



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:21 AM UTC

PDB ID : 6OJ4 / pdb_00006oj4
EMDB ID : EMD-20087
Title : In situ structure of rotavirus VP1 RNA-dependent RNA polymerase (DLP)
Authors : Jenni, S.; Salgado, E.N.; Herrmann, T.; Li, Z.; Grant, T.; Grigorieff, N.;
Trapani, S.; Estrozi, L.F.; Harrison, S.C.
Deposited on : 2019-04-10
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

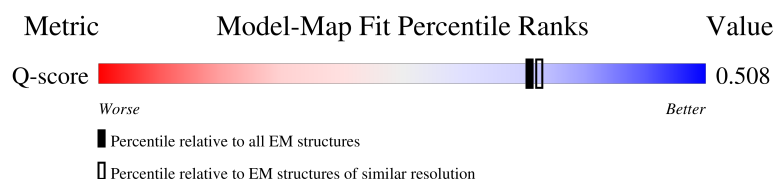
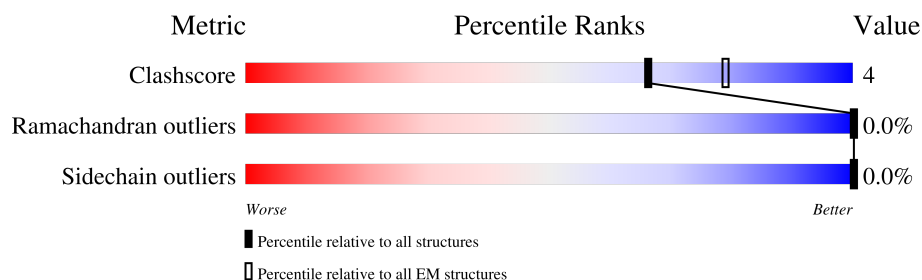
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.30 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	15087 (2.80 - 3.80)

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	887	 78% 10% 12%
1	B	887	 78% 10% 12%
1	C	887	 78% 10% 12%
1	D	887	 82% 11% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	887	 80%10%10%
1	F	887	 81%10%10%
1	G	887	 81%9%10%
1	H	887	 80%10%10%
1	I	887	 82%8%10%
1	J	887	 81%11%8%
2	P	1088	 86%13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 148556 atoms, of which 74461 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 Inner capsid protein VP2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	781	Total	C	H	N	O	S	0	0
			12787	4052	6408	1101	1190	36		
1	B	781	Total	C	H	N	O	S	0	0
			12787	4052	6408	1101	1190	36		
1	C	780	Total	C	H	N	O	S	0	0
			12772	4047	6400	1100	1189	36		
1	D	827	Total	C	H	N	O	S	0	0
			13574	4297	6809	1163	1269	36		
1	E	795	Total	C	H	N	O	S	0	0
			13028	4132	6529	1118	1213	36		
1	F	802	Total	C	H	N	O	S	0	0
			13151	4170	6588	1130	1227	36		
1	G	802	Total	C	H	N	O	S	0	0
			13151	4170	6588	1130	1227	36		
1	H	802	Total	C	H	N	O	S	0	0
			13151	4170	6588	1130	1227	36		
1	I	800	Total	C	H	N	O	S	0	0
			13114	4159	6569	1127	1223	36		
1	J	816	Total	C	H	N	O	S	0	0
			13391	4242	6713	1149	1251	36		

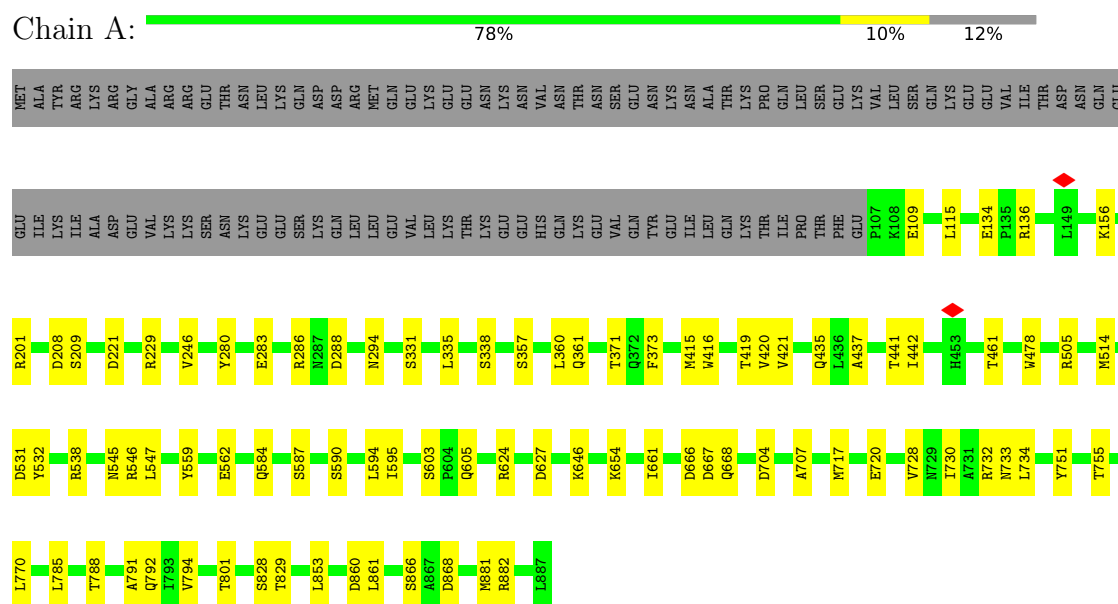
- Molecule 2 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	P	1086	Total	C	H	N	O	S	0	0
			17650	5633	8861	1455	1662	39		

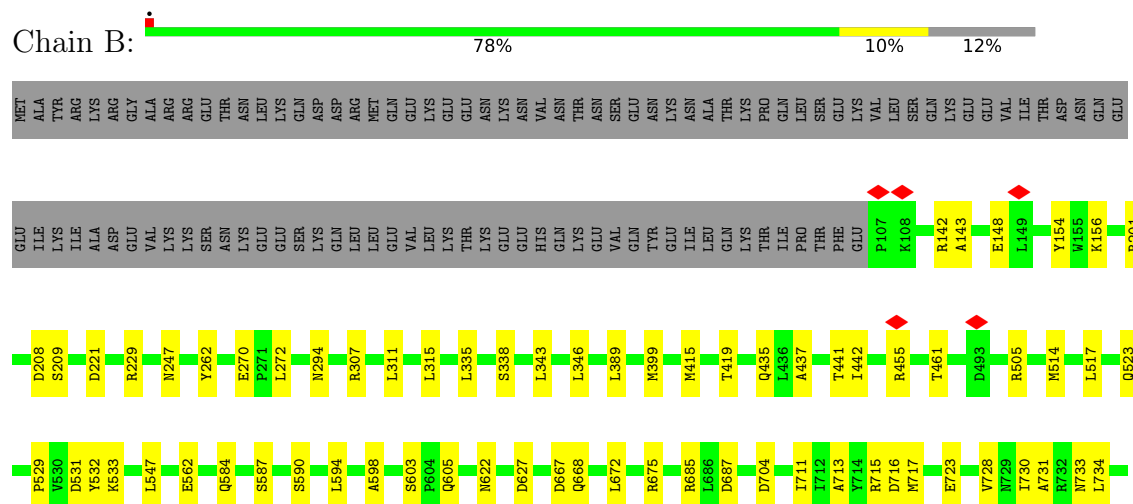
3 Residue-property plots

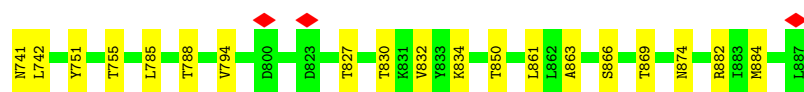
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Inner capsid protein VP2



