53	0.42
1:B:374:ASN:O	2:B:604:HOH:O	2.22	0.42
1:E:67:ARG:HB2	1:E:71:SER:HB3	2.01	0.42
1:E:96:SER:O	1:E:99:VAL:HG22	2.20	0.42
1:F:67:ARG:HB2	1:F:71:SER:HB3	2.01	0.42
1:F:150:MET:HG2	1:F:154:LYS:NZ	2.35	0.42
1:A:154:LYS:HE2	1:E:84:GLN:HE22	1.84	0.41
1:B:93:ILE:HG12	1:B:127:ALA:HB3	2.01	0.41
1:C:414:GLN:O	1:C:417:LEU:N	2.53	0.41
1:D:414:GLN:O	1:D:417:LEU:N	2.53	0.41
1:B:414:GLN:O	1:B:417:LEU:N	2.53	0.41
1:D:93:ILE:HG12	1:D:127:ALA:HB3	2.01	0.41
1:E:404:ASP:O	1:E:408:HIS:ND1	2.32	0.41
1:E:468:ALA:O	1:E:472:ASN:HA	2.20	0.41
1:F:96:SER:O	1:F:99:VAL:HG22	2.20	0.41
1:F:468:ALA:O	1:F:472:ASN:HA	2.20	0.41
1:A:443:ALA:HA	1:A:447:ASP:OD2	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:468:ALA:O	1:D:472:ASN:HA	2.20	0.41
1:E:89:CYS:HB3	1:E:125:ALA:HB2	2.02	0.41
1:F:89:CYS:HB3	1:F:125:ALA:HB2	2.03	0.41
1:B:86:ARG:HD3	2:B:681:HOH:O	2.21	0.41
1:C:84:GLN:HE22	1:F:154:LYS:HE2	1.84	0.41
1:D:96:SER:O	1:D:99:VAL:HG22	2.20	0.41
1:E:93:ILE:HG12	1:E:127:ALA:HB3	2.01	0.41
1:B:96:SER:O	1:B:99:VAL:HG22	2.20	0.41
1:B:468:ALA:O	1:B:472:ASN:HA	2.20	0.41
1:C:154:LYS:HE2	1:F:84:GLN:HE22	1.84	0.41
1:C:374:ASN:O	2:C:604:HOH:O	2.22	0.41
1:C:443:ALA:HA	1:C:447:ASP:OD2	2.20	0.41
1:D:86:ARG:HD3	2:D:680:HOH:O	2.21	0.41
1:E:96:SER:HB3	1:E:99:VAL:HG13	2.02	0.41
1:F:96:SER:HB3	1:F:99:VAL:HG13	2.02	0.41
1:C:86:ARG:HD3	2:C:679:HOH:O	2.21	0.41
1:C:150:MET:HG2	1:C:154:LYS:NZ	2.35	0.41
1:D:89:CYS:HB3	1:D:125:ALA:HB2	2.03	0.41
1:A:86:ARG:HD3	2:A:680:HOH:O	2.21	0.41
1:A:90:LYS:NZ	1:A:164:VAL:HG12	2.36	0.41
1:B:89:CYS:HB3	1:B:125:ALA:HB2	2.03	0.41
1:B:403:ARG:CZ	2:B:616:HOH:O	2.69	0.41
1:C:90:LYS:NZ	1:C:164:VAL:HG12	2.36	0.41
1:D:403:ARG:CZ	2:D:616:HOH:O	2.69	0.41
1:F:93:ILE:HG12	1:F:127:ALA:HB3	2.01	0.41
1:F:404:ASP:O	1:F:408:HIS:ND1	2.32	0.41
1:A:150:MET:HG2	1:A:154:LYS:NZ	2.35	0.41
1:A:408:HIS:HD2	1:F:436:PHE:HB2	1.86	0.41
1:A:374:ASN:O	2:A:604:HOH:O	2.22	0.40
1:B:90:LYS:NZ	1:B:164:VAL:HG12	2.36	0.40
1:D:90:LYS:NZ	1:D:164:VAL:HG12	2.36	0.40
1:E:414:GLN:O	1:E:417:LEU:N	2.53	0.40
1:A:78:TYR:CE1	1:A:101:VAL:HG22	2.57	0.40
1:C:78:TYR:CE1	1:C:101:VAL:HG22	2.57	0.40
1:B:436:PHE:CD1	1:F:408:HIS:HB3	2.56	0.40
1:F:414:GLN:O	1:F:417:LEU:N	2.53	0.40
1:E:424:HIS:O	1:E:424:HIS:ND1	2.55	0.40
1:F:424:HIS:O	1:F:424:HIS:ND1	2.55	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	290/558 (52%)	279 (96%)	11 (4%)	0	100	100
1	B	290/558 (52%)	279 (96%)	11 (4%)	0	100	100
1	C	290/558 (52%)	279 (96%)	11 (4%)	0	100	100
1	D	290/558 (52%)	279 (96%)	11 (4%)	0	100	100
1	E	290/558 (52%)	279 (96%)	11 (4%)	0	100	100
1	F	290/558 (52%)	279 (96%)	11 (4%)	0	100	100
All	All	1740/3348 (52%)	1674 (96%)	66 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	244/456 (54%)	244 (100%)	0	100	100
1	B	244/456 (54%)	244 (100%)	0	100	100
1	C	244/456 (54%)	244 (100%)	0	100	100
1	D	244/456 (54%)	244 (100%)	0	100	100
1	E	244/456 (54%)	244 (100%)	0	100	100
1	F	244/456 (54%)	244 (100%)	0	100	100
All	All	1464/2736 (54%)	1464 (100%)	0	100	100



