



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:38 AM UTC

PDB ID : 6OGY / pdb_00006ogy
EMDB ID : EMD-20059
Title : In situ structure of Rotavirus RNA-dependent RNA polymerase at duplex-open state
Authors : Ding, K.; Chang, T.; Shen, W.; Roy, P.; Zhou, Z.H.
Deposited on : 2019-04-03
Resolution : 3.40 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:

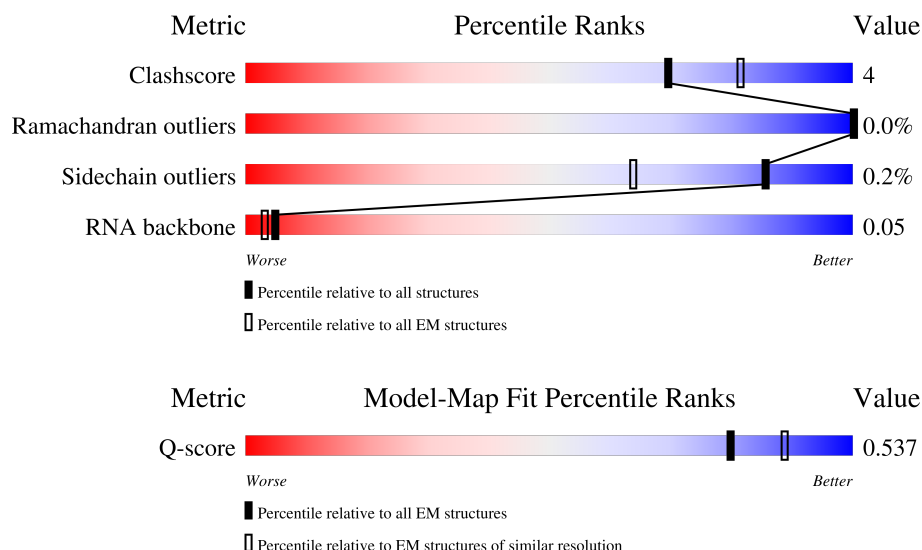
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
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 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



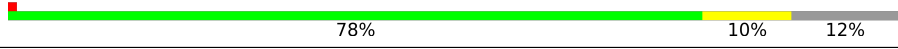
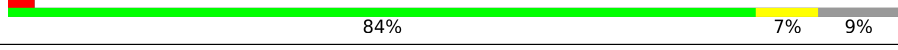
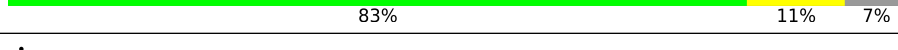
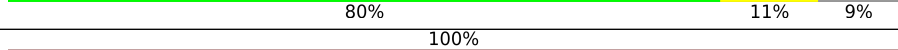
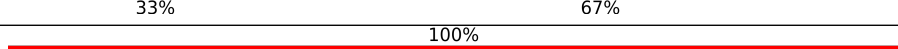
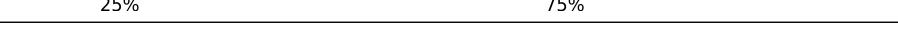
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	1088	
2	C	887	
2	D	887	

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Mol	Chain	Length	Quality of chain
2	E	887	
2	F	887	
2	G	887	
2	H	887	
2	I	887	
2	J	887	
2	K	887	
2	L	887	
3	M	3	
4	N	4	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 74364 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 RNA-dependent RNA polymerase of rotavirus A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1053	Total	C	N	O	S	0	0
			8523	5464	1411	1611	37		

- Molecule 2 is a protein called Inner capsid protein VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	794	Total	C	N	O	S	0	0
			6492	4127	1117	1212	36		
2	D	815	Total	C	N	O	S	0	0
			6670	4238	1147	1249	36		
2	E	781	Total	C	N	O	S	0	0
			6379	4052	1101	1190	36		
2	F	805	Total	C	N	O	S	0	0
			6587	4186	1134	1231	36		
2	G	781	Total	C	N	O	S	0	0
			6379	4052	1101	1190	36		
2	H	805	Total	C	N	O	S	0	0
			6587	4186	1134	1231	36		
2	I	810	Total	C	N	O	S	0	0
			6628	4213	1140	1239	36		
2	J	805	Total	C	N	O	S	0	0
			6587	4186	1134	1231	36		
2	K	827	Total	C	N	O	S	0	0
			6765	4297	1163	1269	36		
2	L	805	Total	C	N	O	S	0	0
			6587	4186	1134	1231	36		

- Molecule 3 is DNA/RNA hybrid called DNA/RNA (5'-D(*(GTG))-R(P*GP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	3	Total	C	N	O	P	0	0
			95	40	18	32	5		

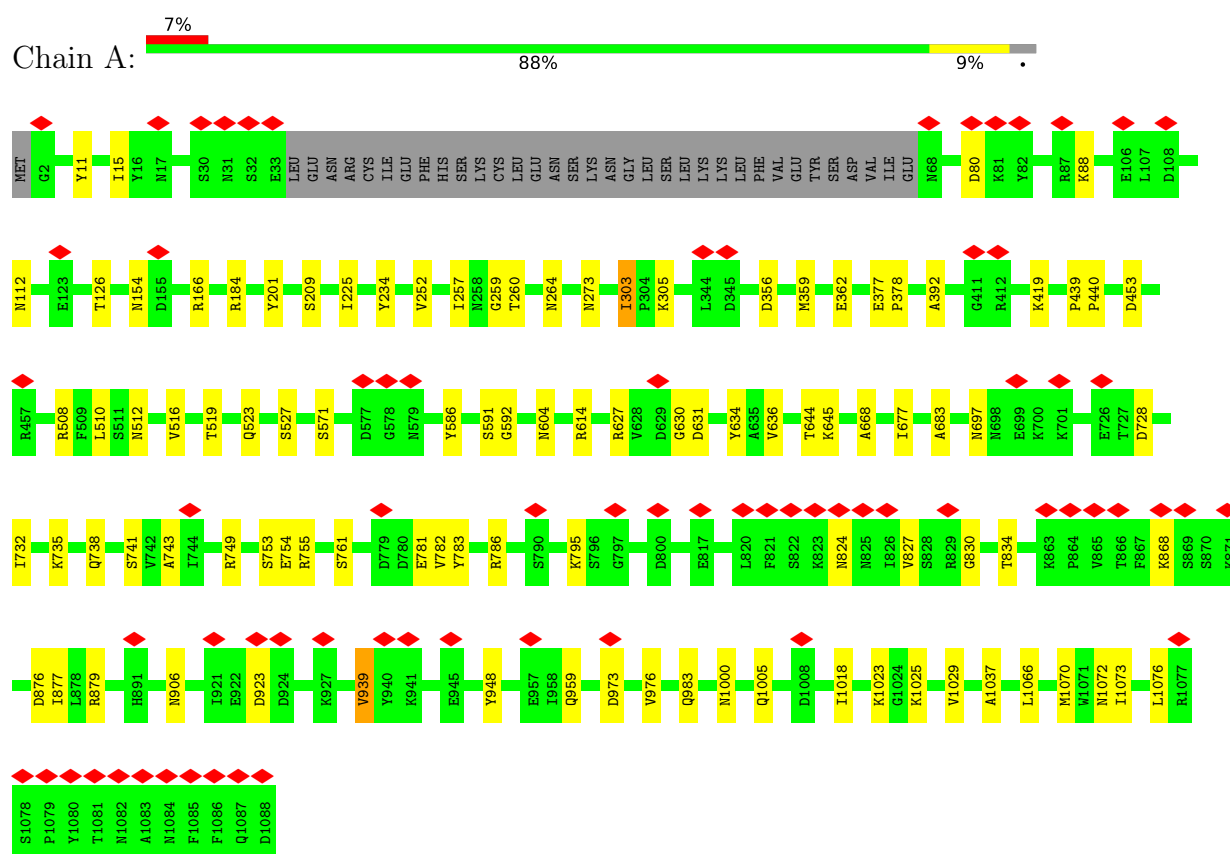
- Molecule 4 is a RNA chain called RNA (5'-R(P*AP*GP*CP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	4	Total	C	N	O	P	0	0
			85	38	16	27	4		

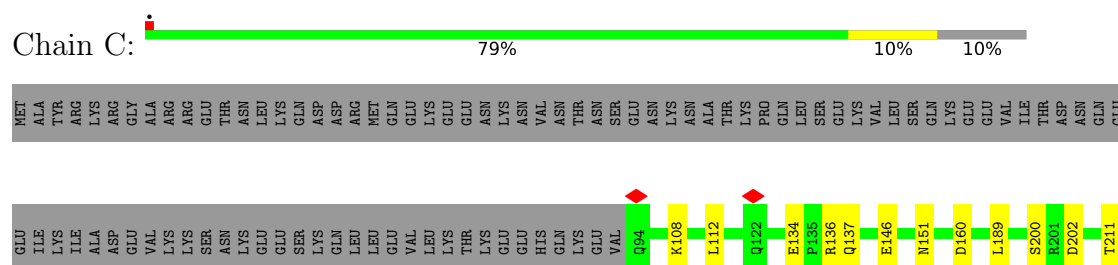
3 Residue-property plots

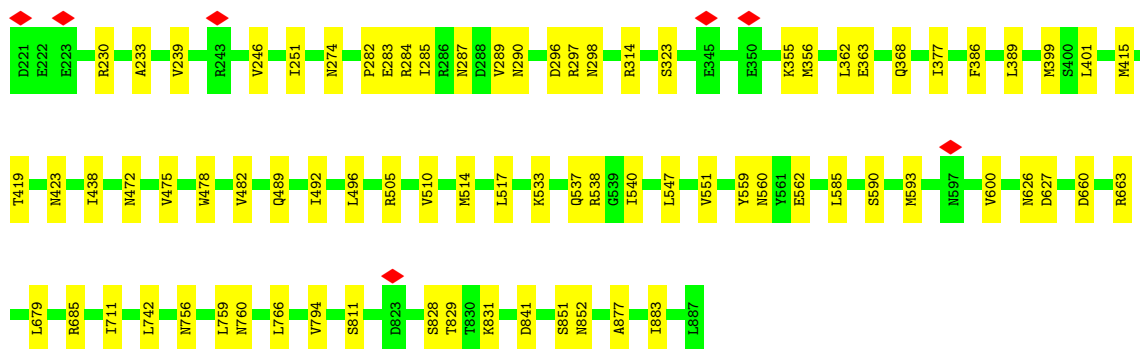
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