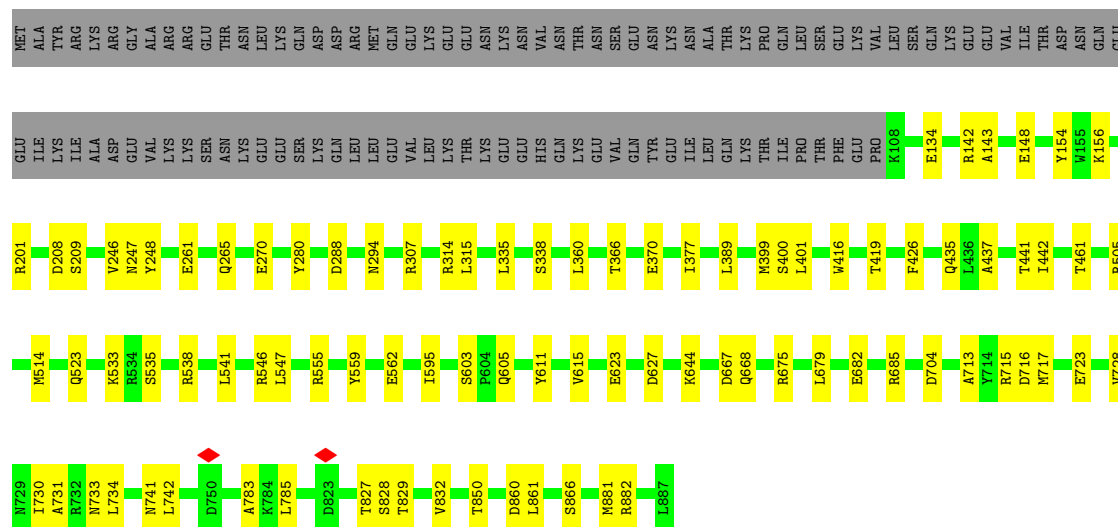
• Molecule 1: Inner capsid protein VP2





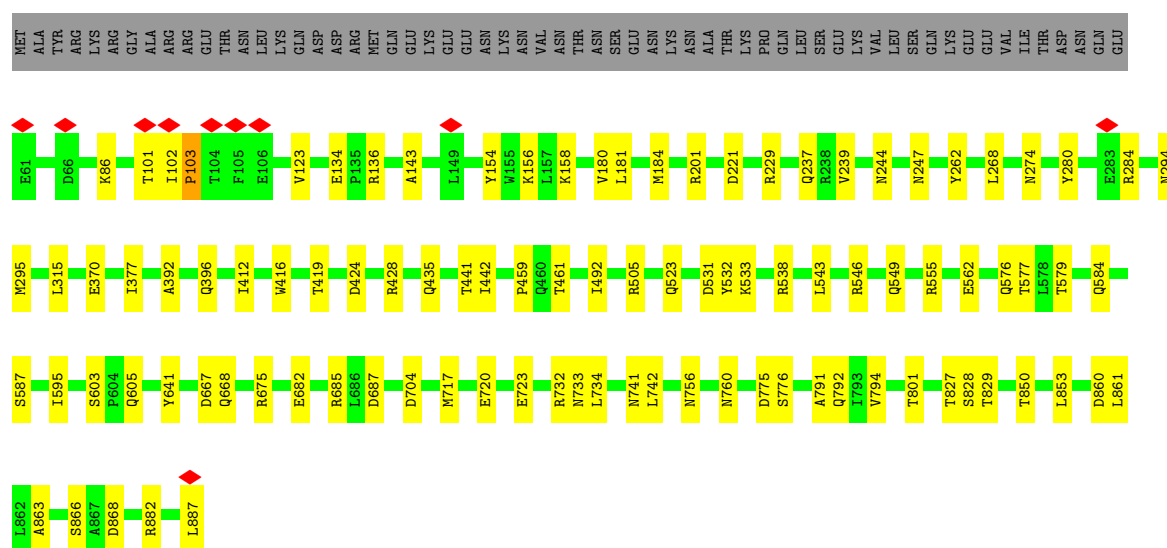
• Molecule 1: Inner capsid protein VP2

Chain C: 78% 10% 12%



• Molecule 1: Inner capsid protein VP2

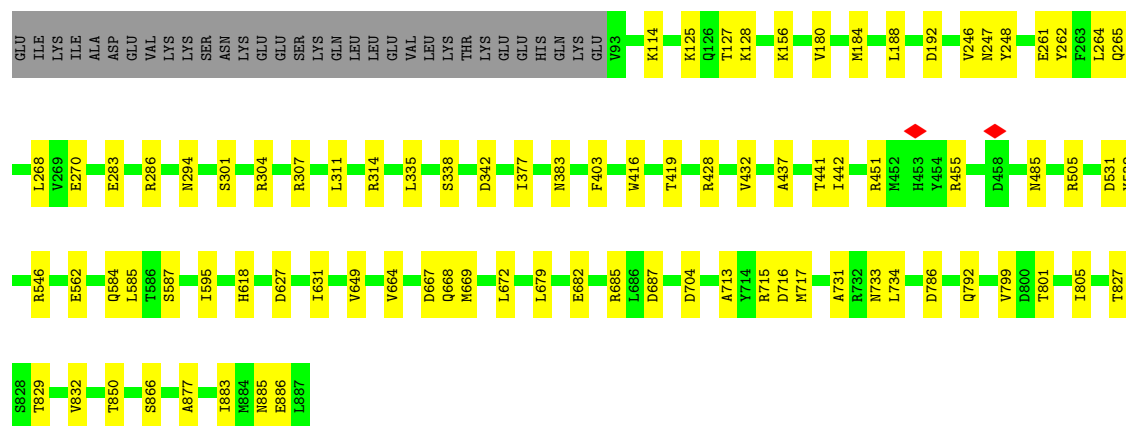
Chain D: 82% 11% 7%



• Molecule 1: Inner capsid protein VP2

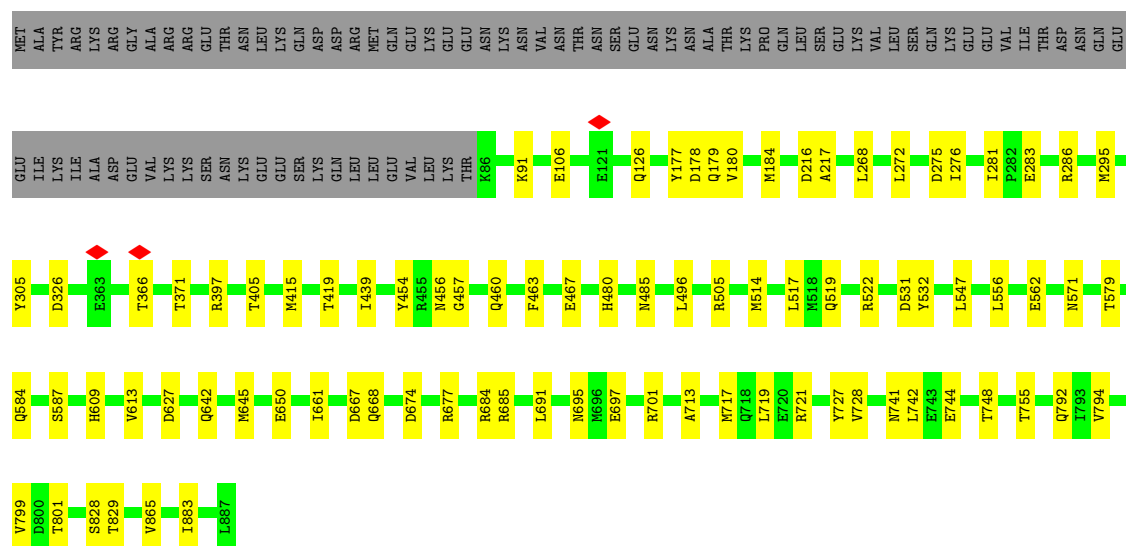
Chain E: 80% 10% 10%





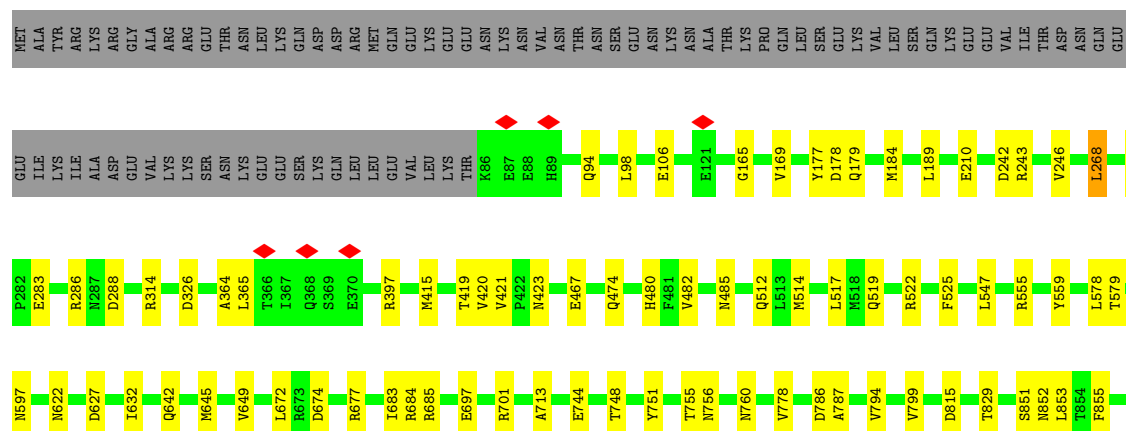
• Molecule 1: Inner capsid protein VP2

Chain F: 81% 10% 10%

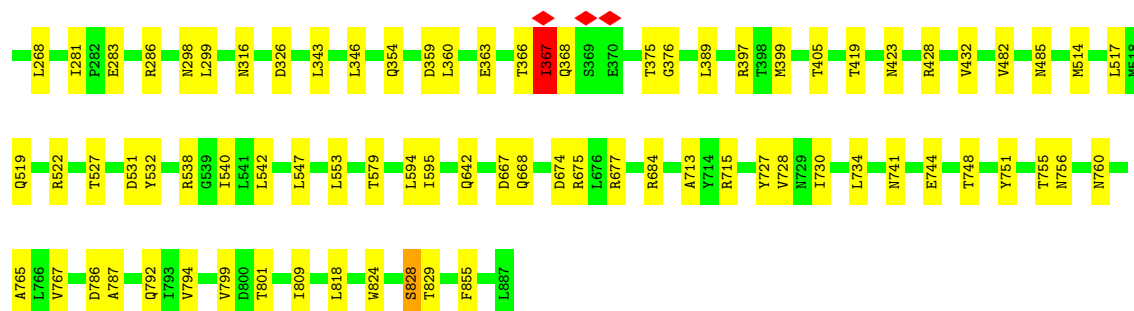


• Molecule 1: Inner capsid protein VP2

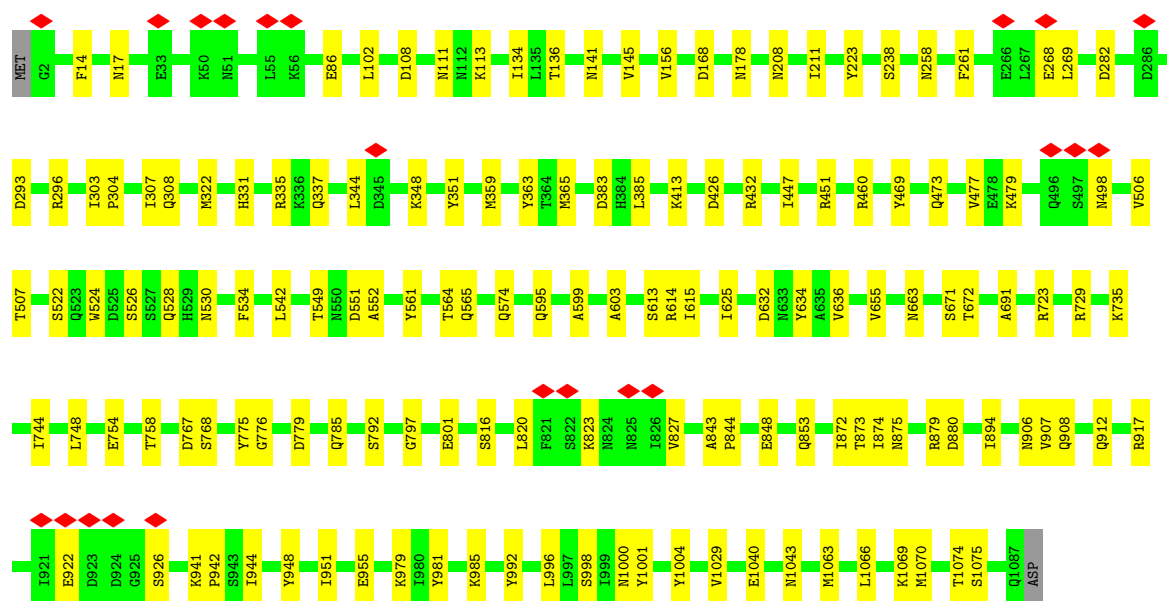
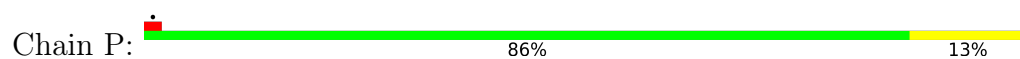
Chain G: 81% 9% 10%



GLU	IIE	LVS	IIE	ASP	GLU	VAL	LVS	SER	N72	K73	E74	E75	S76	K77	Q78	L79	L80	K84	T85	K86	E87	E106	E121	K124	E134	P135	R136	D178	Q179	V180	L181	L182	F183	M184	L189	D192	R201	D216	A217	T224	R229	I232				
MET	ALA	TYR	ARG	LYS	ARG	GLY	ALA	ARG	GLU	THR	ASN	LEU	LYS	GLN	ASP	ASP	ARG	MET	GLN	GLU	GLU	GLY	GLY	ASN	LYS	ASN	ASN	VAL	ASN	THR	ASN	SER	GLU	LYS	GLN	SER	LEU	VAL	GLU	VAL	ILE	THR	ASP	ASN	GLN	GLU



• Molecule 2: RNA-directed RNA polymerase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	50176	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 ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	18.686	Depositor
Minimum map value	-9.790	Depositor
Average map value	0.028	Depositor
Map value standard deviation	0.730	Depositor
Recommended contour level	2	Depositor
Map size (Å)	360.096, 360.096, 360.096	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.023, 1.023, 1.023	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	0.46	0/6495	0.50	0/8810
1	B	0.46	0/6495	0.50	0/8810
1	C	0.46	0/6487	0.49	0/8799
1	D	0.46	0/6885	0.51	0/9332
1	E	0.46	0/6618	0.50	0/8979
1	F	0.46	0/6683	0.49	0/9064
1	G	0.46	0/6683	0.50	0/9064
1	H	0.47	0/6683	0.50	0/9064
1	I	0.47	0/6665	0.50	0/9041
1	J	0.46	0/6798	0.51	2/9217 (0.0%)
2	P	0.36	0/8963	0.49	0/12120
All	All	0.45	0/75455	0.50	2/102300 (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	B	0	1
1	C	0	1
1	D	0	2
1	F	0	1
1	G	0	2
1	H	0	1
1	I	0	3
1	J	0	3
2	P	0	1
All	All	0	15

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	367	ILE	CA-C-N	5.08	130.85	121.70
1	J	367	ILE	C-N-CA	5.08	130.85	121.70

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	143	ALA	Peptide
1	C	143	ALA	Peptide
1	D	102	ILE	Peptide
1	D	143	ALA	Peptide
1	F	106	GLU	Peptide
1	G	106	GLU	Peptide
1	G	525	PHE	Peptide
1	H	106	GLU	Peptide
1	I	106	GLU	Peptide
1	I	143	ALA	Peptide
1	I	579	THR	Peptide
1	J	106	GLU	Peptide
1	J	367	ILE	Peptide
1	J	828	SER	Peptide
2	P	941	LYS	Peptide

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	6379	6408	6408	55	0
1	B	6379	6408	6408	55	0
1	C	6372	6400	6400	54	0
1	D	6765	6809	6809	55	0
1	E	6499	6529	6529	52	0
1	F	6563	6588	6588	49	0
1	G	6563	6588	6588	46	0
1	H	6563	6588	6588	53	0
1	I	6545	6569	6569	44	0
1	J	6678	6713	6713	59	0
2	P	8789	8861	8861	89	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	74095	74461	74461	586	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 4.