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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	HIS
1	A	195	HIS
1	A	209	HIS
1	A	388	ASN
1	A	414	GLN
1	B	189	HIS
1	B	195	HIS
1	B	209	HIS
1	B	388	ASN
1	B	414	GLN
1	C	189	HIS
1	C	195	HIS
1	C	209	HIS
1	C	388	ASN
1	C	414	GLN
1	D	189	HIS
1	D	195	HIS
1	D	209	HIS
1	D	388	ASN
1	D	414	GLN
1	E	189	HIS
1	E	195	HIS
1	E	209	HIS
1	E	388	ASN
1	E	414	GLN
1	F	189	HIS
1	F	195	HIS
1	F	209	HIS
1	F	388	ASN
1	F	414	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](#)

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.

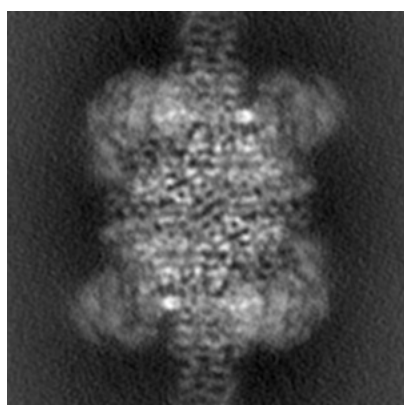
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8194. These allow visual inspection of the internal detail of the map and identification of artifacts.

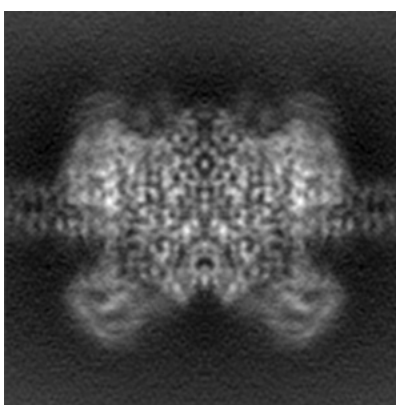
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

