



## Full wwPDB EM Validation Report ⓘ

Mar 19, 2024 – 09:24 PM JST

PDB ID : 6JPQ  
EMDB ID : EMD-9870  
Title : CryoEM structure of Abo1 hexamer - ADP complex  
Authors : Cho, C.; Jang, J.; Song, J.J.  
Deposited on : 2019-03-27  
Resolution : 4.44 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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>.

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

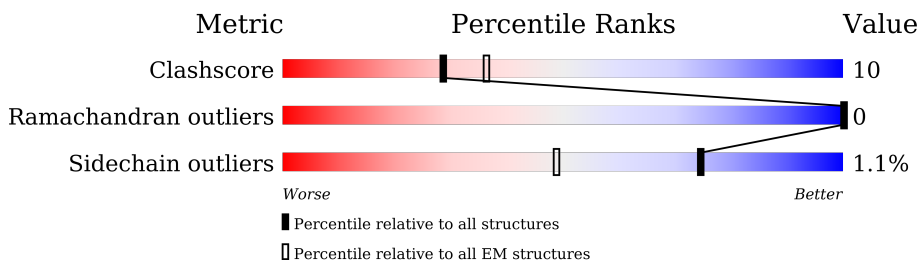
EMDB validation analysis : 0.0.1.dev70  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 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 4.44 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	1198	
1	B	1198	
1	C	1198	
1	D	1198	
1	E	1198	
1	F	1198	

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 27768 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 Uncharacterized AAA domain-containing protein C31G5.19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	577	4628	2963	789	854	22	0	0
1	B	577	4628	2963	789	854	22	0	0
1	C	577	4628	2963	789	854	22	0	0
1	D	577	4628	2963	789	854	22	0	0
1	E	577	4628	2963	789	854	22	0	0
1	F	577	4628	2963	789	854	22	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP O14114
A	-6	ALA	-	expression tag	UNP O14114
A	-5	MET	-	expression tag	UNP O14114
A	-4	GLY	-	expression tag	UNP O14114
A	-3	SER	-	expression tag	UNP O14114
A	-2	GLY	-	expression tag	UNP O14114
A	-1	ILE	-	expression tag	UNP O14114
A	0	GLN	-	expression tag	UNP O14114
B	-7	GLY	-	expression tag	UNP O14114
B	-6	ALA	-	expression tag	UNP O14114
B	-5	MET	-	expression tag	UNP O14114
B	-4	GLY	-	expression tag	UNP O14114
B	-3	SER	-	expression tag	UNP O14114
B	-2	GLY	-	expression tag	UNP O14114
B	-1	ILE	-	expression tag	UNP O14114
B	0	GLN	-	expression tag	UNP O14114
C	-7	GLY	-	expression tag	UNP O14114
C	-6	ALA	-	expression tag	UNP O14114

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	MET	-	expression tag	UNP O14114
C	-4	GLY	-	expression tag	UNP O14114
C	-3	SER	-	expression tag	UNP O14114
C	-2	GLY	-	expression tag	UNP O14114
C	-1	ILE	-	expression tag	UNP O14114
C	0	GLN	-	expression tag	UNP O14114
D	-7	GLY	-	expression tag	UNP O14114
D	-6	ALA	-	expression tag	UNP O14114
D	-5	MET	-	expression tag	UNP O14114
D	-4	GLY	-	expression tag	UNP O14114
D	-3	SER	-	expression tag	UNP O14114
D	-2	GLY	-	expression tag	UNP O14114
D	-1	ILE	-	expression tag	UNP O14114
D	0	GLN	-	expression tag	UNP O14114
E	-7	GLY	-	expression tag	UNP O14114
E	-6	ALA	-	expression tag	UNP O14114
E	-5	MET	-	expression tag	UNP O14114
E	-4	GLY	-	expression tag	UNP O14114
E	-3	SER	-	expression tag	UNP O14114
E	-2	GLY	-	expression tag	UNP O14114
E	-1	ILE	-	expression tag	UNP O14114
E	0	GLN	-	expression tag	UNP O14114
F	-7	GLY	-	expression tag	UNP O14114
F	-6	ALA	-	expression tag	UNP O14114
F	-5	MET	-	expression tag	UNP O14114
F	-4	GLY	-	expression tag	UNP O14114
F	-3	SER	-	expression tag	UNP O14114
F	-2	GLY	-	expression tag	UNP O14114
F	-1	ILE	-	expression tag	UNP O14114
F	0	GLN	-	expression tag	UNP O14114

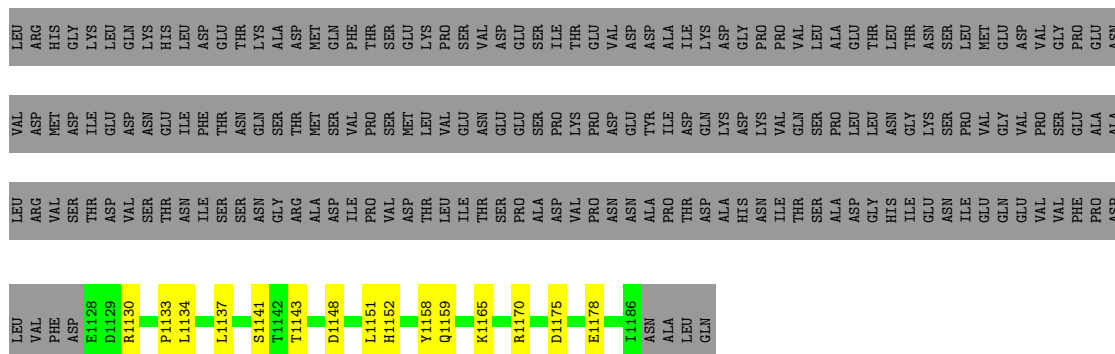




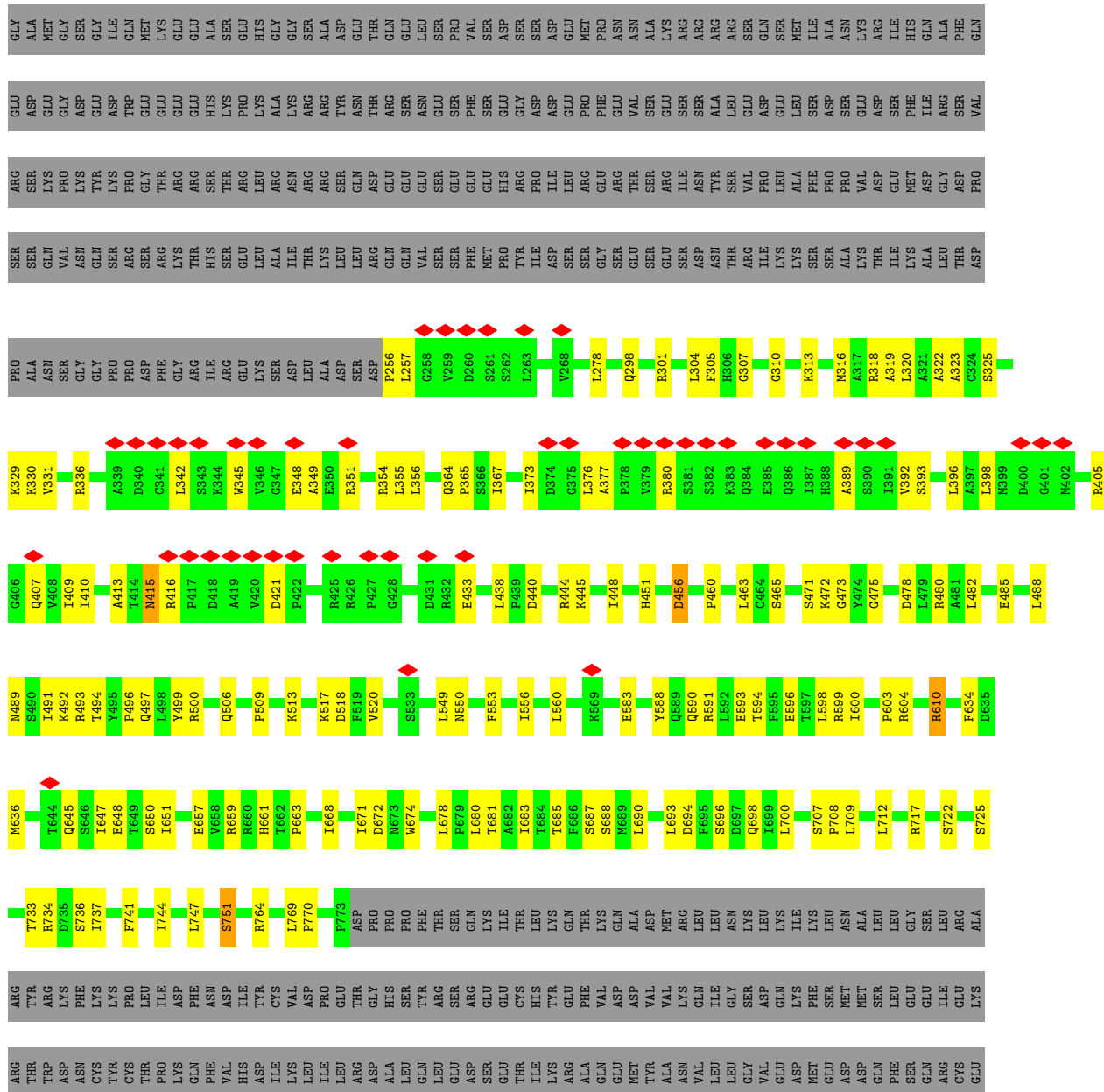
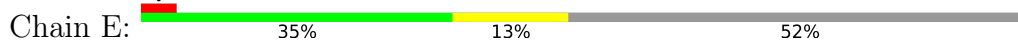








● Molecule 1: Uncharacterized AAA domain-containing protein C31G5.19





HIS	ASN	CYS
ILE	GLY	GLU
GLU	LYS	ARG
ASN	SER	MET
ILE	PRO	ALA
GLU	VAL	LEU
GLN	GLY	ARG
GLU	VAL	GLU
VAL	PRO	ASP
VAL	SER	GLY
PHE	GLU	ARG
PRO	ALA	ARG
ASP	ALA	LYS
LEU	LEU	LEU
VAL	ARG	ARG
PHE	VAL	HIS
ASP	SER	GLY
E1128	THR	LYS
D1129	ASP	LEU
R1130	VAL	GLN
	SER	ASN
P1133	THR	LYS
L1134	ASN	HIS
K1135	ILE	LEU
G1136	SER	PHE
L1137	SER	THR
L1138	ASN	ASN
I1139	GLY	LYS
D1140	ARG	ALA
S1141	ALA	MET
T1142	ASP	GLN
T1143	ILE	PHE
	PRO	THR
	VAL	PRO
D1148	VAL	SER
	ASP	SER
L1151	THR	GLU
H1152	LEU	LYS
	ILE	PRO
K1165	THR	SER
	SER	ASP
R1170	PRO	GLU
	ALA	GLU
D1175	ASP	SER
	VAL	ILE
E1178	PRO	THR
	PRO	LYS
T1186	ASN	ASP
ASN	ALA	VAL
ALA	PRO	GLU
LEU	THR	ASP
GLN	ASP	ILE
	ALA	LYS
	ALA	ASP
	HIS	LYS
	LYS	GLY
	ASN	PRO
	ILE	VAL
	THR	PRO
	SER	VAL
	ALA	LEU
	ASP	ALA
	GLY	GLU
	LEU	LEU
	THR	THR

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53582	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 ( $e^-/\text{\AA}^2$ )	1.02	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	10.447	Depositor
Minimum map value	-5.122	Depositor
Average map value	-0.034	Depositor
Map value standard deviation	0.576	Depositor
Recommended contour level	1.4	Depositor
Map size (Å)	335.0, 335.0, 335.0	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	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	0.36	0/4734	0.58	2/6411 (0.0%)
1	B	0.36	0/4734	0.58	2/6411 (0.0%)
1	C	0.36	0/4734	0.58	2/6411 (0.0%)
1	D	0.36	0/4734	0.58	2/6411 (0.0%)
1	E	0.36	0/4734	0.58	2/6411 (0.0%)
1	F	0.36	0/4734	0.58	2/6411 (0.0%)
All	All	0.36	0/28404	0.58	12/38466 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
All	All	0	12