All (586) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:874:ILE:HD11	2:P:996:LEU:HD13	1.62	0.81
1:A:294:ASN:OD1	1:A:866:SER:OG	2.01	0.78
1:B:201:ARG:O	1:F:642:GLN:NE2	2.17	0.77
1:E:294:ASN:OD1	1:E:866:SER:OG	2.02	0.77
1:J:124:LYS:NZ	1:J:182:THR:O	2.17	0.77
1:F:519:GLN:OE1	1:F:522:ARG:NH2	2.19	0.76
1:C:644:LYS:NZ	1:H:597:ASN:O	2.18	0.75
1:H:326:ASP:OD1	1:H:397:ARG:NH1	2.19	0.75
2:P:1004:TYR:OH	2:P:1043:ASN:OD1	2.04	0.75
1:G:713:ALA:O	1:G:829:THR:OG1	2.03	0.74
2:P:293:ASP:OD1	2:P:296:ARG:NH2	2.19	0.74
2:P:955:GLU:OE2	2:P:979:LYS:NZ	2.21	0.74
2:P:775:TYR:OH	2:P:1040:GLU:OE2	2.05	0.74
1:G:597:ASN:ND2	1:G:886:GLU:O	2.20	0.74
1:I:177:TYR:OH	1:I:685:ARG:O	2.06	0.74
1:C:294:ASN:OD1	1:C:866:SER:OG	2.05	0.73
1:E:342:ASP:OD1	1:E:383:ASN:ND2	2.22	0.73
1:I:326:ASP:OD1	1:I:397:ARG:NH1	2.22	0.73
1:G:519:GLN:OE1	1:G:522:ARG:NH2	2.21	0.73
1:B:584:GLN:O	1:B:587:SER:OG	2.07	0.72
1:I:449:MET:HE1	1:I:470:ILE:HD13	1.70	0.72
1:H:343:LEU:HD13	1:H:346:LEU:HD21	1.72	0.71
1:D:756:ASN:OD1	1:D:760:ASN:ND2	2.23	0.71
2:P:948:TYR:OH	2:P:1070:MET:O	2.09	0.71
1:G:755:THR:HG22	1:G:794:VAL:HG12	1.71	0.71
1:J:354:GLN:HB2	2:P:365:MET:HE1	1.73	0.70
1:B:716:ASP:OD1	1:B:827:THR:OG1	2.09	0.70
2:P:14:PHE:O	2:P:17:ASN:ND2	2.24	0.70
1:F:326:ASP:OD1	1:F:397:ARG:NH1	2.25	0.70
2:P:426:ASP:OD2	2:P:432:ARG:NH2	2.24	0.70
2:P:307:ILE:HA	2:P:322:MET:HE1	1.73	0.70
1:C:360:LEU:O	1:C:538:ARG:NH1	2.25	0.70
1:H:177:TYR:OH	1:H:685:ARG:O	2.08	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:TYR:OH	1:D:723:GLU:OE2	2.10	0.69
1:B:603:SER:OG	1:B:605:GLN:OE1	2.10	0.69
1:B:863:ALA:O	1:F:91:LYS:NZ	2.25	0.69
1:D:603:SER:OG	1:D:605:GLN:OE1	2.09	0.69
1:J:674:ASP:OD1	1:J:677:ARG:NH2	2.25	0.69
1:I:283:GLU:OE1	1:I:286:ARG:NH2	2.25	0.69
1:H:753:GLN:NE2	1:H:757:MET:SD	2.66	0.69
1:I:281:ILE:O	1:I:286:ARG:NH1	2.26	0.69
1:B:154:TYR:OH	1:B:723:GLU:OE2	2.10	0.69
1:D:435:GLN:OE1	1:D:461:THR:OG1	2.10	0.69
1:B:221:ASP:O	1:B:229:ARG:NH2	2.26	0.68
1:F:281:ILE:O	1:F:286:ARG:NH1	2.26	0.68
1:C:603:SER:OG	1:C:605:GLN:OE1	2.12	0.68
1:F:697:GLU:OE2	1:F:701:ARG:NE	2.25	0.68
1:G:697:GLU:OE2	1:G:701:ARG:NE	2.26	0.68
1:J:326:ASP:OD1	1:J:397:ARG:NH1	2.26	0.68
2:P:141:ASN:OD1	2:P:735:LYS:NZ	2.17	0.68
2:P:998:SER:OG	2:P:1001:TYR:O	2.10	0.68
1:F:713:ALA:O	1:F:829:THR:OG1	2.07	0.68
1:H:281:ILE:O	1:H:286:ARG:NH1	2.27	0.68
1:B:441:THR:HG1	1:B:532:TYR:HH	1.23	0.67
1:C:860:ASP:O	1:G:94:GLN:NE2	2.27	0.67
1:D:546:ARG:NH2	1:D:595:ILE:O	2.27	0.67
1:G:326:ASP:OD1	1:G:397:ARG:NH1	2.28	0.67
1:E:441:THR:OG1	1:E:532:TYR:OH	2.10	0.67
1:G:281:ILE:O	1:G:286:ARG:NH1	2.27	0.67
1:F:792:GLN:NE2	1:F:801:THR:O	2.28	0.66
1:E:717:MET:O	1:E:827:THR:OG1	2.07	0.66
1:F:283:GLU:OE1	1:F:286:ARG:NH2	2.28	0.66
1:E:114:LYS:NZ	2:P:549:THR:O	2.29	0.66
1:H:138:LEU:HD13	1:H:724:MET:HE1	1.76	0.66
1:D:244:ASN:O	1:D:853:LEU:N	2.28	0.66
1:F:496:LEU:N	1:F:571:ASN:OD1	2.29	0.65
1:C:261:GLU:OE2	1:C:265:GLN:NE2	2.29	0.65
1:F:674:ASP:OD1	1:F:677:ARG:NH2	2.29	0.65
1:J:343:LEU:HD13	1:J:346:LEU:HD21	1.76	0.65
1:F:744:GLU:O	1:F:748:THR:OG1	2.13	0.65
1:D:416:TRP:O	1:D:419:THR:OG1	2.13	0.65
1:J:134:GLU:OE2	1:J:136:ARG:NH2	2.28	0.65
1:G:314:ARG:NH1	1:G:622:ASN:OD1	2.29	0.65
1:G:514:MET:HG3	1:G:547:LEU:HD13	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:LYS:NZ	1:B:704:ASP:OD2	2.30	0.65
1:J:363:GLU:O	1:J:366:THR:OG1	2.15	0.65
1:H:389:LEU:HD23	1:H:399:MET:HE1	1.78	0.64
1:I:697:GLU:OE2	1:I:701:ARG:NE	2.29	0.64
1:C:201:ARG:O	1:G:642:GLN:NE2	2.29	0.64
1:G:756:ASN:OD1	1:G:760:ASN:ND2	2.30	0.64
1:B:717:MET:O	1:B:827:THR:OG1	2.08	0.64
1:C:370:GLU:OE2	1:C:535:SER:OG	2.07	0.64
1:C:437:ALA:O	1:C:441:THR:HG22	1.98	0.64
1:D:294:ASN:OD1	1:D:866:SER:OG	2.16	0.64
1:D:221:ASP:O	1:D:229:ARG:NH2	2.31	0.64
1:B:731:ALA:N	1:B:832:VAL:O	2.30	0.64
1:C:555:ARG:NH1	1:C:882:ARG:O	2.31	0.64
1:J:755:THR:HG22	1:J:794:VAL:HG12	1.80	0.64
1:J:786:ASP:OD2	1:J:828:SER:OG	2.14	0.64
2:P:108:ASP:OD1	2:P:113:LYS:NZ	2.21	0.63
1:B:523:GLN:O	1:B:533:LYS:NZ	2.31	0.63
1:J:281:ILE:O	1:J:286:ARG:NH1	2.31	0.63
1:B:435:GLN:OE1	1:B:461:THR:OG1	2.16	0.63
1:C:247:ASN:OD1	1:C:850:THR:HG22	1.99	0.63
1:C:627:ASP:OD1	1:C:685:ARG:NH1	2.32	0.63
1:G:419:THR:O	1:G:485:ASN:ND2	2.31	0.63
1:E:188:LEU:HD11	1:E:264:LEU:CD2	2.29	0.63
1:A:707:ALA:N	1:A:770:LEU:O	2.32	0.62
2:P:344:LEU:O	2:P:348:LYS:NZ	2.27	0.62
1:B:247:ASN:OD1	1:B:850:THR:HG22	1.99	0.62
1:G:744:GLU:O	1:G:748:THR:OG1	2.13	0.62
2:P:992:TYR:CE2	2:P:996:LEU:HD11	2.35	0.62
1:C:716:ASP:OD1	1:C:827:THR:OG1	2.17	0.62
1:H:674:ASP:OD1	1:H:677:ARG:NH2	2.32	0.62
1:I:674:ASP:OD1	1:I:677:ARG:NH2	2.33	0.62
1:C:154:TYR:OH	1:C:723:GLU:OE2	2.17	0.62
1:F:326:ASP:OD2	1:F:579:THR:HG22	2.00	0.62
2:P:460:ARG:NH1	2:P:522:SER:O	2.32	0.62
2:P:880:ASP:OD2	2:P:1069:LYS:NZ	2.32	0.62
1:D:717:MET:O	1:D:827:THR:OG1	2.18	0.61
1:G:423:ASN:ND2	1:G:482:VAL:O	2.33	0.61
1:A:201:ARG:O	1:J:642:GLN:NE2	2.32	0.61
1:G:184:MET:SD	1:G:684:ARG:NH2	2.74	0.61
1:I:343:LEU:HD13	1:I:346:LEU:HD21	1.81	0.61
1:C:156:LYS:NZ	1:C:704:ASP:OD2	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:311:LEU:O	1:E:618:HIS:NE2	2.33	0.61
1:I:514:MET:HG3	1:I:547:LEU:HD13	1.82	0.61
1:E:716:ASP:OD1	1:E:827:THR:OG1	2.18	0.61
1:H:283:GLU:OE1	1:H:286:ARG:NH2	2.34	0.61
2:P:754:GLU:OE2	2:P:768:SER:OG	2.16	0.61
1:D:720:GLU:OE2	1:D:732:ARG:NH2	2.34	0.61
1:H:423:ASN:ND2	1:H:482:VAL:O	2.34	0.61
1:F:177:TYR:OH	1:F:685:ARG:O	2.10	0.61
2:P:351:TYR:OH	2:P:526:SER:O	2.16	0.61
1:A:720:GLU:OE2	1:A:732:ARG:NH2	2.34	0.61
1:E:505:ARG:NH2	1:E:562:GLU:OE1	2.34	0.61
1:I:419:THR:O	1:I:485:ASN:ND2	2.34	0.60
2:P:744:ILE:HB	2:P:748:LEU:HD22	1.83	0.60
1:I:423:ASN:ND2	1:I:482:VAL:O	2.34	0.60
1:E:156:LYS:NZ	1:E:704:ASP:OD2	2.33	0.60
1:E:792:GLN:NE2	1:E:801:THR:O	2.33	0.60
2:P:524:TRP:O	2:P:530:ASN:ND2	2.33	0.60
1:H:326:ASP:OD2	1:H:579:THR:HG22	2.01	0.60
1:B:869:THR:O	1:F:405:THR:OG1	2.17	0.60
1:H:713:ALA:O	1:H:829:THR:OG1	2.14	0.60
2:P:792:SER:O	2:P:853:GLN:NE2	2.35	0.60
1:A:717:MET:O	1:A:828:SER:N	2.35	0.59
1:C:360:LEU:HD22	1:C:370:GLU:OE1	2.01	0.59
2:P:951:ILE:HG21	2:P:985:LYS:HG2	1.84	0.59
1:B:514:MET:HG3	1:B:547:LEU:HD13	1.83	0.59
2:P:86:GLU:OE1	2:P:178:ASN:ND2	2.35	0.59
1:E:627:ASP:O	1:E:631:ILE:HD12	2.02	0.59
1:A:360:LEU:O	1:A:538:ARG:NH1	2.34	0.59
1:H:519:GLN:OE1	1:H:522:ARG:NH2	2.34	0.59
1:I:624:ARG:NH2	1:I:627:ASP:OD2	2.35	0.59
1:C:514:MET:HG3	1:C:547:LEU:HD13	1.85	0.59
1:I:134:GLU:OE2	1:I:136:ARG:NH2	2.35	0.59
2:P:874:ILE:CD1	2:P:996:LEU:HD13	2.31	0.59
1:C:435:GLN:OE1	1:C:461:THR:OG1	2.19	0.59
1:C:717:MET:O	1:C:827:THR:OG1	2.14	0.59
1:A:435:GLN:OE1	1:A:461:THR:OG1	2.17	0.58
1:C:623:GLU:OE2	1:C:685:ARG:NH2	2.36	0.58
1:H:244:ASN:OD1	1:H:853:LEU:N	2.36	0.58
1:C:523:GLN:O	1:C:533:LYS:NZ	2.36	0.58
1:E:416:TRP:O	1:E:419:THR:OG1	2.18	0.58
1:J:283:GLU:OE1	1:J:286:ARG:NH2	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:370:GLU:OE2	1:D:538:ARG:NH2	2.36	0.58
1:D:555:ARG:NH1	1:D:882:ARG:O	2.36	0.58
2:P:873:THR:OG1	2:P:1075:SER:OG	2.09	0.58
1:D:134:GLU:OE2	1:D:136:ARG:NH2	2.36	0.58
2:P:528:GLN:OE1	2:P:663:ASN:ND2	2.37	0.58
1:B:598:ALA:N	1:B:884:MET:SD	2.76	0.58
1:F:126:GLN:N	1:F:126:GLN:OE1	2.37	0.58
1:H:777:SER:OG	1:H:815:ASP:OD2	2.19	0.58
1:I:756:ASN:OD1	1:I:760:ASN:ND2	2.37	0.58
2:P:498:ASN:ND2	2:P:922:GLU:OE1	2.37	0.57
1:A:546:ARG:NH2	1:A:595:ILE:O	2.37	0.57
1:I:320:ASN:O	1:I:671:ARG:NH2	2.37	0.57
1:C:505:ARG:NH2	1:C:562:GLU:OE1	2.37	0.57
1:A:420:VAL:HG23	1:A:421:VAL:HG23	1.87	0.57
1:A:134:GLU:OE2	1:A:136:ARG:NH2	2.37	0.57
2:P:785:GLN:OE1	2:P:875:ASN:ND2	2.37	0.57
1:A:717:MET:N	1:A:828:SER:O	2.37	0.57
1:B:874:ASN:OD1	1:B:882:ARG:NH2	2.37	0.57
1:B:315:LEU:O	1:B:675:ARG:NH1	2.38	0.57
1:H:456:ASN:OD1	1:H:457:GLY:N	2.38	0.57
2:P:917:ARG:NH1	2:P:1000:ASN:OD1	2.37	0.56
1:A:751:TYR:O	1:A:755:THR:OG1	2.20	0.56
1:E:437:ALA:O	1:E:441:THR:HG22	2.06	0.56
1:A:785:LEU:O	1:A:788:THR:OG1	2.14	0.56
1:G:283:GLU:OE1	1:G:286:ARG:NH2	2.39	0.56
1:J:744:GLU:O	1:J:748:THR:OG1	2.12	0.56
1:D:505:ARG:NH2	1:D:562:GLU:OE1	2.38	0.56
1:J:79:LEU:HD11	2:P:308:GLN:NE2	2.19	0.56
1:J:741:ASN:ND2	1:J:744:GLU:OE1	2.39	0.56
1:D:584:GLN:O	1:D:587:SER:OG	2.16	0.56
1:J:828:SER:OG	1:J:829:THR:O	2.15	0.56
2:P:872:ILE:O	2:P:1074:THR:OG1	2.18	0.55
1:H:632:ILE:HG23	1:H:645:MET:HE3	1.88	0.55
1:J:354:GLN:CB	2:P:365:MET:HE1	2.35	0.55
2:P:363:TYR:OH	2:P:603:ALA:HB1	2.07	0.55
1:B:415:MET:O	1:B:419:THR:HG23	2.05	0.55
1:F:584:GLN:O	1:F:587:SER:OG	2.20	0.55
1:H:584:GLN:O	1:H:587:SER:OG	2.11	0.55
1:A:584:GLN:O	1:A:587:SER:OG	2.16	0.55
1:J:326:ASP:OD2	1:J:579:THR:HG22	2.06	0.55
1:J:375:THR:HG22	1:J:376:GLY:H	1.72	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:TYR:CG	1:A:861:LEU:HD23	2.42	0.55
1:A:603:SER:OG	1:A:605:GLN:OE1	2.25	0.55
1:J:178:ASP:OD1	1:J:179:GLN:N	2.40	0.55
1:G:288:ASP:OD2	1:G:559:TYR:OH	2.16	0.54
2:P:955:GLU:OE2	2:P:981:TYR:OH	2.24	0.54
1:A:667:ASP:OD1	1:A:668:GLN:N	2.39	0.54
1:E:188:LEU:HD11	1:E:264:LEU:HD23	1.88	0.54
1:D:791:ALA:O	1:D:794:VAL:HG22	2.07	0.54
1:D:863:ALA:O	1:H:91:LYS:NZ	2.40	0.54
1:J:423:ASN:ND2	1:J:482:VAL:O	2.40	0.54
1:E:261:GLU:OE2	1:E:265:GLN:NE2	2.40	0.54
1:A:505:ARG:NH2	1:A:562:GLU:OE1	2.41	0.53
1:C:134:GLU:N	1:C:134:GLU:OE1	2.42	0.53
1:E:127:THR:HG22	1:E:128:LYS:H	1.71	0.53
1:G:751:TYR:O	1:G:755:THR:HG23	2.07	0.53
1:J:224:THR:O	1:J:229:ARG:NH1	2.42	0.53
1:G:98:LEU:HD11	1:G:578:LEU:HD23	1.91	0.53
2:P:922:GLU:OE1	2:P:926:SER:OG	2.19	0.53
1:A:288:ASP:OD2	1:A:559:TYR:OH	2.20	0.53
1:B:441:THR:HG23	1:B:442:ILE:HD12	1.89	0.53
1:F:454:TYR:OH	1:F:460:GLN:O	2.11	0.53
1:E:713:ALA:O	1:E:829:THR:HG23	2.08	0.53
1:G:364:ALA:C	1:G:365:LEU:HD12	2.34	0.53
1:I:532:TYR:CE2	1:I:536:ILE:HD11	2.43	0.53
2:P:168:ASP:OD2	2:P:223:TYR:OH	2.25	0.53
2:P:816:SER:O	2:P:820:LEU:N	2.40	0.53
1:A:441:THR:OG1	1:A:532:TYR:OH	2.13	0.53
1:J:818:LEU:O	1:J:824:TRP:NE1	2.38	0.53
1:I:216:ASP:OD1	1:I:217:ALA:N	2.41	0.53
1:G:177:TYR:OH	1:G:685:ARG:O	2.17	0.53
1:H:697:GLU:OE2	1:H:701:ARG:NE	2.42	0.53
1:J:792:GLN:NE2	1:J:801:THR:O	2.42	0.53
1:C:416:TRP:O	1:C:419:THR:OG1	2.25	0.53
2:P:625:ILE:HG22	2:P:636:VAL:HB	1.91	0.53
1:E:247:ASN:OD1	1:E:850:THR:HG22	2.09	0.52
1:E:283:GLU:OE2	1:E:286:ARG:NH2	2.42	0.52
2:P:906:ASN:OD1	2:P:907:VAL:N	2.42	0.52
1:B:415:MET:SD	1:B:517:LEU:HD21	2.49	0.52
1:B:389:LEU:HD23	1:B:399:MET:HE1	1.92	0.52
1:C:335:LEU:O	1:C:338:SER:OG	2.19	0.52
1:F:216:ASP:OD1	1:F:217:ALA:N	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:246:VAL:HG11	1:G:853:LEU:HD21	1.91	0.52
1:J:751:TYR:O	1:J:755:THR:HG23	2.09	0.52
1:H:343:LEU:CD1	1:H:346:LEU:HD21	2.40	0.52
1:A:415:MET:O	1:A:419:THR:HG23	2.10	0.52
1:D:828:SER:OG	1:D:829:THR:N	2.43	0.52
1:E:403:PHE:HB3	1:E:585:LEU:HD12	1.92	0.52
1:J:553:LEU:HD13	1:J:595:ILE:CD1	2.40	0.52
1:E:301:SER:O	1:E:304:ARG:NH1	2.40	0.52
1:E:125:LYS:NZ	1:E:192:ASP:OD2	2.24	0.51
1:G:178:ASP:OD1	1:G:179:GLN:N	2.43	0.51
1:A:416:TRP:O	1:A:420:VAL:HG22	2.11	0.51
1:I:403:PHE:HB3	1:I:585:LEU:HD12	1.92	0.51
1:E:682:GLU:OE2	1:E:685:ARG:NE	2.42	0.51
1:A:733:ASN:OD1	1:A:734:LEU:N	2.43	0.51
1:G:474:GLN:O	1:G:512:GLN:NE2	2.43	0.51
1:A:514:MET:HG3	1:A:547:LEU:HD13	1.92	0.51
1:A:531:ASP:OD1	1:A:532:TYR:N	2.43	0.51
2:P:359:MET:SD	2:P:614:ARG:NH2	2.84	0.51
1:D:274:ASN:ND2	1:D:295:MET:SD	2.84	0.51
1:E:314:ARG:HB3	1:E:679:LEU:HD21	1.91	0.51
1:J:180:VAL:O	1:J:184:MET:N	2.44	0.51
2:P:506:VAL:HG12	2:P:634:TYR:CE2	2.45	0.50
2:P:797:GLY:N	2:P:848:GLU:OE2	2.42	0.50
1:A:624:ARG:NH2	1:A:627:ASP:OD2	2.43	0.50
1:E:667:ASP:OD1	1:E:668:GLN:N	2.44	0.50
1:E:877:ALA:HB2	1:E:883:ILE:CG2	2.41	0.50
1:J:216:ASP:OD1	1:J:217:ALA:N	2.44	0.50
1:B:713:ALA:O	1:B:715:ARG:N	2.44	0.50
1:J:359:ASP:OD1	1:J:360:LEU:N	2.44	0.50
2:P:729:ARG:NH2	2:P:767:ASP:O	2.44	0.50
1:B:531:ASP:OD1	1:B:532:TYR:N	2.45	0.50
1:C:733:ASN:OD1	1:C:734:LEU:N	2.44	0.50
1:F:556:LEU:HA	1:F:883:ILE:HD11	1.92	0.50
1:G:514:MET:CG	1:G:547:LEU:HD13	2.41	0.50
1:I:283:GLU:O	1:I:287:ASN:ND2	2.44	0.50
1:B:208:ASP:OD1	1:B:209:SER:N	2.44	0.50
1:J:84:LYS:NZ	2:P:282:ASP:OD2	2.44	0.50
1:J:727:TYR:CD2	1:J:809:ILE:HD11	2.47	0.50
2:P:145:VAL:HG21	2:P:211:ILE:HG23	1.94	0.50
1:D:268:LEU:HD12	1:D:268:LEU:O	2.11	0.50
1:I:751:TYR:O	1:I:755:THR:HG23	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:337:GLN:O	2:P:451:ARG:NH1	2.44	0.50
1:B:590:SER:O	1:B:594:LEU:N	2.43	0.50
1:C:828:SER:OG	1:C:829:THR:N	2.45	0.50
1:D:156:LYS:NZ	1:D:704:ASP:OD2	2.45	0.50
1:G:189:LEU:HD21	1:G:855:PHE:CE1	2.47	0.50
1:F:456:ASN:OD1	1:F:457:GLY:N	2.45	0.49
1:H:532:TYR:CE2	1:H:536:ILE:HD11	2.47	0.49
1:D:775:ASP:OD1	1:D:776:SER:N	2.44	0.49
1:J:346:LEU:HD22	1:J:594:LEU:O	2.11	0.49
1:B:262:TYR:OH	1:B:687:ASP:OD2	2.20	0.49
1:H:514:MET:HG3	1:H:547:LEU:HD13	1.94	0.49
2:P:413:LYS:NZ	2:P:801:GLU:OE2	2.22	0.49
1:A:441:THR:HG23	1:A:442:ILE:HD12	1.94	0.49
1:I:584:GLN:O	1:I:587:SER:OG	2.25	0.49
1:D:247:ASN:OD1	1:D:850:THR:HG22	2.12	0.49
1:D:531:ASP:OD1	1:D:532:TYR:N	2.46	0.49
1:H:376:GLY:O	1:H:590:SER:OG	2.30	0.49