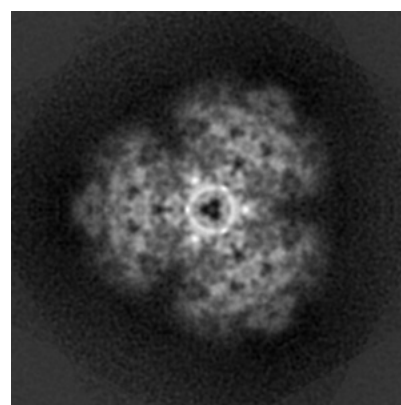
#### 6.1.1 Primary map



X



Y

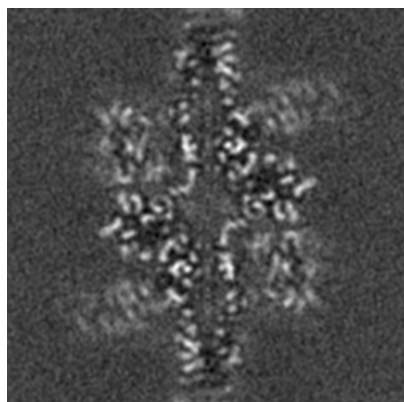


Z

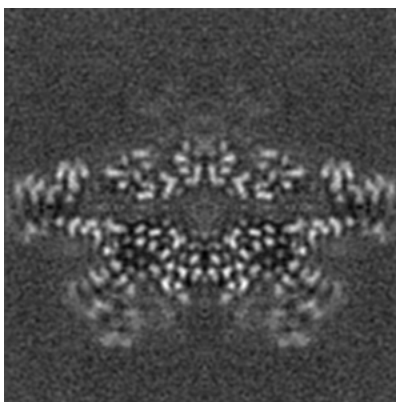
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

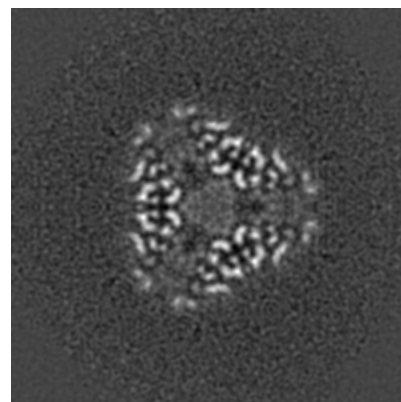
#### 6.2.1 Primary map



X Index: 117



Y Index: 117

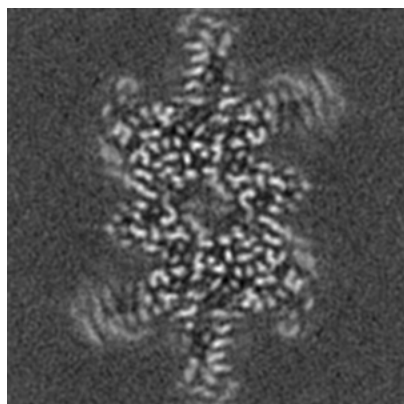


Z Index: 117

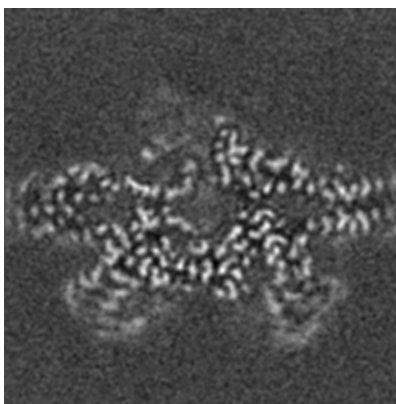
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

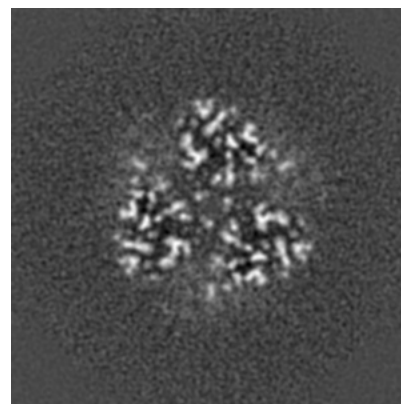
### 6.3.1 Primary map



X Index: 127



Y Index: 112



Z Index: 133

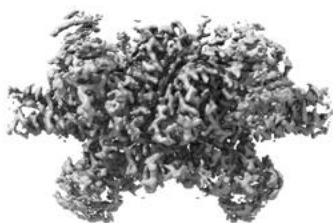
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0085. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

