



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 04:21 AM UTC

PDB ID : 6H9G / pdb_00006h9g
EMDB ID : EMD-0175
Title : Influenza A nucleoprotein docked into 3D helical structure of the wild type ribonucleoprotein complex obtained using cryoEM. Conformation 1.
Authors : Coloma, R.; Arranz, R.; de la Rosa-Trevin, J.M.; Sorzano, C.O.S.; Munier, S.; Carlero, D.; Naffakh, N.; Ortin, J.; Martin-Benito, J.
Deposited on : 2018-08-03
Resolution : 11.00 Å(reported)
Based on initial model : 2IQH

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

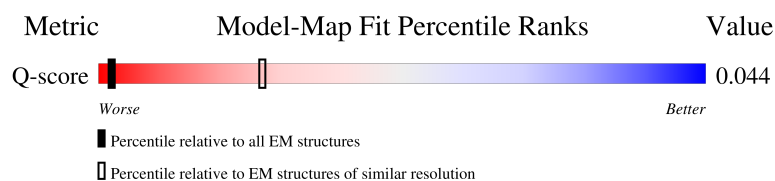
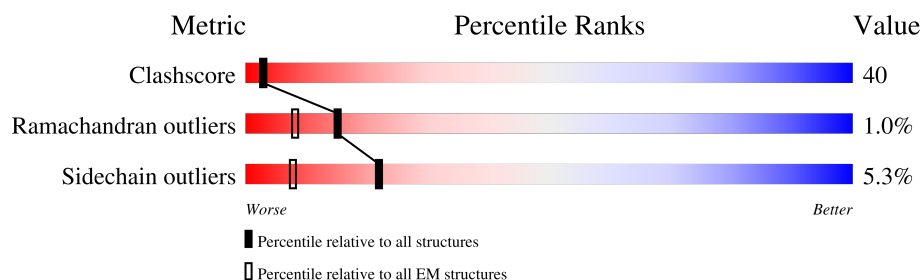
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 11.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	97 (10.50 - 11.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	469	8% 36% 40% 5% 19%
1	C	469	8% 36% 40% 5% 19%
2	B	19	11% 79% 11%
2	D	19	11% 79% 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6320 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 Nucleoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	382	Total	C	N	O	S	0	0
			3012	1871	560	558	23		
1	C	382	Total	C	N	O	S	0	0
			3012	1871	560	558	23		

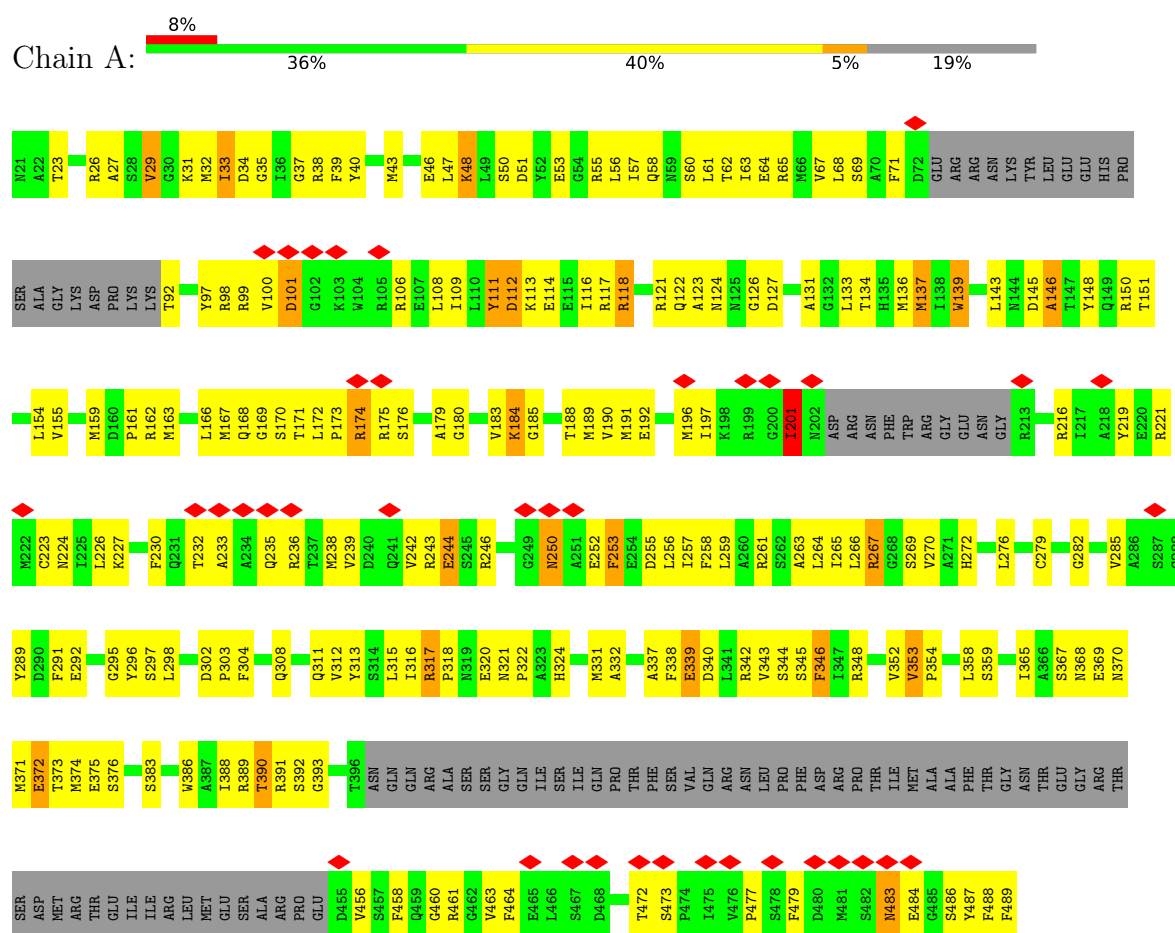
- Molecule 2 is a protein called Polypeptide loop.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	19	Total	C	N	O	0	0
			148	94	26	28		
2	D	19	Total	C	N	O	0	0
			148	94	26	28		

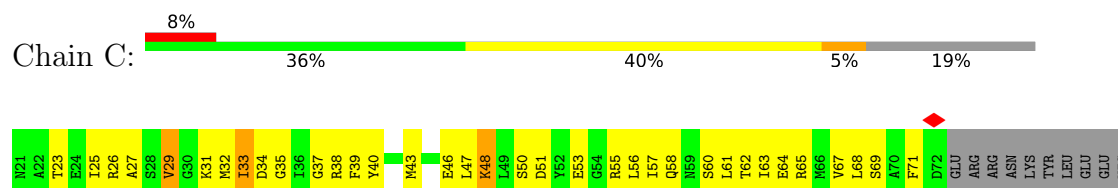
3 Residue-property plots

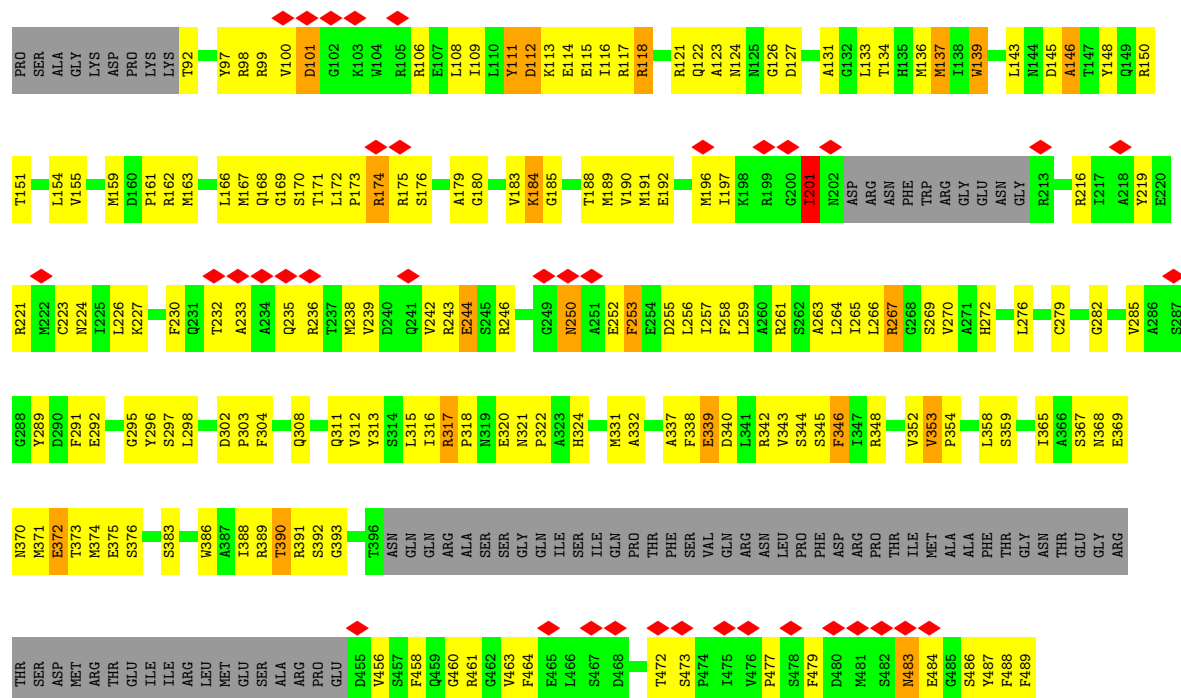
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Nucleoprotein



• Molecule 1: Nucleoprotein





- Molecule 2: Polypeptide loop

Chain B: 11% 79% 11%



- Molecule 2: Polypeptide loop

Chain D: 11% 79% 11%



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-65.39°, rise=33.63 Å, axial sym=D1	Depositor
Number of segments used	2367	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.088	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	271.2, 271.2, 271.2	wwPDB
Map dimensions	120, 120, 120	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.26, 2.26, 2.26	Depositor

5 Model quality

5.1 Standard geometry

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	1.14	3/3060 (0.1%)	1.26	21/4112 (0.5%)
1	C	1.14	3/3060 (0.1%)	1.26	21/4112 (0.5%)
2	B	1.10	0/151	1.38	1/204 (0.5%)
2	D	1.10	0/151	1.38	1/204 (0.5%)
All	All	1.14	6/6422 (0.1%)	1.27	44/8632 (0.5%)