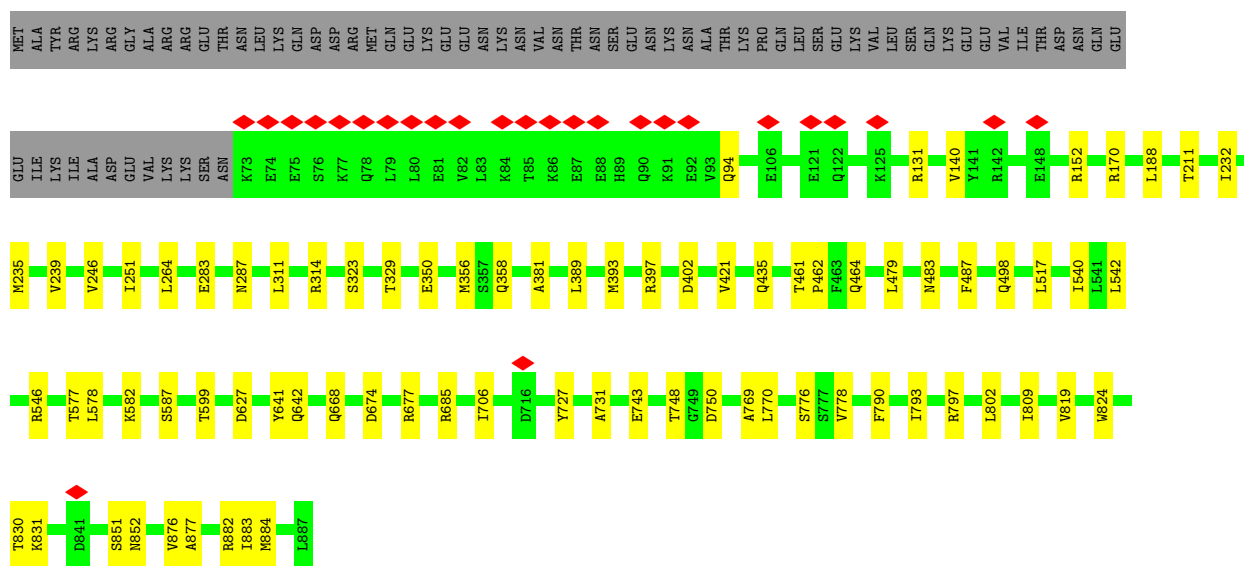
- Molecule 2: Inner capsid protein VP2





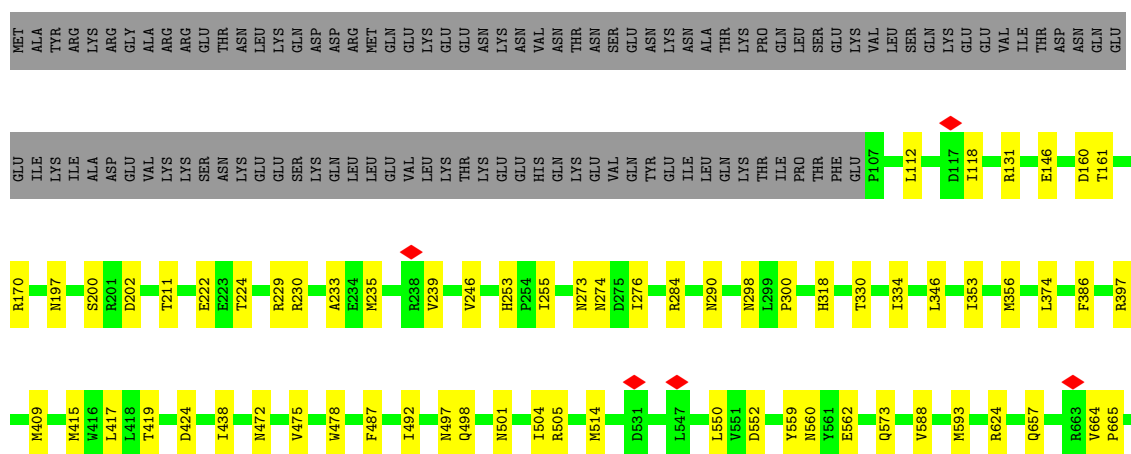
• Molecule 2: Inner capsid protein VP2

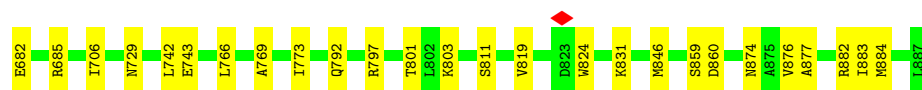
Chain D: 83% 9% 8%



• Molecule 2: Inner capsid protein VP2

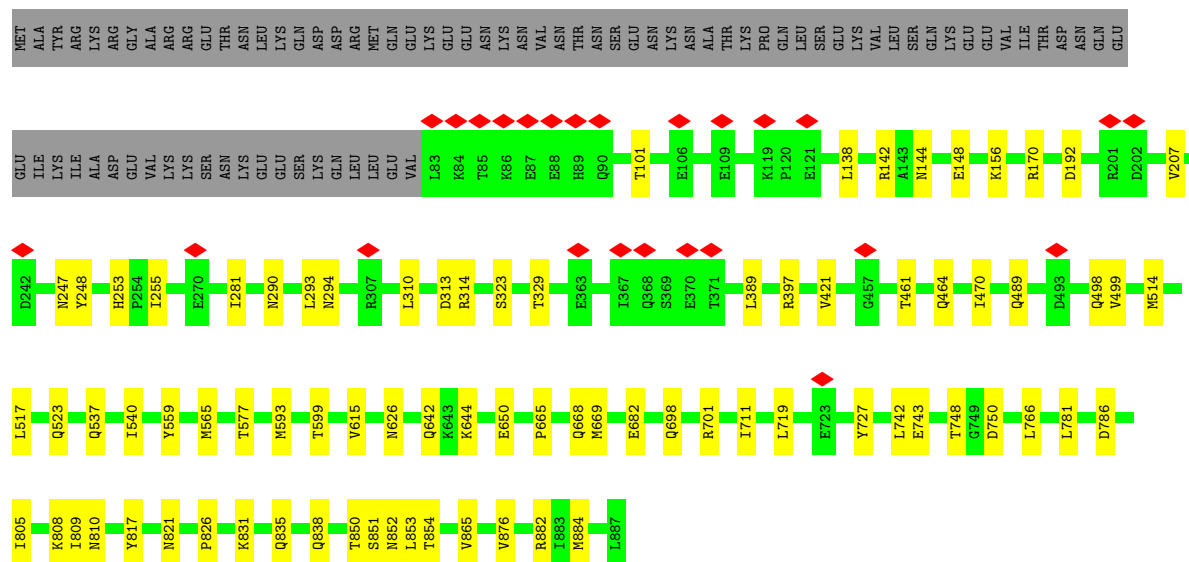
Chain E: 78% 10% 12%





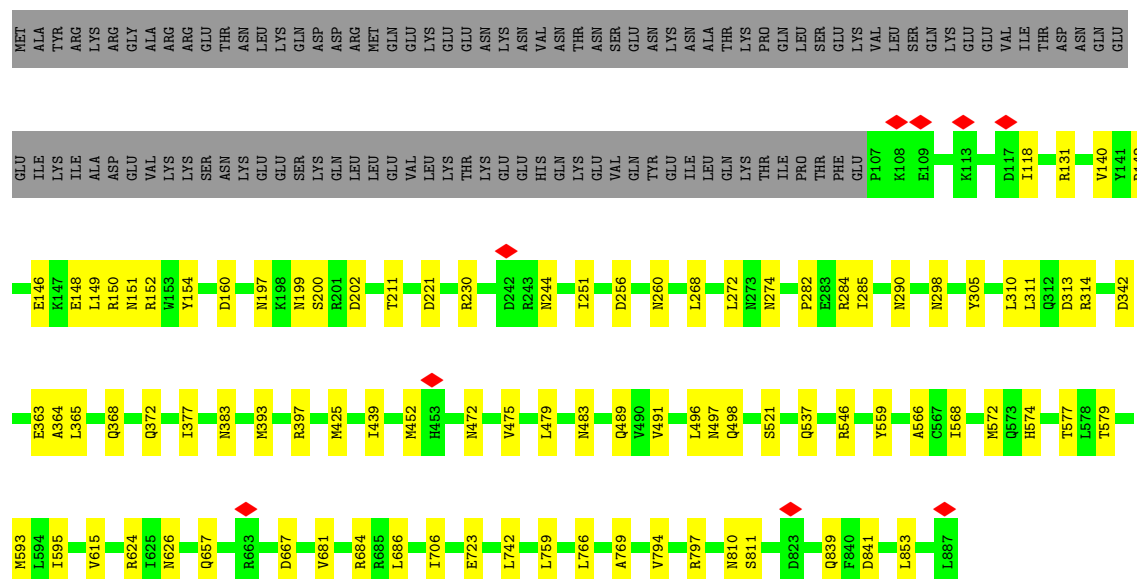
• Molecule 2: Inner capsid protein VP2

Chain F: 82% 9% 9%



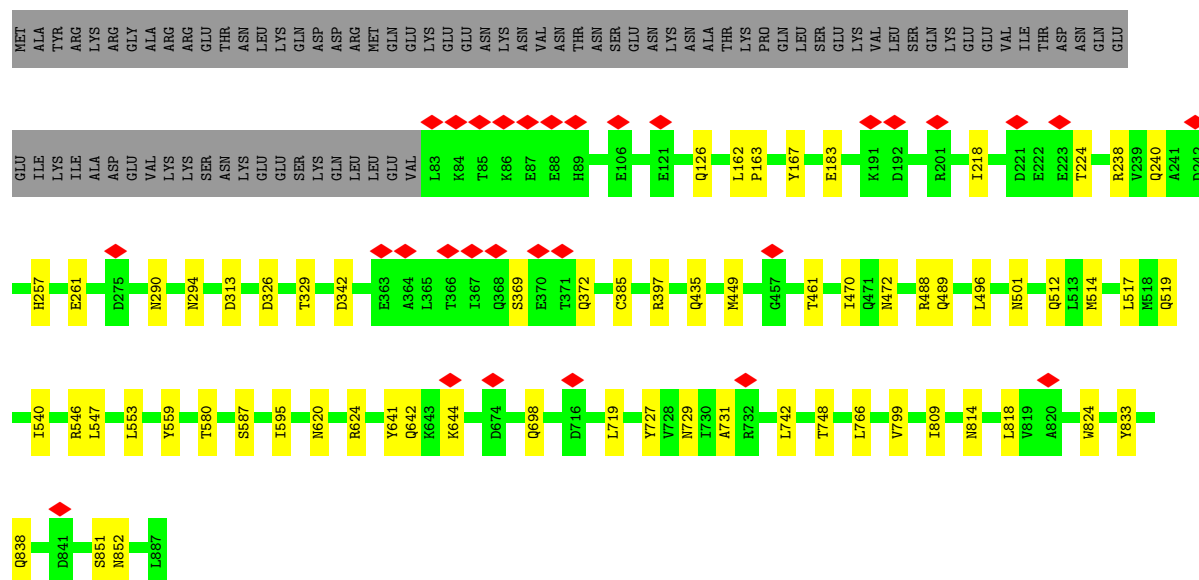
• Molecule 2: Inner capsid protein VP2

Chain G: 78% 10% 12%



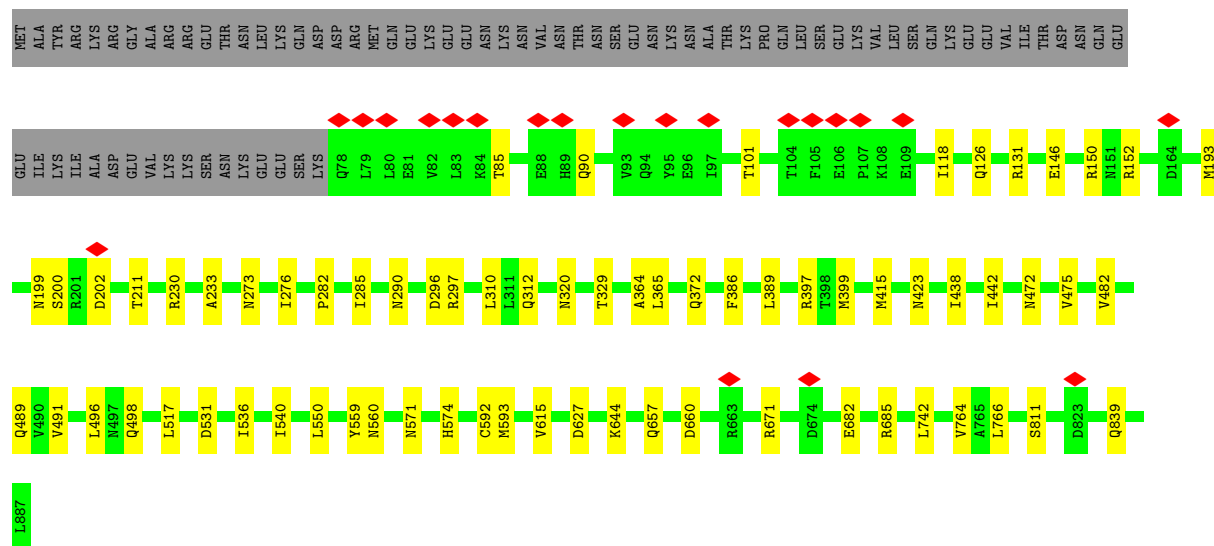
• Molecule 2: Inner capsid protein VP2

Chain H: 84% 7% 9%



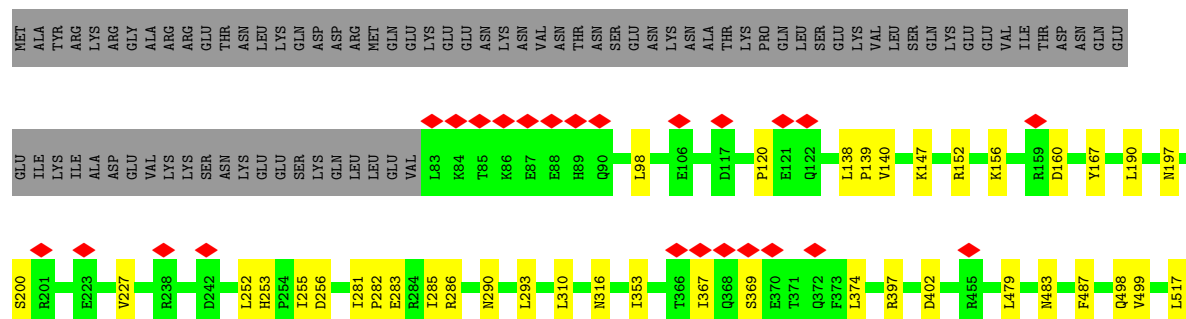
• Molecule 2: Inner capsid protein VP2

Chain I: 84% 8% 9%



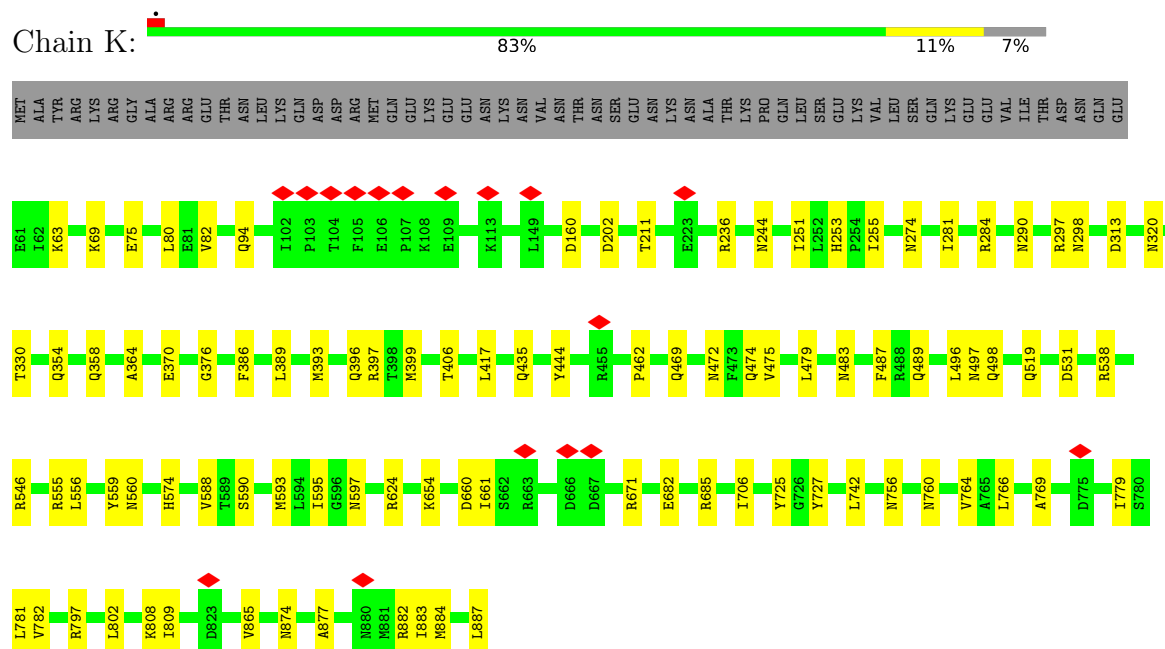
• Molecule 2: Inner capsid protein VP2

Chain J: 83% 8% 9%

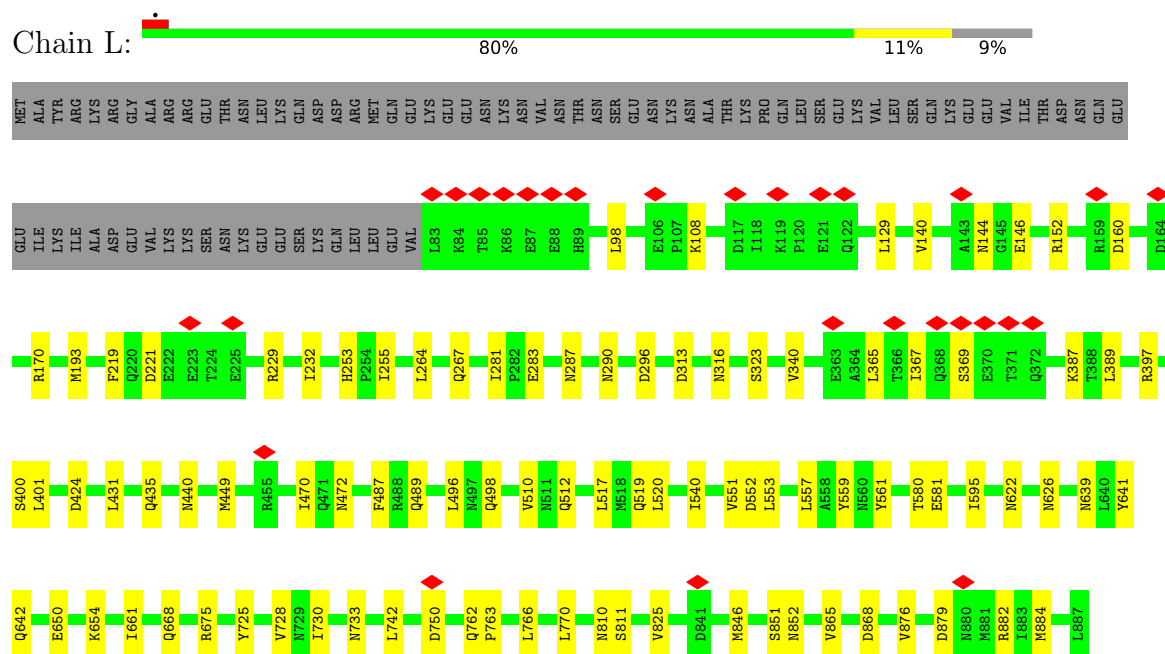




• Molecule 2: Inner capsid protein VP2



• Molecule 2: Inner capsid protein VP2



• Molecule 3: DNA/RNA (5'-D(*(GTG))-R(P*GP*C)-3')



- Molecule 4: RNA (5'-R(P*AP*GP*CP*C)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	798260	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 ($e^-/\text{\AA}^2$)	22	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	0.231	Depositor
Minimum map value	-0.164	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.0311	Depositor
Map size (Å)	342.40002, 342.40002, 342.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GTG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.24	1/8692 (0.0%)	0.41	0/11755
2	C	0.24	0/6611	0.46	0/8969
2	D	0.24	0/6790	0.43	0/9206
2	E	0.25	0/6495	0.44	0/8810
2	F	0.24	0/6707	0.45	0/9096
2	G	0.25	0/6495	0.45	0/8810
2	H	0.23	0/6707	0.44	0/9096
2	I	0.24	0/6748	0.45	0/9152
2	J	0.23	0/6707	0.43	0/9096
2	K	0.24	0/6885	0.44	0/9332
2	L	0.24	0/6707	0.43	0/9096
3	M	0.09	0/47	0.16	0/71
4	N	0.11	0/94	0.33	0/144
All	All	0.24	1/75685 (0.0%)	0.44	0/102633