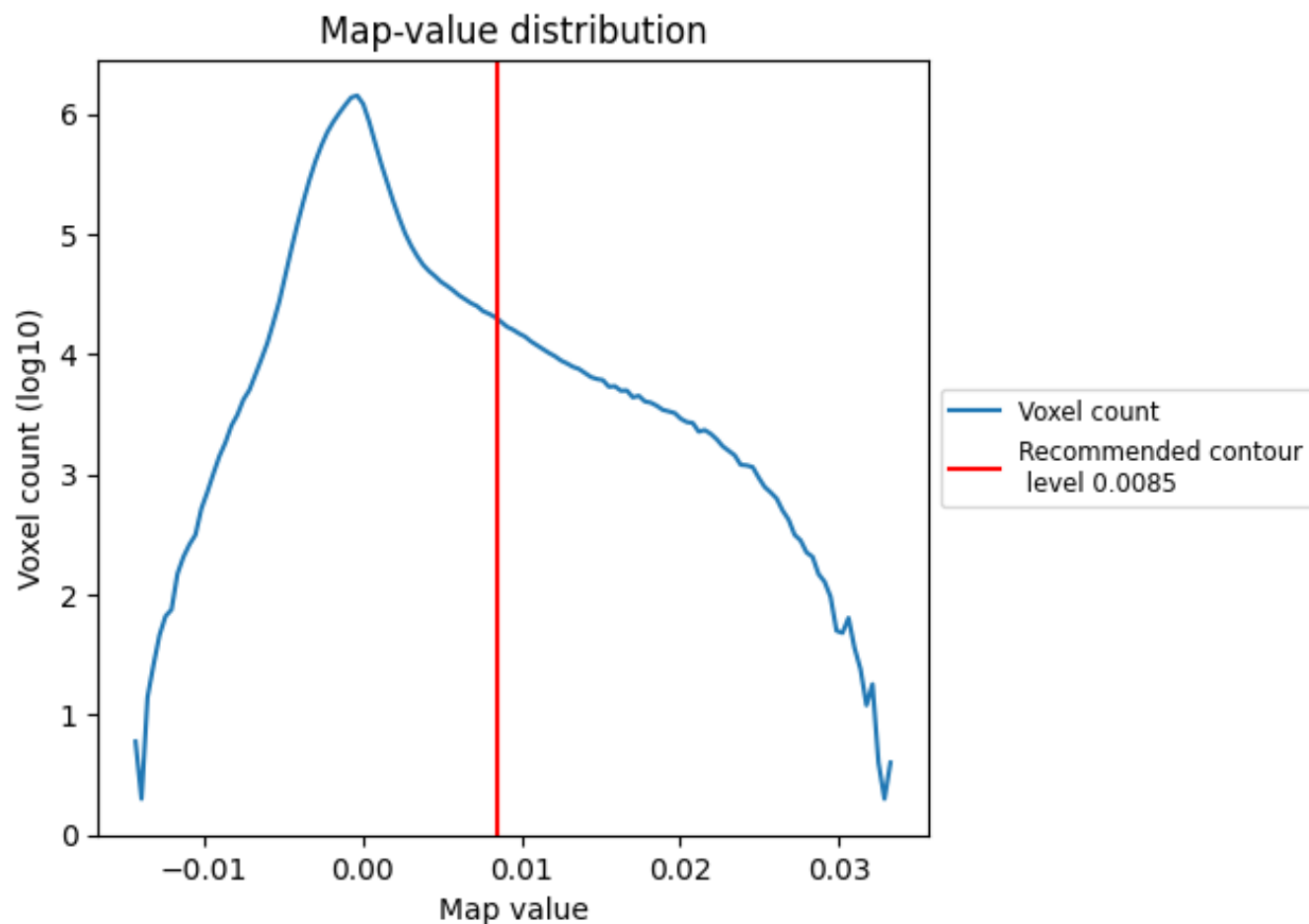
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