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	1
1	C	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	201	ILE	C-N	-8.03	1.22	1.33
1	C	201	ILE	C-N	-8.03	1.22	1.33
1	A	146	ALA	CA-CB	-5.41	1.46	1.53
1	C	146	ALA	CA-CB	-5.41	1.46	1.53
1	A	289	TYR	CA-C	-5.29	1.45	1.52
1	C	289	TYR	CA-C	-5.29	1.45	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	ILE	O-C-N	-8.12	112.80	122.06
1	C	201	ILE	O-C-N	-8.12	112.80	122.06
1	A	179	ALA	N-CA-C	-7.12	104.20	113.17
1	C	179	ALA	N-CA-C	-7.12	104.20	113.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	MET	N-CA-C	-6.82	104.43	112.89
1	C	136	MET	N-CA-C	-6.82	104.43	112.89
1	A	137	MET	N-CA-C	-6.72	104.02	111.82
1	C	137	MET	N-CA-C	-6.72	104.02	111.82
1	A	317	ARG	CA-C-N	6.71	126.22	119.24
1	A	317	ARG	C-N-CA	6.71	126.22	119.24
1	C	317	ARG	CA-C-N	6.71	126.22	119.24
1	C	317	ARG	C-N-CA	6.71	126.22	119.24
1	A	276	LEU	CA-C-N	6.54	126.52	119.78
1	A	276	LEU	C-N-CA	6.54	126.52	119.78
1	C	276	LEU	CA-C-N	6.54	126.52	119.78
1	C	276	LEU	C-N-CA	6.54	126.52	119.78
1	A	139	TRP	N-CA-C	-6.18	104.55	111.28
1	C	139	TRP	N-CA-C	-6.18	104.55	111.28
1	A	353	VAL	CA-C-N	5.73	126.06	119.92
1	A	353	VAL	C-N-CA	5.73	126.06	119.92
1	C	353	VAL	CA-C-N	5.73	126.06	119.92
1	C	353	VAL	C-N-CA	5.73	126.06	119.92
2	B	419	PRO	N-CA-C	5.61	119.28	110.80
2	D	419	PRO	N-CA-C	5.61	119.28	110.80
1	A	372	GLU	N-CA-C	-5.59	105.09	111.07
1	C	372	GLU	N-CA-C	-5.59	105.09	111.07
1	A	312	VAL	CB-CA-C	-5.52	103.34	110.84
1	C	312	VAL	CB-CA-C	-5.52	103.34	110.84
1	A	216	ARG	N-CA-C	5.37	116.94	111.14
1	C	216	ARG	N-CA-C	5.37	116.94	111.14
1	A	338	PHE	N-CA-C	-5.16	104.74	112.54
1	C	338	PHE	N-CA-C	-5.16	104.74	112.54
1	A	473	SER	N-CA-C	5.15	116.87	109.04
1	C	473	SER	N-CA-C	5.15	116.87	109.04
1	A	184	LYS	N-CA-C	5.14	117.69	110.23
1	C	184	LYS	N-CA-C	5.14	117.69	110.23
1	A	392	SER	N-CA-C	5.13	117.48	110.24
1	C	392	SER	N-CA-C	5.13	117.48	110.24
1	A	148	TYR	N-CA-C	5.08	117.88	109.85
1	C	148	TYR	N-CA-C	5.08	117.88	109.85
1	A	346	PHE	N-CA-C	-5.03	105.71	111.14
1	C	346	PHE	N-CA-C	-5.03	105.71	111.14
1	A	29	VAL	N-CA-C	-5.01	105.69	113.16
1	C	29	VAL	N-CA-C	-5.01	105.69	113.16

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	201	ILE	Mainchain
1	C	201	ILE	Mainchain

5.2 Too-close contacts

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	3012	0	3007	237	0
1	C	3012	0	3007	239	0
2	B	148	0	146	35	0
2	D	148	0	146	37	0
All	All	6320	0	6306	498	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 40.