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	303	ILE	C-N	5.73	1.38	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8523	0	8596	63	0
2	C	6492	0	6520	55	0
2	D	6670	0	6707	48	0
2	E	6379	0	6408	59	0
2	F	6587	0	6619	51	0
2	G	6379	0	6408	56	0
2	H	6587	0	6619	38	0
2	I	6628	0	6664	44	0
2	J	6587	0	6619	40	0
2	K	6765	0	6809	59	0
2	L	6587	0	6619	59	0
3	M	95	0	49	3	0
4	N	85	0	45	1	0
All	All	74364	0	74682	531	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 (531) 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:D:94:GLN:HE22	2:E:860:ASP:H	1.40	0.68
2:F:642:GLN:HG2	2:G:202:ASP:HA	1.79	0.65
2:I:150:ARG:HH22	2:I:152:ARG:HH11	1.46	0.64
2:G:498:GLN:HE22	2:G:574:HIS:HB2	1.62	0.63
1:A:377:GLU:HG2	1:A:378:PRO:HD3	1.81	0.63
2:L:650:GLU:HG3	2:L:661:ILE:HG21	1.81	0.63
2:K:211:THR:HG23	2:K:251:ILE:HG22	1.80	0.63
2:D:188:LEU:HD12	2:D:264:LEU:HB3	1.80	0.62
2:C:211:THR:HG23	2:C:251:ILE:HG22	1.80	0.62
2:D:461:THR:H	2:D:464:GLN:HE21	1.47	0.62
1:A:259:GLY:HA2	1:A:273:ASN:HA	1.82	0.61
2:L:367:ILE:HG22	2:L:369:SER:H	1.66	0.61
2:D:402:ASP:HB2	2:D:582:LYS:HD2	1.83	0.61
2:G:365:LEU:HG	2:I:364:ALA:HB3	1.83	0.60
2:L:253:HIS:HD2	2:L:255:ILE:H	1.50	0.59
2:L:742:LEU:HD21	2:L:766:LEU:HD23	1.82	0.59
2:G:479:LEU:O	2:G:483:ASN:ND2	2.36	0.59
1:A:741:SER:OG	1:A:749:ARG:NH1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:498:GLN:HE22	2:I:574:HIS:HB2	1.68	0.59
2:E:552:ASP:HB3	2:E:884:MET:HG2	1.85	0.59
2:F:253:HIS:HD2	2:F:255:ILE:H	1.51	0.58
2:K:253:HIS:HD2	2:K:255:ILE:H	1.50	0.58
2:H:727:TYR:HB2	2:H:809:ILE:HB	1.86	0.58
2:J:727:TYR:HB2	2:J:809:ILE:HB	1.84	0.58
2:I:282:PRO:HG2	2:I:285:ILE:HD12	1.84	0.58
2:H:488:ARG:HE	2:H:501:ASN:HB3	1.68	0.58
2:H:369:SER:HB2	2:H:372:GLN:HB2	1.85	0.57
2:L:552:ASP:HB3	2:L:884:MET:HA	1.86	0.57
1:A:80:ASP:HA	3:M:2:G:H21	1.69	0.57
2:D:727:TYR:HB2	2:D:809:ILE:HB	1.85	0.57
1:A:983:GLN:HE21	2:C:362:LEU:HD13	1.70	0.57
2:L:472:ASN:ND2	2:L:519:GLN:OE1	2.37	0.57
2:C:289:VAL:HG13	2:L:440:ASN:HD21	1.68	0.57
2:K:489:GLN:HB3	2:K:496:LEU:HD11	1.86	0.57
2:L:365:LEU:HB3	2:L:367:ILE:HG12	1.87	0.57
1:A:1023:LYS:HB3	2:G:364:ALA:HB2	1.86	0.57
2:F:517:LEU:HG	2:F:540:ILE:HG23	1.87	0.57
2:I:320:ASN:O	2:I:671:ARG:NH1	2.38	0.57
2:E:197:ASN:ND2	2:E:200:SER:OG	2.38	0.57
2:E:290:ASN:ND2	2:E:559:TYR:OH	2.37	0.57
2:C:386:PHE:HZ	2:C:560:ASN:HD22	1.52	0.57
2:L:219:PHE:O	2:L:229:ARG:NH2	2.37	0.57
2:C:290:ASN:ND2	2:C:559:TYR:OH	2.37	0.56
2:D:94:GLN:NE2	2:E:859:SER:OG	2.38	0.56
2:D:578:LEU:HD21	2:E:300:PRO:HG3	1.87	0.56
2:K:389:LEU:HD23	2:K:399:MET:HE1	1.87	0.56
2:C:282:PRO:HG2	2:C:285:ILE:HD12	1.87	0.56
2:K:706:ILE:HD11	2:K:769:ALA:HB1	1.87	0.56
2:C:283:GLU:OE2	2:C:287:ASN:ND2	2.39	0.56
2:D:876:VAL:HA	2:D:882:ARG:HA	1.87	0.56
2:K:69:LYS:HA	2:K:80:LEU:HD11	1.88	0.56
1:A:604:ASN:HD21	1:A:631:ASP:HA	1.70	0.56
2:G:706:ILE:HD11	2:G:769:ALA:HB1	1.88	0.56
2:K:290:ASN:ND2	2:K:559:TYR:OH	2.39	0.56
1:A:184:ARG:HH22	3:M:1:GTG:HN21	1.54	0.55
2:E:682:GLU:OE1	2:E:685:ARG:NH1	2.40	0.55
2:I:489:GLN:HB3	2:I:496:LEU:HD11	1.88	0.55
2:L:221:ASP:O	2:L:229:ARG:NH1	2.39	0.55
2:J:281:ILE:HD11	2:J:865:VAL:HG21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:253:HIS:HD2	2:E:255:ILE:H	1.54	0.55
2:J:517:LEU:HG	2:J:540:ILE:HG23	1.87	0.55
1:A:264:ASN:O	1:A:508:ARG:NH1	2.40	0.55
2:G:272:LEU:HD22	2:G:305:TYR:HB3	1.88	0.55
2:J:253:HIS:HD2	2:J:255:ILE:H	1.54	0.55
2:C:472:ASN:HB3	2:C:475:VAL:HG12	1.89	0.55
2:I:118:ILE:HG12	2:I:657:GLN:HG3	1.89	0.54
2:K:756:ASN:O	2:K:760:ASN:ND2	2.40	0.54
2:D:599:THR:HB	2:D:884:MET:HG3	1.90	0.54
2:F:727:TYR:HB2	2:F:809:ILE:HB	1.90	0.54
2:K:797:ARG:NH2	2:L:296:ASP:OD1	2.40	0.54
1:A:11:TYR:OH	1:A:738:GLN:NE2	2.40	0.54
2:H:218:ILE:HG23	2:H:224:THR:HG21	1.90	0.54
2:L:397:ARG:HG2	2:L:581:GLU:HG2	1.90	0.54
2:F:290:ASN:ND2	2:F:559:TYR:OH	2.41	0.54
2:G:274:ASN:HD21	2:G:298:ASN:HA	1.73	0.54
2:D:283:GLU:OE2	2:D:287:ASN:ND2	2.41	0.54
2:D:750:ASP:OD2	2:E:230:ARG:NH2	2.41	0.54
2:E:819:VAL:HA	2:E:824:TRP:HE1	1.72	0.54
2:F:138:LEU:HD11	2:F:156:LYS:HD2	1.90	0.54
2:K:330:THR:OG1	2:K:397:ARG:NH1	2.40	0.54
2:L:290:ASN:ND2	2:L:559:TYR:OH	2.40	0.54
2:D:851:SER:OG	2:D:852:ASN:N	2.40	0.54
2:F:698:GLN:HE21	2:F:838:GLN:HE22	1.56	0.54
2:F:851:SER:OG	2:F:852:ASN:N	2.41	0.54
2:H:698:GLN:HE21	2:H:838:GLN:HE21	1.55	0.54
2:G:282:PRO:HG2	2:G:285:ILE:HD12	1.90	0.54
2:K:474:GLN:NE2	2:K:519:GLN:OE1	2.41	0.54
2:E:161:THR:HG23	2:E:161:THR:O	2.08	0.53
2:E:274:ASN:HD21	2:E:298:ASN:HA	1.72	0.53
2:H:449:MET:HE1	2:H:470:ILE:HA	1.90	0.53
2:H:742:LEU:HD21	2:H:766:LEU:HD23	1.90	0.53
2:J:479:LEU:O	2:J:483:ASN:ND2	2.41	0.53
2:K:877:ALA:HB2	2:K:883:ILE:HG23	1.90	0.53
1:A:786:ARG:NH2	1:A:876:ASP:OD2	2.40	0.53
2:C:230:ARG:NH2	2:L:750:ASP:OD2	2.41	0.53
2:D:487:PHE:HB3	2:D:498:GLN:HB3	1.90	0.53
2:G:472:ASN:HB3	2:G:475:VAL:HG12	1.90	0.53
1:A:761:SER:HA	1:A:1076:LEU:HD22	1.89	0.53
2:G:363:GLU:H	2:G:368:GLN:HE22	1.56	0.53
2:K:479:LEU:O	2:K:483:ASN:ND2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:311:LEU:HD11	2:D:314:ARG:HH11	1.73	0.53
2:E:472:ASN:HB3	2:E:475:VAL:HG12	1.90	0.53
2:C:146:GLU:HA	2:C:811:SER:HB2	1.90	0.53
2:J:140:VAL:HG21	2:J:152:ARG:HG3	1.90	0.53
2:C:112:LEU:HD11	2:C:660:ASP:HB3	1.90	0.53
2:C:323:SER:OG	2:D:358:GLN:NE2	2.42	0.53
2:I:312:GLN:HE21	2:I:571:ASN:HB2	1.74	0.53
2:D:131:ARG:NH1	2:D:251:ILE:O	2.40	0.53
1:A:264:ASN:HD21	2:E:346:LEU:HD12	1.72	0.53
2:D:642:GLN:HG2	2:E:202:ASP:HA	1.91	0.53
2:H:326:ASP:OD1	2:H:397:ARG:NH2	2.41	0.53
2:L:146:GLU:HA	2:L:811:SER:HB2	1.91	0.53
1:A:959:GLN:HG2	1:A:976:VAL:HG21	1.90	0.52
2:D:517:LEU:HG	2:D:540:ILE:HG23	1.91	0.52
2:J:546:ARG:NH2	2:J:592:CYS:O	2.42	0.52
2:L:129:LEU:HD13	2:L:193:MET:HE1	1.91	0.52
2:I:627:ASP:OD1	2:I:685:ARG:NH2	2.43	0.52
2:L:725:TYR:O	2:L:810:ASN:ND2	2.40	0.52
2:E:298:ASN:OD1	2:E:298:ASN:N	2.42	0.52
2:J:290:ASN:ND2	2:J:559:TYR:OH	2.43	0.52
2:L:517:LEU:HG	2:L:540:ILE:HG23	1.92	0.52
2:G:742:LEU:HD11	2:G:766:LEU:HD23	1.92	0.52
2:K:284:ARG:HH12	2:K:497:ASN:HD21	1.56	0.52
2:F:750:ASP:OD2	2:G:230:ARG:NH2	2.42	0.52
2:J:138:LEU:HD11	2:J:156:LYS:HD2	1.92	0.52
2:G:546:ARG:NH2	2:G:595:ILE:O	2.43	0.52
2:F:626:ASN:ND2	2:F:682:GLU:OE2	2.42	0.52
2:I:442:ILE:HD13	2:I:536:ILE:HD11	1.91	0.52
2:E:284:ARG:HH12	2:E:497:ASN:HD21	1.57	0.52
1:A:782:VAL:HG21	1:A:879:ARG:HD2	1.92	0.51
2:G:759:LEU:HD21	2:G:794:VAL:HG11	1.91	0.51
2:H:620:ASN:OD1	2:H:624:ARG:NH2	2.43	0.51
2:E:235:MET:HE2	2:E:846:MET:HG3	1.91	0.51
2:G:256:ASP:O	2:G:260:ASN:ND2	2.43	0.51
2:H:514:MET:HG3	2:H:547:LEU:HD22	1.92	0.51
2:I:365:LEU:HG	2:K:364:ALA:HB3	1.91	0.51
2:E:417:LEU:HD11	2:E:588:VAL:HG21	1.92	0.51
2:K:660:ASP:OD1	2:K:660:ASP:N	2.43	0.51
2:E:792:GLN:HE22	2:E:801:THR:HB	1.76	0.51
2:G:118:ILE:HG12	2:G:657:GLN:HG3	1.92	0.51
1:A:604:ASN:ND2	1:A:630:GLY:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:627:ASP:OD1	2:C:685:ARG:NH2	2.44	0.51
2:K:160:ASP:OD1	2:K:160:ASP:N	2.44	0.51
1:A:755:ARG:NH1	1:A:781:GLU:OE1	2.43	0.51
2:D:706:ILE:HD11	2:D:769:ALA:HB1	1.93	0.51
2:J:283:GLU:OE1	2:J:286:ARG:NH2	2.44	0.51
2:K:654:LYS:HE3	2:K:661:ILE:HG13	1.91	0.51
2:G:521:SER:O	2:G:537:GLN:NE2	2.41	0.51
1:A:392:ALA:HA	1:A:939:VAL:HG11	1.93	0.50
2:D:140:VAL:HG11	2:D:152:ARG:HD2	1.93	0.50
2:D:170:ARG:NH2	2:D:743:GLU:OE2	2.45	0.50
2:D:479:LEU:O	2:D:483:ASN:ND2	2.44	0.50
2:F:170:ARG:NH2	2:F:743:GLU:OE2	2.43	0.50
2:G:290:ASN:ND2	2:G:559:TYR:OH	2.44	0.50
2:I:296:ASP:OD2	2:I:297:ARG:NH1	2.44	0.50
2:L:489:GLN:HB3	2:L:496:LEU:HD11	1.93	0.50
2:C:423:ASN:HD21	2:C:482:VAL:HG12	1.75	0.50
2:F:499:VAL:HG12	2:F:565:MET:HE1	1.94	0.50
2:H:517:LEU:HG	2:H:540:ILE:HG23	1.92	0.50
2:K:682:GLU:OE1	2:K:685:ARG:NH1	2.44	0.50
2:E:131:ARG:NH2	2:E:211:THR:OG1	2.44	0.50
2:E:386:PHE:HZ	2:E:560:ASN:HD22	1.58	0.50
2:L:879:ASP:OD1	2:L:879:ASP:N	2.44	0.50
1:A:743:ALA:HB2	1:A:749:ARG:HD2	1.94	0.50
2:C:663:ARG:NH2	2:D:350:GLU:OE1	2.45	0.50
2:F:719:LEU:HD11	2:F:781:LEU:HD11	1.93	0.50
2:G:140:VAL:HG21	2:G:152:ARG:HD3	1.94	0.50
1:A:359:MET:HE2	1:A:614:ARG:HG3	1.92	0.50
1:A:1025:LYS:NZ	2:G:363:GLU:OE2	2.45	0.50
2:D:641:TYR:HD1	2:D:642:GLN:HG3	1.75	0.50
2:F:323:SER:H	2:F:668:GLN:HE22	1.60	0.50
2:I:329:THR:HG23	2:I:397:ARG:HD3	1.93	0.50
2:K:556:LEU:HD22	2:K:884:MET:HE3	1.93	0.50
2:J:316:ASN:O	2:J:675:ARG:NH1	2.45	0.50