1:B:294:ASN:OD1	1:B:866:SER:OG	2.27	0.49
1:B:529:PRO:HD3	1:C:541:LEU:HD11	1.95	0.49
1:E:713:ALA:O	1:E:715:ARG:N	2.46	0.49
1:A:283:GLU:OE2	1:A:286:ARG:NH2	2.45	0.49
1:A:828:SER:OG	1:A:829:THR:N	2.46	0.49
1:F:272:LEU:HD13	1:F:305:TYR:CD1	2.47	0.49
1:H:755:THR:HG22	1:H:794:VAL:HG12	1.94	0.49
1:I:343:LEU:CD1	1:I:346:LEU:HD21	2.43	0.49
2:P:1066:LEU:HG	2:P:1070:MET:HE2	1.95	0.49
1:D:280:TYR:CG	1:D:861:LEU:HD23	2.48	0.49
1:G:165:GLY:O	1:G:169:VAL:HG23	2.13	0.49
1:C:546:ARG:NH2	1:C:595:ILE:O	2.46	0.48
1:F:371:THR:HG22	1:F:371:THR:O	2.13	0.48
1:A:357:SER:O	1:A:361:GLN:N	2.43	0.48
1:B:315:LEU:HD13	1:B:672:LEU:HD11	1.94	0.48
1:F:180:VAL:O	1:F:184:MET:N	2.46	0.48
1:B:733:ASN:OD1	1:B:734:LEU:N	2.47	0.48
1:D:262:TYR:OH	1:D:687:ASP:OD2	2.23	0.48
1:H:124:LYS:NZ	1:H:182:THR:O	2.43	0.48
1:H:288:ASP:OD1	1:H:289:VAL:N	2.46	0.48
1:I:611:TYR:O	1:I:615:VAL:HG23	2.13	0.48
2:P:506:VAL:HG23	2:P:507:THR:HG23	1.95	0.48
1:E:885:ASN:OD1	1:E:886:GLU:N	2.47	0.48
1:I:326:ASP:OD2	1:I:579:THR:HG22	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:268:LEU:HD23	1:J:684:ARG:NH1	2.28	0.48
1:J:389:LEU:HD23	1:J:399:MET:HE1	1.94	0.48
1:A:882:ARG:NH1	1:J:527:THR:HG22	2.29	0.48
1:B:667:ASP:OD1	1:B:668:GLN:N	2.46	0.48
1:C:401:LEU:HD11	1:C:426:PHE:CD1	2.49	0.48
1:D:549:GLN:NE2	1:D:887:LEU:OXT	2.47	0.48
1:F:741:ASN:OD1	1:F:742:LEU:N	2.47	0.48
1:G:242:ASP:OD1	1:G:243:ARG:N	2.47	0.48
1:H:397:ARG:HH22	1:H:579:THR:HG23	1.77	0.48
1:H:667:ASP:OD1	1:H:668:GLN:N	2.47	0.48
2:P:542:LEU:HD11	2:P:561:TYR:HD2	1.78	0.48
1:E:733:ASN:OD1	1:E:734:LEU:N	2.47	0.48
1:A:221:ASP:O	1:A:229:ARG:NH2	2.47	0.48
1:E:428:ARG:O	1:E:432:VAL:HG23	2.14	0.48
1:G:467:GLU:OE2	1:G:480:HIS:ND1	2.44	0.48
1:B:755:THR:HG23	1:B:794:VAL:HG12	1.96	0.47
1:C:731:ALA:N	1:C:832:VAL:O	2.47	0.47
1:E:531:ASP:OD1	1:E:532:TYR:N	2.47	0.47
1:A:246:VAL:CG2	1:A:853:LEU:HD13	2.44	0.47
1:A:860:ASP:OD1	1:A:861:LEU:N	2.45	0.47
1:D:667:ASP:OD1	1:D:668:GLN:N	2.46	0.47
1:E:335:LEU:O	1:E:338:SER:OG	2.30	0.47
1:A:115:LEU:HD11	1:A:331:SER:OG	2.14	0.47
1:A:156:LYS:NZ	1:A:704:ASP:OD2	2.46	0.47
2:P:632:ASP:OD1	2:P:632:ASP:N	2.45	0.47
1:C:667:ASP:OD1	1:C:668:GLN:N	2.48	0.47
1:I:667:ASP:OD1	1:I:668:GLN:N	2.47	0.47
2:P:383:ASP:OD2	2:P:479:LYS:NZ	2.43	0.47
1:D:441:THR:HG23	1:D:442:ILE:HD12	1.96	0.47
1:E:799:VAL:HG23	1:E:799:VAL:O	2.15	0.47
1:H:275:ASP:OD1	1:H:276:ILE:N	2.47	0.47
1:B:627:ASP:OD1	1:B:685:ARG:NH2	2.47	0.47
1:J:531:ASP:OD1	1:J:532:TYR:N	2.48	0.47
1:C:315:LEU:O	1:C:675:ARG:NH1	2.46	0.47
1:I:488:ARG:O	1:I:499:VAL:HG22	2.14	0.47
1:F:755:THR:HG22	1:F:794:VAL:HG12	1.96	0.47
1:G:674:ASP:OD1	1:G:677:ARG:NH2	2.48	0.47
1:I:178:ASP:OD1	1:I:179:GLN:N	2.47	0.47
1:A:335:LEU:O	1:A:338:SER:OG	2.31	0.46
1:I:734:LEU:HD11	1:I:765:ALA:HB1	1.97	0.46
1:F:721:ARG:NH2	1:F:727:TYR:OH	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:577:THR:OG1	1:D:579:THR:O	2.32	0.46
2:P:261:PHE:O	2:P:507:THR:OG1	2.21	0.46
2:P:565:GLN:NE2	2:P:595:GLN:OE1	2.48	0.46
1:D:428:ARG:NH2	1:D:459:PRO:O	2.48	0.46
1:E:731:ALA:N	1:E:832:VAL:O	2.46	0.46
1:C:246:VAL:HG11	1:C:248:TYR:CE2	2.50	0.46
1:F:531:ASP:OD1	1:F:532:TYR:N	2.49	0.46
1:G:778:VAL:N	1:G:815:ASP:OD2	2.44	0.46
2:P:944:ILE:HD12	2:P:944:ILE:H	1.81	0.46
1:D:392:ALA:O	1:D:396:GLN:N	2.48	0.46
1:G:555:ARG:HB3	1:G:883:ILE:HG22	1.98	0.46
2:P:141:ASN:ND2	2:P:208:ASN:OD1	2.48	0.46
1:A:590:SER:O	1:A:594:LEU:N	2.47	0.46
1:B:505:ARG:NE	1:B:562:GLU:OE1	2.49	0.46
1:B:704:ASP:OD1	1:B:834:LYS:NZ	2.44	0.46
1:E:441:THR:HG23	1:E:442:ILE:HD12	1.98	0.46
1:G:632:ILE:HG23	1:G:645:MET:HE3	1.97	0.46
1:H:751:TYR:O	1:H:755:THR:HG23	2.14	0.46
2:P:156:VAL:HG23	2:P:156:VAL:O	2.15	0.46
1:B:751:TYR:O	1:B:755:THR:OG1	2.23	0.46
1:C:208:ASP:OD1	1:C:209:SER:N	2.48	0.46
2:P:843:ALA:HB3	2:P:844:PRO:HD3	1.97	0.46
1:A:646:LYS:NZ	1:A:666:ASP:OD1	2.43	0.46
1:B:785:LEU:O	1:B:788:THR:OG1	2.32	0.46
1:C:288:ASP:OD2	1:C:559:TYR:OH	2.34	0.46
1:C:682:GLU:OE2	1:C:685:ARG:NE	2.46	0.46
1:D:181:LEU:HD13	1:D:685:ARG:HH11	1.81	0.46
2:P:447:ILE:O	2:P:574:GLN:N	2.47	0.46
2:P:613:SER:OG	2:P:614:ARG:NH1	2.49	0.46
1:A:419:THR:HG21	1:A:478:TRP:HE1	1.81	0.45
1:H:792:GLN:NE2	1:H:801:THR:O	2.48	0.45
1:J:799:VAL:O	1:J:799:VAL:HG13	2.16	0.45
1:B:343:LEU:HD13	1:B:346:LEU:HD21	1.98	0.45
1:E:268:LEU:HD12	1:E:268:LEU:O	2.16	0.45
1:F:439:ILE:HD11	1:F:463:PHE:CD1	2.50	0.45
1:J:367:ILE:N	1:J:368:GLN:HA	2.31	0.45
2:P:268:GLU:C	2:P:269:LEU:HD12	2.41	0.45
2:P:779:ASP:OD1	2:P:879:ARG:NH2	2.50	0.45
2:P:908:GLN:O	2:P:912:GLN:N	2.46	0.45
1:C:441:THR:HG23	1:C:442:ILE:HD12	1.98	0.45
1:H:329:THR:HG23	1:H:395:SER:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ASP:OD1	1:A:209:SER:N	2.49	0.45
1:D:792:GLN:NE2	1:D:801:THR:O	2.49	0.45
1:G:786:ASP:OD1	1:G:787:ALA:N	2.49	0.45
1:J:298:ASN:OD1	1:J:299:LEU:N	2.50	0.45
1:J:514:MET:HG3	1:J:547:LEU:HD13	1.99	0.45
2:P:534:PHE:HZ	2:P:599:ALA:HB1	1.82	0.45
1:A:545:ASN:OD1	1:E:451:ARG:NH1	2.49	0.45
1:E:246:VAL:HG11	1:E:248:TYR:CE2	2.52	0.45
1:H:346:LEU:HD22	1:H:594:LEU:O	2.17	0.45
1:H:419:THR:O	1:H:485:ASN:ND2	2.50	0.45
1:J:419:THR:O	1:J:485:ASN:ND2	2.49	0.45
2:P:615:ILE:HD11	2:P:655:VAL:HG22	1.99	0.45
1:I:275:ASP:OD1	1:I:276:ILE:N	2.50	0.45
1:J:538:ARG:O	1:J:542:LEU:HD13	2.16	0.45
1:B:311:LEU:O	1:B:622:ASN:ND2	2.50	0.45
1:D:201:ARG:NH2	1:H:748:THR:HG23	2.32	0.45
1:D:682:GLU:OE2	1:D:685:ARG:NE	2.49	0.45
1:F:419:THR:O	1:F:485:ASN:ND2	2.50	0.45
1:B:272:LEU:HD11	1:B:861:LEU:HD11	1.98	0.45
1:D:237:GLN:OE1	1:D:239:VAL:HG13	2.17	0.45
1:F:505:ARG:NH2	1:F:562:GLU:OE1	2.49	0.45
1:I:627:ASP:OD1	1:I:685:ARG:NE	2.50	0.45
1:J:727:TYR:HD2	1:J:809:ILE:HD11	1.80	0.45
2:P:469:TYR:HD1	2:P:564:THR:HG23	1.81	0.45
1:C:400:SER:C	1:C:401:LEU:HD12	2.42	0.44
1:E:377:ILE:O	1:E:377:ILE:HG22	2.16	0.44
1:H:333:TYR:OH	1:H:388:THR:HG23	2.17	0.44
1:J:756:ASN:OD1	1:J:760:ASN:ND2	2.50	0.44
1:C:728:VAL:HG23	1:C:730:ILE:HG22	1.99	0.44
1:D:134:GLU:OE1	1:D:158:LYS:N	2.50	0.44
1:F:717:MET:N	1:F:828:SER:O	2.50	0.44
1:J:553:LEU:HD13	1:J:595:ILE:HD13	2.00	0.44
1:J:667:ASP:OD1	1:J:668:GLN:N	2.50	0.44
1:A:881:MET:HE3	1:E:455:ARG:NH2	2.33	0.44
1:E:649:VAL:HG13	1:E:672:LEU:HD23	2.00	0.44
1:F:667:ASP:OD1	1:F:668:GLN:N	2.50	0.44
1:E:262:TYR:OH	1:E:687:ASP:OD2	2.23	0.44
1:I:755:THR:HG22	1:I:794:VAL:HG12	2.00	0.44
1:A:654:LYS:HG2	1:A:661:ILE:HD13	1.99	0.44
1:A:654:LYS:CG	1:A:661:ILE:HD13	2.48	0.44
1:G:799:VAL:HG13	1:G:799:VAL:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:316:ASN:O	1:J:675:ARG:NH1	2.50	0.44
1:B:437:ALA:O	1:B:441:THR:HG22	2.18	0.44
1:F:178:ASP:OD1	1:F:179:GLN:N	2.50	0.44
1:H:799:VAL:O	1:H:799:VAL:HG13	2.18	0.44
1:B:270:GLU:OE1	1:B:307:ARG:NH2	2.50	0.44
1:C:280:TYR:CG	1:C:861:LEU:HD23	2.53	0.44
1:C:611:TYR:O	1:C:615:VAL:HG23	2.17	0.44
1:I:138:LEU:HD13	1:I:724:MET:HE1	2.00	0.44
1:G:851:SER:OG	1:G:852:ASN:N	2.51	0.44
1:C:270:GLU:OE1	1:C:307:ARG:NH2	2.50	0.44
1:C:314:ARG:HB3	1:C:679:LEU:HD21	2.00	0.44
2:P:469:TYR:CD1	2:P:564:THR:HG23	2.53	0.44
1:B:415:MET:HE1	1:B:442:ILE:HG21	1.98	0.43
1:H:713:ALA:O	1:H:715:ARG:N	2.50	0.43
1:I:444:TYR:CE1	1:I:470:ILE:HD11	2.53	0.43
2:P:268:GLU:O	2:P:269:LEU:HD12	2.17	0.43
2:P:303:ILE:HG23	2:P:304:PRO:HD3	1.99	0.43
2:P:776:GLY:N	2:P:875:ASN:OD1	2.45	0.43
1:A:371:THR:O	1:A:373:PHE:N	2.51	0.43
1:A:661:ILE:HD12	1:A:661:ILE:H	1.82	0.43
1:A:791:ALA:O	1:A:794:VAL:HG22	2.18	0.43
1:B:346:LEU:HD22	1:B:594:LEU:O	2.17	0.43
1:C:377:ILE:O	1:C:377:ILE:HG22	2.18	0.43
1:E:180:VAL:O	1:E:184:MET:N	2.49	0.43
1:E:270:GLU:OE1	1:E:307:ARG:NH2	2.51	0.43
1:E:419:THR:O	1:E:485:ASN:ND2	2.51	0.43
1:E:664:VAL:HG13	1:E:669:MET:HE3	2.01	0.43
1:F:275:ASP:OD1	1:F:276:ILE:N	2.51	0.43
1:D:424:ASP:OD1	1:D:576:GLN:NE2	2.51	0.43
1:I:511:ASN:OD1	1:I:547:LEU:HD11	2.18	0.43
2:P:238:SER:O	2:P:335:ARG:NH1	2.52	0.43
1:G:326:ASP:OD2	1:G:579:THR:HG22	2.18	0.43
1:J:359:ASP:OD2	1:J:542:LEU:HD11	2.19	0.43
1:J:734:LEU:HD11	1:J:765:ALA:HB1	2.01	0.43
1:C:142:ARG:NE	1:C:148:GLU:OE2	2.52	0.43
1:G:420:VAL:HG23	1:G:421:VAL:HG23	2.01	0.43
1:H:818:LEU:O	1:H:824:TRP:NE1	2.44	0.43
1:D:123:VAL:HG23	1:D:123:VAL:O	2.19	0.43
1:D:641:TYR:O	1:I:882:ARG:NH1	2.52	0.43
1:D:868:ASP:OD2	1:H:405:THR:HG22	2.19	0.43
1:F:514:MET:HG3	1:F:547:LEU:HD13	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:691:LEU:O	1:F:695:ASN:ND2	2.52	0.43
1:J:734:LEU:HD21	1:J:767:VAL:CG1	2.49	0.43
1:F:268:LEU:HD23	1:F:684:ARG:NH1	2.34	0.43
1:F:799:VAL:HG13	1:F:799:VAL:O	2.19	0.43
1:G:210:GLU:OE1	1:G:210:GLU:N	2.52	0.43
1:G:744:GLU:N	1:G:744:GLU:OE1	2.52	0.43
1:H:246:VAL:HG11	1:H:853:LEU:HD21	2.00	0.43
1:I:799:VAL:HG13	1:I:799:VAL:O	2.18	0.43
1:E:584:GLN:O	1:E:587:SER:OG	2.32	0.43
1:I:717:MET:HE1	1:I:831:LYS:HE2	2.01	0.43
1:A:437:ALA:O	1:A:441:THR:HG22	2.19	0.42
1:B:343:LEU:CD1	1:B:346:LEU:HD21	2.48	0.42
1:D:741:ASN:OD1	1:D:742:LEU:N	2.50	0.42
1:H:624:ARG:NH2	1:H:627:ASP:OD2	2.48	0.42
1:I:366:THR:HG22	1:I:366:THR:O	2.18	0.42
2:P:691:ALA:HB2	2:P:723:ARG:HB2	2.00	0.42
1:D:412:ILE:HG22	1:D:543:LEU:HD22	2.00	0.42
1:F:650:GLU:HB2	1:F:661:ILE:HG21	2.02	0.42
1:G:415:MET:SD	1:G:517:LEU:HD21	2.59	0.42
1:A:792:GLN:NE2	1:A:801:THR:O	2.47	0.42
1:F:366:THR:HG22	1:F:366:THR:O	2.19	0.42
2:P:691:ALA:HB2	2:P:723:ARG:CB	2.49	0.42
1:C:713:ALA:O	1:C:715:ARG:N	2.50	0.42
1:H:446:ALA:HB1	1:H:523:GLN:OE1	2.20	0.42
1:I:453:HIS:O	1:I:455:ARG:NH1	2.51	0.42
1:H:683:ILE:HD12	1:H:683:ILE:H	1.83	0.42
2:P:671:SER:OG	2:P:672:THR:N	2.52	0.42
1:A:109:GLU:O	2:P:258:ASN:ND2	2.50	0.42
1:D:180:VAL:O	1:D:184:MET:N	2.51	0.42
1:I:531:ASP:OD1	1:I:532:TYR:N	2.53	0.42
1:B:441:THR:OG1	1:B:532:TYR:OH	2.02	0.42
1:D:733:ASN:OD1	1:D:734:LEU:N	2.52	0.42
1:G:683:ILE:HD12	1:G:683:ILE:H	1.85	0.42
1:J:713:ALA:O	1:J:715:ARG:N	2.49	0.42
2:P:473:GLN:O	2:P:477:VAL:HG23	2.20	0.42
1:B:728:VAL:HG23	1:B:730:ILE:HG22	2.02	0.42
1:D:134:GLU:OE1	1:D:134:GLU:N	2.53	0.42
1:G:268:LEU:O	1:G:268:LEU:HD12	2.20	0.42
1:H:299:LEU:HD21	1:H:864:PHE:CE1	2.55	0.42
2:P:335:ARG:O	2:P:337:GLN:N	2.52	0.42
2:P:551:ASP:OD1	2:P:552:ALA:N	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:728:VAL:HG23	1:A:730:ILE:HG22	2.02	0.42
1:E:546:ARG:NH2	1:E:595:ILE:O	2.50	0.42
1:H:246:VAL:CG1	1:H:853:LEU:HD21	2.50	0.42
2:P:823:LYS:HB2	2:P:827:VAL:HG22	2.02	0.42
2:P:894:ILE:HG23	2:P:912:GLN:HG2	2.02	0.42
2:P:134:ILE:HG12	2:P:136:THR:HG22	2.02	0.42
2:P:534:PHE:CE1	2:P:603:ALA:HB2	2.54	0.42
1:B:335:LEU:O	1:B:338:SER:OG	2.34	0.41
1:D:523:GLN:O	1:D:533:LYS:NZ	2.53	0.41
1:G:627:ASP:OD1	1:G:685:ARG:NE	2.47	0.41
1:C:366:THR:O	1:D:86:LYS:NZ	2.48	0.41
1:D:377:ILE:HG22	1:D:377:ILE:O	2.18	0.41
1:F:609:HIS:O	1:F:613:VAL:HG23	2.20	0.41
1:H:383:ASN:OD1	1:H:384:ASP:N	2.53	0.41
1:C:389:LEU:HD23	1:C:399:MET:HE1	2.02	0.41
1:C:860:ASP:OD1	1:C:861:LEU:N	2.51	0.41
1:C:783:ALA:HB3	1:C:785:LEU:CD1	2.50	0.41
1:D:101:THR:HG22	1:D:103:PRO:HD3	2.02	0.41
1:F:415:MET:SD	1:F:517:LEU:HD21	2.60	0.41
1:F:645:MET:HE1	1:F:677:ARG:HD3	2.02	0.41
1:H:298:ASN:OD1	1:H:299:LEU:N	2.54	0.41
1:B:142:ARG:NE	1:B:148:GLU:OE2	2.53	0.41
1:F:439:ILE:HD11	1:F:463:PHE:HD1	1.84	0.41
1:G:649:VAL:CG1	1:G:672:LEU:HD23	2.50	0.41
2:P:1029:VAL:HG11	2:P:1063:MET:SD	2.60	0.41
1:A:868:ASP:OD2	1:J:405:THR:HG22	2.19	0.41
1:C:741:ASN:OD1	1:C:742:LEU:N	2.52	0.41
1:F:467:GLU:OE2	1:F:480:HIS:ND1	2.47	0.41
1:H:786:ASP:OD2	1:H:828:SER:OG	2.38	0.41
1:I:346:LEU:HD22	1:I:594:LEU:O	2.21	0.41
1:J:189:LEU:HD21	1:J:855:PHE:CE1	2.55	0.41
1:D:315:LEU:O	1:D:675:ARG:NH1	2.47	0.41
1:D:860:ASP:OD1	1:D:861:LEU:N	2.51	0.41
1:E:403:PHE:CB	1:E:585:LEU:HD12	2.50	0.41
1:H:611:TYR:O	1:H:615:VAL:HG23	2.21	0.41
1:H:744:GLU:OE1	1:H:744:GLU:N	2.54	0.41
1:J:232:ILE:HA	1:J:235:MET:HE2	2.02	0.41
1:J:517:LEU:HD22	1:J:540:ILE:HG23	2.03	0.41
1:B:455:ARG:HH22	1:C:881:MET:HE3	1.86	0.41
1:B:711:ILE:O	1:B:830:THR:HG23	2.21	0.41
1:B:741:ASN:OD1	1:B:742:LEU:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:786:ASP:OD1	1:E:805:ILE:N	2.50	0.41
1:F:295:MET:HE1	1:F:865:VAL:HG22	2.03	0.41
1:I:383:ASN:OD1	1:I:384:ASP:N	2.54	0.41
1:I:717:MET:O	1:I:828:SER:N	2.52	0.41
1:A:881:MET:HE3	1:E:455:ARG:HH22	1.86	0.40
1:D:284:ARG:HH21	1:D:492:ILE:HG21	1.85	0.40
1:J:519:GLN:OE1	1:J:522:ARG:NH2	2.54	0.40
2:P:331:HIS:NE2	2:P:691:ALA:O	2.51	0.40
2:P:385:LEU:HD23	2:P:479:LYS:HE2	2.04	0.40
1:J:428:ARG:O	1:J:432:VAL:HG23	2.21	0.40
1:J:728:VAL:HG23	1:J:730:ILE:HG22	2.02	0.40
1:B:713:ALA:HB3	1:B:717:MET:HE2	2.03	0.40
1:A:514:MET:CG	1:A:547:LEU:HD13	2.51	0.40
1:C:514:MET:CG	1:C:547:LEU:HD13	2.48	0.40
1:F:627:ASP:OD1	1:F:685:ARG:NE	2.54	0.40
1:F:719:LEU:HD22	1:F:728:VAL:C	2.45	0.40
1:I:731:ALA:N	1:I:832:VAL:O	2.48	0.40
1:J:786:ASP:OD1	1:J:787:ALA:N	2.54	0.40
2:P:102:LEU:O	2:P:111:ASN:ND2	2.55	0.40
2:P:754:GLU:O	2:P:758:THR:OG1	2.22	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	779/887 (88%)	713 (92%)	66 (8%)	0	100	100
1	B	779/887 (88%)	713 (92%)	66 (8%)	0	100	100
1	C	778/887 (88%)	705 (91%)	73 (9%)	0	100	100
1	D	825/887 (93%)	751 (91%)	73 (9%)	1 (0%)	48	75