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	355	LEU	CA-CB-CG	6.26	129.70	115.30
1	D	355	LEU	CA-CB-CG	6.26	129.70	115.30
1	E	355	LEU	CA-CB-CG	6.26	129.70	115.30
1	F	355	LEU	CA-CB-CG	6.26	129.69	115.30
1	A	355	LEU	CA-CB-CG	6.25	129.68	115.30
1	B	355	LEU	CA-CB-CG	6.25	129.67	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	709	LEU	CA-CB-CG	5.14	127.12	115.30
1	D	709	LEU	CA-CB-CG	5.14	127.11	115.30
1	E	709	LEU	CA-CB-CG	5.13	127.11	115.30
1	B	709	LEU	CA-CB-CG	5.13	127.11	115.30
1	A	709	LEU	CA-CB-CG	5.13	127.10	115.30
1	F	709	LEU	CA-CB-CG	5.12	127.08	115.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	298	GLN	Peptide
1	A	751	SER	Peptide
1	B	298	GLN	Peptide
1	B	751	SER	Peptide
1	C	298	GLN	Peptide
1	C	751	SER	Peptide
1	D	298	GLN	Peptide
1	D	751	SER	Peptide
1	E	298	GLN	Peptide
1	E	751	SER	Peptide
1	F	298	GLN	Peptide
1	F	751	SER	Peptide

## 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	4628	0	4700	101	0
1	B	4628	0	4700	109	0
1	C	4628	0	4700	109	0
1	D	4628	0	4700	99	0
1	E	4628	0	4700	98	0
1	F	4628	0	4700	99	0
All	All	27768	0	28200	584	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 10.