2:K:742:LEU:HD11	2:K:766:LEU:HD23	1.92	0.50
1:A:519:THR:HG22	1:A:668:ALA:HA	1.94	0.50
2:I:372:GLN:HE22	2:K:358:GLN:HE22	1.59	0.50
2:J:310:LEU:HD21	2:J:615:VAL:HG13	1.92	0.50
2:E:146:GLU:HA	2:E:811:SER:HB2	1.94	0.50
2:C:202:ASP:OD1	2:C:202:ASP:N	2.44	0.50
1:A:959:GLN:NE2	1:A:973:ASP:OD1	2.39	0.49
2:C:533:LYS:NZ	2:C:537:GLN:OE1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:131:ARG:NH2	2:D:211:THR:OG1	2.45	0.49
2:D:748:THR:HB	2:E:230:ARG:HG3	1.93	0.49
2:J:353:ILE:HG23	2:J:374:LEU:HD23	1.94	0.49
2:D:776:SER:O	2:D:776:SER:OG	2.29	0.49
2:D:819:VAL:HA	2:D:824:TRP:HE1	1.77	0.49
2:E:200:SER:HA	2:E:233:ALA:HA	1.93	0.49
2:F:742:LEU:HD21	2:F:766:LEU:HD23	1.95	0.49
2:F:144:ASN:ND2	2:F:727:TYR:OH	2.45	0.49
2:F:599:THR:HB	2:F:884:MET:HG3	1.95	0.49
2:J:734:LEU:O	2:J:735:ASP:OD1	2.30	0.49
2:C:538:ARG:NH2	2:K:531:ASP:OD2	2.43	0.49
2:D:329:THR:HG21	2:D:577:THR:HG21	1.94	0.49
2:F:748:THR:HG22	2:F:750:ASP:H	1.76	0.49
2:G:568:ILE:HD13	2:G:572:MET:HE3	1.94	0.49
2:K:472:ASN:HB3	2:K:475:VAL:HG12	1.95	0.49
2:L:264:LEU:O	2:L:267:GLN:NE2	2.43	0.49
2:C:363:GLU:H	2:C:368:GLN:HE22	1.60	0.49
2:E:706:ILE:HD11	2:E:769:ALA:HB1	1.95	0.49
2:K:281:ILE:HD11	2:K:865:VAL:HG21	1.95	0.49
1:A:948:TYR:OH	1:A:1070:MET:O	2.30	0.49
2:C:134:GLU:OE2	2:C:136:ARG:NH1	2.46	0.49
2:C:274:ASN:HD21	2:C:298:ASN:HA	1.77	0.49
2:E:415:MET:HG2	2:E:438:ILE:HD13	1.94	0.49
2:G:197:ASN:ND2	2:G:200:SER:OG	2.45	0.49
2:K:94:GLN:HE22	2:K:354:GLN:HE21	1.60	0.49
2:E:224:THR:O	2:E:229:ARG:NH2	2.45	0.49
2:I:644:LYS:HB3	2:J:887:LEU:HB2	1.94	0.49
2:C:759:LEU:HD21	2:C:794:VAL:HG11	1.94	0.49
2:J:701:ARG:HD2	2:J:835:GLN:HG3	1.94	0.49
2:C:517:LEU:HB2	2:C:540:ILE:HD11	1.94	0.48
2:K:320:ASN:O	2:K:671:ARG:NH1	2.35	0.48
2:K:386:PHE:HZ	2:K:560:ASN:HD22	1.61	0.48
1:A:112:ASN:ND2	1:A:234:TYR:O	2.36	0.48
2:C:202:ASP:HA	2:L:642:GLN:HG2	1.95	0.48
2:E:773:ILE:HG23	2:E:803:LYS:HD2	1.94	0.48
2:G:667:ASP:OD1	2:H:546:ARG:NH1	2.45	0.48
2:H:290:ASN:ND2	2:H:559:TYR:OH	2.45	0.48
2:I:101:THR:HB	2:K:63:LYS:HG2	1.95	0.48
1:A:166:ARG:NH2	1:A:728:ASP:OD1	2.46	0.48
1:A:824:ASN:HB2	1:A:827:VAL:HG12	1.95	0.48
2:G:397:ARG:NH2	2:G:579:THR:OG1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:385:CYS:SG	2:H:587:SER:OG	2.61	0.48
2:J:282:PRO:HG2	2:J:285:ILE:HD12	1.95	0.48
2:L:851:SER:OG	2:L:852:ASN:N	2.47	0.48
2:F:786:ASP:HA	2:F:805:ILE:HD13	1.95	0.48
2:F:808:LYS:HE2	2:F:810:ASN:HD21	1.77	0.48
2:K:444:TYR:OH	2:K:469:GLN:NE2	2.47	0.48
2:F:701:ARG:HD2	2:F:835:GLN:HG3	1.95	0.48
2:G:131:ARG:NH1	2:G:251:ILE:O	2.43	0.48
2:K:417:LEU:HD11	2:K:588:VAL:HG21	1.96	0.48
2:K:555:ARG:HB3	2:K:883:ILE:HG22	1.94	0.48
2:K:597:ASN:ND2	2:K:887:LEU:O	2.44	0.48
2:D:329:THR:HG22	2:D:397:ARG:HD2	1.95	0.48
2:H:719:LEU:HD22	2:H:729:ASN:HB3	1.96	0.48
2:K:725:TYR:HD1	2:K:808:LYS:HD3	1.77	0.48
2:L:641:TYR:HD1	2:L:642:GLN:HG3	1.77	0.48
1:A:209:SER:OG	1:A:697:ASN:ND2	2.46	0.48
2:H:851:SER:OG	2:H:852:ASN:N	2.46	0.48
2:J:629:VAL:HG12	2:J:681:VAL:HG12	1.96	0.48
1:A:453:ASP:OD1	1:A:453:ASP:N	2.47	0.48
2:C:314:ARG:NH1	2:C:626:ASN:OD1	2.47	0.48
2:C:314:ARG:HB2	2:C:679:LEU:HD21	1.96	0.48
2:D:778:VAL:HG22	2:D:809:ILE:HD12	1.96	0.48
2:G:314:ARG:NH1	2:G:626:ASN:OD1	2.45	0.48
2:J:397:ARG:HE	2:J:581:GLU:HG2	1.79	0.48
2:C:377:ILE:HA	2:C:590:SER:HB2	1.96	0.47
2:D:435:GLN:HG3	2:D:462:PRO:HG2	1.95	0.47
2:E:424:ASP:OD1	2:E:424:ASP:N	2.45	0.47
2:G:150:ARG:O	2:G:151:ASN:ND2	2.47	0.47
2:C:841:ASP:OD1	2:C:841:ASP:N	2.39	0.47
2:D:389:LEU:HD11	2:D:421:VAL:HG21	1.96	0.47
2:F:314:ARG:NH1	2:F:626:ASN:OD1	2.40	0.47
2:I:472:ASN:HB3	2:I:475:VAL:HG12	1.95	0.47
2:J:579:THR:HG22	2:K:297:ARG:HE	1.78	0.47
2:L:323:SER:OG	2:L:668:GLN:OE1	2.31	0.47
1:A:877:ILE:HD12	1:A:1073:ILE:HD12	1.95	0.47
2:K:376:GLY:O	2:K:590:SER:OG	2.32	0.47
2:F:142:ARG:HG2	2:F:148:GLU:HB2	1.96	0.47
1:A:1029:VAL:HG13	1:A:1066:LEU:HD23	1.96	0.47
2:I:423:ASN:HD21	2:I:482:VAL:HG12	1.80	0.47
2:K:274:ASN:HD21	2:K:298:ASN:HA	1.80	0.47
2:D:674:ASP:OD1	2:D:677:ARG:NH2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:126:GLN:HG3	2:I:193:MET:HE1	1.95	0.47
2:I:290:ASN:ND2	2:I:559:TYR:OH	2.48	0.47
2:I:660:ASP:OD1	2:I:660:ASP:N	2.44	0.47
2:L:170:ARG:NH1	2:L:639:ASN:O	2.41	0.47
2:G:310:LEU:HD21	2:G:615:VAL:HG13	1.96	0.47
2:J:877:ALA:HB2	2:J:883:ILE:HG23	1.97	0.47
2:C:202:ASP:HB3	2:L:641:TYR:HB2	1.97	0.47
2:D:393:MET:HE2	2:D:421:VAL:HG13	1.96	0.47
2:F:310:LEU:HD11	2:F:615:VAL:HG13	1.96	0.47
2:F:461:THR:HB	2:F:464:GLN:HG3	1.96	0.47
2:K:487:PHE:HB3	2:K:498:GLN:HB3	1.97	0.47
2:F:389:LEU:HD11	2:F:421:VAL:HG21	1.97	0.47
2:G:154:TYR:OH	2:G:723:GLU:OE2	2.32	0.47
2:D:877:ALA:HB2	2:D:883:ILE:HG23	1.97	0.46
2:K:781:LEU:HD13	2:K:809:ILE:HD11	1.97	0.46
2:C:160:ASP:OD1	2:C:160:ASP:N	2.49	0.46
2:C:401:LEU:HD22	2:C:585:LEU:HD13	1.96	0.46
2:F:329:THR:HG21	2:F:577:THR:HG21	1.96	0.46
2:E:170:ARG:NH2	2:E:743:GLU:OE1	2.47	0.46
2:G:284:ARG:HD2	2:G:566:ALA:HB2	1.97	0.46
2:H:642:GLN:HB3	2:I:202:ASP:HA	1.97	0.46
2:L:283:GLU:OE2	2:L:287:ASN:ND2	2.48	0.46
2:G:284:ARG:HH12	2:G:497:ASN:HD21	1.63	0.46
1:A:753:SER:OG	1:A:754:GLU:N	2.49	0.46
2:C:108:LYS:O	2:C:663:ARG:NH1	2.49	0.46
2:E:514:MET:HE1	2:E:550:LEU:HD22	1.97	0.46
2:H:238:ARG:HH22	2:H:240:GLN:HE21	1.63	0.46
2:I:146:GLU:HA	2:I:811:SER:HB2	1.96	0.46
2:F:329:THR:HG22	2:F:397:ARG:HD2	1.97	0.46
2:I:364:ALA:HB2	2:K:82:VAL:HG22	1.98	0.46
1:A:591:SER:OG	1:A:592:GLY:N	2.46	0.46
2:C:415:MET:HG2	2:C:438:ILE:HD13	1.98	0.46
2:E:624:ARG:HA	2:E:624:ARG:HD3	1.79	0.46
2:G:797:ARG:HE	2:H:294:ASN:HD22	1.64	0.46
2:H:580:THR:OG1	2:I:296:ASP:OD1	2.33	0.46
2:J:369:SER:O	2:J:369:SER:OG	2.33	0.46
2:D:356:MET:HG3	2:D:542:LEU:HD13	1.98	0.46
2:E:353:ILE:HG23	2:E:374:LEU:HD13	1.98	0.46
2:L:622:ASN:O	2:L:626:ASN:ND2	2.49	0.46
2:E:330:THR:OG1	2:E:397:ARG:NH1	2.48	0.46
2:F:281:ILE:HD13	2:F:293:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:786:ASP:OD1	2:J:786:ASP:N	2.47	0.46
2:G:393:MET:HA	2:G:425:MET:HE1	1.97	0.45
2:C:239:VAL:HG22	2:C:246:VAL:HG12	1.99	0.45
2:C:514:MET:HG2	2:C:547:LEU:HD22	1.99	0.45
2:I:682:GLU:OE2	2:I:685:ARG:NH1	2.50	0.45
1:A:571:SER:OG	1:A:586:TYR:O	2.32	0.45
2:F:247:ASN:HB3	2:F:850:THR:HG22	1.99	0.45
2:G:146:GLU:HA	2:G:811:SER:HB2	1.98	0.45
2:J:167:TYR:OH	2:J:641:TYR:O	2.29	0.45
2:C:742:LEU:HD11	2:C:766:LEU:HD23	1.99	0.45
2:F:650:GLU:HG3	2:F:669:MET:HE1	1.97	0.45
2:K:202:ASP:OD2	2:K:236:ARG:NE	2.48	0.45
2:J:487:PHE:HB3	2:J:498:GLN:HB3	1.99	0.45
2:F:281:ILE:HD11	2:F:865:VAL:HG21	1.97	0.45
2:H:257:HIS:NE2	2:H:261:GLU:OE2	2.50	0.45
2:H:472:ASN:ND2	2:H:519:GLN:OE1	2.47	0.45
2:J:98:LEU:HD23	2:K:297:ARG:HD3	1.98	0.45
2:G:268:LEU:HD21	2:G:684:ARG:HD2	1.99	0.45
2:G:489:GLN:HG2	2:G:498:GLN:HG2	1.99	0.45
2:J:367:ILE:HG22	2:J:369:SER:H	1.82	0.45
1:A:830:GLY:O	1:A:834:THR:OG1	2.34	0.45
2:D:770:LEU:HD13	2:D:802:LEU:HD22	1.98	0.45
2:F:489:GLN:NE2	2:F:498:GLN:OE1	2.49	0.45
2:G:491:VAL:HG12	2:G:496:LEU:HB2	1.98	0.45
2:G:593:MET:HB3	2:G:593:MET:HE2	1.84	0.45
2:H:553:LEU:HD12	2:H:595:ILE:HG21	1.98	0.45
2:J:253:HIS:CD2	2:J:255:ILE:H	2.35	0.45
2:F:781:LEU:HD13	2:F:809:ILE:HD11	1.99	0.45
2:G:841:ASP:OD1	2:G:841:ASP:N	2.50	0.45
1:A:225:ILE:HG23	1:A:303:ILE:HD11	1.99	0.45
1:A:783:TYR:OH	1:A:868:LYS:NZ	2.50	0.45
2:C:505:ARG:NE	2:C:562:GLU:OE1	2.50	0.45
2:L:140:VAL:HG11	2:L:152:ARG:HD2	1.99	0.45
1:A:88:LYS:HE3	1:A:88:LYS:HB2	1.79	0.44
2:C:284:ARG:HH11	2:C:492:ILE:HD12	1.81	0.44
2:E:877:ALA:HB2	2:E:883:ILE:HG23	1.99	0.44
2:F:593:MET:HE2	2:F:593:MET:HB3	1.79	0.44
2:L:389:LEU:HD23	2:L:557:LEU:HD21	1.98	0.44
2:L:449:MET:HE1	2:L:470:ILE:HA	1.99	0.44
1:A:126:THR:O	1:A:201:TYR:OH	2.34	0.44
1:A:516:VAL:HG13	1:A:636:VAL:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:239:VAL:HA	2:D:246:VAL:HG23	1.99	0.44
2:G:342:ASP:HB2	2:G:383:ASN:HD21	1.81	0.44
1:A:735:LYS:HA	1:A:735:LYS:HD2	1.80	0.44
2:D:232:ILE:HA	2:D:235:MET:HG2	1.99	0.44
2:D:790:PHE:HE2	2:D:830:THR:HG21	1.83	0.44
2:E:160:ASP:OD1	2:E:160:ASP:N	2.51	0.44
2:E:593:MET:HE2	2:E:593:MET:HB3	1.79	0.44
2:F:748:THR:HG23	2:G:230:ARG:HG3	2.00	0.44
2:L:160:ASP:OD1	2:L:160:ASP:N	2.40	0.44
2:G:244:ASN:HB2	2:G:853:LEU:HB2	2.00	0.44
2:C:593:MET:HE2	2:C:593:MET:HB3	1.86	0.44
2:D:381:ALA:HB1	2:D:587:SER:HB2	1.98	0.44
2:G:342:ASP:OD1	2:G:342:ASP:N	2.44	0.44
2:I:386:PHE:HZ	2:I:560:ASN:HD22	1.66	0.44