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	793/887 (89%)	724 (91%)	69 (9%)	0	100	100
1	F	800/887 (90%)	713 (89%)	87 (11%)	0	100	100
1	G	800/887 (90%)	723 (90%)	77 (10%)	0	100	100
1	H	800/887 (90%)	716 (90%)	83 (10%)	1 (0%)	48	75
1	I	798/887 (90%)	725 (91%)	72 (9%)	1 (0%)	48	75
1	J	814/887 (92%)	736 (90%)	78 (10%)	0	100	100
2	P	1084/1088 (100%)	986 (91%)	97 (9%)	1 (0%)	48	75
All	All	9050/9958 (91%)	8205 (91%)	841 (9%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	942	PRO
1	H	107	PRO
1	D	103	PRO
1	I	107	PRO

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	717/818 (88%)	717 (100%)	0	100	100
1	B	717/818 (88%)	717 (100%)	0	100	100
1	C	716/818 (88%)	716 (100%)	0	100	100
1	D	762/818 (93%)	762 (100%)	0	100	100
1	E	731/818 (89%)	731 (100%)	0	100	100
1	F	738/818 (90%)	738 (100%)	0	100	100
1	G	738/818 (90%)	737 (100%)	1 (0%)	88	90
1	H	738/818 (90%)	738 (100%)	0	100	100
1	I	736/818 (90%)	736 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	752/818 (92%)	752 (100%)	0	100	100
2	P	986/989 (100%)	986 (100%)	0	100	100
All	All	8331/9169 (91%)	8330 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	268	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	HIS
1	A	274	ASN
1	A	464	GLN
1	A	847	HIS
1	B	266	HIS
1	C	267	GLN
1	C	847	HIS
1	D	94	GLN
1	D	298	ASN
1	D	318	HIS
1	D	407	ASN
1	E	253	HIS
1	E	874	ASN
1	F	274	ASN
1	F	508	HIS
1	F	605	GLN
1	F	695	ASN
1	G	294	ASN
1	G	616	ASN
1	H	257	HIS
1	H	294	ASN
1	H	318	HIS
1	H	453	HIS
1	H	508	HIS
1	I	407	ASN
1	J	523	GLN
1	J	792	GLN
2	P	51	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	111	ASN
2	P	152	HIS
2	P	563	GLN
2	P	638	GLN
2	P	1044	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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.