All (584) 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:E:319:ALA:O	1:E:323:ALA:HB2	1.91	0.71
1:F:319:ALA:O	1:F:323:ALA:HB2	1.91	0.71
1:D:319:ALA:O	1:D:323:ALA:HB2	1.91	0.71
1:A:319:ALA:O	1:A:323:ALA:HB2	1.91	0.70
1:B:319:ALA:O	1:B:323:ALA:HB2	1.91	0.70
1:C:319:ALA:O	1:C:323:ALA:HB2	1.91	0.70
1:C:599:ARG:HG2	1:D:1158:TYR:HB3	1.75	0.68
1:E:438:LEU:HD21	1:E:473:GLY:HA2	1.77	0.67
1:D:438:LEU:HD21	1:D:473:GLY:HA2	1.77	0.67
1:B:438:LEU:HD21	1:B:473:GLY:HA2	1.77	0.66
1:C:438:LEU:HD21	1:C:473:GLY:HA2	1.77	0.66
1:F:304:LEU:HB2	1:F:433:GLU:HG2	1.79	0.65
1:F:438:LEU:HD21	1:F:473:GLY:HA2	1.77	0.65
1:A:438:LEU:HD21	1:A:473:GLY:HA2	1.77	0.65
1:B:599:ARG:HE	1:C:1159:GLN:HA	1.62	0.65
1:D:304:LEU:HB2	1:D:433:GLU:HG2	1.79	0.65
1:B:304:LEU:HB2	1:B:433:GLU:HG2	1.79	0.65
1:E:304:LEU:HB2	1:E:433:GLU:HG2	1.79	0.65
1:C:304:LEU:HB2	1:C:433:GLU:HG2	1.78	0.64
1:A:304:LEU:HB2	1:A:433:GLU:HG2	1.79	0.64
1:A:307:GLY:O	1:A:415:ASN:ND2	2.32	0.63
1:F:307:GLY:O	1:F:415:ASN:ND2	2.32	0.63
1:D:307:GLY:O	1:D:415:ASN:ND2	2.31	0.63
1:B:599:ARG:O	1:C:1159:GLN:NE2	2.32	0.63
1:E:307:GLY:O	1:E:415:ASN:ND2	2.32	0.63
1:B:307:GLY:O	1:B:415:ASN:ND2	2.31	0.62
1:C:307:GLY:O	1:C:415:ASN:ND2	2.32	0.62
1:A:310:GLY:H	1:A:313:LYS:HB2	1.65	0.62
1:B:599:ARG:HG2	1:C:1158:TYR:HB3	1.82	0.61
1:C:310:GLY:H	1:C:313:LYS:HB2	1.65	0.61
1:F:663:PRO:HB3	1:F:698:GLN:HB2	1.83	0.61
1:F:405:ARG:HH11	1:F:410:ILE:HD12	1.66	0.61
1:D:405:ARG:HH11	1:D:410:ILE:HD12	1.66	0.61
1:D:310:GLY:H	1:D:313:LYS:HB2	1.65	0.61
1:F:310:GLY:H	1:F:313:LYS:HB2	1.65	0.61
1:B:663:PRO:HB3	1:B:698:GLN:HB2	1.83	0.61
1:D:663:PRO:HB3	1:D:698:GLN:HB2	1.83	0.61
1:A:405:ARG:HH11	1:A:410:ILE:HD12	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:405:ARG:HH11	1:E:410:ILE:HD12	1.66	0.60
1:E:663:PRO:HB3	1:E:698:GLN:HB2	1.83	0.60
1:C:663:PRO:HB3	1:C:698:GLN:HB2	1.83	0.60
1:E:310:GLY:H	1:E:313:LYS:HB2	1.65	0.60
1:A:456:ASP:OD1	1:A:456:ASP:N	2.34	0.60
1:D:456:ASP:N	1:D:456:ASP:OD1	2.34	0.60
1:B:310:GLY:H	1:B:313:LYS:HB2	1.65	0.59
1:B:1175:ASP:OD1	1:B:1175:ASP:N	2.35	0.59
1:A:663:PRO:HB3	1:A:698:GLN:HB2	1.83	0.59
1:F:492:LYS:NZ	1:F:496:PRO:O	2.35	0.59
1:B:440:ASP:O	1:B:472:LYS:NZ	2.36	0.59
1:B:405:ARG:HH11	1:B:410:ILE:HD12	1.66	0.59
1:C:492:LYS:NZ	1:C:496:PRO:O	2.35	0.59
1:F:1175:ASP:N	1:F:1175:ASP:OD1	2.35	0.59
1:E:594:THR:HA	1:E:598:LEU:HD13	1.85	0.59
1:C:405:ARG:HH11	1:C:410:ILE:HD12	1.66	0.59
1:C:603:PRO:HB2	1:C:700:LEU:HA	1.85	0.59
1:D:603:PRO:HB2	1:D:700:LEU:HA	1.85	0.59
1:B:594:THR:HA	1:B:598:LEU:HD13	1.85	0.59
1:D:492:LYS:NZ	1:D:496:PRO:O	2.35	0.59
1:D:1175:ASP:N	1:D:1175:ASP:OD1	2.35	0.59
1:A:337:LYS:O	1:F:393:SER:OG	2.20	0.58
1:B:603:PRO:HB2	1:B:700:LEU:HA	1.85	0.58
1:C:456:ASP:OD1	1:C:456:ASP:N	2.34	0.58
1:E:456:ASP:OD1	1:E:456:ASP:N	2.34	0.58
1:E:734:ARG:HH22	1:E:1143:THR:HA	1.69	0.58
1:B:492:LYS:NZ	1:B:496:PRO:O	2.35	0.58
1:A:594:THR:HA	1:A:598:LEU:HD13	1.85	0.58
1:B:734:ARG:HH22	1:B:1143:THR:HA	1.69	0.58
1:D:734:ARG:HH22	1:D:1143:THR:HA	1.69	0.58
1:C:440:ASP:O	1:C:472:LYS:NZ	2.36	0.58
1:F:734:ARG:HH22	1:F:1143:THR:HA	1.69	0.58
1:B:380:ARG:HH21	1:C:375:GLY:HA3	1.68	0.57
1:F:603:PRO:HB2	1:F:700:LEU:HA	1.85	0.57
1:C:594:THR:HA	1:C:598:LEU:HD13	1.85	0.57
1:C:734:ARG:HH22	1:C:1143:THR:HA	1.68	0.57
1:A:603:PRO:HB2	1:A:700:LEU:HA	1.85	0.57
1:E:603:PRO:HB2	1:E:700:LEU:HA	1.85	0.57
1:A:1175:ASP:N	1:A:1175:ASP:OD1	2.35	0.57
1:D:594:THR:HA	1:D:598:LEU:HD13	1.85	0.57
1:F:456:ASP:N	1:F:456:ASP:OD1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:594:THR:HA	1:F:598:LEU:HD13	1.85	0.56
1:A:734:ARG:HH22	1:A:1143:THR:HA	1.69	0.56
1:B:456:ASP:OD1	1:B:456:ASP:N	2.34	0.56
1:A:393:SER:OG	1:B:337:LYS:O	2.19	0.56
1:E:331:VAL:HA	1:E:365:PRO:HB2	1.88	0.56
1:E:1175:ASP:OD1	1:E:1175:ASP:N	2.35	0.56
1:C:1137:LEU:O	1:C:1141:SER:OG	2.24	0.55
1:D:331:VAL:HA	1:D:365:PRO:HB2	1.88	0.55
1:D:1137:LEU:O	1:D:1141:SER:OG	2.24	0.55
1:E:492:LYS:NZ	1:E:496:PRO:O	2.35	0.55
1:F:331:VAL:HA	1:F:365:PRO:HB2	1.88	0.55
1:F:1137:LEU:O	1:F:1141:SER:OG	2.24	0.55
1:A:492:LYS:NZ	1:A:496:PRO:O	2.35	0.55
1:A:1137:LEU:O	1:A:1141:SER:OG	2.24	0.55
1:E:1137:LEU:O	1:E:1141:SER:OG	2.24	0.55
1:C:1175:ASP:OD1	1:C:1175:ASP:N	2.35	0.55
1:B:331:VAL:HA	1:B:365:PRO:HB2	1.88	0.54
1:A:331:VAL:HA	1:A:365:PRO:HB2	1.88	0.54
1:D:440:ASP:O	1:D:472:LYS:NZ	2.36	0.54
1:E:440:ASP:O	1:E:472:LYS:NZ	2.36	0.54
1:B:1137:LEU:O	1:B:1141:SER:OG	2.24	0.54
1:F:444:ARG:NH1	1:F:471:SER:O	2.41	0.54
1:C:331:VAL:HA	1:C:365:PRO:HB2	1.88	0.54
1:C:444:ARG:NH1	1:C:471:SER:O	2.41	0.54
1:E:444:ARG:NH1	1:E:471:SER:O	2.41	0.54
1:A:636:MET:SD	1:A:636:MET:N	2.80	0.54
1:B:444:ARG:NH1	1:B:471:SER:O	2.41	0.54
1:B:636:MET:SD	1:B:636:MET:N	2.80	0.54
1:C:636:MET:SD	1:C:636:MET:N	2.80	0.54
1:C:751:SER:OG	1:C:1165:LYS:O	2.26	0.53
1:B:751:SER:OG	1:B:1165:LYS:O	2.26	0.53
1:D:751:SER:OG	1:D:1165:LYS:O	2.26	0.53
1:A:444:ARG:NH1	1:A:471:SER:O	2.41	0.53
1:B:506:GLN:HE21	1:B:770:PRO:HG2	1.74	0.53
1:D:444:ARG:NH1	1:D:471:SER:O	2.41	0.53
1:E:451:HIS:CG	1:E:480:ARG:HE	2.26	0.53
1:A:451:HIS:CG	1:A:480:ARG:HE	2.26	0.53
1:D:294:ARG:NH1	1:E:509:PRO:O	2.41	0.53
1:A:440:ASP:O	1:A:472:LYS:NZ	2.36	0.53
1:F:451:HIS:CG	1:F:480:ARG:HE	2.26	0.53
1:C:506:GLN:HE21	1:C:770:PRO:HG2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:751:SER:OG	1:A:1165:LYS:O	2.26	0.53
1:D:451:HIS:CG	1:D:480:ARG:HE	2.26	0.53
1:D:634:PHE:HB2	1:D:668:ILE:HG12	1.91	0.53
1:E:751:SER:OG	1:E:1165:LYS:O	2.26	0.53
1:C:451:HIS:CG	1:C:480:ARG:HE	2.26	0.53
1:C:634:PHE:HB2	1:C:668:ILE:HG12	1.91	0.53
1:C:733:THR:HG23	1:C:736:SER:H	1.75	0.53
1:D:506:GLN:HE21	1:D:770:PRO:HG2	1.74	0.53
1:B:451:HIS:CG	1:B:480:ARG:HE	2.26	0.52
1:F:751:SER:HB3	1:F:1170:ARG:HH22	1.74	0.52
1:E:506:GLN:HE21	1:E:770:PRO:HG2	1.74	0.52
1:A:751:SER:HB3	1:A:1170:ARG:HH22	1.74	0.52
1:D:636:MET:N	1:D:636:MET:SD	2.80	0.52
1:D:751:SER:HB3	1:D:1170:ARG:HH22	1.74	0.52
1:E:634:PHE:HB2	1:E:668:ILE:HG12	1.91	0.52
1:E:751:SER:HB3	1:E:1170:ARG:HH22	1.74	0.52
1:F:588:TYR:HA	1:F:591:ARG:HD2	1.92	0.52
1:F:751:SER:OG	1:F:1165:LYS:O	2.26	0.52
1:C:751:SER:HB3	1:C:1170:ARG:HH22	1.74	0.52
1:B:751:SER:HB3	1:B:1170:ARG:HH22	1.74	0.52
1:D:733:THR:HG23	1:D:736:SER:H	1.75	0.52
1:F:733:THR:HG23	1:F:736:SER:H	1.74	0.52
1:A:506:GLN:HE21	1:A:770:PRO:HG2	1.74	0.52
1:A:588:TYR:HA	1:A:591:ARG:HD2	1.92	0.52
1:B:380:ARG:HH12	1:C:372:GLU:HG2	1.74	0.52
1:A:733:THR:HG23	1:A:736:SER:H	1.75	0.52
1:B:588:TYR:HA	1:B:591:ARG:HD2	1.92	0.52
1:D:588:TYR:HA	1:D:591:ARG:HD2	1.92	0.51
1:A:671:ILE:HA	1:A:674:TRP:HB3	1.92	0.51
1:B:634:PHE:HB2	1:B:668:ILE:HG12	1.91	0.51
1:B:1148:ASP:O	1:B:1152:HIS:ND1	2.42	0.51
1:A:497:GLN:HB3	1:A:769:LEU:HD12	1.93	0.51
1:A:634:PHE:HB2	1:A:668:ILE:HG12	1.91	0.51
1:B:590:GLN:HA	1:B:593:GLU:HB2	1.91	0.51
1:E:671:ILE:HA	1:E:674:TRP:HB3	1.92	0.51
1:F:345:TRP:HB2	1:F:348:GLU:HB2	1.93	0.51
1:B:671:ILE:HA	1:B:674:TRP:HB3	1.92	0.51
1:B:733:THR:HG23	1:B:736:SER:H	1.75	0.51
1:C:671:ILE:HA	1:C:674:TRP:HB3	1.93	0.51
1:E:497:GLN:HB3	1:E:769:LEU:HD12	1.93	0.51
1:F:590:GLN:HA	1:F:593:GLU:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:TRP:HB2	1:B:348:GLU:HB2	1.93	0.51
1:C:590:GLN:HA	1:C:593:GLU:HB2	1.91	0.51
1:A:590:GLN:HA	1:A:593:GLU:HB2	1.91	0.51
1:E:590:GLN:HA	1:E:593:GLU:HB2	1.91	0.51
1:F:634:PHE:HB2	1:F:668:ILE:HG12	1.91	0.51
1:D:345:TRP:HB2	1:D:348:GLU:HB2	1.93	0.51
1:D:590:GLN:HA	1:D:593:GLU:HB2	1.91	0.51
1:E:588:TYR:HA	1:E:591:ARG:HD2	1.92	0.51
1:E:610:ARG:HA	1:E:708:PRO:HD3	1.93	0.51
1:B:610:ARG:HA	1:B:708:PRO:HD3	1.93	0.51
1:D:497:GLN:HB3	1:D:769:LEU:HD12	1.93	0.51
1:E:733:THR:HG23	1:E:736:SER:H	1.74	0.51
1:E:1148:ASP:O	1:E:1152:HIS:ND1	2.42	0.51
1:A:338:GLY:HA3	1:F:380:ARG:HH22	1.76	0.50
1:A:610:ARG:HA	1:A:708:PRO:HD3	1.93	0.50
1:A:328:ASN:HB3	1:B:504:ARG:HH11	1.77	0.50
1:C:588:TYR:HA	1:C:591:ARG:HD2	1.92	0.50
1:F:497:GLN:HB3	1:F:769:LEU:HD12	1.93	0.50
1:F:506:GLN:HE21	1:F:770:PRO:HG2	1.74	0.50
1:F:685:THR:O	1:F:688:SER:OG	2.26	0.50
1:C:685:THR:O	1:C:688:SER:OG	2.26	0.50
1:D:671:ILE:HA	1:D:674:TRP:HB3	1.92	0.50
1:A:680:LEU:HA	1:A:683:ILE:HB	1.93	0.50
1:B:645:GLN:NE2	1:B:650:SER:OG	2.44	0.50
1:C:497:GLN:HB3	1:C:769:LEU:HD12	1.93	0.50
1:A:1148:ASP:O	1:A:1152:HIS:ND1	2.42	0.50
1:B:497:GLN:HB3	1:B:769:LEU:HD12	1.93	0.50
1:C:610:ARG:HA	1:C:708:PRO:HD3	1.93	0.50
1:E:345:TRP:HB2	1:E:348:GLU:HB2	1.93	0.50
1:F:671:ILE:HA	1:F:674:TRP:HB3	1.92	0.50
1:A:345:TRP:HB2	1:A:348:GLU:HB2	1.93	0.50
1:C:345:TRP:HB2	1:C:348:GLU:HB2	1.93	0.50
1:C:680:LEU:HA	1:C:683:ILE:HB	1.93	0.50
1:B:680:LEU:HA	1:B:683:ILE:HB	1.93	0.50
1:F:440:ASP:O	1:F:472:LYS:NZ	2.36	0.50
1:F:680:LEU:HA	1:F:683:ILE:HB	1.93	0.50
1:A:645:GLN:NE2	1:A:650:SER:OG	2.44	0.49
1:E:583:GLU:O	1:F:515:LYS:NZ	2.33	0.49
1:D:599:ARG:HG2	1:E:1158:TYR:HB3	1.93	0.49
1:D:610:ARG:HA	1:D:708:PRO:HD3	1.93	0.49