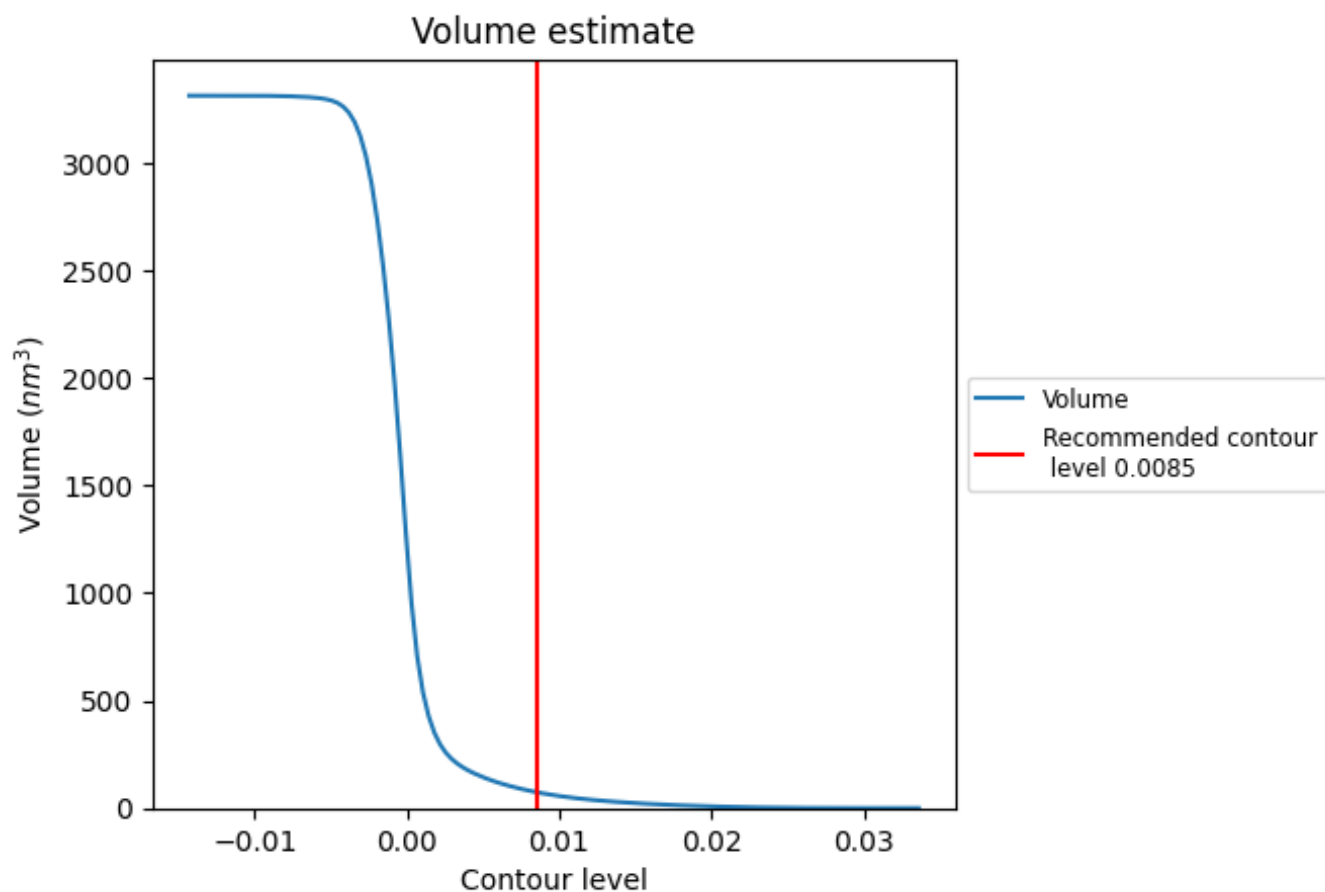
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