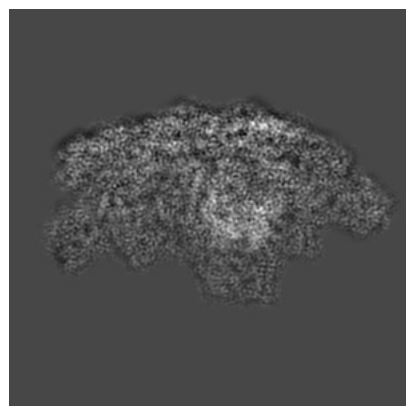
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20087. These allow visual inspection of the internal detail of the map and identification of artifacts.

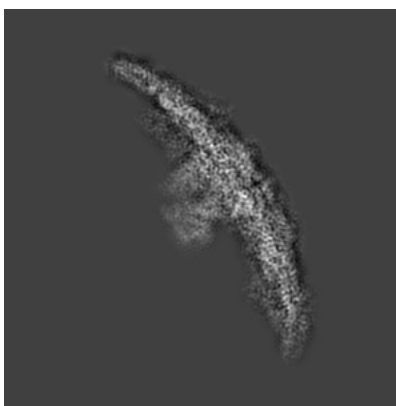
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

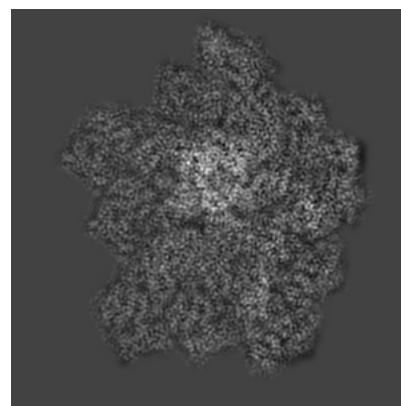
6.1.1 Primary map



X

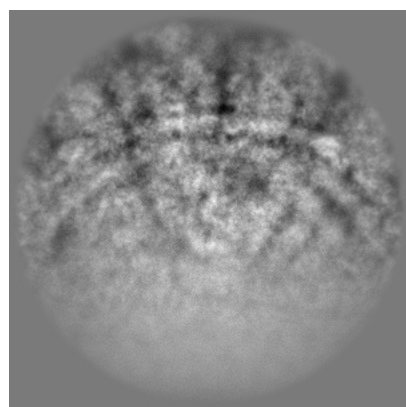


Y

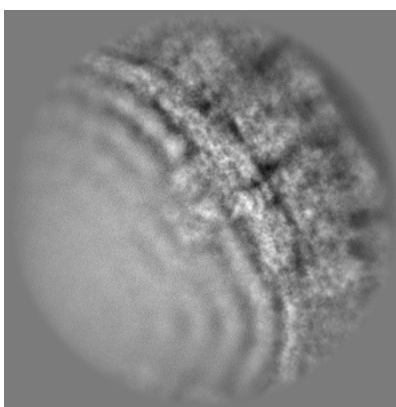


Z

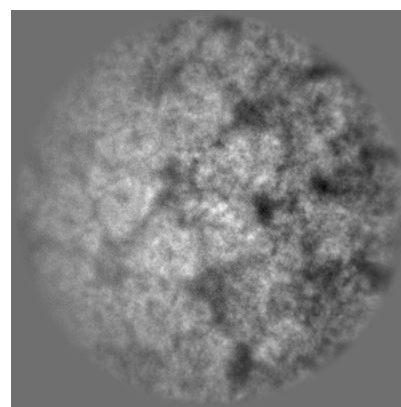
6.1.2 Raw map



X



Y

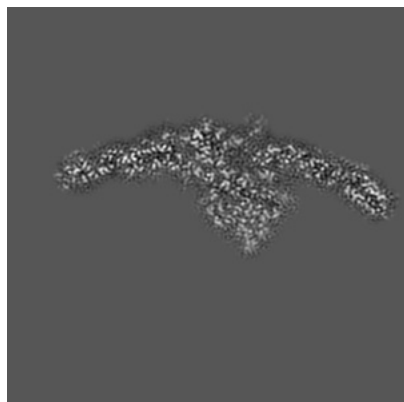


Z

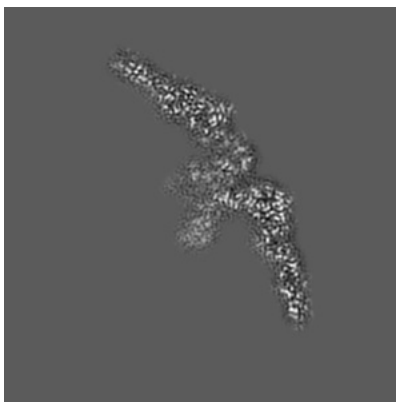
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

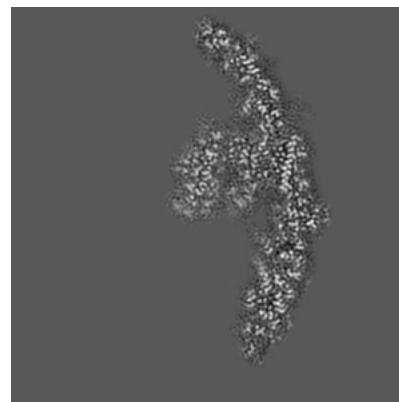
6.2.1 Primary map



X Index: 176

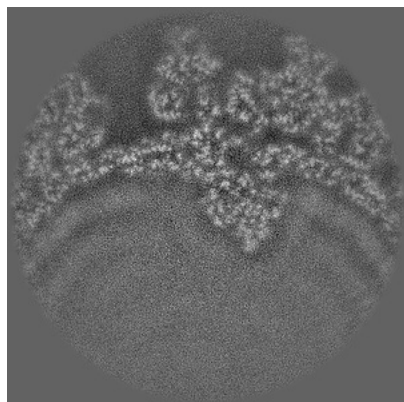


Y Index: 176

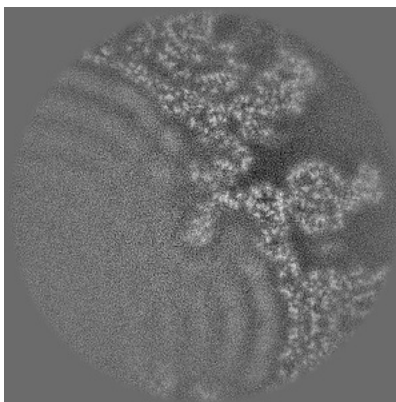


Z Index: 176

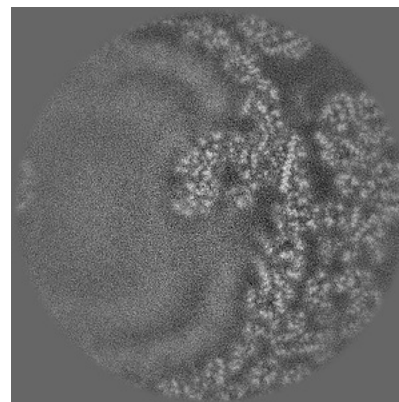
6.2.2 Raw map



X Index: 176



Y Index: 176



Z Index: 176

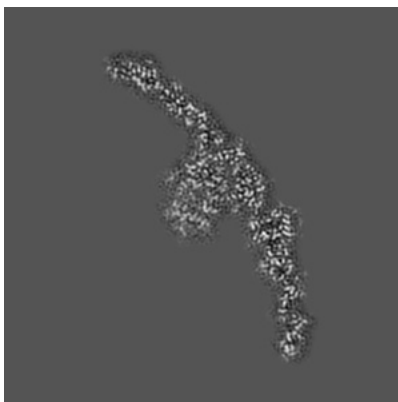
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 174

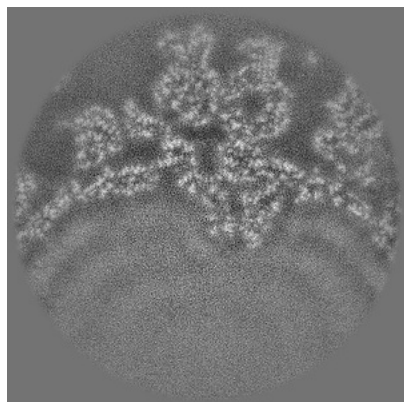


Y Index: 222

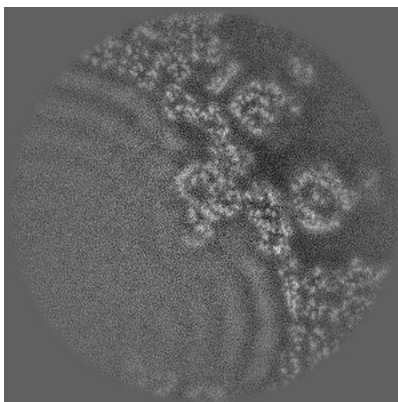


Z Index: 233

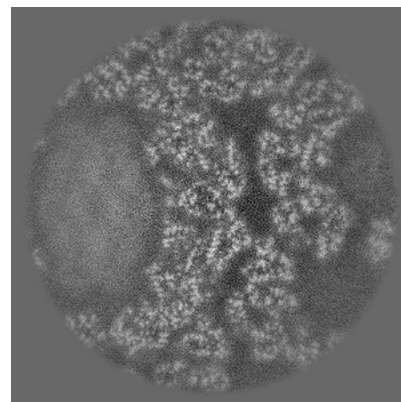
6.3.2 Raw map



X Index: 199



Y Index: 181

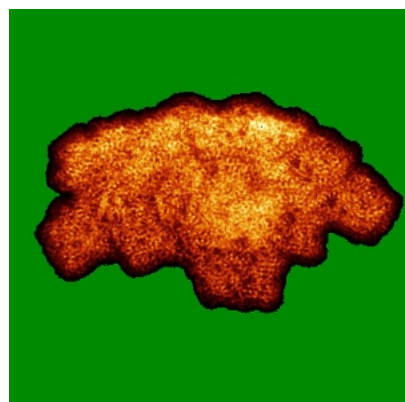


Z Index: 228

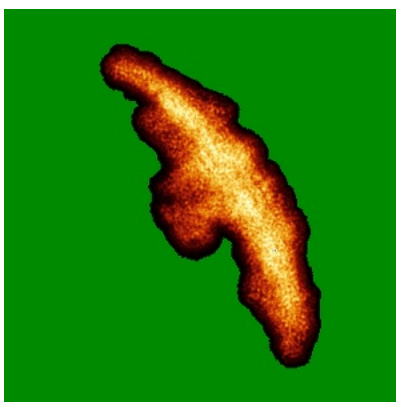
The images above show the largest variance slices of the map in three orthogonal directions.