All (498) 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:C:111:TYR:HB3	1:C:116:ILE:HD11	1.47	0.97
1:A:111:TYR:HB3	1:A:116:ILE:HD11	1.47	0.97
1:C:483:ASN:HD22	1:C:483:ASN:H	1.09	0.94
1:A:483:ASN:H	1:A:483:ASN:HD22	1.09	0.94
1:C:226:LEU:HD13	1:C:230:PHE:HE1	1.31	0.94
1:A:226:LEU:HD13	1:A:230:PHE:HE1	1.31	0.94
1:C:58:GLN:HG3	1:C:315:LEU:HG	1.50	0.93
1:A:58:GLN:HG3	1:A:315:LEU:HG	1.50	0.93
1:A:238:MET:HE3	1:A:255:ASP:OD1	1.73	0.88
1:C:238:MET:HE3	1:C:255:ASP:OD1	1.73	0.88
1:A:163:MET:HE3	1:A:261:ARG:HG2	1.56	0.85
1:C:163:MET:HE3	1:C:261:ARG:HG2	1.56	0.85
1:A:238:MET:HE1	1:A:258:PHE:HD2	1.43	0.83
1:C:238:MET:HE1	1:C:258:PHE:HD2	1.43	0.83
1:C:250:ASN:HA	1:C:253:PHE:HB3	1.58	0.83
1:A:250:ASN:HA	1:A:253:PHE:HB3	1.58	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:GLN:HE22	1:A:383:SER:H	1.24	0.83
1:C:308:GLN:HE22	1:C:383:SER:H	1.24	0.83
1:C:189:MET:HE2	1:C:192:GLU:OE1	1.80	0.82
1:A:189:MET:HE2	1:A:192:GLU:OE1	1.80	0.82
1:C:196:MET:HE1	1:C:219:TYR:HB2	1.61	0.81
1:A:196:MET:HE1	1:A:219:TYR:HB2	1.61	0.81
1:A:461:ARG:HG3	2:B:413:SER:OG	1.82	0.80
1:C:121:ARG:HG2	1:C:121:ARG:HH11	1.47	0.80
1:A:121:ARG:HG2	1:A:121:ARG:HH11	1.47	0.80
1:C:461:ARG:HG3	2:D:413:SER:OG	1.82	0.80
1:A:324:HIS:HD2	1:A:359:SER:H	1.30	0.79
1:C:324:HIS:HD2	1:C:359:SER:H	1.30	0.79
1:C:114:GLU:HA	1:C:117:ARG:HE	1.47	0.78
1:A:71:PHE:HE1	1:A:117:ARG:HA	1.48	0.78
1:A:114:GLU:HA	1:A:117:ARG:HE	1.47	0.78
1:C:71:PHE:HE1	1:C:117:ARG:HA	1.48	0.78
1:A:272:HIS:CD2	2:B:411:THR:HA	2.19	0.78
1:C:227:LYS:HE3	1:C:236:ARG:HB3	1.65	0.78
1:C:272:HIS:CD2	2:D:411:THR:HA	2.19	0.78
1:C:483:ASN:HD22	1:C:483:ASN:N	1.82	0.78
1:A:483:ASN:HD22	1:A:483:ASN:N	1.82	0.78
1:A:227:LYS:HE3	1:A:236:ARG:HB3	1.65	0.77
1:A:317:ARG:HD3	1:A:369:GLU:OE1	1.83	0.77
1:C:317:ARG:HD3	1:C:369:GLU:OE1	1.83	0.77
1:C:114:GLU:HB3	1:C:117:ARG:HH21	1.46	0.77
1:A:111:TYR:HB3	1:A:116:ILE:CD1	2.15	0.77
1:C:111:TYR:HB3	1:C:116:ILE:CD1	2.15	0.77
1:A:114:GLU:HB3	1:A:117:ARG:HH21	1.46	0.77
1:A:238:MET:HE1	1:A:258:PHE:CD2	2.19	0.76
1:C:340:ASP:O	1:C:343:VAL:HG12	1.85	0.76
1:A:340:ASP:O	1:A:343:VAL:HG12	1.85	0.76
1:C:238:MET:HE1	1:C:258:PHE:CD2	2.19	0.76
1:A:114:GLU:CB	1:A:117:ARG:HH21	1.97	0.76
1:A:390:THR:HG22	1:A:391:ARG:H	1.50	0.76
1:C:114:GLU:CB	1:C:117:ARG:HH21	1.97	0.76
1:A:242:VAL:HG11	1:A:256:LEU:HD21	1.68	0.76
1:C:242:VAL:HG11	1:C:256:LEU:HD21	1.68	0.76
1:C:390:THR:HG22	1:C:391:ARG:H	1.50	0.75
1:A:232:THR:OG1	1:A:235:GLN:HG3	1.87	0.75
1:C:232:THR:OG1	1:C:235:GLN:HG3	1.87	0.75
1:A:342:ARG:HB3	1:A:479:PHE:CE2	2.23	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:ARG:HB3	1:C:479:PHE:CE2	2.23	0.73
1:C:486:SER:HB3	2:D:408:ILE:HD11	1.70	0.73
1:A:486:SER:HB3	2:B:408:ILE:HD11	1.70	0.73
1:C:71:PHE:CE1	1:C:117:ARG:HA	2.24	0.72
1:A:71:PHE:CE1	1:A:117:ARG:HA	2.24	0.72
1:A:174:ARG:HD3	1:A:174:ARG:N	2.03	0.72
1:C:174:ARG:N	1:C:174:ARG:HD3	2.03	0.72
1:C:324:HIS:CD2	1:C:359:SER:H	2.09	0.71
1:A:324:HIS:CD2	1:A:359:SER:H	2.09	0.71
1:A:267:ARG:HG3	1:A:393:GLY:O	1.92	0.70
1:C:267:ARG:HG3	1:C:393:GLY:O	1.92	0.70
1:A:235:GLN:O	1:A:239:VAL:HG23	1.91	0.70
1:A:296:TYR:CD1	1:A:302:ASP:HB3	2.26	0.70
2:B:412:PHE:H	2:B:416:ARG:NH2	1.90	0.70
1:C:296:TYR:CD1	1:C:302:ASP:HB3	2.26	0.70
1:C:235:GLN:O	1:C:239:VAL:HG23	1.91	0.70
2:D:412:PHE:H	2:D:416:ARG:NH2	1.90	0.70
1:A:340:ASP:HB2	2:B:408:ILE:HD13	1.74	0.70
1:A:460:GLY:H	2:B:415:GLN:HE21	1.40	0.69
1:C:340:ASP:HB2	2:D:408:ILE:HD13	1.74	0.69
1:C:460:GLY:H	2:D:415:GLN:HE21	1.40	0.69
1:A:226:LEU:HD13	1:A:230:PHE:CE1	2.22	0.69
1:C:489:PHE:HB2	2:D:405:GLN:HG3	1.73	0.69
1:A:489:PHE:HB2	2:B:405:GLN:HG3	1.73	0.69
1:C:226:LEU:HD13	1:C:230:PHE:CE1	2.22	0.69
1:C:461:ARG:HG3	2:D:413:SER:HG	1.54	0.68
1:A:37:GLY:HA3	1:A:285:VAL:HG21	1.75	0.67
1:A:92:THR:N	1:A:113:LYS:HG2	2.09	0.67
1:C:37:GLY:HA3	1:C:285:VAL:HG21	1.75	0.67
1:C:92:THR:N	1:C:113:LYS:HG2	2.09	0.67
1:A:151:THR:HG23	1:A:161:PRO:HB3	1.77	0.67
1:C:151:THR:HG23	1:C:161:PRO:HB3	1.77	0.67
1:A:375:GLU:N	1:A:375:GLU:OE1	2.30	0.65
1:C:375:GLU:N	1:C:375:GLU:OE1	2.30	0.65
1:A:26:ARG:HH11	1:A:295:GLY:HA3	1.62	0.64
1:A:111:TYR:CB	1:A:116:ILE:HD11	2.26	0.64
1:C:111:TYR:CB	1:C:116:ILE:HD11	2.26	0.64
1:C:26:ARG:HH11	1:C:295:GLY:HA3	1.62	0.64
1:C:244:GLU:OE1	1:C:244:GLU:HA	1.95	0.64
1:A:244:GLU:OE1	1:A:244:GLU:HA	1.95	0.64
1:A:62:THR:O	1:A:65:ARG:HG2	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:THR:O	1:C:65:ARG:HG2	1.98	0.64
1:A:242:VAL:HG13	1:A:252:GLU:HG3	1.78	0.64
1:C:315:LEU:HD12	1:C:365:ILE:HD13	1.78	0.64
1:C:242:VAL:HG13	1:C:252:GLU:HG3	1.78	0.63
1:A:315:LEU:HD12	1:A:365:ILE:HD13	1.78	0.63
1:C:342:ARG:HB3	1:C:479:PHE:CD2	2.34	0.63
1:A:342:ARG:HB3	1:A:479:PHE:CD2	2.34	0.63
1:C:344:SER:O	1:C:348:ARG:HB2	1.99	0.63
1:A:344:SER:O	1:A:348:ARG:HB2	1.99	0.63
1:A:58:GLN:HG3	1:A:315:LEU:CG	2.26	0.63
1:C:58:GLN:HG3	1:C:315:LEU:CG	2.26	0.63
1:C:340:ASP:CB	2:D:408:ILE:HD13	2.29	0.63
1:A:340:ASP:CB	2:B:408:ILE:HD13	2.29	0.62
1:A:227:LYS:HB2	1:A:239:VAL:HG11	1.79	0.62
1:C:227:LYS:HB2	1:C:239:VAL:HG11	1.79	0.62
1:C:176:SER:OG	1:C:180:GLY:HA3	1.99	0.62
1:A:197:ILE:HG23	1:A:201:ILE:HG13	1.80	0.62
1:A:176:SER:OG	1:A:180:GLY:HA3	1.99	0.62
1:C:197:ILE:HG23	1:C:201:ILE:HG13	1.80	0.62
1:A:121:ARG:HG2	1:A:121:ARG:NH1	2.15	0.61
1:A:180:GLY:O	1:A:183:VAL:HG12	2.00	0.61
1:C:121:ARG:HG2	1:C:121:ARG:NH1	2.15	0.61
1:C:180:GLY:O	1:C:183:VAL:HG12	2.00	0.61
2:B:411:THR:H	2:B:416:ARG:HH22	1.49	0.61
2:D:411:THR:H	2:D:416:ARG:HH22	1.49	0.61
1:C:242:VAL:HG11	1:C:256:LEU:CD2	2.31	0.61
1:A:97:TYR:CE2	1:A:106:ARG:HG3	2.35	0.61
1:A:154:LEU:HD21	1:A:167:MET:HG2	1.81	0.61
1:A:242:VAL:HG11	1:A:256:LEU:CD2	2.31	0.61
1:C:154:LEU:HD21	1:C:167:MET:HG2	1.81	0.61
1:A:121:ARG:HB3	1:A:126:GLY:HA2	1.82	0.61
1:C:97:TYR:CE2	1:C:106:ARG:HG3	2.35	0.61
1:C:121:ARG:HB3	1:C:126:GLY:HA2	1.82	0.61
1:A:43:MET:O	1:A:47:LEU:HD23	2.02	0.60
1:A:483:ASN:H	1:A:483:ASN:ND2	1.86	0.60
1:C:43:MET:O	1:C:47:LEU:HD23	2.02	0.60
1:C:483:ASN:H	1:C:483:ASN:ND2	1.86	0.60
1:C:92:THR:N	1:C:113:LYS:HZ3	1.99	0.60
1:A:162:ARG:HD3	2:B:402:SER:HB2	1.83	0.59
1:A:339:GLU:HG3	2:B:411:THR:HB	1.83	0.59
1:C:32:MET:HE2	1:C:131:ALA:HB1	1.82	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:GLU:HG3	2:D:411:THR:HB	1.83	0.59
1:A:32:MET:HE2	1:A:131:ALA:HB1	1.82	0.59
1:C:162:ARG:HD3	2:D:402:SER:HB2	1.83	0.59
1:A:92:THR:N	1:A:113:LYS:HZ3	1.99	0.59
1:A:321:ASN:HB3	1:A:324:HIS:HB2	1.83	0.59
1:A:255:ASP:O	1:A:258:PHE:HB3	2.02	0.59
1:C:321:ASN:HB3	1:C:324:HIS:HB2	1.83	0.59
1:C:255:ASP:O	1:C:258:PHE:HB3	2.02	0.59
1:C:253:PHE:C	1:C:253:PHE:CD2	2.81	0.58
1:A:253:PHE:C	1:A:253:PHE:CD2	2.81	0.58
1:A:61:LEU:HA	1:A:64:GLU:OE1	2.04	0.58
1:A:267:ARG:NH1	2:B:407:SER:OG	2.36	0.58
1:C:61:LEU:HA	1:C:64:GLU:OE1	2.04	0.58
1:C:298:LEU:N	1:C:298:LEU:HD12	2.19	0.58
1:A:298:LEU:N	1:A:298:LEU:HD12	2.19	0.58
1:C:267:ARG:NH1	2:D:407:SER:OG	2.36	0.58
1:A:163:MET:HE3	1:A:261:ARG:CG	2.32	0.57
1:C:321:ASN:HD22	1:C:322:PRO:HD2	1.70	0.57
1:A:71:PHE:CE1	1:A:117:ARG:HG2	2.40	0.57
1:A:100:VAL:O	1:A:101:ASP:C	2.48	0.57
1:A:321:ASN:HD22	1:A:322:PRO:HD2	1.70	0.57
1:C:71:PHE:CE1	1:C:117:ARG:HG2	2.40	0.57
1:A:150:ARG:O	1:A:154:LEU:HG	2.04	0.57
1:C:100:VAL:O	1:C:101:ASP:C	2.48	0.57
1:C:163:MET:HE3	1:C:261:ARG:CG	2.32	0.57
2:D:417:ASN:O	2:D:419:PRO:HD3	2.04	0.57
2:B:417:ASN:O	2:B:419:PRO:HD3	2.04	0.57