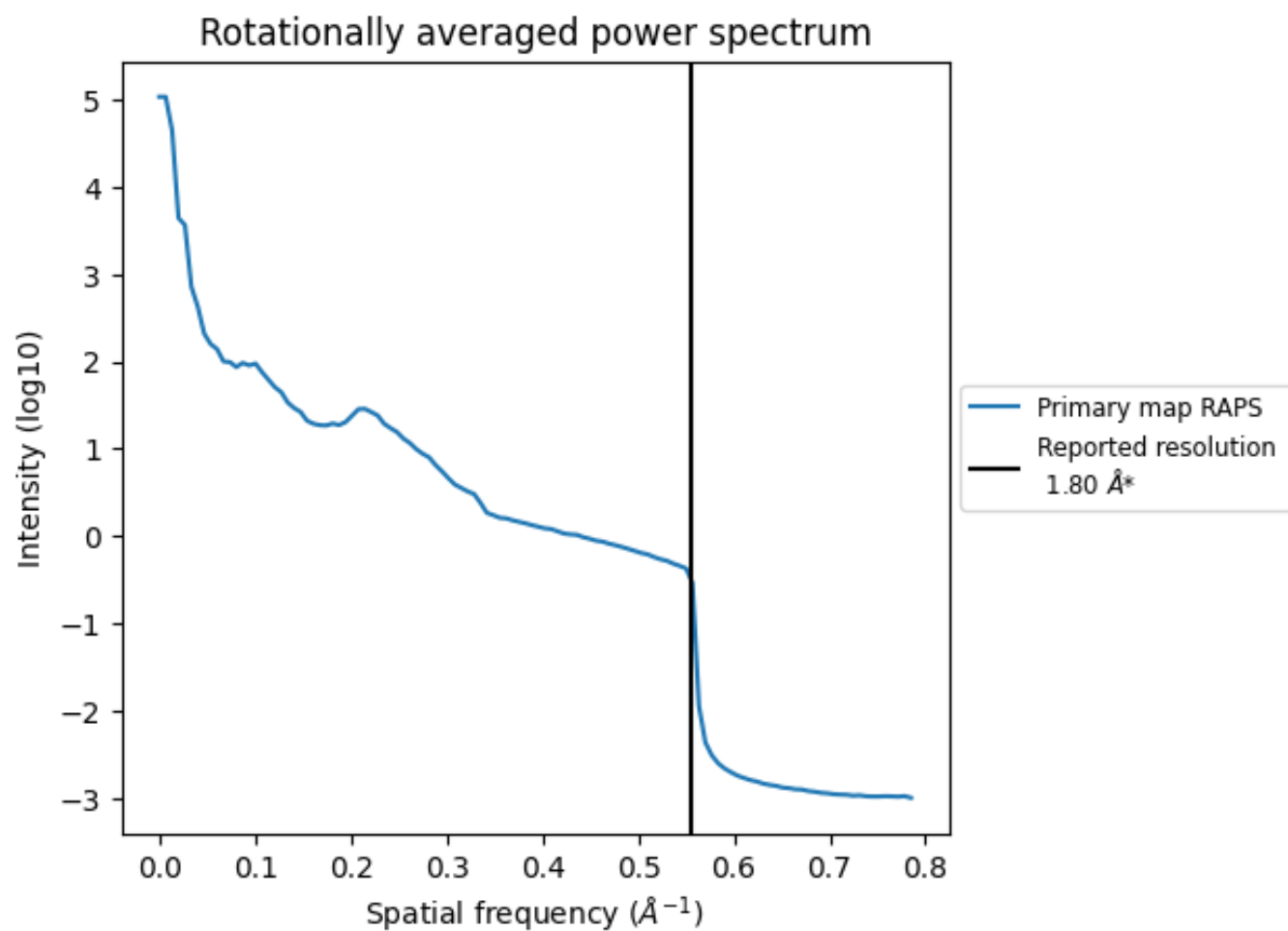
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 74 nm<sup>3</sup>; this corresponds to an approximate mass of 67 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.556 Å<sup>-1</sup>



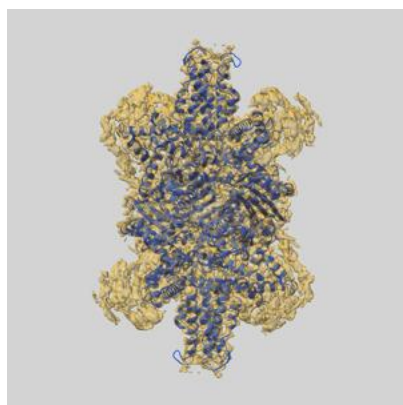
## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

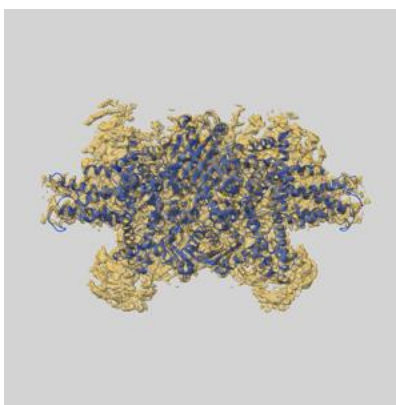
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8194 and PDB model 5K12. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