2:L:253:HIS:CD2	2:L:255:ILE:H	2.33	0.44
2:C:828:SER:OG	2:C:829:THR:N	2.51	0.44
2:I:131:ARG:NH2	2:I:211:THR:OG1	2.50	0.44
2:I:491:VAL:HG22	2:I:496:LEU:HB2	2.00	0.44
2:I:550:LEU:HD21	2:I:592:CYS:HB3	1.98	0.44
2:L:219:PHE:HB2	2:L:232:ILE:HD11	1.99	0.44
2:D:731:ALA:HB2	2:D:831:LYS:HD3	2.00	0.44
2:G:152:ARG:HH21	2:G:839:GLN:HE22	1.65	0.44
2:L:281:ILE:HD11	2:L:865:VAL:HG11	1.98	0.44
2:E:253:HIS:CD2	2:E:255:ILE:H	2.35	0.43
2:F:711:ILE:HG23	2:F:831:LYS:HG3	2.00	0.43
2:L:498:GLN:O	2:L:561:TYR:OH	2.33	0.43
1:A:732:ILE:HD13	1:A:732:ILE:HA	1.89	0.43
1:A:906:ASN:OD1	1:A:906:ASN:N	2.50	0.43
2:H:435:GLN:OE1	2:H:461:THR:OG1	2.32	0.43
2:L:340:VAL:HG13	2:L:387:LYS:HG2	2.00	0.43
2:L:424:ASP:OD1	2:L:424:ASP:N	2.49	0.43
2:E:664:VAL:HA	2:E:665:PRO:HD3	1.90	0.43
2:I:415:MET:HG2	2:I:438:ILE:HD13	2.00	0.43
2:J:227:VAL:HG21	2:J:843:ARG:HH22	1.83	0.43
2:K:779:ILE:HA	2:K:782:VAL:HG12	1.99	0.43
2:L:144:ASN:OD1	2:L:144:ASN:N	2.51	0.43
1:A:795:LYS:HB2	1:A:795:LYS:HE2	1.78	0.43
2:C:756:ASN:OD1	2:C:760:ASN:ND2	2.51	0.43
2:E:273:ASN:H	2:E:276:ILE:HG22	1.84	0.43
2:F:644:LYS:HD3	2:F:644:LYS:HA	1.72	0.43
1:A:257:ILE:CG2	1:A:260:THR:CG2	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:118:ILE:HG12	2:E:657:GLN:HG3	2.00	0.43
2:F:253:HIS:CD2	2:F:255:ILE:H	2.35	0.43
2:J:281:ILE:HD13	2:J:293:LEU:HD13	2.00	0.43
2:L:512:GLN:O	2:L:512:GLN:NE2	2.51	0.43
2:D:546:ARG:HE	2:D:546:ARG:HB3	1.68	0.43
2:D:797:ARG:HH12	2:E:222:GLU:HG3	1.82	0.43
2:G:439:ILE:HG21	2:G:452:MET:HE3	2.00	0.43
2:H:167:TYR:OH	2:H:641:TYR:O	2.36	0.43
2:I:85:THR:OG1	2:I:90:GLN:NE2	2.47	0.43
2:I:200:SER:HA	2:I:233:ALA:HA	2.00	0.43
1:A:15:ILE:HD13	3:M:1:GTG:H3'	2.00	0.43
2:C:510:VAL:HB	2:C:551:VAL:HG22	2.00	0.43
2:F:853:LEU:HG	2:F:854:THR:HG23	2.01	0.43
2:H:126:GLN:NE2	2:H:183:GLU:O	2.52	0.43
2:C:877:ALA:HB2	2:C:883:ILE:HG23	2.00	0.43
2:E:742:LEU:HD11	2:E:766:LEU:HD23	2.01	0.43
2:H:814:ASN:OD1	2:H:814:ASN:N	2.51	0.43
2:K:874:ASN:OD1	2:K:882:ARG:NH1	2.40	0.43
1:A:677:ILE:HD12	1:A:677:ILE:HA	1.85	0.43
1:A:923:ASP:OD1	1:A:1000:ASN:ND2	2.51	0.43
2:G:199:ASN:OD1	2:G:199:ASN:N	2.51	0.43
2:H:742:LEU:HD22	2:H:799:VAL:HG21	2.00	0.43
2:K:593:MET:HE2	2:K:593:MET:HB3	1.84	0.43
2:L:654:LYS:HE3	2:L:654:LYS:HB2	1.78	0.43
2:I:152:ARG:HE	2:I:839:GLN:NE2	2.17	0.43
1:A:439:PRO:HA	1:A:440:PRO:HD3	1.92	0.42
2:F:719:LEU:HD12	2:F:826:PRO:HB2	2.01	0.42
2:G:624:ARG:HA	2:G:624:ARG:HD3	1.83	0.42
2:H:162:LEU:HA	2:H:163:PRO:HD3	1.92	0.42
2:G:160:ASP:OD1	2:G:160:ASP:N	2.48	0.42
2:K:435:GLN:HB3	2:K:462:PRO:HG2	2.01	0.42
2:C:137:GLN:HG2	2:C:151:ASN:HD22	1.84	0.42
2:F:817:TYR:O	2:F:821:ASN:ND2	2.52	0.42
2:L:846:MET:HE3	2:L:846:MET:HB2	1.97	0.42
2:C:355:LYS:HD3	2:K:406:THR:HG22	2.02	0.42
2:C:851:SER:OG	2:C:852:ASN:N	2.48	0.42
2:E:318:HIS:CE1	2:E:573:GLN:HE21	2.37	0.42
2:F:192:ASP:OD1	2:F:192:ASP:N	2.53	0.42
2:G:131:ARG:NH2	2:G:211:THR:OG1	2.52	0.42
2:G:313:ASP:N	2:G:313:ASP:OD1	2.53	0.42
2:J:402:ASP:HB2	2:J:582:LYS:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:499:VAL:HG12	2:J:565:MET:HE1	2.00	0.42
2:K:393:MET:O	2:K:396:GLN:NE2	2.53	0.42
2:K:624:ARG:HD3	2:K:624:ARG:HA	1.82	0.42
2:C:419:THR:HB	2:C:478:TRP:HE1	1.83	0.42
2:H:313:ASP:N	2:H:313:ASP:OD1	2.50	0.42
2:I:199:ASN:OD1	2:I:199:ASN:N	2.52	0.42
2:I:517:LEU:HB2	2:I:540:ILE:HD11	2.02	0.42
2:I:593:MET:HE2	2:I:593:MET:HB3	1.71	0.42
2:K:370:GLU:OE1	2:K:538:ARG:NH1	2.52	0.42
1:A:512:ASN:OD1	1:A:512:ASN:N	2.48	0.42
2:F:313:ASP:OD1	2:F:313:ASP:N	2.49	0.42
2:G:311:LEU:HD11	2:G:314:ARG:HH21	1.84	0.42
2:C:356:MET:HE3	2:C:356:MET:HB2	1.89	0.42
2:F:523:GLN:O	2:F:537:GLN:NE2	2.52	0.42
2:I:389:LEU:HD23	2:I:399:MET:HE1	2.01	0.42
2:K:244:ASN:OD1	2:K:244:ASN:N	2.48	0.42
2:L:762:GLN:HA	2:L:763:PRO:HD3	1.94	0.42
2:F:207:VAL:HG22	2:F:248:TYR:HB2	2.02	0.42
2:G:372:GLN:HE21	2:K:75:GLU:HG2	1.85	0.42
2:H:748:THR:HB	2:I:230:ARG:HG3	2.02	0.42
1:A:305:LYS:HD3	1:A:305:LYS:HA	1.78	0.41
2:E:284:ARG:HH11	2:E:492:ILE:HD12	1.84	0.41
2:E:409:MET:HE2	2:E:593:MET:HE1	2.01	0.41
1:A:356:ASP:OD1	1:A:356:ASP:N	2.54	0.41
2:I:310:LEU:HD21	2:I:615:VAL:HG13	2.02	0.41
2:I:742:LEU:HD11	2:I:766:LEU:HD23	2.01	0.41
2:J:252:LEU:HD22	2:J:256:ASP:HB3	2.02	0.41
2:K:727:TYR:HB2	2:K:809:ILE:HB	2.02	0.41
2:L:313:ASP:N	2:L:313:ASP:OD1	2.53	0.41
2:L:316:ASN:O	2:L:675:ARG:NH1	2.53	0.41
1:A:362:GLU:OE1	1:A:614:ARG:NH2	2.37	0.41
1:A:1018:ILE:HD12	1:A:1037:ALA:HB1	2.02	0.41
2:D:323:SER:OG	2:D:668:GLN:OE1	2.38	0.41
2:H:489:GLN:HB3	2:H:496:LEU:HD11	2.01	0.41
2:J:190:LEU:HB2	2:J:851:SER:HB3	2.03	0.41
2:J:197:ASN:ND2	2:J:200:SER:OG	2.53	0.41
2:J:729:ASN:HB2	2:J:831:LYS:HB3	2.02	0.41
2:K:546:ARG:NH2	2:K:595:ILE:O	2.53	0.41
2:L:108:LYS:NZ	2:L:581:GLU:OE1	2.53	0.41
1:A:510:LEU:HD23	1:A:510:LEU:HA	1.85	0.41
2:C:297:ARG:HD3	2:L:98:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:627:ASP:OD1	2:D:685:ARG:NE	2.54	0.41
2:D:793:ILE:H	2:D:793:ILE:HG13	1.75	0.41
2:E:552:ASP:HB3	2:E:884:MET:HA	2.03	0.41
2:H:342:ASP:OD1	2:H:342:ASP:N	2.47	0.41
1:A:627:ARG:HD3	1:A:634:TYR:HE1	1.85	0.41
2:C:189:LEU:HD23	2:C:189:LEU:HA	1.85	0.41
2:E:419:THR:HB	2:E:478:TRP:HE1	1.85	0.41
2:E:729:ASN:HB2	2:E:831:LYS:HB3	2.01	0.41
2:I:273:ASN:H	2:I:276:ILE:HG22	1.84	0.41
2:E:501:ASN:HB3	2:E:504:ILE:HG13	2.03	0.41
2:E:874:ASN:OD1	2:E:882:ARG:NH1	2.54	0.41
2:F:101:THR:HG23	2:F:665:PRO:HG3	2.02	0.41
2:H:644:LYS:HE3	2:H:644:LYS:HB3	1.92	0.41
2:K:397:ARG:HD2	2:K:397:ARG:HA	1.86	0.41
2:L:167:TYR:OH	2:L:641:TYR:O	2.30	0.41
1:A:523:GLN:O	1:A:527:SER:OG	2.38	0.41
2:E:876:VAL:HA	2:E:882:ARG:HA	2.03	0.41
2:H:731:ALA:HB3	2:H:833:TYR:HA	2.03	0.41
2:L:431:LEU:HD11	2:L:435:GLN:HE21	1.86	0.41
1:A:154:ASN:OD1	1:A:154:ASN:N	2.51	0.41
1:A:257:ILE:HG23	1:A:260:THR:CG2	2.50	0.41
2:C:489:GLN:HB3	2:C:496:LEU:HD11	2.02	0.41
2:E:487:PHE:HB3	2:E:498:GLN:HB3	2.02	0.41
2:E:505:ARG:NE	2:E:562:GLU:OE2	2.54	0.41
2:F:876:VAL:HA	2:F:882:ARG:HA	2.02	0.41
2:G:142:ARG:HE	2:G:148:GLU:HG3	1.86	0.41
2:I:423:ASN:ND2	2:I:482:VAL:O	2.54	0.41
2:K:498:GLN:HE22	2:K:574:HIS:HB2	1.86	0.41
2:K:802:LEU:HD12	2:K:802:LEU:HA	1.91	0.41
2:L:876:VAL:HA	2:L:882:ARG:HA	2.03	0.41
2:C:200:SER:HA	2:C:233:ALA:HA	2.02	0.41
2:C:389:LEU:HD23	2:C:399:MET:HE1	2.03	0.41
2:H:329:THR:HG22	2:H:397:ARG:HD3	2.02	0.41
2:J:139:PRO:HB3	2:J:147:LYS:HE2	2.03	0.41
2:J:160:ASP:OD1	2:J:160:ASP:N	2.41	0.41
2:L:553:LEU:HD12	2:L:595:ILE:HG21	2.03	0.41
1:A:252:VAL:HG12	1:A:683:ALA:HB2	2.03	0.40
1:A:1005:GLN:H	1:A:1005:GLN:HG3	1.70	0.40
2:C:296:ASP:OD1	2:L:580:THR:OG1	2.39	0.40
2:H:512:GLN:O	2:H:512:GLN:NE2	2.54	0.40
2:J:706:ILE:HD11	2:J:769:ALA:HB1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:510:VAL:HB	2:L:551:VAL:HG22	2.02	0.40
2:L:728:VAL:HG13	2:L:730:ILE:HG12	2.03	0.40
2:L:868:ASP:O	2:L:868:ASP:OD1	2.39	0.40
1:A:644:THR:OG1	1:A:645:LYS:N	2.54	0.40
2:E:797:ARG:HH21	2:F:294:ASN:HB3	1.86	0.40
2:G:681:VAL:HG13	2:G:686:LEU:HB2	2.04	0.40
1:A:419:LYS:HE3	4:N:2:C:H41	1.86	0.40
2:C:711:ILE:HD11	2:C:831:LYS:HG3	2.03	0.40
2:E:112:LEU:HD12	2:E:334:ILE:HG22	2.04	0.40
2:E:239:VAL:HG22	2:E:246:VAL:HG12	2.03	0.40
2:J:253:HIS:HB3	2:J:256:ASP:HB2	2.03	0.40
2:K:313:ASP:OD1	2:K:313:ASP:N	2.51	0.40
2:L:733:ASN:OD1	2:L:733:ASN:N	2.53	0.40
2:F:514:MET:HE3	2:F:514:MET:HB3	1.98	0.40
2:H:818:LEU:C	2:H:824:TRP:HE1	2.30	0.40
2:L:487:PHE:HB3	2:L:498:GLN:HB3	2.03	0.40
2:E:356:MET:HE3	2:E:356:MET:HB2	1.94	0.40
2:F:470:ILE:HD13	2:F:470:ILE:HA	1.92	0.40
2:G:489:GLN:HB3	2:G:496:LEU:HD11	2.03	0.40
2:I:531:ASP:OD2	2:K:538:ARG:NH2	2.40	0.40
2:L:400:SER:OG	2:L:401:LEU:N	2.54	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	1049/1088 (96%)	1007 (96%)	42 (4%)	0	100	100
2	C	792/887 (89%)	759 (96%)	33 (4%)	0	100	100
2	D	813/887 (92%)	786 (97%)	27 (3%)	0	100	100
2	E	779/887 (88%)	749 (96%)	30 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	803/887 (90%)	769 (96%)	34 (4%)	0	100	100
2	G	779/887 (88%)	751 (96%)	28 (4%)	0	100	100
2	H	803/887 (90%)	773 (96%)	30 (4%)	0	100	100
2	I	808/887 (91%)	774 (96%)	34 (4%)	0	100	100
2	J	803/887 (90%)	781 (97%)	21 (3%)	1 (0%)	48	78
2	K	825/887 (93%)	792 (96%)	33 (4%)	0	100	100
2	L	803/887 (90%)	767 (96%)	36 (4%)	0	100	100
All	All	9057/9958 (91%)	8708 (96%)	348 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	120	PRO