1:C:150:ARG:O	1:C:154:LEU:HG	2.04	0.57
1:A:267:ARG:HB2	1:A:393:GLY:HA3	1.86	0.56
1:C:267:ARG:HB2	1:C:393:GLY:HA3	1.86	0.56
1:A:31:LYS:HD3	1:A:292:GLU:OE2	2.05	0.56
1:A:238:MET:O	1:A:242:VAL:HG23	2.06	0.56
1:A:346:PHE:CE2	1:A:477:PRO:HB3	2.39	0.56
1:C:31:LYS:HD3	1:C:292:GLU:OE2	2.05	0.56
1:C:238:MET:O	1:C:242:VAL:HG23	2.06	0.56
1:A:46:GLU:O	1:A:48:LYS:HG2	2.05	0.56
1:C:346:PHE:CE2	1:C:477:PRO:HB3	2.39	0.56
1:C:46:GLU:O	1:C:48:LYS:HG2	2.05	0.56
1:C:370:ASN:HD22	1:C:372:GLU:HB3	1.70	0.56
1:A:230:PHE:HB3	1:A:235:GLN:HB3	1.88	0.56
1:A:263:ALA:HA	1:A:266:LEU:O	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ASN:HD22	1:A:372:GLU:HB3	1.70	0.56
1:C:263:ALA:HA	1:C:266:LEU:O	2.06	0.56
1:C:230:PHE:HB3	1:C:235:GLN:HB3	1.88	0.56
1:A:353:VAL:HG13	1:A:354:PRO:HD2	1.88	0.56
1:A:390:THR:OG1	2:B:413:SER:HB2	2.05	0.56
1:C:353:VAL:HG13	1:C:354:PRO:HD2	1.88	0.56
1:A:243:ARG:O	1:A:243:ARG:HG2	2.06	0.55
1:C:390:THR:OG1	2:D:413:SER:HB2	2.05	0.55
1:C:243:ARG:O	1:C:243:ARG:HG2	2.06	0.55
1:A:321:ASN:HD22	1:A:322:PRO:CD	2.20	0.55
1:C:321:ASN:HD22	1:C:322:PRO:CD	2.20	0.55
1:A:97:TYR:CD1	1:A:97:TYR:N	2.74	0.55
1:C:97:TYR:N	1:C:97:TYR:CD1	2.74	0.55
2:D:411:THR:N	2:D:416:ARG:HH22	2.03	0.55
1:A:311:GLN:HG3	1:A:313:TYR:CZ	2.42	0.55
2:B:411:THR:N	2:B:416:ARG:HH22	2.03	0.55
1:C:311:GLN:HG3	1:C:313:TYR:CZ	2.42	0.55
1:C:196:MET:CE	1:C:219:TYR:HB2	2.35	0.54
1:A:39:PHE:CZ	1:A:67:VAL:HG21	2.42	0.54
1:C:39:PHE:CZ	1:C:67:VAL:HG21	2.42	0.54
1:C:189:MET:CE	1:C:192:GLU:OE1	2.53	0.54
1:C:252:GLU:O	1:C:255:ASP:N	2.40	0.54
1:A:196:MET:CE	1:A:219:TYR:HB2	2.35	0.54
1:A:252:GLU:O	1:A:255:ASP:N	2.40	0.54
1:A:189:MET:CE	1:A:192:GLU:OE1	2.53	0.54
1:C:100:VAL:HG12	1:C:101:ASP:N	2.22	0.54
1:C:162:ARG:HD3	2:D:402:SER:CB	2.38	0.54
1:A:100:VAL:HG12	1:A:101:ASP:N	2.22	0.54
1:A:162:ARG:HD3	2:B:402:SER:CB	2.38	0.54
1:A:342:ARG:HB3	1:A:479:PHE:HE2	1.73	0.54
2:B:416:ARG:HD2	2:B:418:LEU:CD2	2.38	0.54
1:C:342:ARG:HB3	1:C:479:PHE:HE2	1.73	0.54
2:D:416:ARG:HD2	2:D:418:LEU:CD2	2.38	0.54
1:A:339:GLU:OE1	1:A:340:ASP:N	2.35	0.53
1:C:339:GLU:OE1	1:C:340:ASP:N	2.35	0.53
1:C:53:GLU:OE2	1:C:99:ARG:N	2.41	0.53
1:A:53:GLU:OE2	1:A:99:ARG:N	2.41	0.53
1:A:167:MET:HG3	1:A:170:SER:HB3	1.91	0.53
1:C:167:MET:HG3	1:C:170:SER:HB3	1.91	0.53
1:C:270:VAL:N	1:C:391:ARG:O	2.42	0.52
1:A:270:VAL:N	1:A:391:ARG:O	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:GLU:OE1	2:B:416:ARG:NH1	2.43	0.52
1:C:339:GLU:OE1	2:D:416:ARG:NH1	2.43	0.52
1:A:370:ASN:ND2	1:A:372:GLU:HB3	2.25	0.52
1:C:343:VAL:HG13	1:C:344:SER:N	2.24	0.52
1:C:370:ASN:ND2	1:C:372:GLU:HB3	2.25	0.52
1:A:317:ARG:HB2	1:A:320:GLU:HG3	1.91	0.52
1:A:343:VAL:HG13	1:A:344:SER:N	2.24	0.52
1:C:69:SER:OG	1:C:92:THR:HG21	2.10	0.52
1:A:69:SER:OG	1:A:92:THR:HG21	2.10	0.52
1:A:71:PHE:CD1	1:A:117:ARG:HG2	2.44	0.52
1:A:297:SER:C	1:A:298:LEU:HD12	2.35	0.52
1:A:460:GLY:H	2:B:415:GLN:NE2	2.07	0.52
1:C:297:SER:C	1:C:298:LEU:HD12	2.35	0.52
1:C:317:ARG:HB2	1:C:320:GLU:HG3	1.91	0.52
1:A:29:VAL:O	1:A:32:MET:HG3	2.10	0.52
1:C:29:VAL:O	1:C:32:MET:HG3	2.10	0.52
1:C:71:PHE:CD1	1:C:117:ARG:HG2	2.44	0.52
1:C:460:GLY:H	2:D:415:GLN:NE2	2.07	0.52
1:A:146:ALA:HB2	1:A:337:ALA:HB2	1.92	0.52
1:C:315:LEU:HB2	1:C:365:ILE:HD11	1.92	0.52
1:A:106:ARG:NH2	1:A:371:MET:HE3	2.25	0.51
1:A:111:TYR:CD2	1:A:116:ILE:HD11	2.45	0.51
1:A:315:LEU:HB2	1:A:365:ILE:HD11	1.92	0.51
1:C:39:PHE:CE2	1:C:67:VAL:HG21	2.45	0.51
1:C:106:ARG:NH2	1:C:371:MET:HE3	2.25	0.51
1:C:146:ALA:HB2	1:C:337:ALA:HB2	1.92	0.51
1:A:296:TYR:CE1	1:A:302:ASP:HB3	2.46	0.51
2:B:406:ILE:O	2:B:420:PHE:HA	2.10	0.51
1:C:111:TYR:CD2	1:C:116:ILE:HD11	2.45	0.51
1:C:296:TYR:CE1	1:C:302:ASP:HB3	2.46	0.51
1:A:38:ARG:NH1	1:A:123:ALA:O	2.44	0.51
1:A:39:PHE:CE2	1:A:67:VAL:HG21	2.45	0.51
1:A:168:GLN:O	1:A:184:LYS:HA	2.10	0.51
1:C:38:ARG:NH1	1:C:123:ALA:O	2.44	0.51
1:C:168:GLN:O	1:C:184:LYS:HA	2.10	0.51
2:D:406:ILE:O	2:D:420:PHE:HA	2.10	0.51
1:C:232:THR:O	1:C:236:ARG:HG3	2.09	0.51
1:C:238:MET:HE2	1:C:259:LEU:HD13	1.92	0.51
1:A:238:MET:HE2	1:A:259:LEU:HD13	1.92	0.51
1:A:232:THR:O	1:A:236:ARG:HG3	2.09	0.51
1:A:35:GLY:HA3	1:A:124:ASN:OD1	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:THR:O	1:A:173:PRO:HD3	2.11	0.51
1:A:189:MET:HE2	1:A:189:MET:HA	1.92	0.51
1:C:35:GLY:HA3	1:C:124:ASN:OD1	2.11	0.51
1:C:171:THR:O	1:C:173:PRO:HD3	2.11	0.51
1:C:189:MET:HE2	1:C:189:MET:HA	1.92	0.51
1:C:321:ASN:HD22	1:C:322:PRO:N	2.09	0.51
1:C:342:ARG:HH22	2:D:417:ASN:ND2	2.08	0.51
1:A:253:PHE:O	1:A:257:ILE:HG13	2.11	0.51
1:A:321:ASN:HD22	1:A:322:PRO:N	2.09	0.51
1:C:253:PHE:O	1:C:257:ILE:HG13	2.11	0.51
1:A:196:MET:HE1	1:A:219:TYR:CB	2.38	0.50
1:A:302:ASP:HB2	1:A:303:PRO:HD3	1.93	0.50
1:A:342:ARG:HH22	2:B:417:ASN:ND2	2.08	0.50
1:C:134:THR:O	1:C:137:MET:HB3	2.10	0.50
1:C:302:ASP:HB2	1:C:303:PRO:HD3	1.93	0.50
1:A:106:ARG:NH1	1:A:367:SER:HA	2.26	0.50
1:A:134:THR:O	1:A:137:MET:HB3	2.10	0.50
2:B:408:ILE:O	2:B:408:ILE:HG22	2.09	0.50
2:B:416:ARG:HD2	2:B:418:LEU:HD23	1.92	0.50
1:C:106:ARG:NH1	1:C:367:SER:HA	2.26	0.50
1:C:196:MET:HE1	1:C:219:TYR:CB	2.38	0.50
1:C:223:CYS:O	1:C:226:LEU:HB3	2.11	0.50
1:A:223:CYS:O	1:A:226:LEU:HB3	2.11	0.50
1:A:291:PHE:O	1:A:295:GLY:N	2.42	0.50
1:C:291:PHE:O	1:C:295:GLY:N	2.42	0.50
2:D:416:ARG:HD2	2:D:418:LEU:HD23	1.92	0.50
1:A:63:ILE:O	1:A:67:VAL:HG23	2.12	0.50
1:C:63:ILE:O	1:C:67:VAL:HG23	2.12	0.50
2:D:408:ILE:HG22	2:D:408:ILE:O	2.09	0.50
1:A:137:MET:CE	1:A:175:ARG:HE	2.25	0.50
1:C:137:MET:CE	1:C:175:ARG:HE	2.25	0.50
1:A:308:GLN:HE22	1:A:383:SER:N	2.01	0.50
1:A:311:GLN:HG3	1:A:313:TYR:OH	2.12	0.50
1:C:311:GLN:HG3	1:C:313:TYR:OH	2.12	0.50
1:A:458:PHE:HB2	2:B:414:VAL:O	2.11	0.50
1:C:118:ARG:HH21	1:C:122:GLN:HG3	1.77	0.50
1:C:458:PHE:HB2	2:D:414:VAL:O	2.11	0.50
1:A:118:ARG:HH21	1:A:122:GLN:HG3	1.77	0.50
1:C:308:GLN:HE22	1:C:383:SER:N	2.01	0.49
1:A:56:LEU:O	1:A:57:ILE:C	2.54	0.49
1:C:56:LEU:O	1:C:57:ILE:C	2.54	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:GLN:HE21	1:A:58:GLN:HA	1.77	0.49
1:C:58:GLN:HA	1:C:58:GLN:HE21	1.77	0.49
1:A:166:LEU:HD21	1:A:264:LEU:HD23	1.95	0.49
1:C:166:LEU:HD21	1:C:264:LEU:HD23	1.95	0.49
1:C:162:ARG:HG2	2:D:404:GLY:O	2.13	0.49
1:A:162:ARG:HG2	2:B:404:GLY:O	2.13	0.49
1:A:298:LEU:N	1:A:298:LEU:CD1	2.76	0.48
1:C:298:LEU:N	1:C:298:LEU:CD1	2.76	0.48
1:C:345:SER:HA	1:C:352:VAL:HG23	1.95	0.48
1:A:345:SER:HA	1:A:352:VAL:HG23	1.95	0.48
1:C:226:LEU:HD12	1:C:239:VAL:HG13	1.95	0.48
1:A:226:LEU:HD12	1:A:239:VAL:HG13	1.95	0.48
1:A:232:THR:HG1	1:A:235:GLN:HG3	1.77	0.48
1:C:189:MET:HB2	1:C:226:LEU:HD23	1.95	0.48
1:A:26:ARG:NH1	1:A:295:GLY:C	2.71	0.48
1:A:189:MET:HB2	1:A:226:LEU:HD23	1.95	0.48
1:C:26:ARG:NH1	1:C:295:GLY:C	2.71	0.48
1:C:232:THR:HG1	1:C:235:GLN:HG3	1.77	0.48
1:A:267:ARG:HH21	2:B:418:LEU:CB	2.27	0.48
1:C:267:ARG:HH21	2:D:418:LEU:CB	2.27	0.48
1:C:487:TYR:HB3	2:D:405:GLN:HB2	1.96	0.48
1:A:487:TYR:HB3	2:B:405:GLN:HB2	1.96	0.48
1:C:267:ARG:HH21	2:D:418:LEU:HB2	1.77	0.47
1:C:316:ILE:HG22	1:C:376:SER:HA	1.95	0.47
1:C:318:PRO:HD3	1:C:373:THR:O	2.14	0.47
1:A:197:ILE:HG23	1:A:201:ILE:CG1	2.45	0.47
1:A:267:ARG:HH21	2:B:418:LEU:HB2	1.77	0.47
1:A:316:ILE:HG22	1:A:376:SER:HA	1.95	0.47
1:A:318:PRO:HD3	1:A:373:THR:O	2.14	0.47
1:A:112:ASP:O	1:A:113:LYS:C	2.56	0.47
1:C:112:ASP:O	1:C:113:LYS:C	2.56	0.47
1:C:197:ILE:HG23	1:C:201:ILE:CG1	2.45	0.47