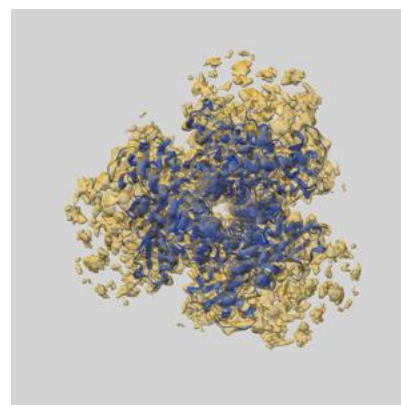
### 9.1 Map-model overlay [i](#)



X



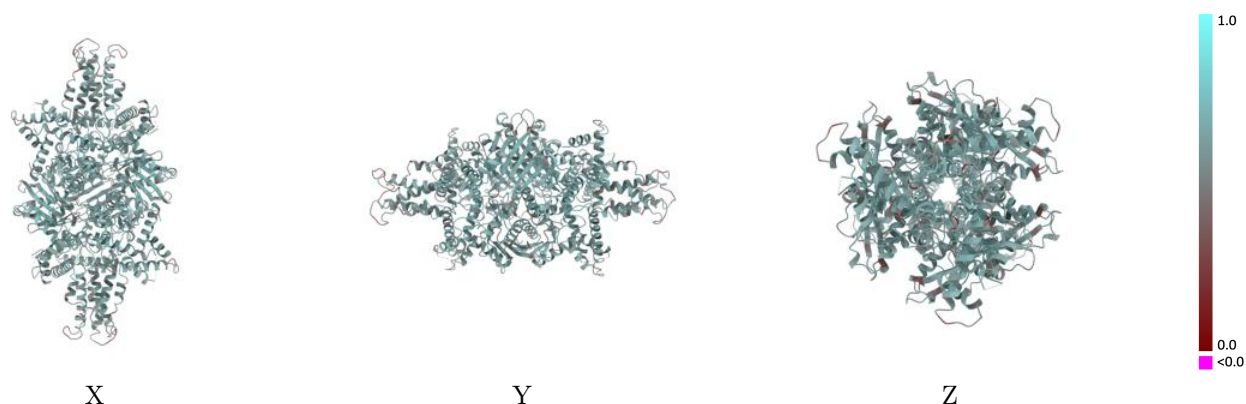
Y



Z

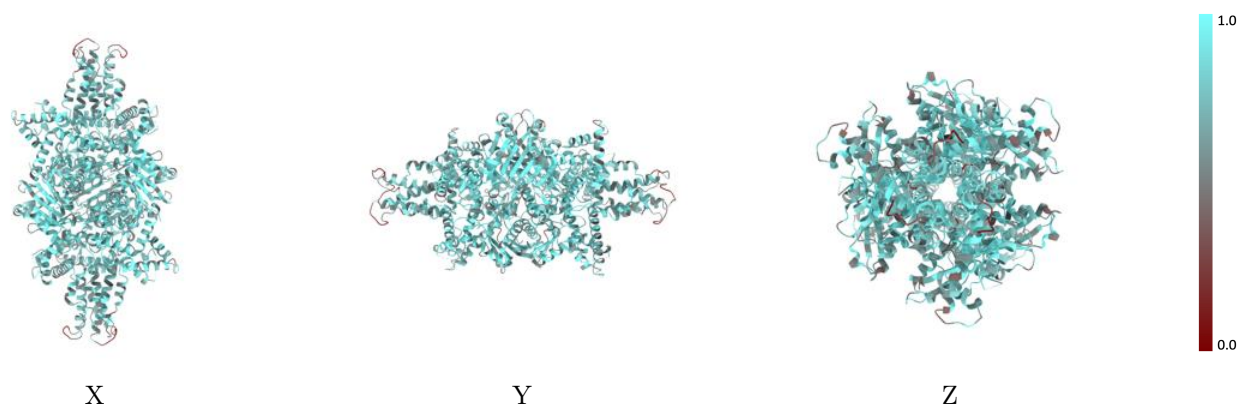
The images above show the 3D surface view of the map at the recommended contour level 0.0085 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