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	199/989 (20%)	197 (99%)	2 (1%)	68	75
2	C	730/818 (89%)	729 (100%)	1 (0%)	88	89
2	D	751/818 (92%)	751 (100%)	0	100	100
2	E	717/818 (88%)	717 (100%)	0	100	100
2	F	741/818 (91%)	741 (100%)	0	100	100
2	G	717/818 (88%)	712 (99%)	5 (1%)	76	78
2	H	741/818 (91%)	741 (100%)	0	100	100
2	I	746/818 (91%)	745 (100%)	1 (0%)	88	89
2	J	741/818 (91%)	741 (100%)	0	100	100
2	K	762/818 (93%)	761 (100%)	1 (0%)	88	89
2	L	741/818 (91%)	738 (100%)	3 (0%)	84	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	7586/9169 (83%)	7573 (100%)	13 (0%)	85 85

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	939	VAL
1	A	1072	ASN
2	C	600	VAL
2	G	149	LEU
2	G	221	ASP
2	G	377	ILE
2	G	577	THR
2	G	810	ASN
2	I	764	VAL
2	K	764	VAL
2	L	520	LEU
2	L	770	LEU
2	L	825	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (178) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	920	GLN
1	A	983	GLN
1	A	1034	HIS
1	A	1048	ASN
1	A	1082	ASN
2	C	126	GLN
2	C	247	ASN
2	C	274	ASN
2	C	368	GLN
2	C	396	GLN
2	C	423	ASN
2	C	450	GLN
2	C	456	ASN
2	C	545	ASN
2	C	560	ASN
2	C	573	GLN
2	C	574	HIS
2	C	614	ASN
2	C	733	ASN

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Mol	Chain	Res	Type
2	C	760	ASN
2	C	835	GLN
2	D	94	GLN
2	D	175	ASN
2	D	287	ASN
2	D	312	GLN
2	D	320	ASN
2	D	358	GLN
2	D	464	GLN
2	D	483	ASN
2	D	573	GLN
2	D	574	HIS
2	D	609	HIS
2	D	620	ASN
2	D	756	ASN
2	D	760	ASN
2	D	821	ASN
2	D	847	HIS
2	D	880	ASN
2	E	175	ASN
2	E	197	ASN
2	E	273	ASN
2	E	274	ASN
2	E	287	ASN
2	E	290	ASN
2	E	396	GLN
2	E	469	GLN
2	E	471	GLN
2	E	483	ASN
2	E	560	ASN
2	E	573	GLN
2	E	574	HIS
2	E	614	ASN
2	E	792	GLN
2	E	810	ASN
2	E	880	ASN
2	F	90	GLN
2	F	99	GLN
2	F	144	ASN
2	F	279	ASN
2	F	290	ASN
2	F	316	ASN

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Mol	Chain	Res	Type
2	F	320	ASN
2	F	352	GLN
2	F	469	GLN
2	F	484	ASN
2	F	489	GLN
2	F	498	GLN
2	F	512	GLN
2	F	523	GLN
2	F	695	ASN
2	F	738	GLN
2	F	762	GLN
2	F	821	ASN
2	F	838	GLN
2	F	852	ASN
2	G	151	ASN
2	G	240	GLN
2	G	253	HIS
2	G	273	ASN
2	G	274	ASN
2	G	368	GLN
2	G	383	ASN
2	G	483	ASN
2	G	498	GLN
2	G	511	ASN
2	G	573	GLN
2	G	609	HIS
2	G	614	ASN
2	G	835	GLN
2	G	839	GLN
2	H	90	GLN
2	H	126	GLN
2	H	265	GLN
2	H	267	GLN
2	H	274	ASN
2	H	287	ASN
2	H	290	ASN
2	H	294	ASN
2	H	298	ASN
2	H	309	ASN
2	H	318	HIS
2	H	352	GLN
2	H	354	GLN

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Mol	Chain	Res	Type
2	H	407	ASN
2	H	469	GLN
2	H	474	GLN
2	H	484	ASN
2	H	523	GLN
2	H	573	GLN
2	H	695	ASN
2	H	698	GLN
2	H	810	ASN
2	I	137	GLN
2	I	175	ASN
2	I	240	GLN
2	I	257	HIS
2	I	312	GLN
2	I	368	GLN
2	I	423	ASN
2	I	498	GLN
2	I	506	ASN
2	I	545	ASN
2	I	549	GLN
2	I	560	ASN
2	I	573	GLN
2	I	574	HIS
2	I	614	ASN
2	I	636	ASN
2	I	708	GLN
2	I	733	ASN
2	I	810	ASN
2	I	835	GLN
2	J	94	GLN
2	J	175	ASN
2	J	197	ASN
2	J	294	ASN
2	J	309	ASN
2	J	318	HIS
2	J	352	GLN
2	J	372	GLN
2	J	423	ASN
2	J	480	HIS
2	J	484	ASN
2	J	523	GLN
2	J	573	GLN

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Mol	Chain	Res	Type
2	J	695	ASN
2	J	708	GLN
2	J	762	GLN
2	J	810	ASN
2	J	880	ASN
2	K	90	GLN
2	K	94	GLN
2	K	99	GLN
2	K	126	GLN
2	K	266	HIS
2	K	274	ASN
2	K	358	GLN
2	K	396	GLN
2	K	469	GLN
2	K	483	ASN
2	K	498	GLN
2	K	573	GLN
2	K	574	HIS
2	K	614	ASN
2	K	636	ASN
2	K	760	ASN
2	K	810	ASN
2	L	247	ASN
2	L	320	ASN
2	L	368	GLN
2	L	407	ASN
2	L	469	GLN
2	L	484	ASN
2	L	506	ASN
2	L	523	GLN
2	L	573	GLN
2	L	753	GLN
2	L	761	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	M	1/3 (33%)	0	0
4	N	3/4 (75%)	2 (66%)	0
All	All	4/7 (57%)	2 (50%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	N	1	G
4	N	3	C

There are no RNA pucker outliers to report.

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.