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

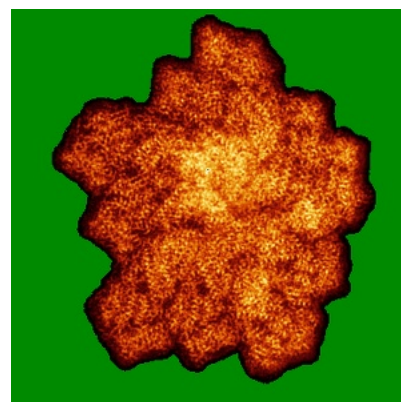
6.4.1 Primary map



X

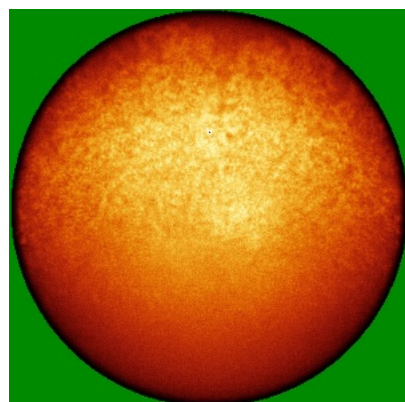


Y

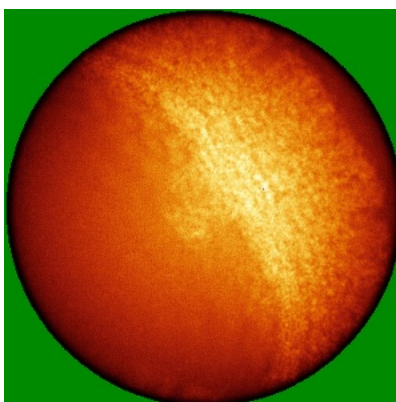


Z

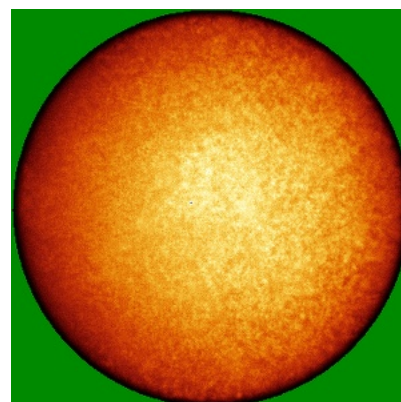
6.4.2 Raw map



X



Y

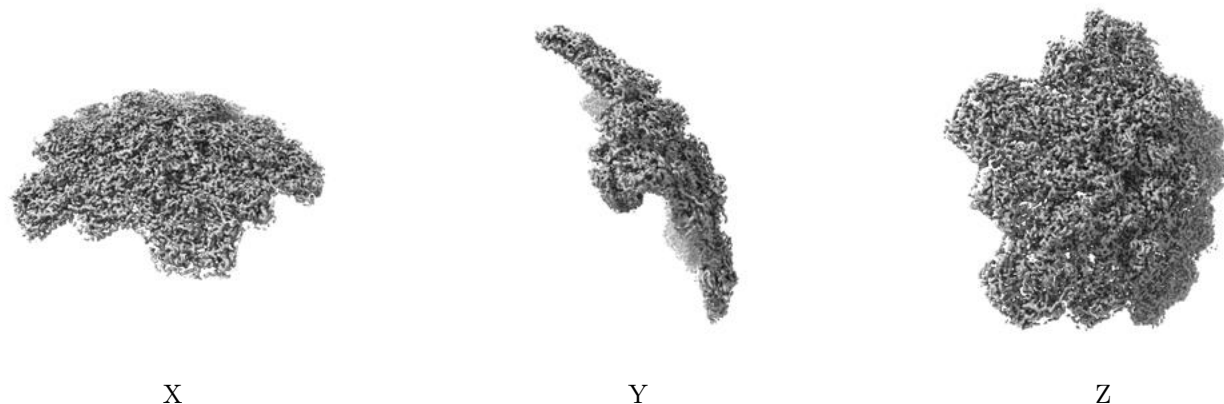


Z

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

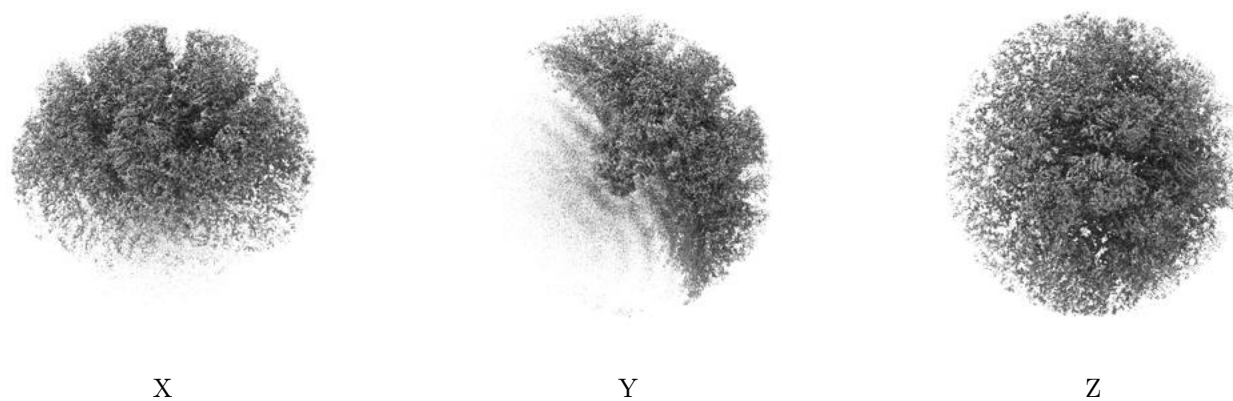
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

6.6 Mask visualisation [i](#)

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

A mask typically either:

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

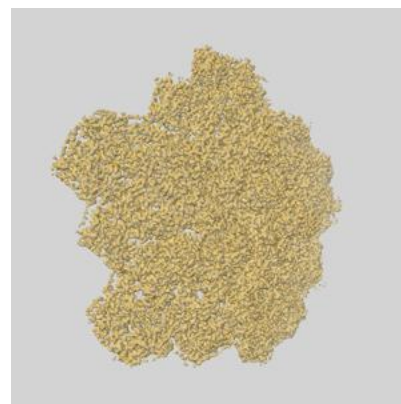
6.6.1 emd_20087_msk_1.map [i](#)



X



Y

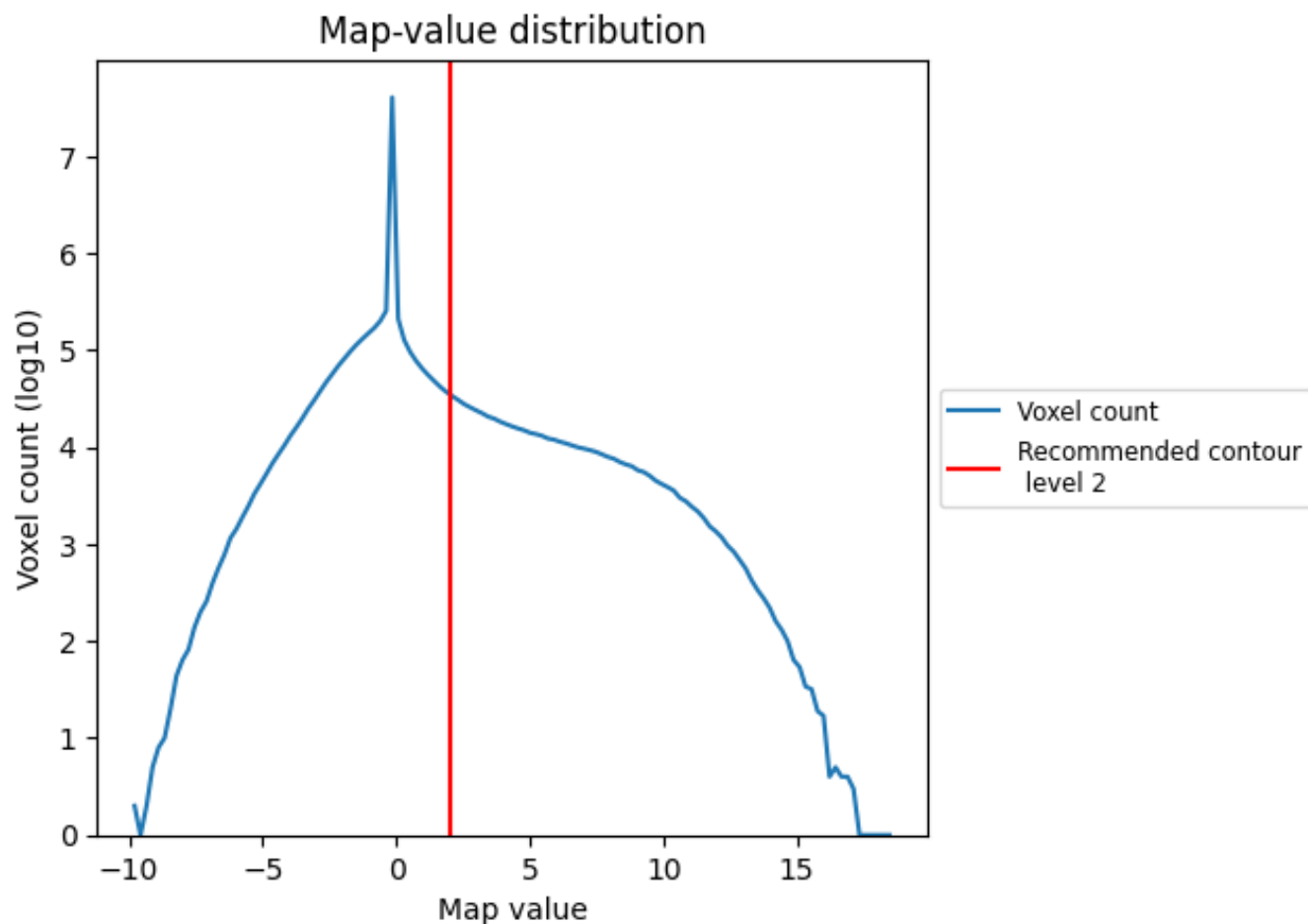


Z

7 Map analysis [i](#)

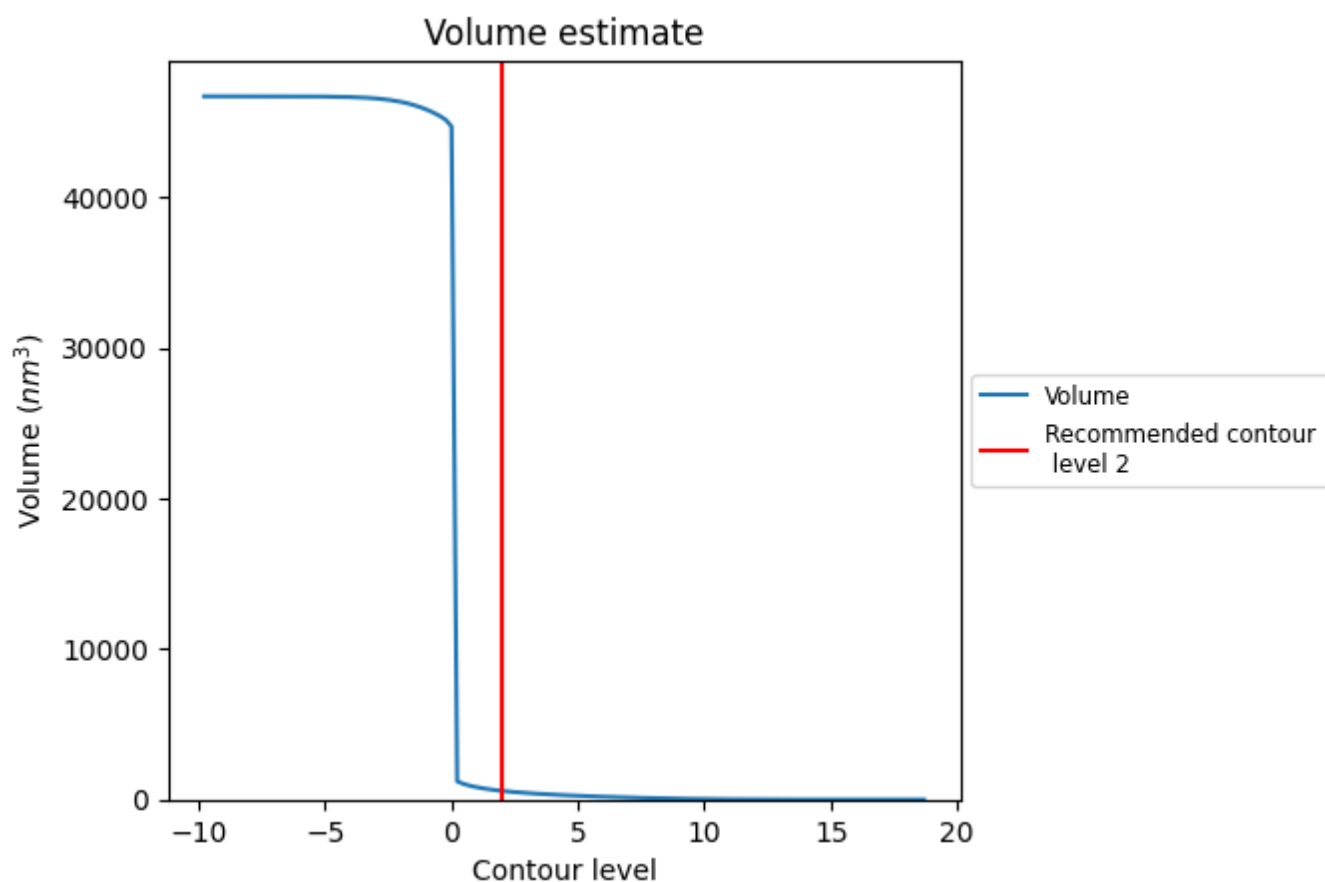
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