1:C:56:LEU:HG	1:C:58:GLN:HG2	1.95	0.47
1:A:56:LEU:HG	1:A:58:GLN:HG2	1.95	0.47
1:A:143:LEU:HA	1:A:332:ALA:HB2	1.96	0.47
1:C:143:LEU:HA	1:C:332:ALA:HB2	1.96	0.47
1:A:106:ARG:HH12	1:A:367:SER:HA	1.80	0.47
1:A:170:SER:HA	1:A:188:THR:HG23	1.97	0.47
1:A:365:ILE:HG12	1:A:374:MET:HE3	1.96	0.47
1:C:365:ILE:HG12	1:C:374:MET:HE3	1.96	0.47
1:C:170:SER:HA	1:C:188:THR:HG23	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:ARG:HH12	1:C:367:SER:HA	1.80	0.47
1:A:253:PHE:C	1:A:253:PHE:HD2	2.21	0.46
1:A:297:SER:O	1:A:303:PRO:HG3	2.15	0.46
1:C:267:ARG:H	1:C:267:ARG:HG2	1.42	0.46
1:C:297:SER:O	1:C:303:PRO:HG3	2.15	0.46
1:A:477:PRO:HG3	2:B:414:VAL:HG11	1.96	0.46
1:C:174:ARG:HD3	1:C:175:ARG:H	1.80	0.46
1:C:253:PHE:C	1:C:253:PHE:HD2	2.21	0.46
1:A:174:ARG:HD3	1:A:175:ARG:H	1.80	0.46
1:C:304:PHE:CE2	1:C:386:TRP:HA	2.50	0.46
1:C:477:PRO:HG3	2:D:414:VAL:HG11	1.96	0.46
1:A:39:PHE:CZ	1:A:67:VAL:CG2	2.99	0.46
1:A:304:PHE:CE2	1:A:386:TRP:HA	2.50	0.46
1:C:39:PHE:CZ	1:C:67:VAL:CG2	2.99	0.46
1:C:368:ASN:N	1:C:368:ASN:HD22	2.13	0.46
1:A:368:ASN:N	1:A:368:ASN:HD22	2.13	0.46
1:A:386:TRP:NE1	1:A:464:PHE:HB2	2.30	0.46
1:A:232:THR:OG1	1:A:235:GLN:CG	2.60	0.45
2:B:408:ILE:HD12	2:B:419:PRO:HB2	1.98	0.45
1:C:232:THR:OG1	1:C:235:GLN:CG	2.60	0.45
1:C:386:TRP:NE1	1:C:464:PHE:HB2	2.30	0.45
1:A:121:ARG:O	1:A:122:GLN:C	2.60	0.45
2:D:408:ILE:HD12	2:D:419:PRO:HB2	1.98	0.45
1:C:121:ARG:O	1:C:122:GLN:C	2.60	0.45
1:C:184:LYS:HD3	1:C:189:MET:HE3	1.98	0.45
1:A:184:LYS:HD3	1:A:189:MET:HE3	1.98	0.45
1:A:269:SER:HA	1:A:391:ARG:O	2.16	0.45
1:C:324:HIS:HD2	1:C:358:LEU:HA	1.81	0.45
1:C:53:GLU:OE2	1:C:98:ARG:HA	2.15	0.45
1:C:269:SER:HA	1:C:391:ARG:O	2.16	0.45
1:A:53:GLU:OE2	1:A:98:ARG:HA	2.15	0.45
1:A:324:HIS:HD2	1:A:358:LEU:HA	1.81	0.45
1:C:56:LEU:O	1:C:58:GLN:N	2.49	0.45
1:C:342:ARG:HH22	2:D:417:ASN:HD21	1.64	0.45
1:A:40:TYR:CE2	1:A:279:CYS:HA	2.50	0.45
1:A:56:LEU:O	1:A:58:GLN:N	2.49	0.45
1:A:68:LEU:HD21	1:A:133:LEU:O	2.17	0.45
1:A:342:ARG:HH22	2:B:417:ASN:HD21	1.64	0.45
1:C:68:LEU:HD21	1:C:133:LEU:O	2.17	0.45
1:C:92:THR:CA	1:C:113:LYS:HZ3	2.30	0.45
1:C:39:PHE:CE1	1:C:43:MET:HE2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:TYR:CE2	1:C:279:CYS:HA	2.50	0.45
1:A:39:PHE:CE1	1:A:43:MET:HE2	2.52	0.44
1:A:143:LEU:HA	1:A:332:ALA:CB	2.47	0.44
1:C:388:ILE:O	1:C:389:ARG:C	2.60	0.44
1:A:388:ILE:O	1:A:389:ARG:C	2.60	0.44
1:C:143:LEU:HA	1:C:332:ALA:CB	2.47	0.44
1:A:386:TRP:CE2	1:A:464:PHE:HB2	2.53	0.44
1:C:386:TRP:CE2	1:C:464:PHE:HB2	2.53	0.44
1:C:487:TYR:N	1:C:487:TYR:CD2	2.84	0.44
1:A:50:SER:OG	1:A:53:GLU:HG3	2.18	0.44
1:C:50:SER:OG	1:C:53:GLU:HG3	2.18	0.44
1:A:92:THR:CA	1:A:113:LYS:HZ3	2.30	0.44
1:A:487:TYR:N	1:A:487:TYR:CD2	2.84	0.44
1:A:47:LEU:HD11	1:A:109:ILE:CD1	2.48	0.44
1:C:47:LEU:HD11	1:C:109:ILE:CD1	2.48	0.44
1:C:174:ARG:CD	1:C:175:ARG:H	2.30	0.44
1:A:174:ARG:CD	1:A:175:ARG:H	2.30	0.44
1:C:34:ASP:OD2	1:C:291:PHE:HB2	2.17	0.44
1:A:34:ASP:OD2	1:A:291:PHE:HB2	2.17	0.43
1:A:159:MET:HE3	1:A:190:VAL:HG12	1.99	0.43
1:C:145:ASP:OD2	1:C:169:GLY:N	2.48	0.43
1:C:264:LEU:HD23	1:C:264:LEU:HA	1.73	0.43
1:A:145:ASP:OD2	1:A:169:GLY:N	2.48	0.43
1:C:111:TYR:HD2	1:C:116:ILE:HD11	1.81	0.43
1:C:172:LEU:HD12	1:C:173:PRO:HD2	2.00	0.43
1:A:111:TYR:HD2	1:A:116:ILE:HD11	1.81	0.43
1:A:172:LEU:HD12	1:A:173:PRO:HD2	2.00	0.43
1:A:321:ASN:HD22	1:A:321:ASN:C	2.25	0.43
1:C:159:MET:HE3	1:C:190:VAL:HG12	1.99	0.43
1:C:321:ASN:HD22	1:C:321:ASN:C	2.25	0.43
1:A:51:ASP:O	1:A:55:ARG:HG3	2.19	0.43
1:A:272:HIS:NE2	2:B:410:PRO:O	2.51	0.43
1:C:51:ASP:O	1:C:55:ARG:HG3	2.19	0.43
1:C:235:GLN:HE21	1:C:266:LEU:HB2	1.83	0.43
1:A:264:LEU:HD23	1:A:264:LEU:HA	1.73	0.43
1:C:272:HIS:NE2	2:D:410:PRO:O	2.51	0.43
1:A:235:GLN:HE21	1:A:266:LEU:HB2	1.83	0.43
1:A:317:ARG:HB3	1:A:318:PRO:HD2	2.01	0.43
1:A:40:TYR:CE1	1:A:63:ILE:HD12	2.54	0.43
1:C:40:TYR:CE1	1:C:63:ILE:HD12	2.54	0.43
1:C:317:ARG:HB3	1:C:318:PRO:HD2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:GLN:HA	1:A:58:GLN:NE2	2.34	0.43
1:A:185:GLY:HA2	1:A:270:VAL:HG21	2.00	0.43
1:C:33:ILE:HG22	1:C:34:ASP:N	2.34	0.43
1:C:58:GLN:HA	1:C:58:GLN:NE2	2.34	0.43
1:A:33:ILE:HG22	1:A:34:ASP:N	2.34	0.43
1:C:185:GLY:HA2	1:C:270:VAL:HG21	2.00	0.43
1:C:487:TYR:O	1:C:488:PHE:C	2.61	0.43
1:A:487:TYR:O	1:A:488:PHE:C	2.61	0.42
2:B:412:PHE:H	2:B:416:ARG:HH22	1.65	0.42
2:D:412:PHE:H	2:D:416:ARG:HH22	1.65	0.42
1:A:230:PHE:CE2	1:A:259:LEU:HG	2.55	0.42
1:C:230:PHE:CE2	1:C:259:LEU:HG	2.55	0.42
1:A:121:ARG:NH1	1:A:121:ARG:CG	2.83	0.42
1:A:159:MET:SD	1:A:191:MET:HG3	2.60	0.42
1:C:121:ARG:NH1	1:C:121:ARG:CG	2.83	0.42
1:C:159:MET:SD	1:C:191:MET:HG3	2.60	0.42
1:A:303:PRO:HD2	1:A:389:ARG:HH22	1.84	0.42
1:A:317:ARG:HB2	1:A:320:GLU:CG	2.49	0.42
1:C:122:GLN:HA	1:C:122:GLN:OE1	2.20	0.42
1:C:303:PRO:HD2	1:C:389:ARG:HH22	1.84	0.42
1:C:324:HIS:HD2	1:C:359:SER:N	2.08	0.42
1:A:33:ILE:HG21	1:A:291:PHE:CG	2.54	0.41
1:A:122:GLN:HA	1:A:122:GLN:OE1	2.20	0.41
1:A:124:ASN:O	1:A:127:ASP:HB2	2.20	0.41
1:A:317:ARG:HD3	1:A:369:GLU:CD	2.45	0.41
1:C:33:ILE:HG21	1:C:291:PHE:CG	2.54	0.41
1:C:317:ARG:HD3	1:C:369:GLU:CD	2.45	0.41
1:C:317:ARG:HB2	1:C:320:GLU:CG	2.49	0.41
1:A:60:SER:O	1:A:64:GLU:HG3	2.20	0.41
1:C:124:ASN:O	1:C:127:ASP:HB2	2.20	0.41
1:C:60:SER:O	1:C:64:GLU:HG3	2.20	0.41
1:C:168:GLN:HE21	1:C:183:VAL:HG22	1.85	0.41
1:A:168:GLN:HE21	1:A:183:VAL:HG22	1.85	0.41
1:A:324:HIS:HD2	1:A:359:SER:N	2.08	0.41
1:C:114:GLU:O	1:C:115:GLU:C	2.64	0.41
1:A:324:HIS:CD2	1:A:358:LEU:HA	2.55	0.41
1:A:114:GLU:HB3	1:A:117:ARG:NH2	2.26	0.41
1:A:331:MET:HE1	1:A:488:PHE:CD1	2.54	0.41
1:C:324:HIS:CD2	1:C:358:LEU:HA	2.55	0.41
1:C:346:PHE:HE2	1:C:463:VAL:HG21	1.85	0.41
1:C:151:THR:O	1:C:155:VAL:HG22	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:MET:HE1	1:C:488:PHE:CD1	2.54	0.41
1:C:460:GLY:N	2:D:415:GLN:HE21	2.14	0.41
1:A:151:THR:O	1:A:155:VAL:HG22	2.20	0.41
1:A:221:ARG:O	1:A:224:ASN:N	2.53	0.41
1:A:346:PHE:HE2	1:A:463:VAL:HG21	1.85	0.41
1:C:221:ARG:O	1:C:224:ASN:N	2.53	0.41
1:A:302:ASP:N	1:A:303:PRO:CD	2.84	0.41
1:C:114:GLU:HB3	1:C:117:ARG:NH2	2.26	0.41
1:A:223:CYS:O	1:A:227:LYS:N	2.45	0.40
1:C:23:THR:O	1:C:27:ALA:HB3	2.21	0.40
1:C:223:CYS:O	1:C:227:LYS:N	2.45	0.40
1:C:265:ILE:HD13	2:D:420:PHE:CD1	2.56	0.40
1:C:302:ASP:N	1:C:303:PRO:CD	2.84	0.40
1:A:23:THR:O	1:A:27:ALA:HB3	2.21	0.40
1:A:264:LEU:O	1:A:267:ARG:NH1	2.54	0.40
1:A:265:ILE:HD13	2:B:420:PHE:CD1	2.56	0.40
2:B:406:ILE:HD13	2:B:406:ILE:HA	1.96	0.40
1:C:25:ILE:H	1:C:25:ILE:HG13	1.73	0.40
1:C:116:ILE:N	1:C:116:ILE:HD12	2.36	0.40
1:C:264:LEU:O	1:C:267:ARG:NH1	2.54	0.40
1:A:37:GLY:HA2	1:A:282:GLY:HA2	2.03	0.40
1:A:114:GLU:HA	1:A:117:ARG:NE	2.24	0.40
1:A:116:ILE:N	1:A:116:ILE:HD12	2.36	0.40
1:A:368:ASN:N	1:A:368:ASN:ND2	2.69	0.40
1:A:168:GLN:NE2	1:A:183:VAL:HG22	2.36	0.40
1:A:230:PHE:CZ	1:A:259:LEU:HG	2.55	0.40
1:A:365:ILE:N	1:A:365:ILE:HD12	2.37	0.40
1:C:37:GLY:HA2	1:C:282:GLY:HA2	2.03	0.40
1:C:168:GLN:NE2	1:C:183:VAL:HG22	2.36	0.40
1:C:365:ILE:N	1:C:365:ILE:HD12	2.37	0.40
2:D:406:ILE:HD13	2:D:406:ILE:HA	1.96	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	374/469 (80%)	324 (87%)	46 (12%)	4 (1%)	11	46
1	C	374/469 (80%)	324 (87%)	46 (12%)	4 (1%)	11	46
2	B	17/19 (90%)	15 (88%)	2 (12%)	0	100	100
2	D	17/19 (90%)	15 (88%)	2 (12%)	0	100	100
All	All	782/976 (80%)	678 (87%)	96 (12%)	8 (1%)	15	49