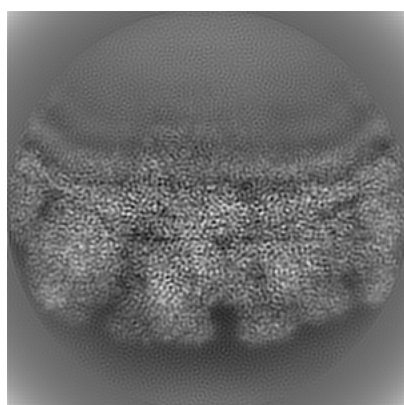
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20059. These allow visual inspection of the internal detail of the map and identification of artifacts.

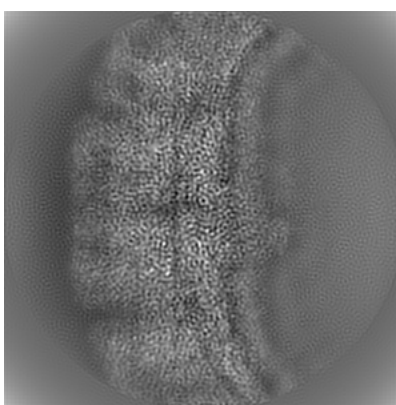
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

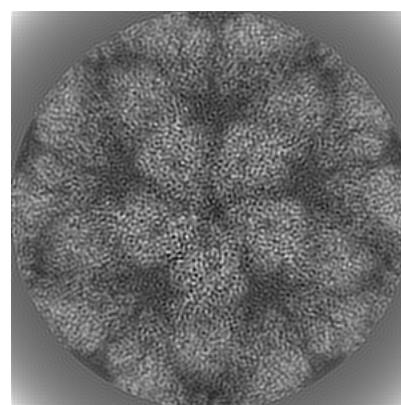
6.1.1 Primary map



X



Y

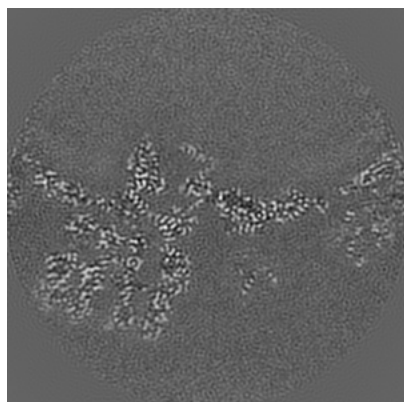


Z

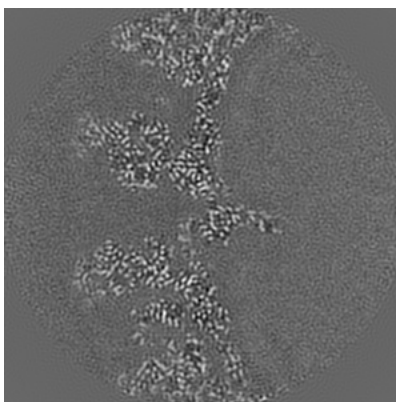
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

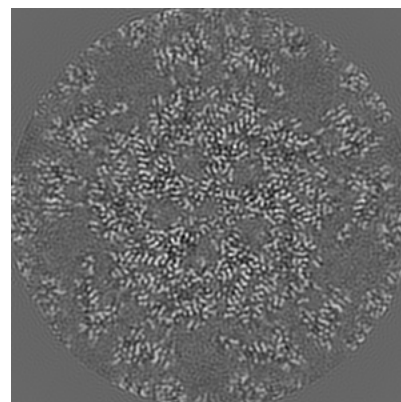
6.2.1 Primary map



X Index: 160



Y Index: 160

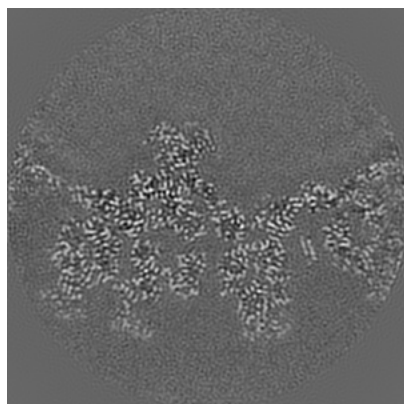


Z Index: 160

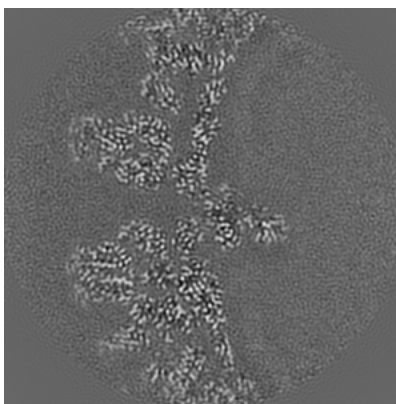
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

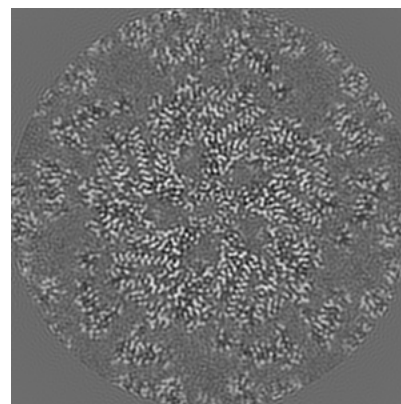
6.3.1 Primary map



X Index: 141



Y Index: 153

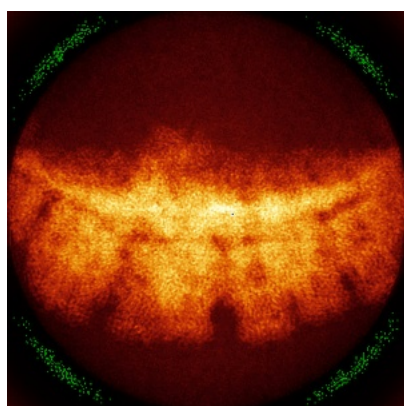


Z Index: 161

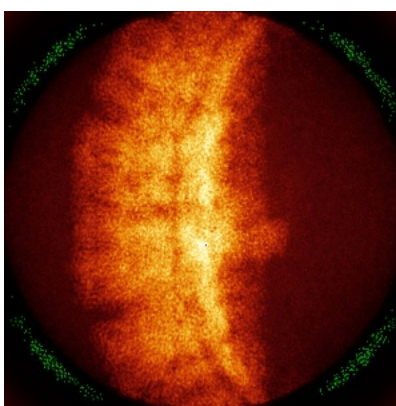
The images above show the largest variance slices of the map in three orthogonal directions.

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

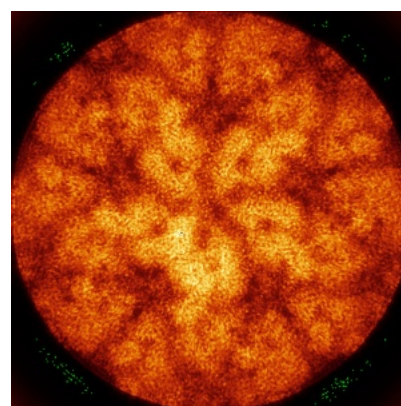
6.4.1 Primary map



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

This section was not generated.

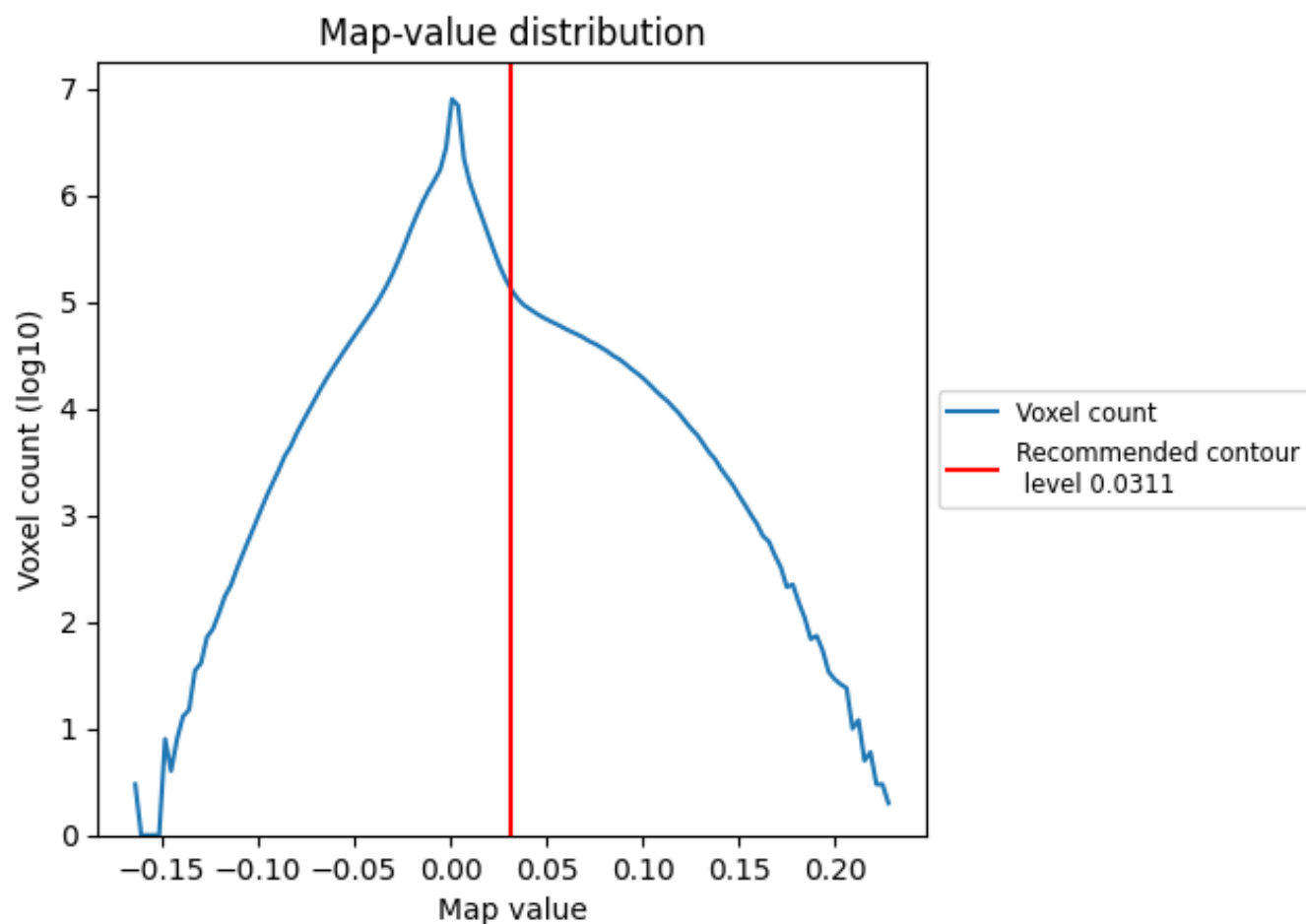
6.6 Mask visualisation

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

7 Map analysis [i](#)

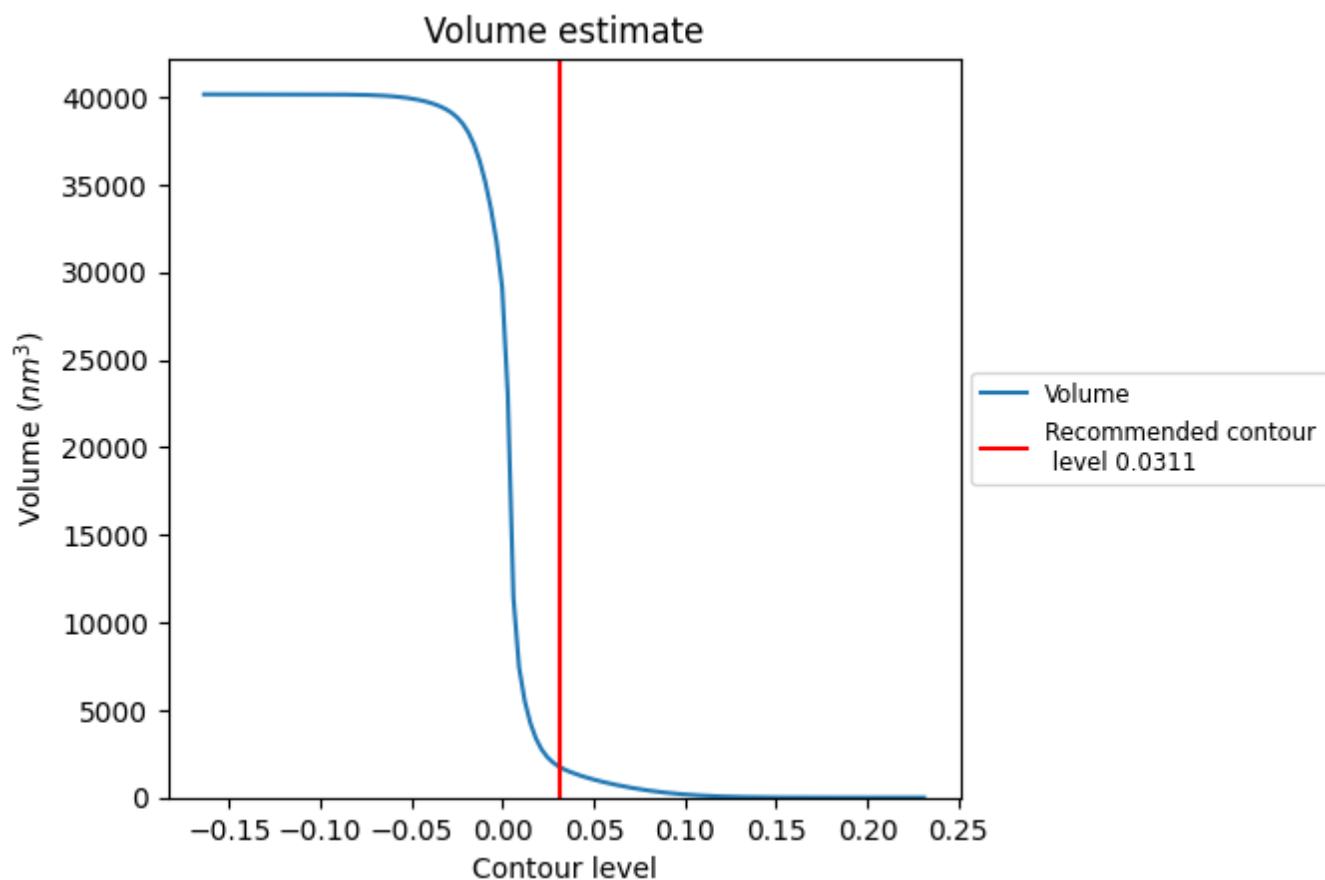
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