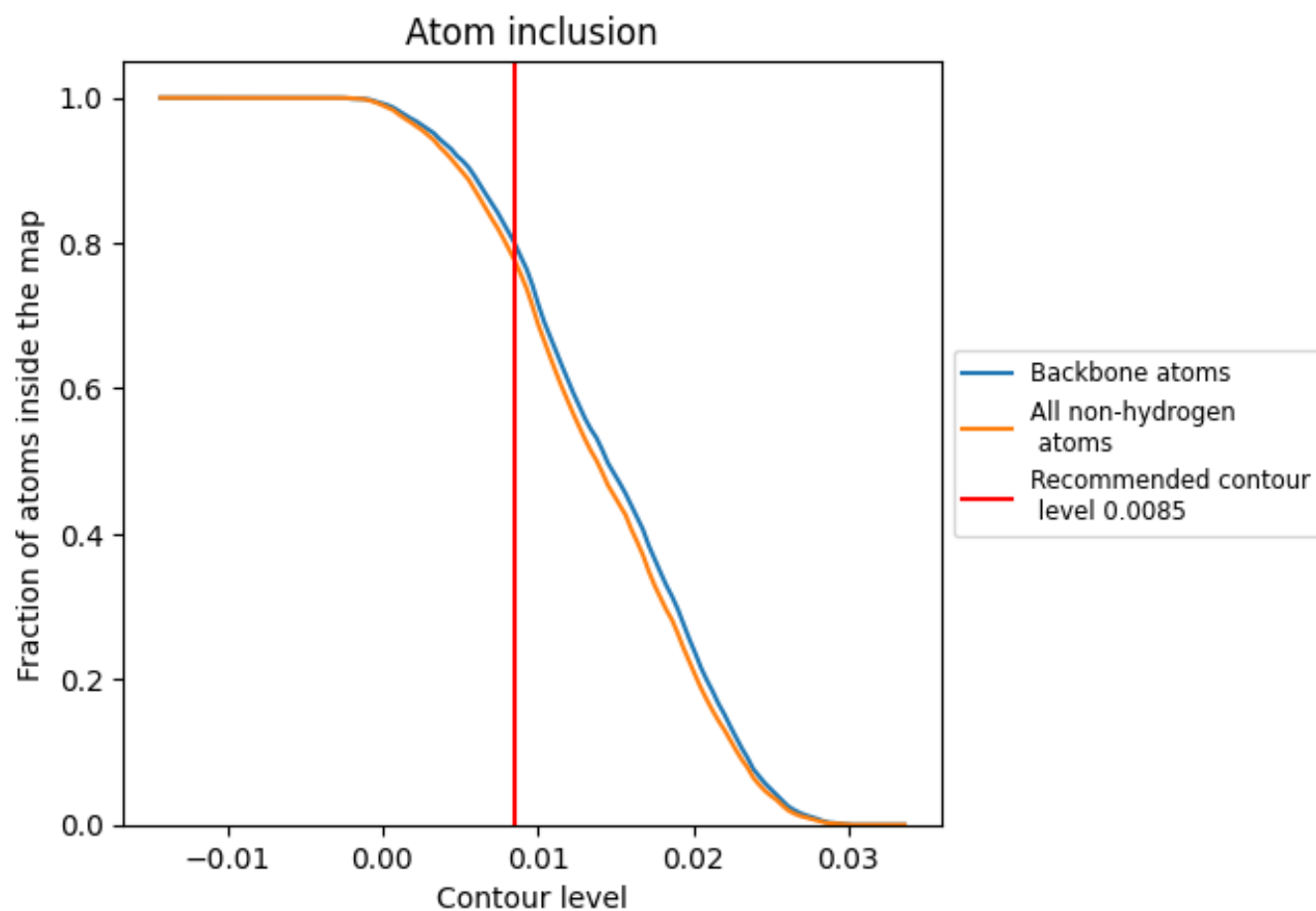
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0085).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0085) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7766	<div><div></div></div> 0.5980
A	<div><div></div></div> 0.7850	<div><div></div></div> 0.5960
B	<div><div></div></div> 0.7864	<div><div></div></div> 0.5980
C	<div><div></div></div> 0.7859	<div><div></div></div> 0.5970
D	<div><div></div></div> 0.7846	<div><div></div></div> 0.5980
E	<div><div></div></div> 0.7864	<div><div></div></div> 0.5970
F	<div><div></div></div> 0.7868	<div><div></div></div> 0.5980

1.0

0.0

<0.0