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	ALA
1	A	472	THR
1	C	233	ALA
1	C	472	THR
1	A	101	ASP
1	A	250	ASN
1	C	101	ASP
1	C	250	ASN

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	322/398 (81%)	305 (95%)	17 (5%)	20	41
1	C	322/398 (81%)	305 (95%)	17 (5%)	20	41
2	B	18/18 (100%)	17 (94%)	1 (6%)	19	40
2	D	18/18 (100%)	17 (94%)	1 (6%)	19	40
All	All	680/832 (82%)	644 (95%)	36 (5%)	22	41

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

Mol	Chain	Res	Type
1	A	33	ILE
1	A	48	LYS
1	A	108	LEU
1	A	111	TYR
1	A	112	ASP
1	A	118	ARG
1	A	139	TRP
1	A	174	ARG
1	A	244	GLU
1	A	246	ARG
1	A	253	PHE
1	A	267	ARG
1	A	339	GLU
1	A	390	THR
1	A	456	VAL
1	A	483	ASN
1	A	484	GLU
2	B	408	ILE
1	C	33	ILE
1	C	48	LYS
1	C	108	LEU
1	C	111	TYR
1	C	112	ASP
1	C	118	ARG
1	C	139	TRP
1	C	174	ARG
1	C	244	GLU
1	C	246	ARG
1	C	253	PHE
1	C	267	ARG
1	C	339	GLU
1	C	390	THR
1	C	456	VAL
1	C	483	ASN
1	C	484	GLU
2	D	408	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	168	GLN
1	A	224	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	272	HIS
1	A	308	GLN
1	A	319	ASN
1	A	321	ASN
1	A	324	HIS
1	A	368	ASN
1	A	370	ASN
1	A	459	GLN
1	A	483	ASN
2	B	415	GLN
1	C	21	ASN
1	C	168	GLN
1	C	224	ASN
1	C	272	HIS
1	C	308	GLN
1	C	319	ASN
1	C	321	ASN
1	C	324	HIS
1	C	368	ASN
1	C	370	ASN
1	C	459	GLN
1	C	483	ASN
2	D	415	GLN

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 oligosaccharides 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.

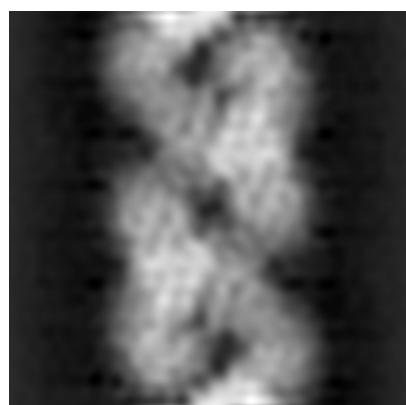
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0175. These allow visual inspection of the internal detail of the map and identification of artifacts.

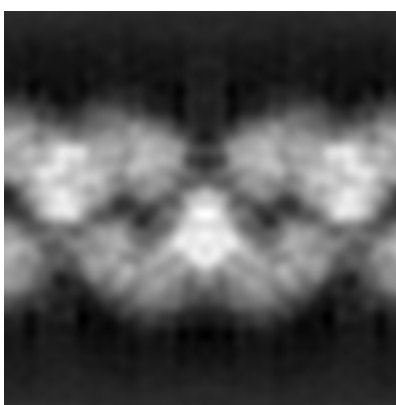
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

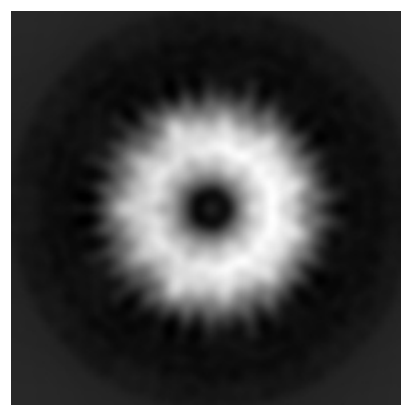
6.1.1 Primary map



X



Y

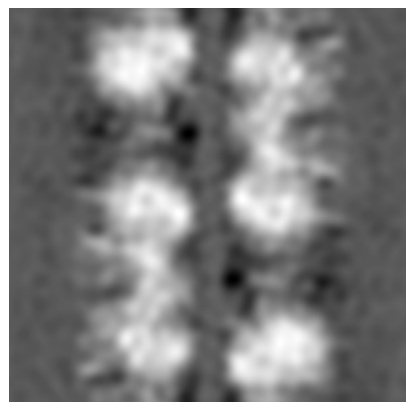


Z

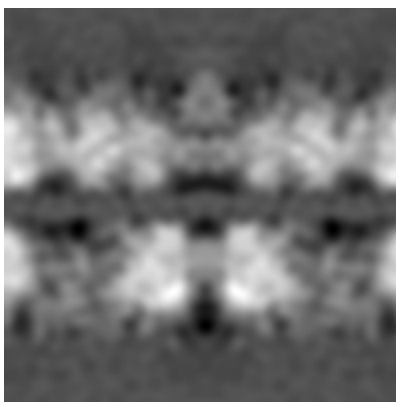
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

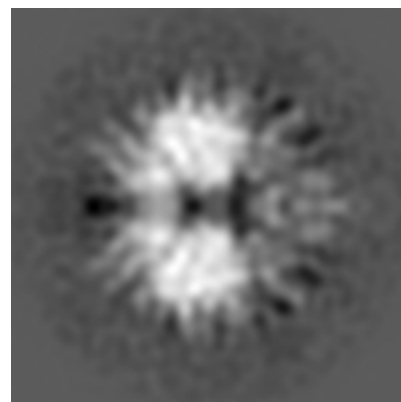
6.2.1 Primary map



X Index: 60



Y Index: 60

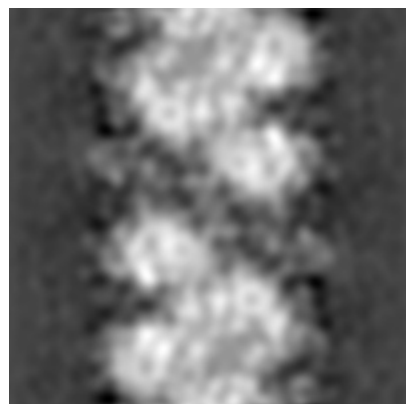


Z Index: 60

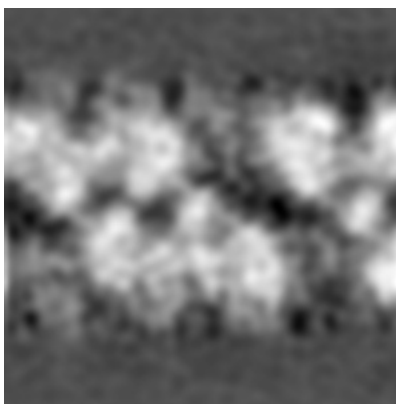
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 76



Y Index: 52

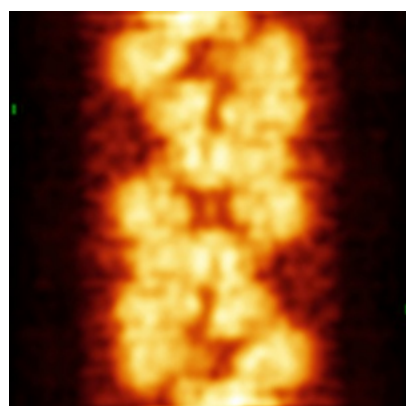


Z Index: 2

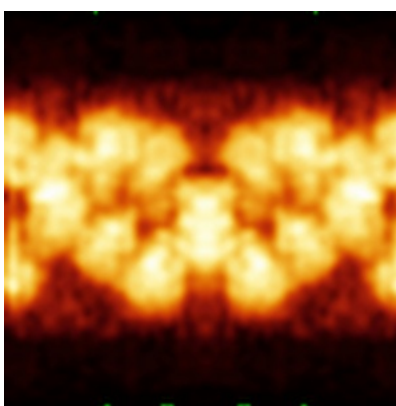
The images above show the largest variance slices of the map in three orthogonal directions.