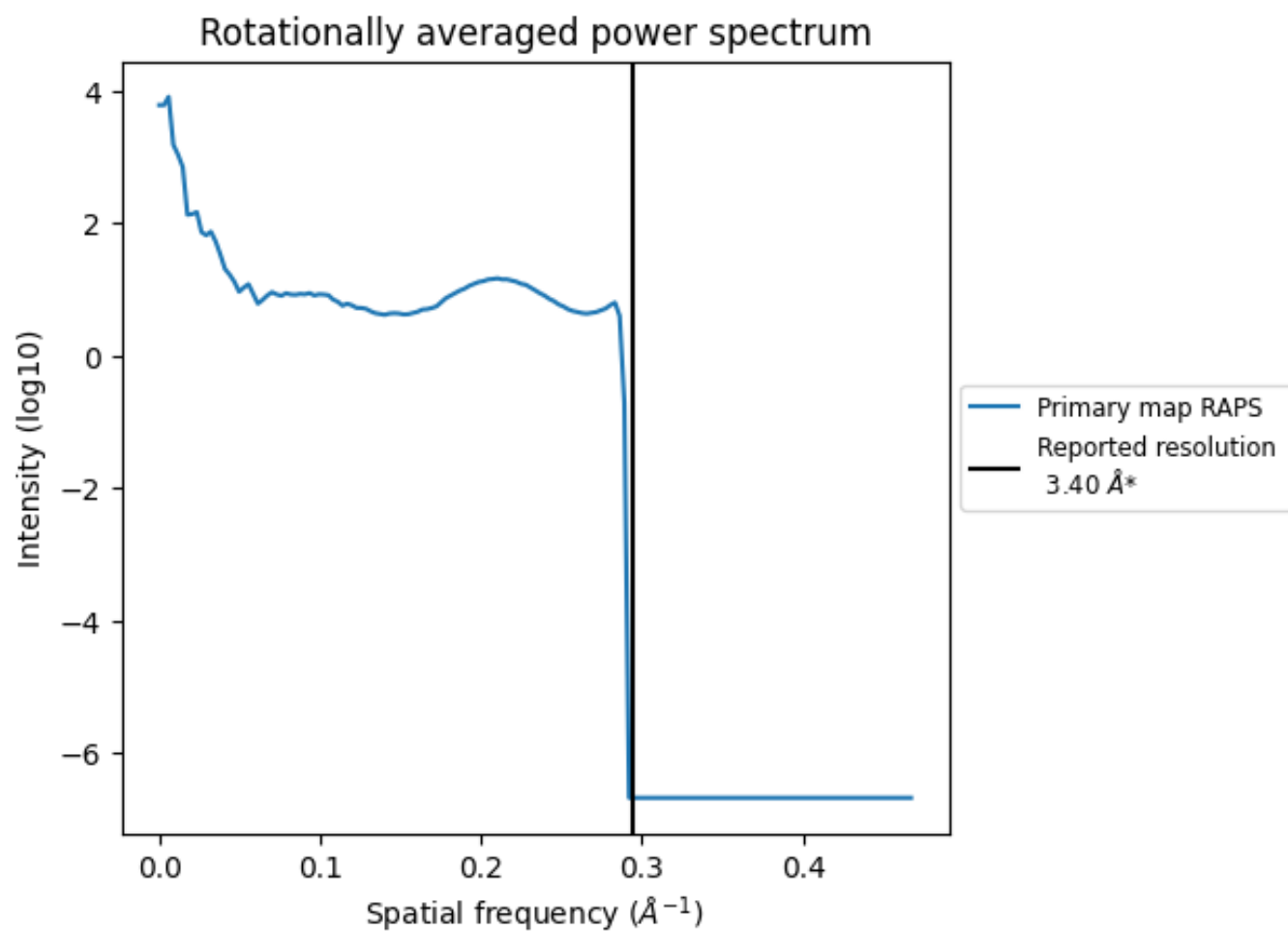
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1759 nm³; this corresponds to an approximate mass of 1589 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 0.294 Å⁻¹

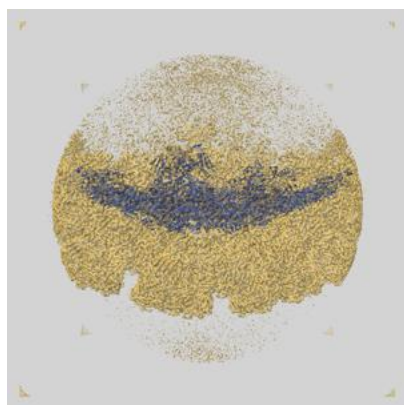
8 Fourier-Shell correlation

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

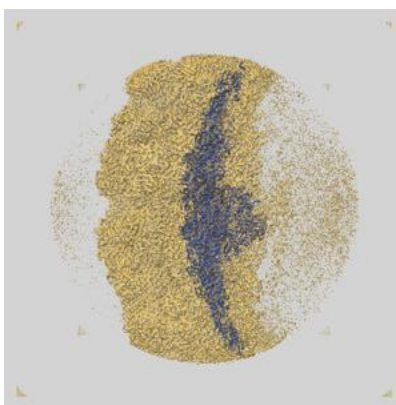
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20059 and PDB model 6OGY. Per-residue inclusion information can be found in section [3](#) on page [6](#).

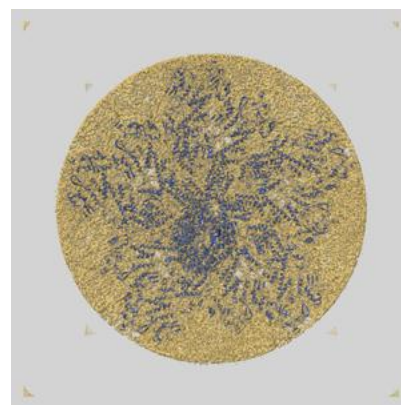
9.1 Map-model overlay [i](#)



X



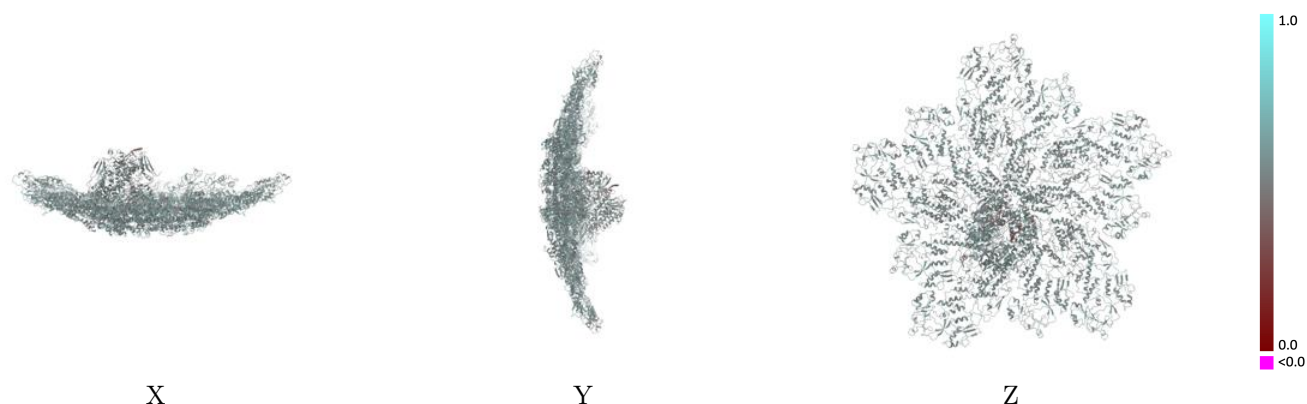
Y



Z

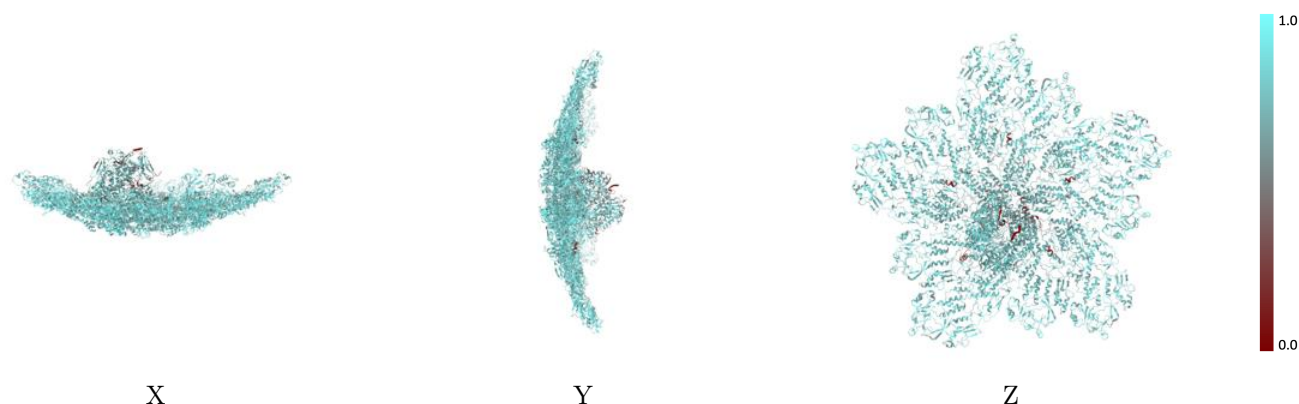
The images above show the 3D surface view of the map at the recommended contour level 0.0311 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



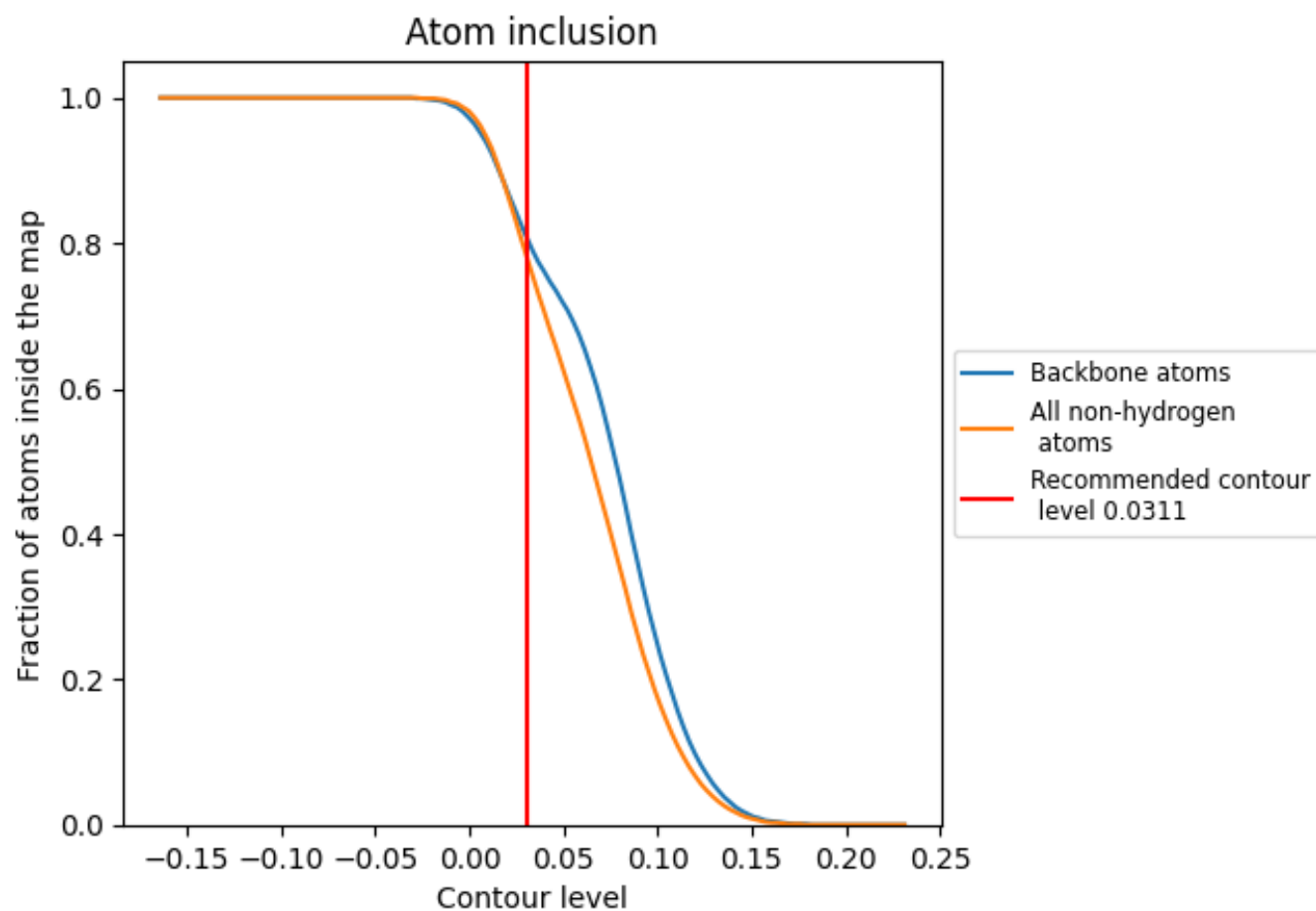
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0311).

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0311) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7770	0.5370
A	0.7370	0.5330
C	0.7950	0.5430
D	0.7770	0.5360
E	0.8010	0.5430
F	0.7820	0.5360
G	0.7920	0.5420
H	0.7750	0.5300
I	0.7800	0.5410
J	0.7790	0.5360
K	0.7890	0.5420
L	0.7740	0.5370
M	0.1470	0.3470
N	0.0000	0.2730

1.0

0.0

<0.0