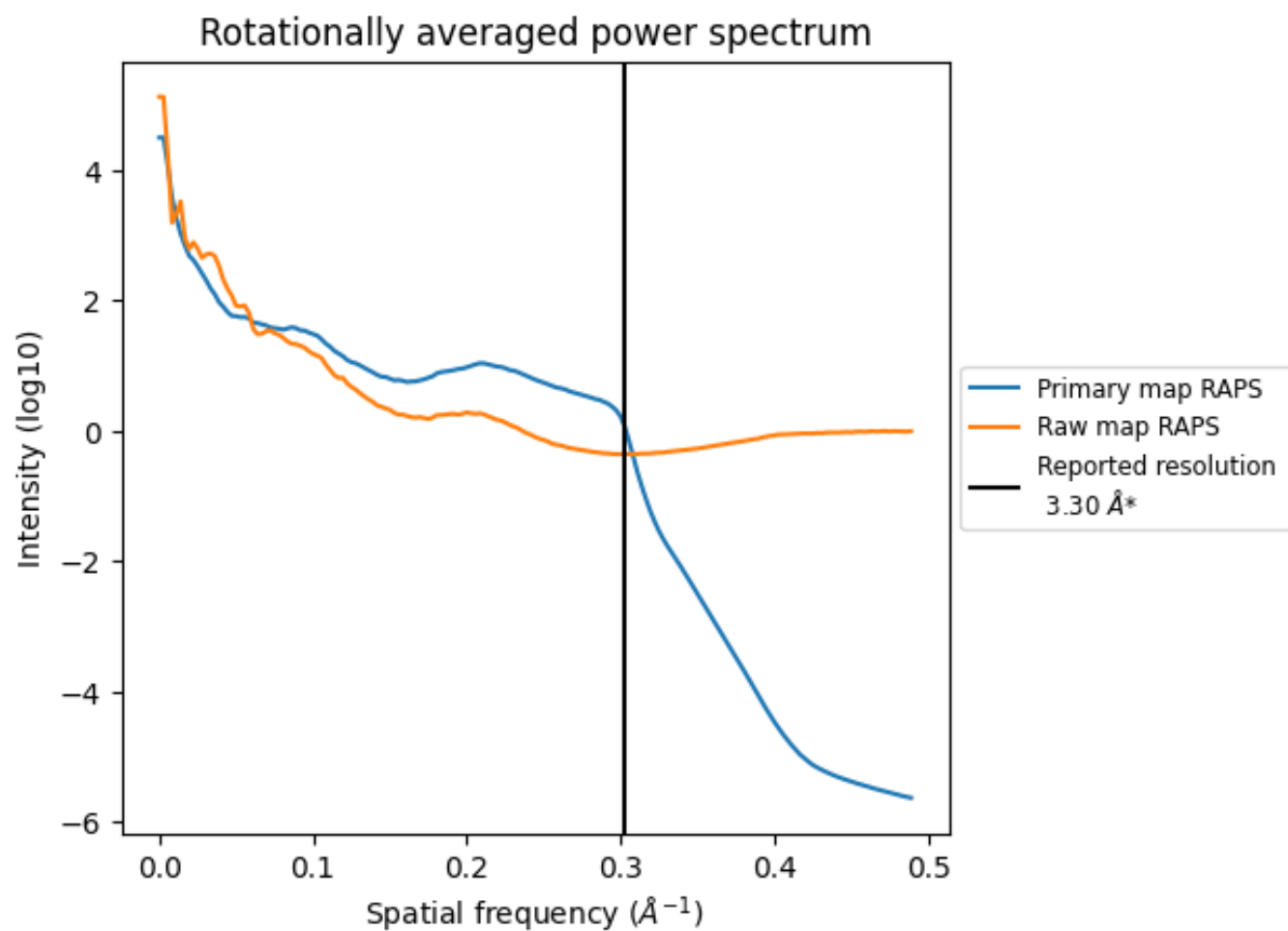
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 575 nm³; this corresponds to an approximate mass of 520 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 ⓘ

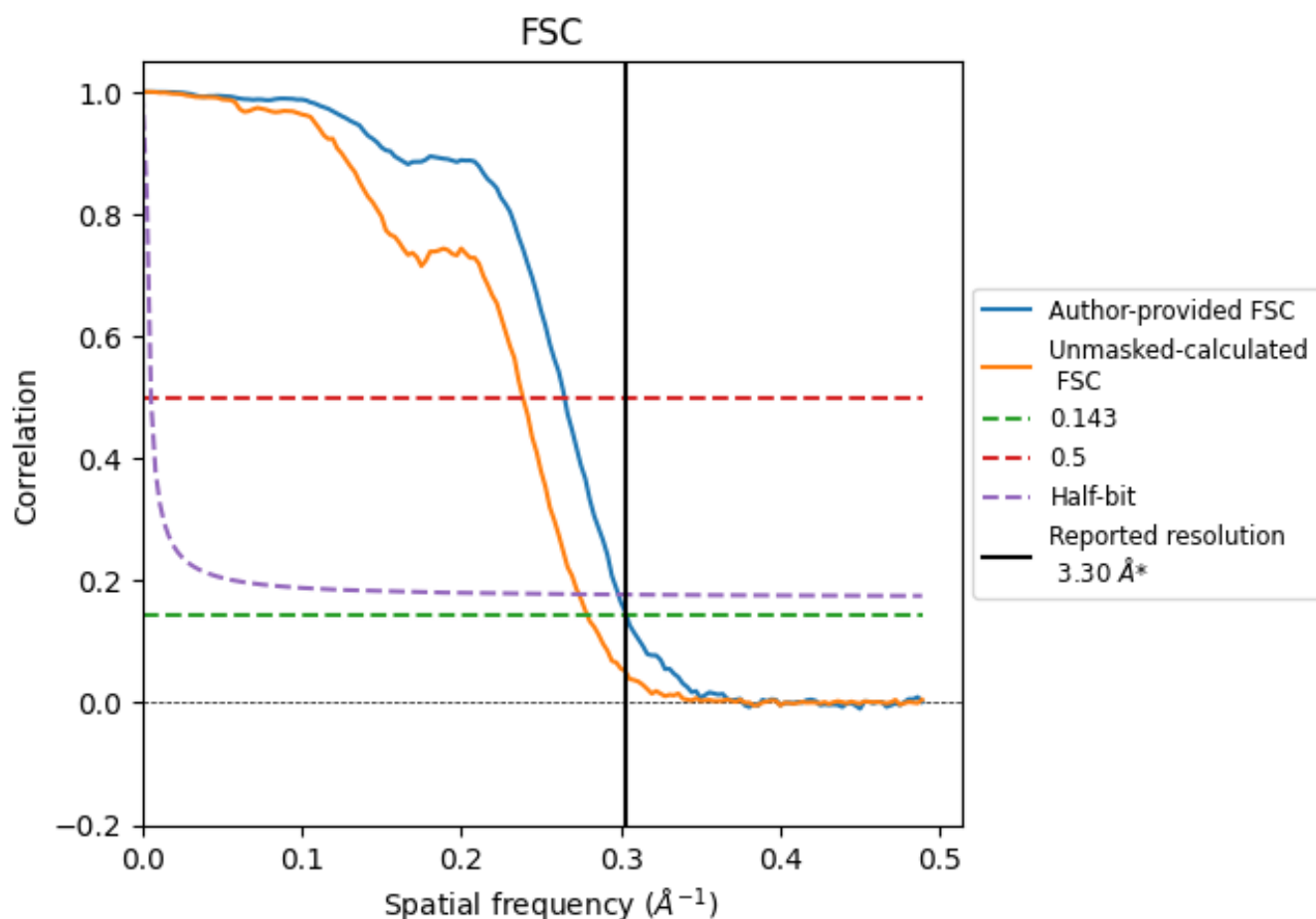


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.29	3.78	3.35
Unmasked-calculated*	3.59	4.19	3.65

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

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20087 and PDB model 6OJ4. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

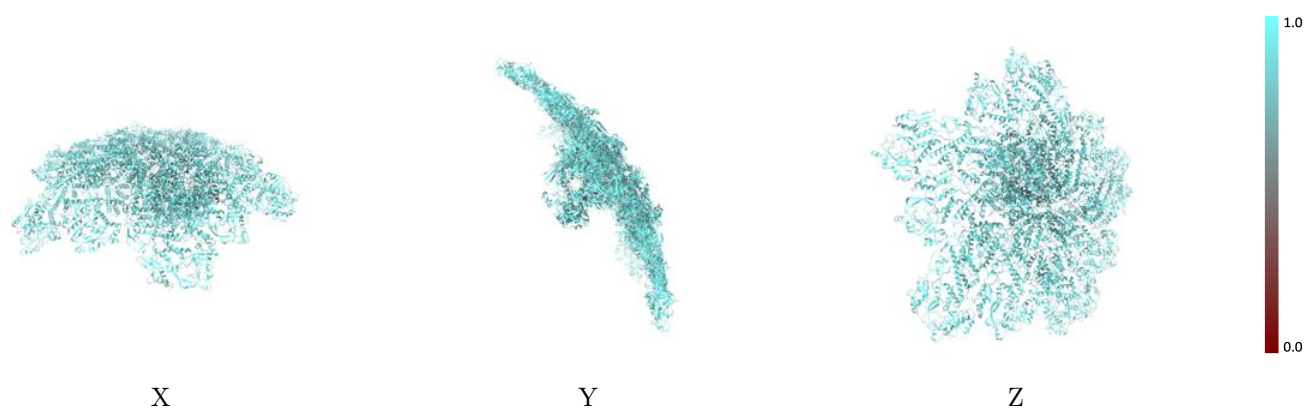
This section was not generated.

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



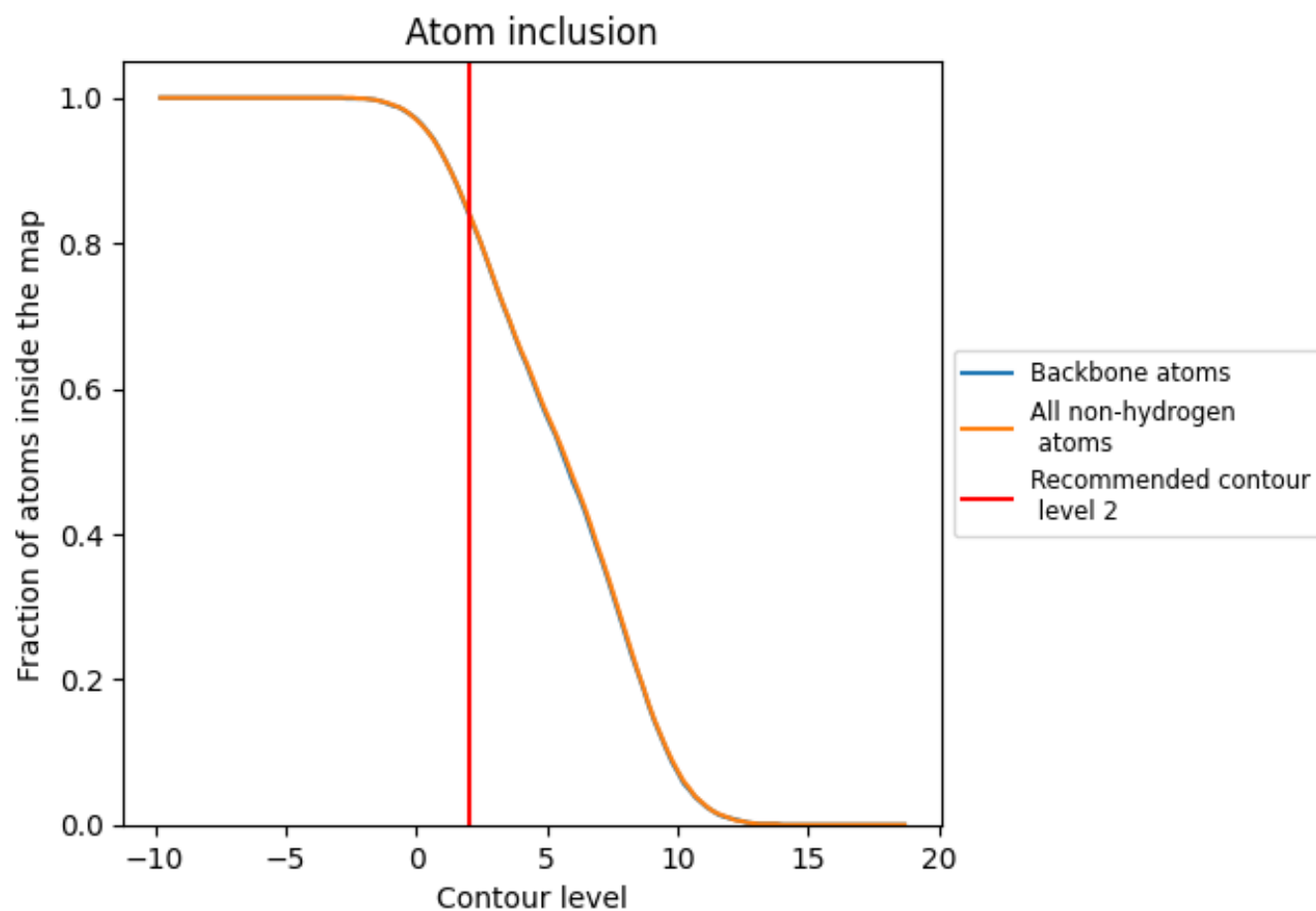
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 84% 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 (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8430	0.5080
A	0.8470	0.5160
B	0.8530	0.5110
C	0.8570	0.5130
D	0.8350	0.5060
E	0.8510	0.5120
F	0.8600	0.5200
G	0.8530	0.5120
H	0.8470	0.5130
I	0.8420	0.5100
J	0.8390	0.5070
P	0.8490	0.4750

1.0

0.0

<0.0