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

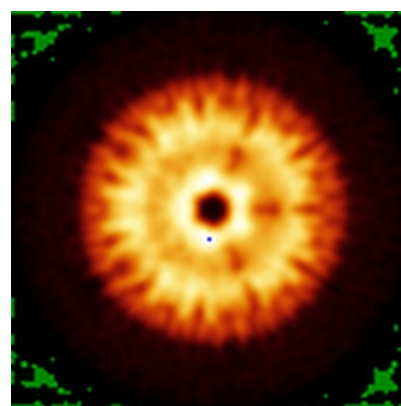
6.4.1 Primary map



X



Y

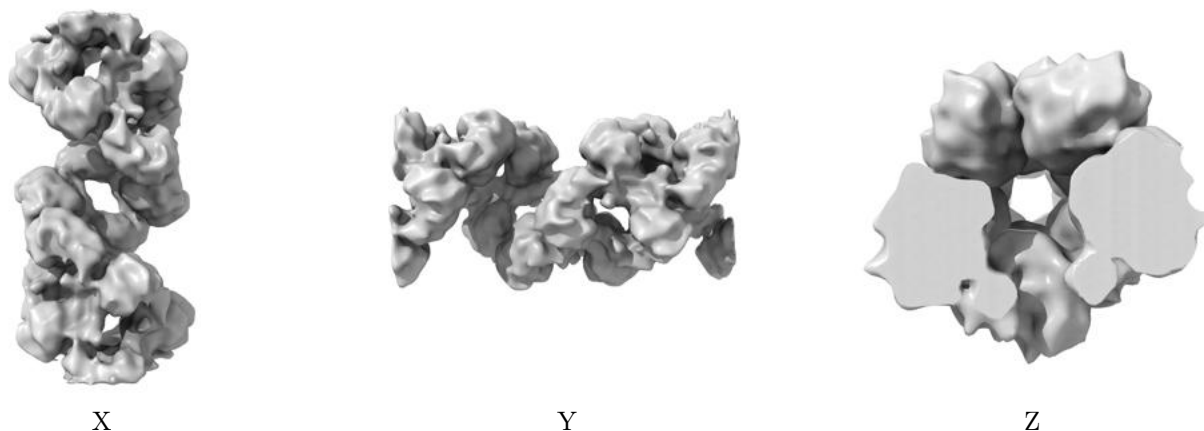


Z

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

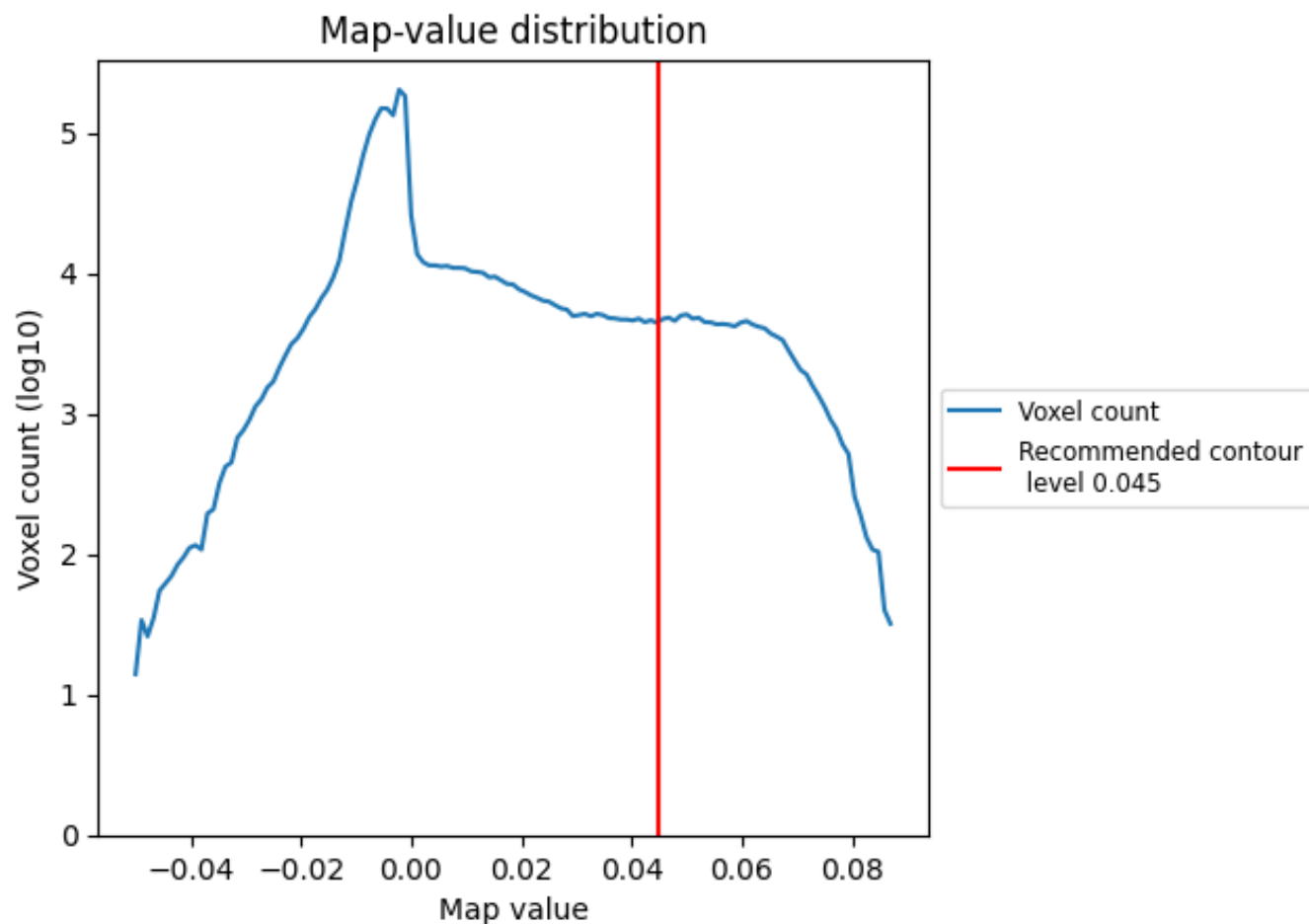
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

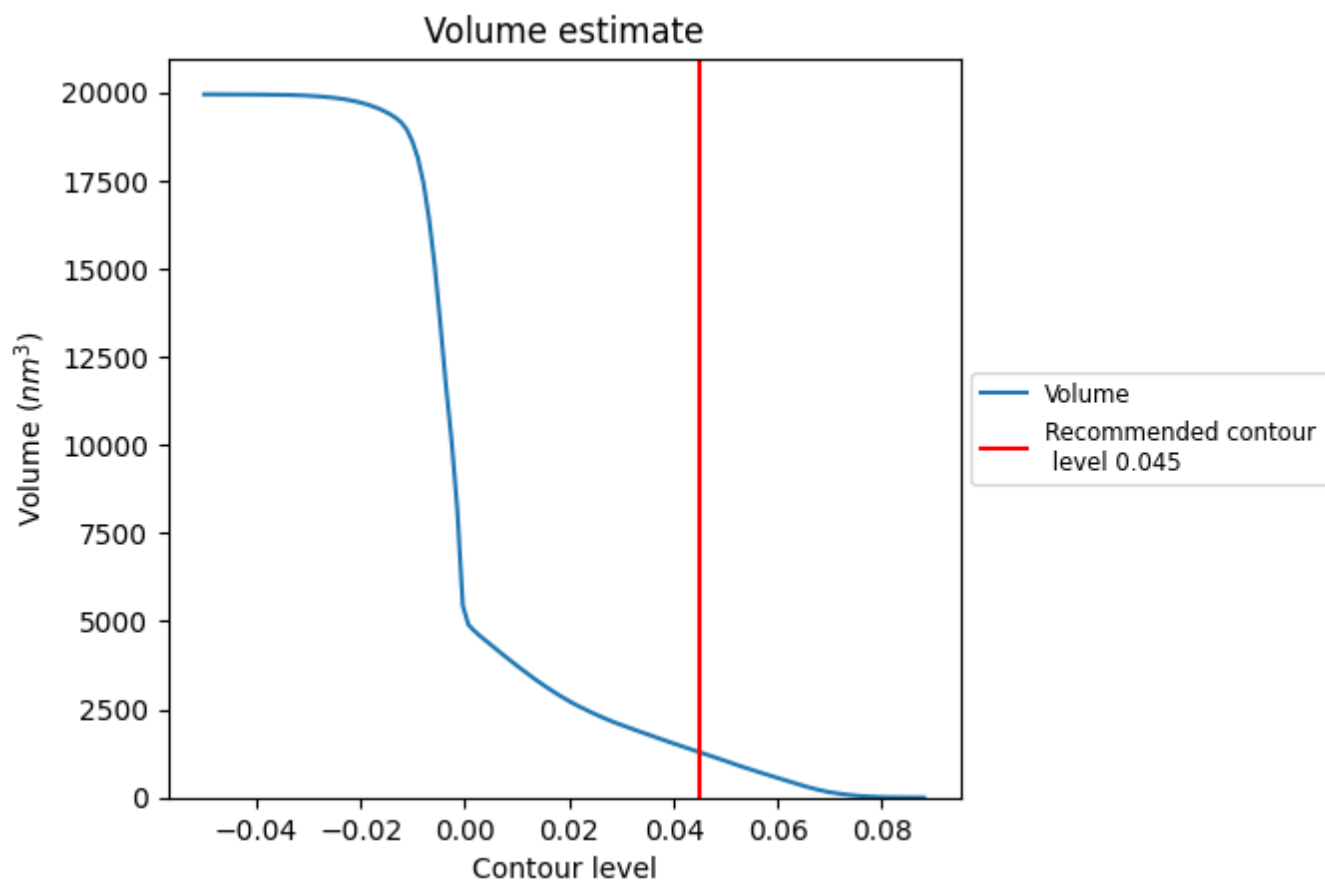
This section contains the results of statistical analysis of the map.

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.

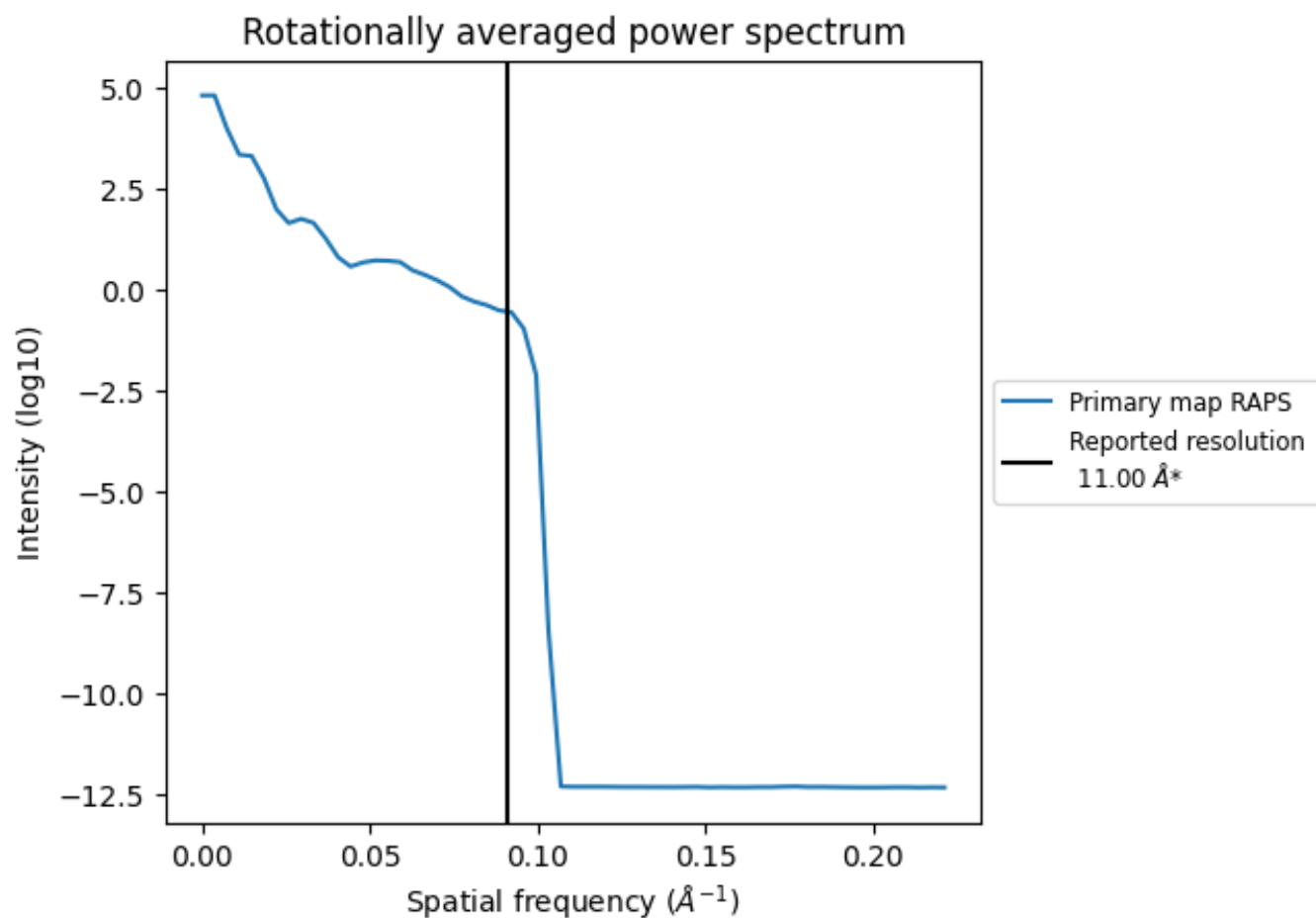
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1291 nm³; this corresponds to an approximate mass of 1166 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 0.091 Å⁻¹