1:E:636:MET:SD	1:E:636:MET:N	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:SER:O	1:A:329:LYS:NZ	2.38	0.49
1:B:364:GLN:HA	1:B:407:GLN:HE21	1.77	0.49
1:A:364:GLN:HA	1:A:407:GLN:HE21	1.77	0.49
1:E:373:ILE:HD13	1:E:376:LEU:HD12	1.95	0.49
1:E:1148:ASP:OD1	1:E:1148:ASP:N	2.46	0.49
1:A:373:ILE:HD13	1:A:376:LEU:HD12	1.95	0.49
1:C:364:GLN:HA	1:C:407:GLN:HE21	1.78	0.49
1:D:364:GLN:HA	1:D:407:GLN:HE21	1.78	0.49
1:D:482:LEU:HA	1:D:485:GLU:HG2	1.95	0.49
1:D:680:LEU:HA	1:D:683:ILE:HB	1.93	0.49
1:F:694:ASP:OD2	1:F:696:SER:OG	2.29	0.49
1:C:482:LEU:HA	1:C:485:GLU:HG2	1.95	0.49
1:D:600:ILE:HD13	1:D:698:GLN:HG3	1.95	0.49
1:F:610:ARG:HA	1:F:708:PRO:HD3	1.93	0.49
1:A:647:ILE:HD13	1:A:678:LEU:HD11	1.95	0.49
1:B:319:ALA:O	1:B:323:ALA:CB	2.59	0.49
1:C:600:ILE:HD13	1:C:698:GLN:HG3	1.95	0.49
1:F:373:ILE:HD13	1:F:376:LEU:HD12	1.95	0.49
1:F:636:MET:SD	1:F:636:MET:N	2.80	0.49
1:C:319:ALA:O	1:C:323:ALA:CB	2.59	0.49
1:A:319:ALA:O	1:A:323:ALA:CB	2.59	0.48
1:A:377:ALA:HB1	1:A:392:VAL:HG22	1.95	0.48
1:B:1148:ASP:OD1	1:B:1148:ASP:N	2.46	0.48
1:D:694:ASP:OD2	1:D:696:SER:OG	2.29	0.48
1:F:1148:ASP:N	1:F:1148:ASP:OD1	2.46	0.48
1:B:600:ILE:HD13	1:B:698:GLN:HG3	1.95	0.48
1:E:319:ALA:O	1:E:323:ALA:CB	2.59	0.48
1:E:647:ILE:HD13	1:E:678:LEU:HD11	1.95	0.48
1:F:645:GLN:NE2	1:F:650:SER:OG	2.44	0.48
1:B:377:ALA:HB1	1:B:392:VAL:HG22	1.95	0.48
1:B:482:LEU:HA	1:B:485:GLU:HG2	1.95	0.48
1:E:482:LEU:HA	1:E:485:GLU:HG2	1.95	0.48
1:E:680:LEU:HA	1:E:683:ILE:HB	1.93	0.48
1:C:599:ARG:HE	1:D:1159:GLN:HA	1.78	0.48
1:C:647:ILE:HD13	1:C:678:LEU:HD11	1.95	0.48
1:D:377:ALA:HB1	1:D:392:VAL:HG22	1.96	0.48
1:D:645:GLN:NE2	1:D:650:SER:OG	2.44	0.48
1:F:647:ILE:HD13	1:F:678:LEU:HD11	1.95	0.48
1:A:600:ILE:HD13	1:A:698:GLN:HG3	1.95	0.48
1:D:647:ILE:HD13	1:D:678:LEU:HD11	1.95	0.48
1:E:645:GLN:NE2	1:E:650:SER:OG	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:364:GLN:HA	1:F:407:GLN:HE21	1.78	0.48
1:F:687:SER:HA	1:F:690:LEU:HD12	1.96	0.48
1:B:386:GLN:HG2	1:C:388:HIS:CE1	2.49	0.48
1:C:377:ALA:HB1	1:C:392:VAL:HG22	1.95	0.48
1:F:377:ALA:HB1	1:F:392:VAL:HG22	1.96	0.48
1:A:489:ASN:O	1:A:493:ARG:CB	2.62	0.48
1:B:426:ARG:HH22	1:C:309:PRO:HG2	1.79	0.48
1:B:723:LYS:HE3	1:C:1186:ILE:HD12	1.96	0.48
1:E:364:GLN:HA	1:E:407:GLN:HE21	1.78	0.48
1:F:489:ASN:O	1:F:493:ARG:CB	2.62	0.48
1:B:373:ILE:HD13	1:B:376:LEU:HD12	1.95	0.48
1:D:1148:ASP:O	1:D:1152:HIS:ND1	2.42	0.48
1:E:489:ASN:O	1:E:493:ARG:CB	2.62	0.48
1:F:319:ALA:O	1:F:323:ALA:CB	2.59	0.48
1:A:482:LEU:HA	1:A:485:GLU:HG2	1.95	0.48
1:C:373:ILE:HD13	1:C:376:LEU:HD12	1.95	0.48
1:B:647:ILE:HD13	1:B:678:LEU:HD11	1.95	0.48
1:D:319:ALA:O	1:D:323:ALA:CB	2.59	0.48
1:D:489:ASN:O	1:D:493:ARG:HB2	2.14	0.48
1:D:373:ILE:HD13	1:D:376:LEU:HD12	1.95	0.47
1:E:685:THR:O	1:E:688:SER:OG	2.26	0.47
1:D:687:SER:HA	1:D:690:LEU:HD12	1.96	0.47
1:A:489:ASN:O	1:A:493:ARG:HB2	2.14	0.47
1:C:489:ASN:O	1:C:493:ARG:CB	2.62	0.47
1:E:687:SER:HA	1:E:690:LEU:HD12	1.96	0.47
1:A:685:THR:O	1:A:688:SER:OG	2.26	0.47
1:A:687:SER:HA	1:A:690:LEU:HD12	1.96	0.47
1:B:295:PHE:HB3	1:C:455:TRP:HE1	1.79	0.47
1:C:489:ASN:O	1:C:493:ARG:HB2	2.14	0.47
1:C:645:GLN:NE2	1:C:650:SER:OG	2.44	0.47
1:D:648:GLU:HA	1:D:651:ILE:HD12	1.97	0.47
1:E:600:ILE:HD13	1:E:698:GLN:HG3	1.95	0.47
1:F:600:ILE:HD13	1:F:698:GLN:HG3	1.95	0.47
1:C:648:GLU:HA	1:C:651:ILE:HD12	1.97	0.47
1:D:489:ASN:O	1:D:493:ARG:CB	2.62	0.47
1:E:751:SER:H	1:E:1170:ARG:HH22	1.63	0.47
1:F:482:LEU:HA	1:F:485:GLU:HG2	1.95	0.47
1:C:550:ASN:HA	1:C:553:PHE:HB3	1.96	0.47
1:C:694:ASP:OD2	1:C:696:SER:OG	2.29	0.47
1:D:1148:ASP:OD1	1:D:1148:ASP:N	2.46	0.47
1:E:648:GLU:HA	1:E:651:ILE:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:ASN:HA	1:A:553:PHE:HB3	1.96	0.47
1:B:325:SER:O	1:B:329:LYS:NZ	2.38	0.47
1:B:694:ASP:OD2	1:B:696:SER:OG	2.29	0.47
1:D:685:THR:O	1:D:688:SER:OG	2.26	0.47
1:E:489:ASN:O	1:E:493:ARG:HB2	2.14	0.47
1:A:577:MET:O	1:B:764:ARG:N	2.37	0.47
1:D:751:SER:H	1:D:1170:ARG:HH22	1.63	0.47
1:A:496:PRO:HB3	1:A:764:ARG:HH11	1.80	0.47
1:A:648:GLU:HA	1:A:651:ILE:HD12	1.97	0.47
1:C:496:PRO:HB3	1:C:764:ARG:HH11	1.80	0.47
1:F:329:LYS:HA	1:F:330:LYS:HA	1.70	0.47
1:A:445:LYS:HA	1:A:448:ILE:HG22	1.97	0.47
1:A:694:ASP:OD2	1:A:696:SER:OG	2.29	0.47
1:B:489:ASN:O	1:B:493:ARG:CB	2.62	0.47
1:B:550:ASN:HA	1:B:553:PHE:HB3	1.96	0.47
1:B:648:GLU:HA	1:B:651:ILE:HD12	1.97	0.47
1:C:1148:ASP:OD1	1:C:1148:ASP:N	2.46	0.47
1:F:751:SER:H	1:F:1170:ARG:HH22	1.63	0.47
1:B:687:SER:HA	1:B:690:LEU:HD12	1.96	0.46
1:E:445:LYS:HA	1:E:448:ILE:HG22	1.97	0.46
1:B:489:ASN:O	1:B:493:ARG:HB2	2.14	0.46
1:D:550:ASN:HA	1:D:553:PHE:HB3	1.96	0.46
1:F:496:PRO:HB3	1:F:764:ARG:HH11	1.80	0.46
1:D:445:LYS:HA	1:D:448:ILE:HG22	1.97	0.46
1:D:496:PRO:HB3	1:D:764:ARG:HH11	1.80	0.46
1:F:325:SER:O	1:F:329:LYS:NZ	2.38	0.46
1:F:657:GLU:O	1:F:661:HIS:ND1	2.42	0.46
1:A:1148:ASP:N	1:A:1148:ASP:OD1	2.46	0.46
1:D:672:ASP:OD2	1:D:707:SER:N	2.49	0.46
1:E:550:ASN:HA	1:E:553:PHE:HB3	1.96	0.46
1:F:489:ASN:O	1:F:493:ARG:HB2	2.14	0.46
1:F:672:ASP:OD2	1:F:707:SER:N	2.49	0.46
1:A:751:SER:H	1:A:1170:ARG:HH22	1.63	0.46
1:B:556:ILE:O	1:B:560:LEU:HB2	2.16	0.46
1:D:556:ILE:O	1:D:560:LEU:HB2	2.16	0.46
1:E:377:ALA:HB1	1:E:392:VAL:HG22	1.96	0.46
1:F:550:ASN:HA	1:F:553:PHE:HB3	1.96	0.46
1:F:648:GLU:HA	1:F:651:ILE:HD12	1.97	0.46
1:C:445:LYS:HA	1:C:448:ILE:HG22	1.97	0.46
1:E:744:ILE:HA	1:E:747:LEU:HB2	1.98	0.46
1:A:517:LYS:HA	1:A:520:VAL:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:ILE:O	1:A:560:LEU:HB2	2.16	0.46
1:B:1134:LEU:HD11	1:B:1178:GLU:HB3	1.98	0.46
1:C:325:SER:O	1:C:329:LYS:NZ	2.38	0.46
1:C:672:ASP:OD2	1:C:707:SER:N	2.48	0.46
1:E:325:SER:O	1:E:329:LYS:NZ	2.38	0.46
1:F:744:ILE:HA	1:F:747:LEU:HB2	1.98	0.46
1:B:596:GLU:HA	1:B:599:ARG:HD3	1.98	0.45
1:B:657:GLU:O	1:B:661:HIS:ND1	2.42	0.45
1:B:744:ILE:HA	1:B:747:LEU:HB2	1.98	0.45
1:B:751:SER:H	1:B:1170:ARG:HH22	1.63	0.45
1:D:517:LYS:HA	1:D:520:VAL:HG12	1.98	0.45
1:D:744:ILE:HA	1:D:747:LEU:HB2	1.98	0.45
1:D:1134:LEU:HD11	1:D:1178:GLU:HB3	1.98	0.45
1:F:445:LYS:HA	1:F:448:ILE:HG22	1.97	0.45
1:A:734:ARG:HA	1:A:737:ILE:HD12	1.99	0.45
1:B:496:PRO:HB3	1:B:764:ARG:HH11	1.80	0.45
1:C:556:ILE:O	1:C:560:LEU:HB2	2.16	0.45
1:C:671:ILE:HG23	1:C:674:TRP:HE3	1.82	0.45
1:C:687:SER:HA	1:C:690:LEU:HD12	1.96	0.45
1:E:556:ILE:O	1:E:560:LEU:HB2	2.16	0.45
1:F:517:LYS:HA	1:F:520:VAL:HG12	1.99	0.45
1:B:685:THR:O	1:B:688:SER:OG	2.26	0.45
1:C:734:ARG:HA	1:C:737:ILE:HD12	1.99	0.45
1:E:496:PRO:HB3	1:E:764:ARG:HH11	1.80	0.45
1:F:556:ILE:O	1:F:560:LEU:HB2	2.16	0.45
1:A:1134:LEU:HD11	1:A:1178:GLU:HB3	1.98	0.45
1:B:517:LYS:HA	1:B:520:VAL:HG12	1.98	0.45
1:C:553:PHE:HA	1:C:556:ILE:HD12	1.98	0.45
1:C:1134:LEU:HD11	1:C:1178:GLU:HB3	1.98	0.45
1:E:517:LYS:HA	1:E:520:VAL:HG12	1.98	0.45
1:E:553:PHE:HA	1:E:556:ILE:HD12	1.98	0.45
1:E:694:ASP:OD2	1:E:696:SER:OG	2.29	0.45
1:C:517:LYS:HA	1:C:520:VAL:HG12	1.98	0.45
1:C:751:SER:H	1:C:1170:ARG:HH22	1.63	0.45
1:F:596:GLU:HA	1:F:599:ARG:HD3	1.98	0.45
1:F:1134:LEU:HD11	1:F:1178:GLU:HB3	1.98	0.45
1:D:596:GLU:HA	1:D:599:ARG:HD3	1.99	0.45
1:E:671:ILE:HG23	1:E:674:TRP:HE3	1.82	0.45
1:B:445:LYS:HA	1:B:448:ILE:HG22	1.97	0.45
1:B:734:ARG:HA	1:B:737:ILE:HD12	1.99	0.45
1:C:659:ARG:HH11	1:C:693:LEU:HD22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:PHE:HA	1:A:556:ILE:HD12	1.98	0.45
1:A:672:ASP:OD2	1:A:707:SER:N	2.49	0.45
1:B:488:LEU:HA	1:B:491:ILE:HD12	1.99	0.45
1:C:657:GLU:O	1:C:661:HIS:ND1	2.42	0.45
1:C:744:ILE:HA	1:C:747:LEU:HB2	1.98	0.45
1:D:553:PHE:HA	1:D:556:ILE:HD12	1.98	0.45
1:E:596:GLU:HA	1:E:599:ARG:HD3	1.98	0.45
1:A:488:LEU:HA	1:A:491:ILE:HD12	1.99	0.45
1:D:671:ILE:HG23	1:D:674:TRP:HE3	1.82	0.45
1:E:672:ASP:OD2	1:E:707:SER:N	2.49	0.45
1:A:596:GLU:HA	1:A:599:ARG:HD3	1.98	0.45
1:A:671:ILE:HG23	1:A:674:TRP:HE3	1.82	0.44
1:E:329:LYS:HA	1:E:330:LYS:HA	1.70	0.44
1:E:488:LEU:HA	1:E:491:ILE:HD12	1.99	0.44
1:E:1134:LEU:HD11	1:E:1178:GLU:HB3	1.98	0.44
1:F:671:ILE:HG23	1:F:674:TRP:HE3	1.82	0.44
1:C:488:LEU:HA	1:C:491:ILE:HD12	1.99	0.44
1:E:659:ARG:HH11	1:E:693:LEU:HD22	1.82	0.44
1:A:744:ILE:HA	1:A:747:LEU:HB2	1.98	0.44
1:B:295:PHE:O	1:C:455:TRP:NE1	2.50	0.44
1:B:671:ILE:HG23	1:B:674:TRP:HE3	1.82	0.44
1:D:734:ARG:HA	1:D:737:ILE:HD12	1.99	0.44
1:B:553:PHE:HA	1:B:556:ILE:HD12	1.98	0.44
1:B:672:ASP:OD2	1:B:707:SER:N	2.48	0.44
1:E:734:ARG:HA	1:E:737:ILE:HD12	1.99	0.44
1:F:659:ARG:HH11	1:F:693:LEU:HD22	1.82	0.44
1:F:734:ARG:HA	1:F:737:ILE:HD12	1.99	0.44
1:A:336:ARG:HD2	1:A:356:LEU:HD11	1.99	0.44
1:D:659:ARG:HH11	1:D:693:LEU:HD22	1.82	0.44
1:F:336:ARG:HD2	1:F:356:LEU:HD11	1.99	0.44
1:F:553:PHE:HA	1:F:556:ILE:HD12	1.98	0.44
1:A:681:THR:O	1:A:685:THR:OG1	2.25	0.44
1:B:316:MET:HA	1:B:319:ALA:HB3	2.00	0.44
1:B:659:ARG:HH11	1:B:693:LEU:HD22	1.82	0.44
1:C:741:PHE:HD1	1:C:744:ILE:HD11	1.83	0.44