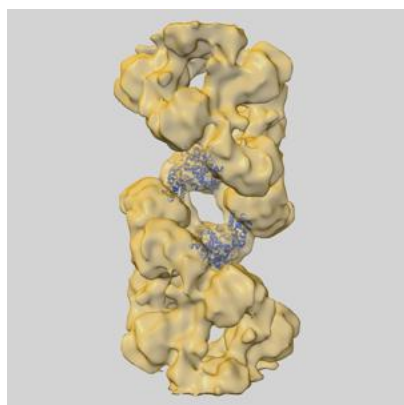
8 Fourier-Shell correlation

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

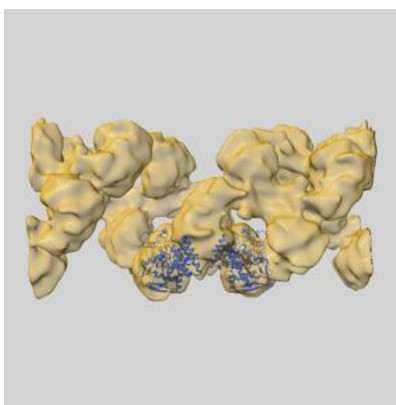
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0175 and PDB model 6H9G. Per-residue inclusion information can be found in section 3 on page 4.

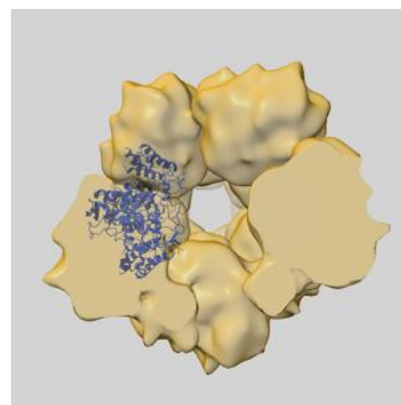
9.1 Map-model overlay [i](#)



X



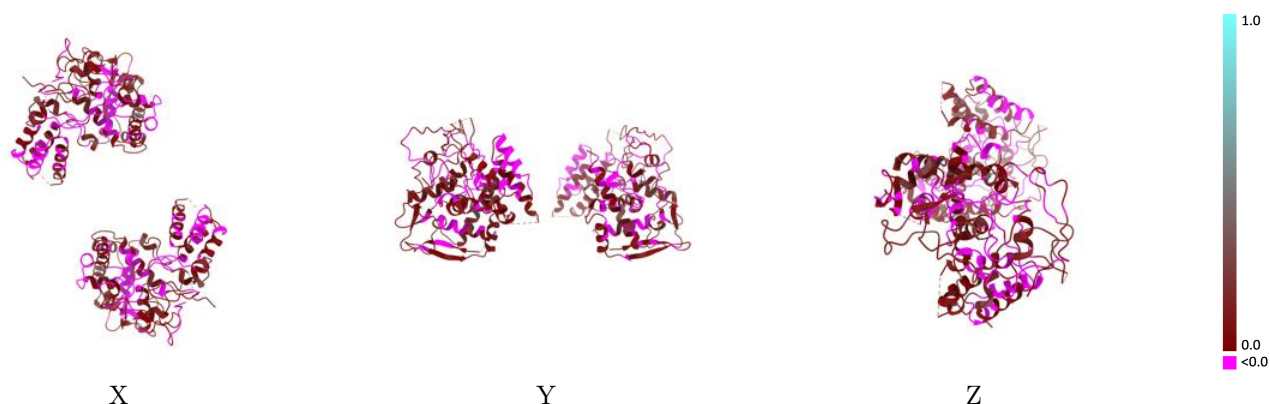
Y



Z

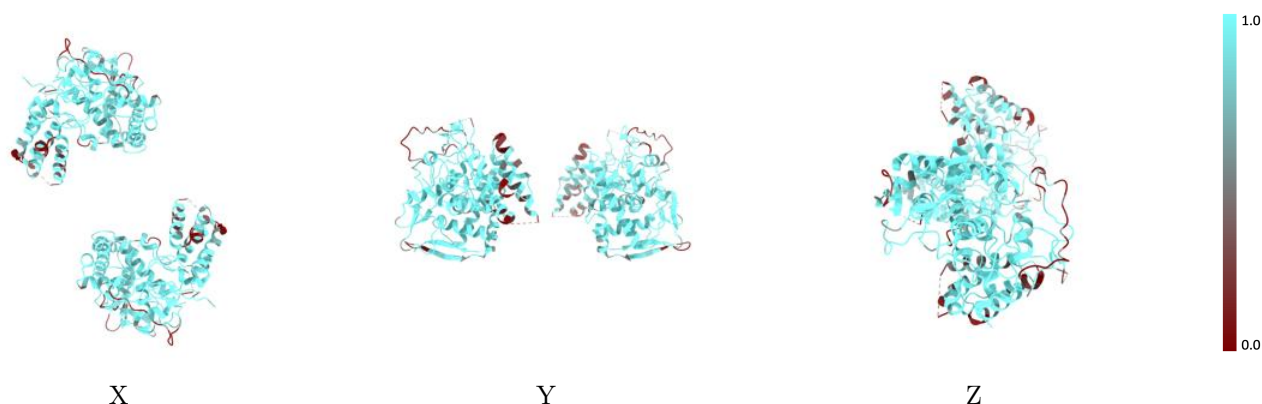
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



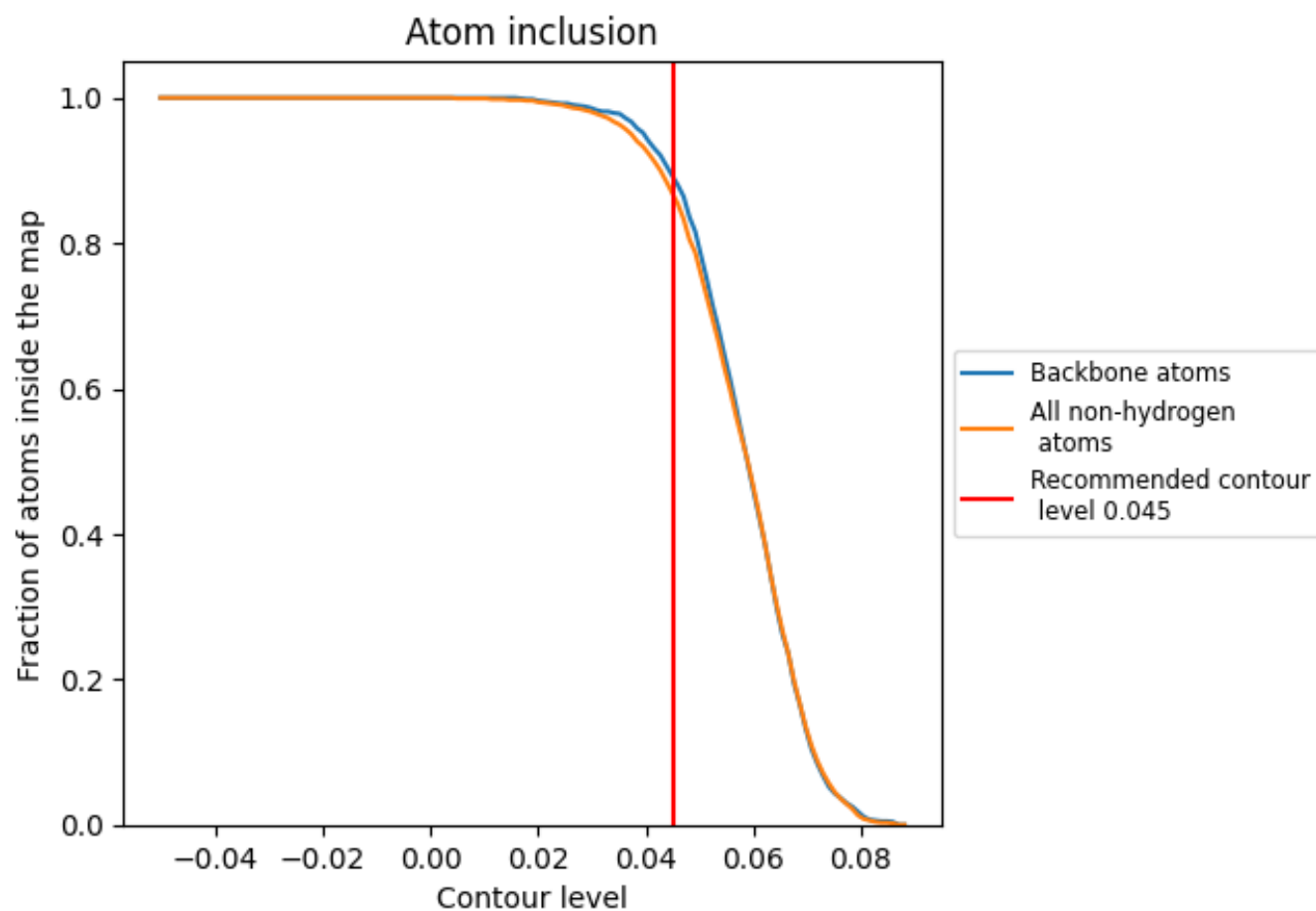
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.045).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 87% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8680	0.0440
A	0.8650	0.0430
B	0.9450	0.0830
C	0.8650	0.0410
D	0.9450	0.0760