1:F:488:LEU:HA	1:F:491:ILE:HD12	1.99	0.44
1:B:336:ARG:HD2	1:B:356:LEU:HD11	2.00	0.44
1:C:596:GLU:HA	1:C:599:ARG:HD3	1.98	0.44
1:C:1148:ASP:O	1:C:1152:HIS:ND1	2.42	0.44
1:D:657:GLU:O	1:D:661:HIS:ND1	2.42	0.44
1:D:712:LEU:H	1:D:717:ARG:NH2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:380:ARG:HG3	1:F:389:ALA:HA	2.00	0.44
1:D:316:MET:HA	1:D:319:ALA:HB3	2.00	0.43
1:D:488:LEU:HA	1:D:491:ILE:HD12	1.99	0.43
1:A:659:ARG:HH11	1:A:693:LEU:HD22	1.82	0.43
1:B:386:GLN:HG2	1:C:388:HIS:HE1	1.82	0.43
1:B:712:LEU:H	1:B:717:ARG:NH2	2.16	0.43
1:C:336:ARG:HD2	1:C:356:LEU:HD11	2.00	0.43
1:E:741:PHE:HD1	1:E:744:ILE:HD11	1.83	0.43
1:F:316:MET:HA	1:F:319:ALA:HB3	2.00	0.43
1:E:342:LEU:HD13	1:E:349:ALA:HB1	2.01	0.43
1:E:380:ARG:HG3	1:E:389:ALA:HA	2.00	0.43
1:B:342:LEU:HD13	1:B:349:ALA:HB1	2.01	0.43
1:B:595:PHE:HE2	1:C:756:PRO:HD2	1.83	0.43
1:A:257:LEU:HB3	1:F:298:GLN:O	2.17	0.43
1:A:712:LEU:H	1:A:717:ARG:NH2	2.16	0.43
1:C:577:MET:HG3	1:D:763:ARG:HE	1.84	0.43
1:C:712:LEU:H	1:C:717:ARG:NH2	2.16	0.43
1:D:336:ARG:HD2	1:D:356:LEU:HD11	1.99	0.43
1:D:741:PHE:HD1	1:D:744:ILE:HD11	1.83	0.43
1:E:712:LEU:H	1:E:717:ARG:NH2	2.16	0.43
1:F:741:PHE:HD1	1:F:744:ILE:HD11	1.83	0.43
1:A:316:MET:HA	1:A:319:ALA:HB3	2.00	0.43
1:A:380:ARG:HG3	1:A:389:ALA:HA	2.00	0.43
1:C:342:LEU:HD13	1:C:349:ALA:HB1	2.01	0.43
1:C:595:PHE:HE2	1:D:756:PRO:HD2	1.83	0.43
1:E:336:ARG:HD2	1:E:356:LEU:HD11	1.99	0.43
1:E:499:TYR:HD2	1:E:500:ARG:HE	1.66	0.43
1:C:465:SER:O	1:C:465:SER:OG	2.35	0.43
1:D:421:ASP:OD1	1:D:421:ASP:N	2.52	0.43
1:D:499:TYR:HD2	1:D:500:ARG:HE	1.66	0.43
1:F:712:LEU:H	1:F:717:ARG:NH2	2.16	0.43
1:F:1148:ASP:O	1:F:1152:HIS:ND1	2.42	0.43
1:D:325:SER:O	1:D:329:LYS:NZ	2.38	0.43
1:E:421:ASP:OD1	1:E:421:ASP:N	2.52	0.43
1:A:421:ASP:OD1	1:A:421:ASP:N	2.52	0.42
1:C:305:PHE:HB2	1:C:413:ALA:HA	2.01	0.42
1:C:499:TYR:HD2	1:C:500:ARG:HE	1.66	0.42
1:E:305:PHE:HB2	1:E:413:ALA:HA	2.01	0.42
1:F:489:ASN:ND2	1:F:518:ASP:HA	2.34	0.42
1:A:555:ASP:O	1:A:559:THR:OG1	2.34	0.42
1:B:380:ARG:HG3	1:B:389:ALA:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:ASP:OD1	1:B:421:ASP:N	2.52	0.42
1:B:681:THR:O	1:B:685:THR:OG1	2.25	0.42
1:B:741:PHE:HD1	1:B:744:ILE:HD11	1.83	0.42
1:B:1148:ASP:HA	1:B:1151:LEU:HD12	2.01	0.42
1:A:722:SER:HB3	1:A:725:SER:HB3	2.02	0.42
1:B:722:SER:HB3	1:B:725:SER:HB3	2.02	0.42
1:C:316:MET:HA	1:C:319:ALA:HB3	2.00	0.42
1:D:380:ARG:HG3	1:D:389:ALA:HA	2.00	0.42
1:D:489:ASN:ND2	1:D:518:ASP:HA	2.34	0.42
1:E:722:SER:HB3	1:E:725:SER:HB3	2.02	0.42
1:A:499:TYR:HD2	1:A:500:ARG:HE	1.66	0.42
1:B:489:ASN:ND2	1:B:518:ASP:HA	2.34	0.42
1:D:342:LEU:HD13	1:D:349:ALA:HB1	2.01	0.42
1:E:316:MET:HA	1:E:319:ALA:HB3	2.00	0.42
1:F:722:SER:HB3	1:F:725:SER:HB3	2.02	0.42
1:A:577:MET:HG3	1:B:763:ARG:HE	1.82	0.42
1:B:499:TYR:HD2	1:B:500:ARG:HE	1.66	0.42
1:B:734:ARG:HD3	1:B:737:ILE:HD12	2.02	0.42
1:D:681:THR:O	1:D:685:THR:OG1	2.25	0.42
1:E:734:ARG:HD3	1:E:737:ILE:HD12	2.02	0.42
1:A:460:PRO:HD2	1:A:463:LEU:HD21	2.02	0.42
1:A:489:ASN:ND2	1:A:518:ASP:HA	2.34	0.42
1:B:460:PRO:HD2	1:B:463:LEU:HD21	2.02	0.42
1:C:380:ARG:HG3	1:C:389:ALA:HA	2.00	0.42
1:D:734:ARG:HD3	1:D:737:ILE:HD12	2.02	0.42
1:E:489:ASN:ND2	1:E:518:ASP:HA	2.34	0.42
1:E:1139:ILE:HD12	1:E:1139:ILE:HA	1.96	0.42
1:A:741:PHE:HD1	1:A:744:ILE:HD11	1.83	0.42
1:A:1148:ASP:HA	1:A:1151:LEU:HD12	2.01	0.42
1:B:329:LYS:HA	1:B:330:LYS:HA	1.70	0.42
1:D:460:PRO:HD2	1:D:463:LEU:HD21	2.02	0.42
1:D:1148:ASP:HA	1:D:1151:LEU:HD12	2.01	0.42
1:B:475:GLY:N	1:B:478:ASP:OD1	2.53	0.42
1:C:1148:ASP:HA	1:C:1151:LEU:HD12	2.01	0.42
1:D:256:PRO:HB2	1:D:257:LEU:H	1.72	0.42
1:F:301:ARG:H	1:F:405:ARG:NH2	2.18	0.42
1:F:342:LEU:HD13	1:F:349:ALA:HB1	2.01	0.42
1:F:1148:ASP:HA	1:F:1151:LEU:HD12	2.01	0.42
1:E:475:GLY:N	1:E:478:ASP:OD1	2.53	0.42
1:E:1148:ASP:HA	1:E:1151:LEU:HD12	2.01	0.42
1:F:499:TYR:HD2	1:F:500:ARG:HE	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:734:ARG:HD3	1:F:737:ILE:HD12	2.02	0.42
1:A:305:PHE:HB2	1:A:413:ALA:HA	2.01	0.42
1:A:475:GLY:N	1:A:478:ASP:OD1	2.53	0.42
1:F:305:PHE:HB2	1:F:413:ALA:HA	2.01	0.42
1:F:367:ILE:HG22	1:F:409:ILE:HB	2.02	0.42
1:F:460:PRO:HD2	1:F:463:LEU:HD21	2.02	0.42
1:A:278:LEU:HD22	1:A:320:LEU:HD21	2.02	0.41
1:A:342:LEU:HD13	1:A:349:ALA:HB1	2.01	0.41
1:B:348:GLU:HA	1:B:351:ARG:HG2	2.02	0.41
1:B:367:ILE:HG22	1:B:409:ILE:HB	2.02	0.41
1:C:301:ARG:H	1:C:405:ARG:NH2	2.18	0.41
1:C:380:ARG:NH1	1:D:372:GLU:HG2	2.35	0.41
1:C:489:ASN:ND2	1:C:518:ASP:HA	2.34	0.41
1:E:256:PRO:HB2	1:E:257:LEU:H	1.72	0.41
1:B:301:ARG:H	1:B:405:ARG:NH2	2.18	0.41
1:B:751:SER:H	1:B:1170:ARG:NH2	2.18	0.41
1:D:475:GLY:N	1:D:478:ASP:OD1	2.53	0.41
1:D:549:LEU:O	1:D:553:PHE:HB2	2.20	0.41
1:E:460:PRO:HD2	1:E:463:LEU:HD21	2.02	0.41
1:B:549:LEU:O	1:B:553:PHE:HB2	2.20	0.41
1:C:734:ARG:HD3	1:C:737:ILE:HD12	2.02	0.41
1:F:1139:ILE:HD12	1:F:1139:ILE:HA	1.96	0.41
1:A:579:ASP:OD1	1:B:762:LYS:HG3	2.21	0.41
1:A:751:SER:H	1:A:1170:ARG:NH2	2.18	0.41
1:C:348:GLU:HA	1:C:351:ARG:HG2	2.02	0.41
1:D:1130:ARG:HA	1:D:1133:PRO:HD2	2.02	0.41
1:E:301:ARG:H	1:E:405:ARG:NH2	2.18	0.41
1:A:549:LEU:O	1:A:553:PHE:HB2	2.20	0.41
1:A:1130:ARG:HA	1:A:1133:PRO:HD2	2.02	0.41
1:B:1130:ARG:HA	1:B:1133:PRO:HD2	2.02	0.41
1:C:278:LEU:HD22	1:C:320:LEU:HD21	2.02	0.41
1:C:460:PRO:HD2	1:C:463:LEU:HD21	2.02	0.41
1:C:578:TYR:CD1	1:D:761:ARG:HG3	2.55	0.41
1:C:1130:ARG:HA	1:C:1133:PRO:HD2	2.02	0.41
1:D:305:PHE:HB2	1:D:413:ALA:HA	2.02	0.41
1:E:278:LEU:HD22	1:E:320:LEU:HD21	2.02	0.41
1:E:318:ARG:O	1:E:322:ALA:HB3	2.21	0.41
1:E:445:LYS:HG3	1:E:465:SER:HB2	2.03	0.41
1:A:572:PRO:HA	1:A:575:GLU:HB3	2.03	0.41
1:C:572:PRO:HA	1:C:575:GLU:HB3	2.03	0.41
1:D:301:ARG:H	1:D:405:ARG:NH2	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:ARG:O	1:D:322:ALA:HB3	2.20	0.41
1:E:751:SER:H	1:E:1170:ARG:NH2	2.18	0.41
1:F:348:GLU:HA	1:F:351:ARG:HG2	2.02	0.41
1:A:318:ARG:O	1:A:322:ALA:HB3	2.21	0.41
1:D:751:SER:H	1:D:1170:ARG:NH2	2.18	0.41
1:E:348:GLU:HA	1:E:351:ARG:HG2	2.02	0.41
1:E:367:ILE:HG22	1:E:409:ILE:HB	2.02	0.41
1:E:549:LEU:O	1:E:553:PHE:HB2	2.20	0.41
1:E:681:THR:O	1:E:685:THR:OG1	2.25	0.41
1:F:307:GLY:O	1:F:313:LYS:NZ	2.46	0.41
1:A:348:GLU:HA	1:A:351:ARG:HG2	2.02	0.41
1:C:445:LYS:HG3	1:C:465:SER:HB2	2.03	0.41
1:D:348:GLU:HA	1:D:351:ARG:HG2	2.02	0.41
1:F:318:ARG:O	1:F:322:ALA:HB3	2.21	0.41
1:F:475:GLY:N	1:F:478:ASP:OD1	2.53	0.41
1:F:549:LEU:O	1:F:553:PHE:HB2	2.20	0.41
1:F:1130:ARG:HA	1:F:1133:PRO:HD2	2.02	0.41
1:A:268:VAL:HB	1:A:315:LEU:HB3	2.03	0.41
1:A:764:ARG:HB2	1:F:579:ASP:HB3	2.02	0.41
1:B:445:LYS:HG3	1:B:465:SER:HB2	2.03	0.41
1:B:572:PRO:HA	1:B:575:GLU:HB3	2.03	0.41
1:C:475:GLY:N	1:C:478:ASP:OD1	2.53	0.41
1:C:549:LEU:O	1:C:553:PHE:HB2	2.20	0.41
1:D:278:LEU:HD22	1:D:320:LEU:HD21	2.02	0.41
1:D:318:ARG:HE	1:D:322:ALA:HB2	1.86	0.41
1:D:722:SER:HB3	1:D:725:SER:HB3	2.02	0.41
1:E:393:SER:HA	1:E:396:LEU:HD12	2.03	0.41
1:F:268:VAL:HB	1:F:315:LEU:HB3	2.03	0.41
1:F:421:ASP:OD1	1:F:421:ASP:N	2.52	0.41
1:F:751:SER:H	1:F:1170:ARG:NH2	2.18	0.41
1:A:301:ARG:H	1:A:405:ARG:NH2	2.18	0.41
1:A:393:SER:HA	1:A:396:LEU:HD12	2.03	0.41
1:A:445:LYS:HG3	1:A:465:SER:HB2	2.03	0.41
1:B:345:TRP:CZ3	1:C:344:LYS:HB3	2.55	0.41
1:C:393:SER:HA	1:C:396:LEU:HD12	2.03	0.41
1:C:722:SER:HB3	1:C:725:SER:HB3	2.02	0.41
1:D:445:LYS:HG3	1:D:465:SER:HB2	2.03	0.41
1:E:657:GLU:O	1:E:661:HIS:ND1	2.42	0.41
1:F:1135:LYS:HD2	1:F:1138:LEU:HD11	2.03	0.41
1:B:305:PHE:HB2	1:B:413:ALA:HA	2.01	0.40
1:B:494:THR:HG22	1:B:513:LYS:HD2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:494:THR:HG22	1:E:513:LYS:HD2	2.03	0.40
1:F:555:ASP:O	1:F:559:THR:OG1	2.34	0.40
1:A:734:ARG:HD3	1:A:737:ILE:HD12	2.02	0.40
1:E:318:ARG:HE	1:E:322:ALA:HB2	1.86	0.40
1:F:278:LEU:HD22	1:F:320:LEU:HD21	2.02	0.40
1:A:367:ILE:HG22	1:A:409:ILE:HB	2.02	0.40
1:B:318:ARG:O	1:B:322:ALA:HB3	2.21	0.40
1:C:318:ARG:O	1:C:322:ALA:HB3	2.21	0.40
1:C:751:SER:H	1:C:1170:ARG:NH2	2.18	0.40
1:C:1135:LYS:HD2	1:C:1138:LEU:HD11	2.04	0.40
1:E:398:LEU:HD23	1:E:398:LEU:HA	1.97	0.40
1:D:367:ILE:HG22	1:D:409:ILE:HB	2.02	0.40
1:F:572:PRO:HA	1:F:575:GLU:HB3	2.03	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	573/1198 (48%)	521 (91%)	52 (9%)	0	100	100
1	B	573/1198 (48%)	521 (91%)	52 (9%)	0	100	100
1	C	573/1198 (48%)	521 (91%)	52 (9%)	0	100	100
1	D	573/1198 (48%)	521 (91%)	52 (9%)	0	100	100
1	E	573/1198 (48%)	521 (91%)	52 (9%)	0	100	100
1	F	573/1198 (48%)	521 (91%)	52 (9%)	0	100	100
All	All	3438/7188 (48%)	3126 (91%)	312 (9%)	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	522/1086 (48%)	516 (99%)	6 (1%)	73	85
1	B	522/1086 (48%)	516 (99%)	6 (1%)	73	85
1	C	522/1086 (48%)	516 (99%)	6 (1%)	73	85
1	D	522/1086 (48%)	516 (99%)	6 (1%)	73	85
1	E	522/1086 (48%)	516 (99%)	6 (1%)	73	85
1	F	522/1086 (48%)	516 (99%)	6 (1%)	73	85
All	All	3132/6516 (48%)	3096 (99%)	36 (1%)	74	85

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	354	ARG
1	A	415	ASN
1	A	416	ARG
1	A	456	ASP
1	A	604	ARG
1	A	610	ARG
1	B	354	ARG
1	B	415	ASN
1	B	416	ARG
1	B	456	ASP
1	B	604	ARG
1	B	610	ARG
1	C	354	ARG
1	C	415	ASN
1	C	416	ARG
1	C	456	ASP
1	C	604	ARG
1	C	610	ARG
1	D	354	ARG
1	D	415	ASN
1	D	416	ARG
1	D	456	ASP

*Continued on next page...*

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Mol	Chain	Res	Type
1	D	604	ARG
1	D	610	ARG
1	E	354	ARG
1	E	415	ASN
1	E	416	ARG
1	E	456	ASP
1	E	604	ARG
1	E	610	ARG
1	F	354	ARG
1	F	415	ASN
1	F	416	ARG
1	F	456	ASP
1	F	604	ARG
1	F	610	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	384	GLN
1	A	415	ASN
1	A	489	ASN
1	A	497	GLN
1	A	506	GLN
1	A	645	GLN
1	A	653	HIS
1	A	1163	ASN
1	B	384	GLN
1	B	415	ASN
1	B	489	ASN
1	B	497	GLN
1	B	506	GLN
1	B	645	GLN
1	B	653	HIS
1	B	1163	ASN
1	C	384	GLN
1	C	388	HIS
1	C	415	ASN
1	C	489	ASN
1	C	497	GLN
1	C	506	GLN
1	C	645	GLN
1	C	653	HIS

*Continued on next page...*

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Mol	Chain	Res	Type
1	C	1163	ASN
1	D	384	GLN
1	D	415	ASN
1	D	489	ASN
1	D	497	GLN
1	D	506	GLN
1	D	645	GLN
1	D	653	HIS
1	D	1163	ASN
1	E	384	GLN
1	E	415	ASN
1	E	489	ASN
1	E	497	GLN
1	E	506	GLN
1	E	589	GLN
1	E	645	GLN
1	E	653	HIS
1	E	1163	ASN
1	F	384	GLN
1	F	415	ASN
1	F	489	ASN
1	F	497	GLN
1	F	506	GLN
1	F	589	GLN
1	F	645	GLN
1	F	653	HIS
1	F	1163	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.



## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

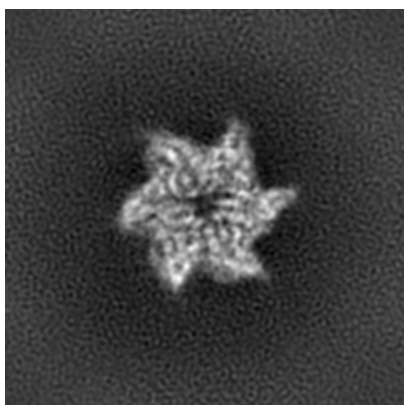
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9870. These allow visual inspection of the internal detail of the map and identification of artifacts.

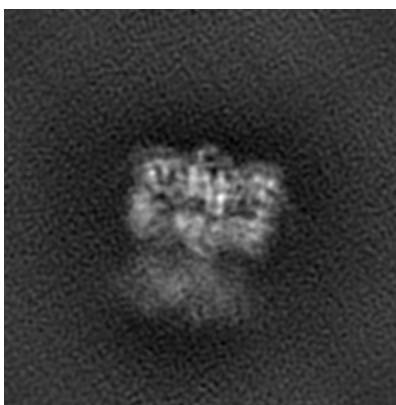
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

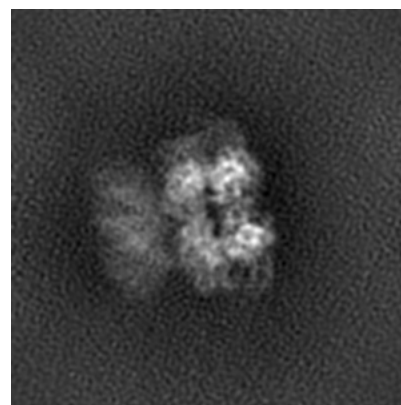
#### 6.1.1 Primary map



X



Y

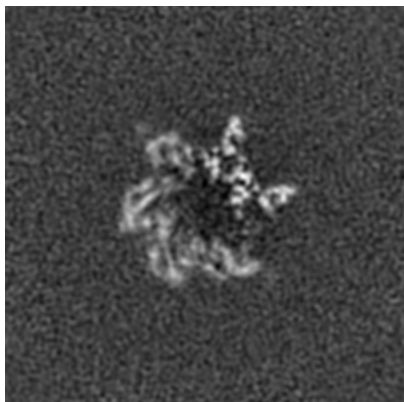


Z

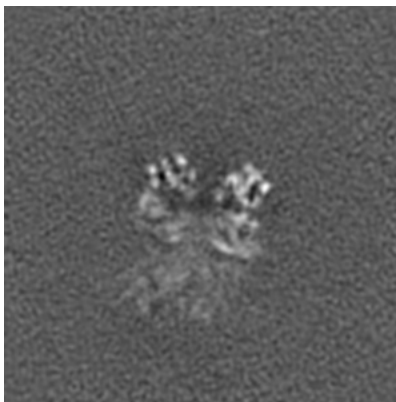
The images above show the map projected in three orthogonal directions.

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

#### 6.2.1 Primary map



X Index: 125



Y Index: 125

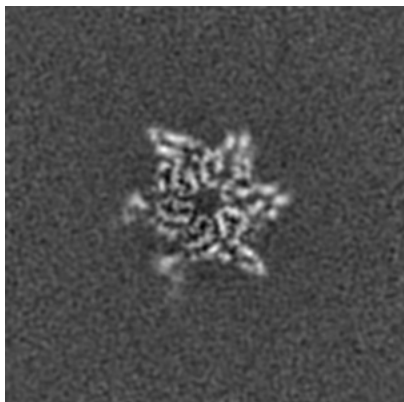


Z Index: 125

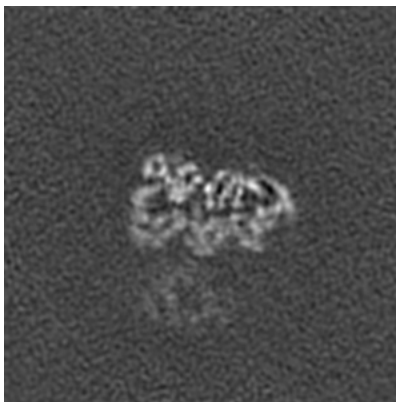
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 141



Y Index: 144

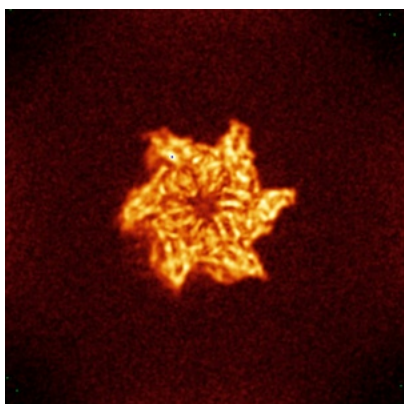


Z Index: 135

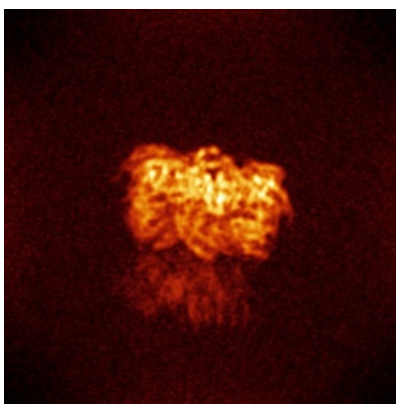
The images above show the largest variance slices of the map in three orthogonal directions.

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

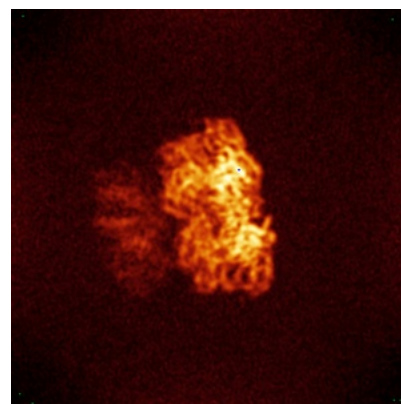
### 6.4.1 Primary map



X



Y

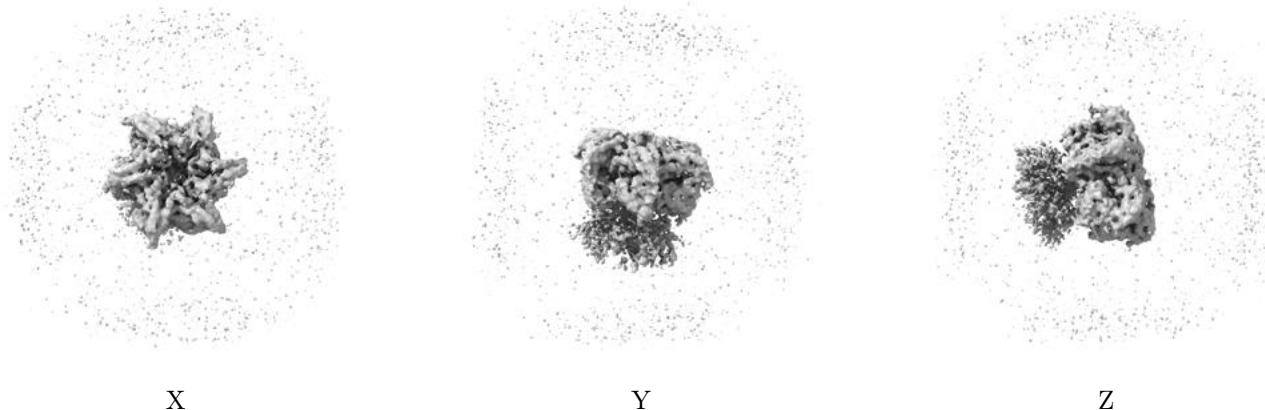


Z

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 1.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

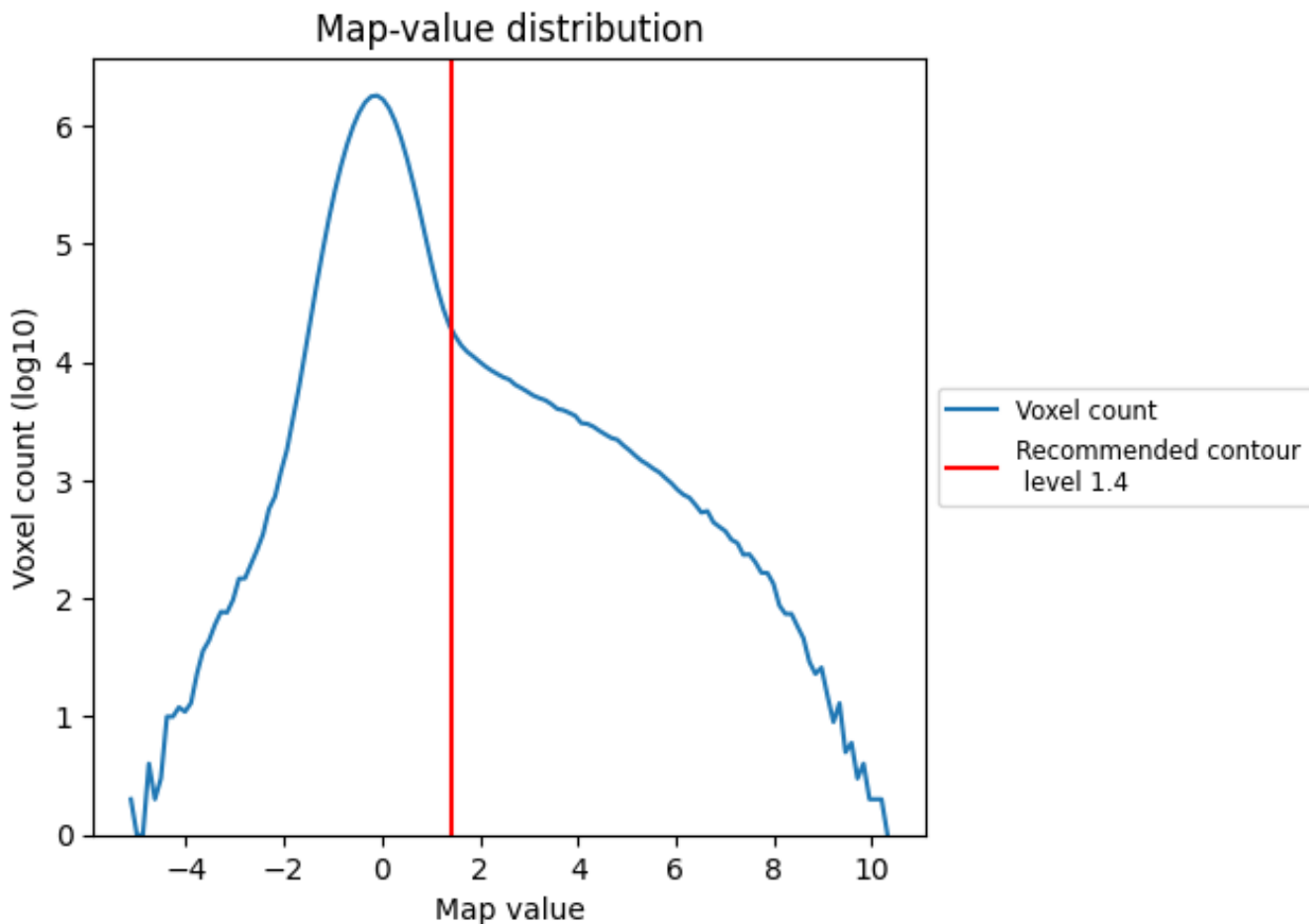
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

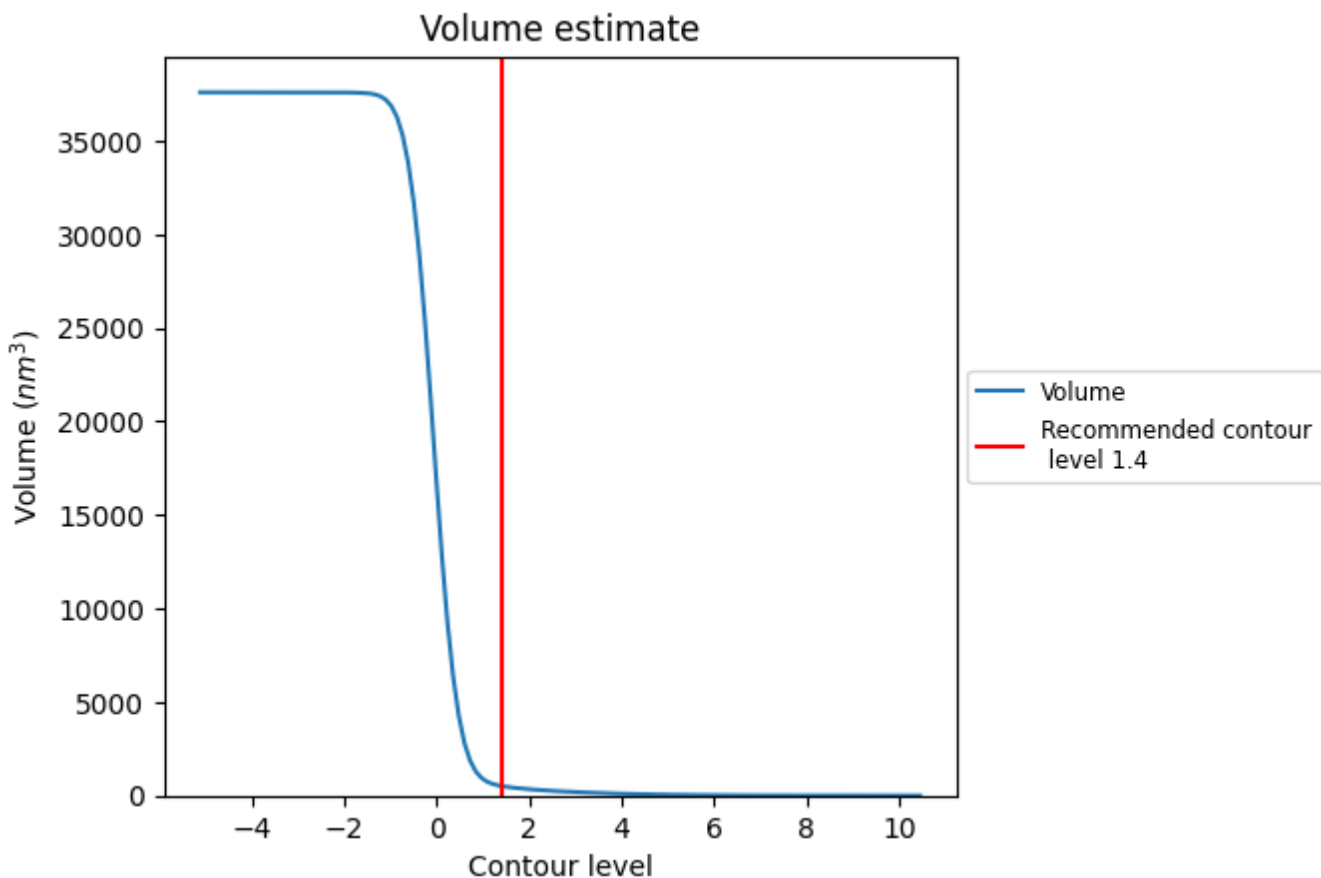
This section contains the results of statistical analysis of the map.

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



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

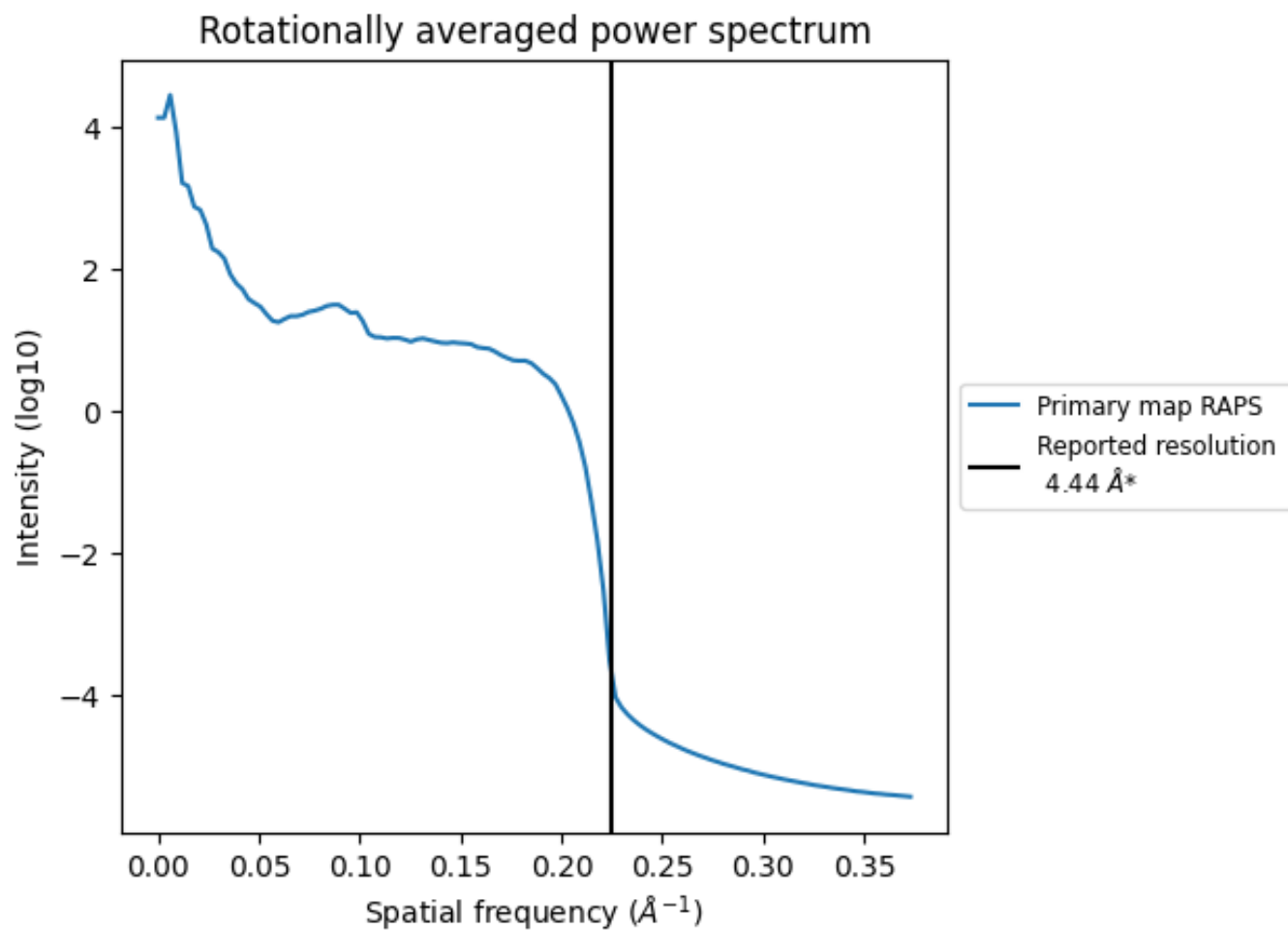
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 510  $\text{nm}^3$ ; this corresponds to an approximate mass of 460 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  $0.225 \text{\AA}^{-1}$

## 8 Fourier-Shell correlation

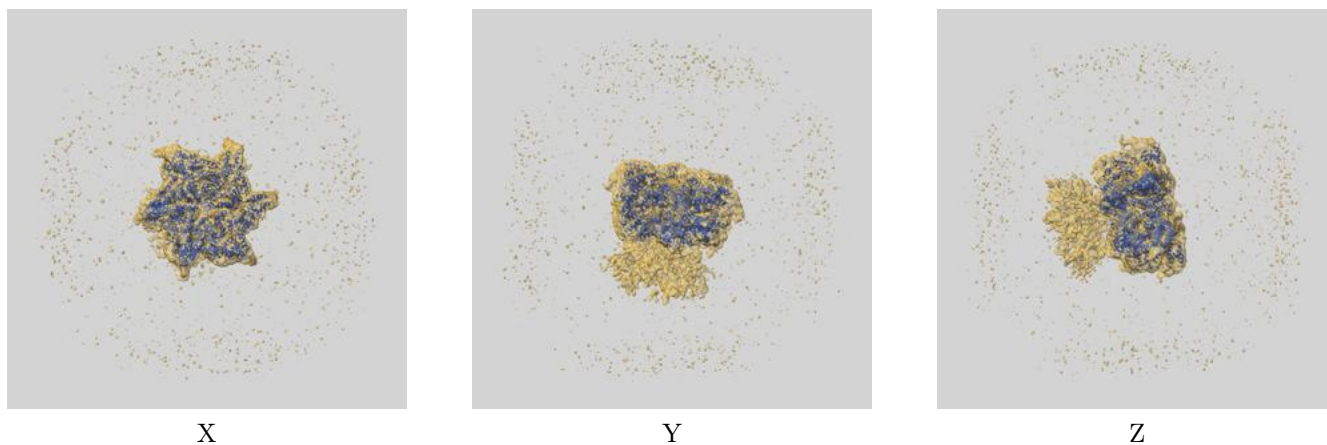
This section was not generated. No FSC curve or half-maps provided.



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

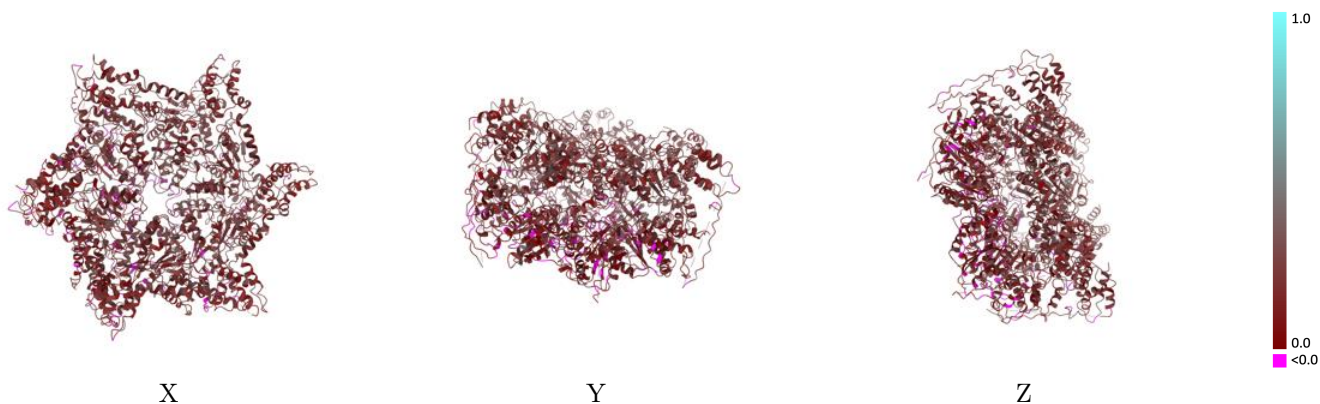
This section contains information regarding the fit between EMDB map EMD-9870 and PDB model 6JPQ. Per-residue inclusion information can be found in section 3 on page 5.

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



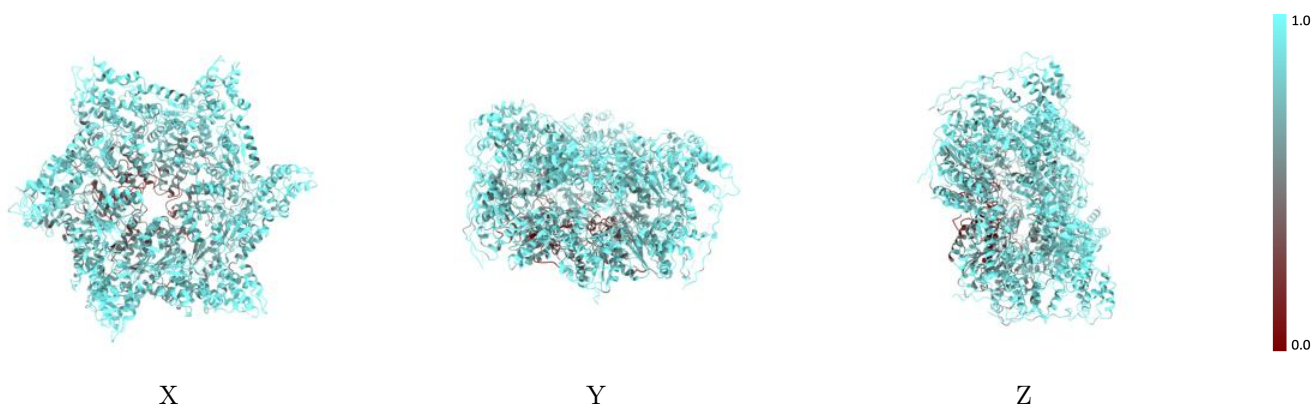
The images above show the 3D surface view of the map at the recommended contour level 1.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



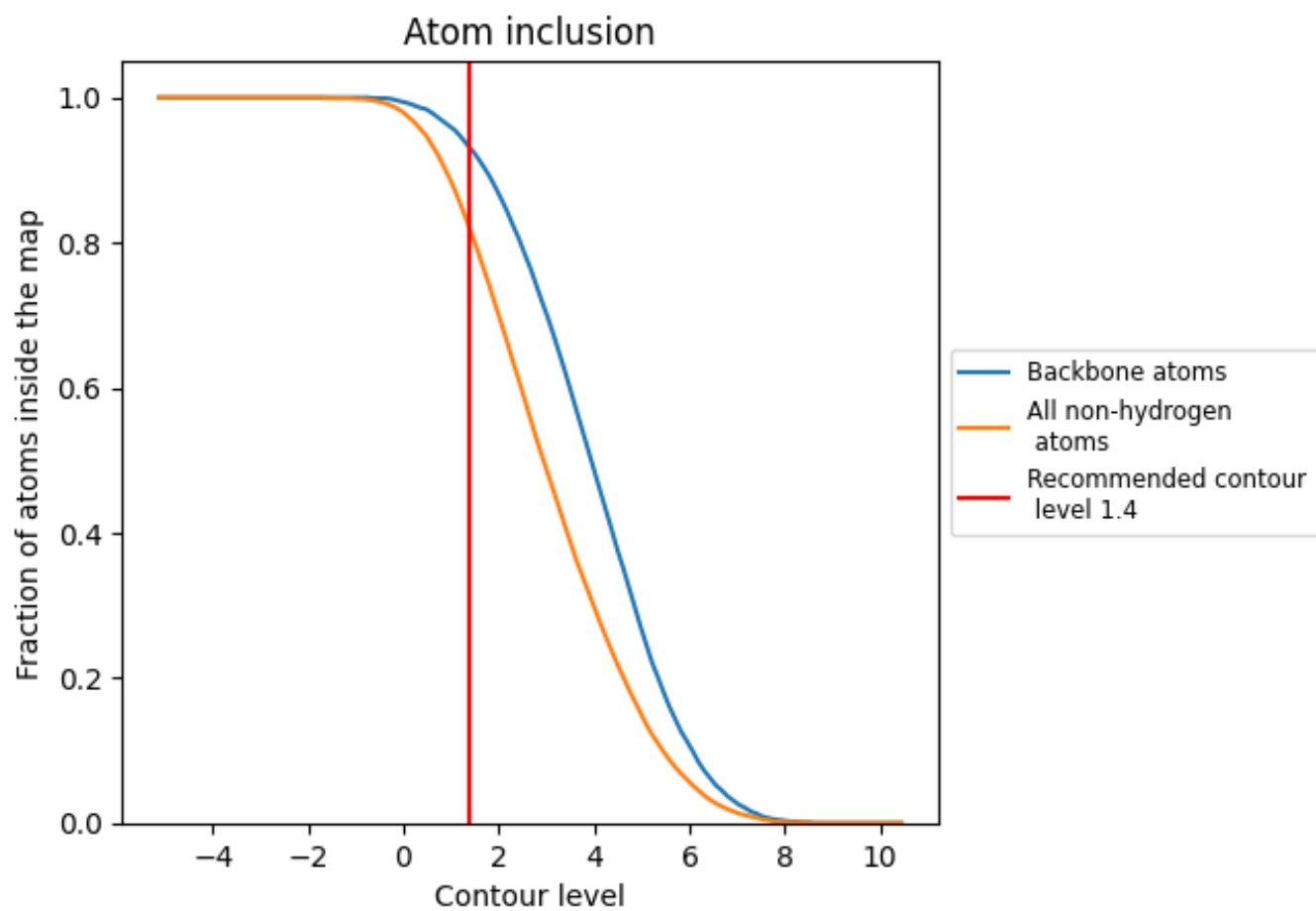
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.4).















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 82% 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 (1.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8180	 0.1880
A	 0.7740	 0.1790
B	 0.8510	 0.2030
C	 0.8630	 0.1970
D	 0.8230	 0.1890
E	 0.8060	 0.1850
F	 0.7890	 0.1770

