



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 02:25 AM UTC

PDB ID : 8IHP / pdb_00008ihp
EMDB ID : EMD-35451
Title : Structure of Semliki Forest virus VLP in complex with the receptor VLDLR-LA3
Authors : Cao, D.; Ma, B.; Cao, Z.; Zhang, X.; Xiang, Y.
Deposited on : 2023-02-23
Resolution : 3.00 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

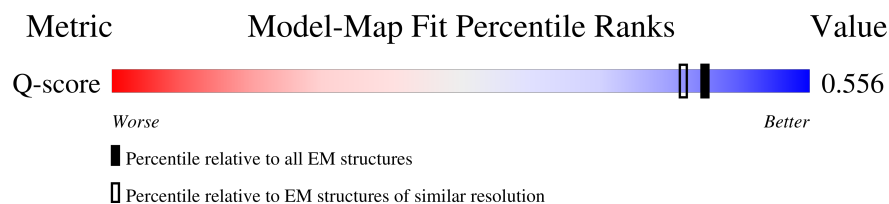
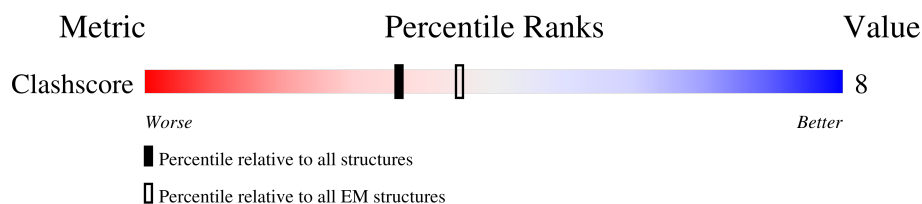
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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



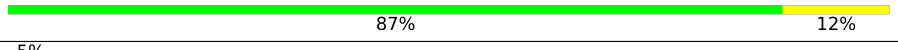
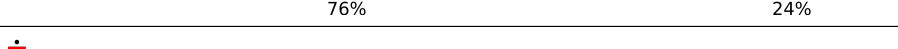
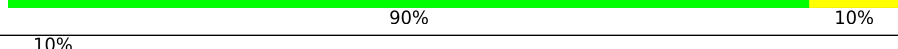
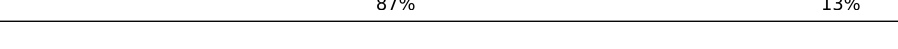
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Q-score	-	25397	14081 (2.50 - 3.50)

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

Mol	Chain	Length	Quality of chain
1	A	422	 80% 19% .
1	D	422	 83% 15% .
1	G	422	 80% 18% .
1	J	422	 83% 16% .
2	B	438	 86% 14%
2	E	438	 80% 19%

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Mol	Chain	Length	Quality of chain
2	H	438	 86%13%
2	K	438	 87%12%
3	C	162	 5%76%24%
3	F	162	 67%33%5%
3	I	162	 22%73%27%
3	L	162	 9%69%31%
4	M	39	 79%21%5%
4	N	39	 10%90%10%
4	O	39	 10%87%13%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 32337 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 Spike glycoprotein E2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	417	Total	C	N	O	S	0	0
			3250	2053	574	598	25		
1	D	417	Total	C	N	O	S	0	0
			3250	2053	574	598	25		
1	G	417	Total	C	N	O	S	0	0
			3250	2053	574	598	25		
1	J	417	Total	C	N	O	S	0	0
			3250	2053	574	598	25		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	162	LYS	GLU	conflict	UNP P03315
D	162	LYS	GLU	conflict	UNP P03315
G	162	LYS	GLU	conflict	UNP P03315
J	162	LYS	GLU	conflict	UNP P03315

- Molecule 2 is a protein called Spike glycoprotein E1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	437	Total	C	N	O	S	0	0
			3318	2103	555	635	25		
2	E	437	Total	C	N	O	S	0	0
			3318	2103	555	635	25		
2	H	437	Total	C	N	O	S	0	0
			3318	2103	555	635	25		
2	K	437	Total	C	N	O	S	0	0
			3318	2103	555	635	25		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	323	ASP	ASN	variant	UNP P03315

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Chain	Residue	Modelled	Actual	Comment	Reference
E	323	ASP	ASN	variant	UNP P03315
H	323	ASP	ASN	variant	UNP P03315
K	323	ASP	ASN	variant	UNP P03315

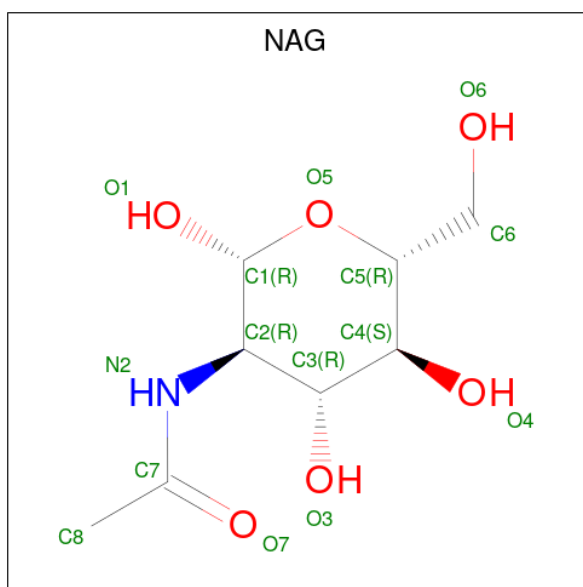
- Molecule 3 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	162	Total	C	N	O	S	0	0
			1250	781	227	233	9		
3	F	162	Total	C	N	O	S	0	0
			1250	781	227	233	9		
3	I	162	Total	C	N	O	S	0	0
			1250	781	227	233	9		
3	L	162	Total	C	N	O	S	0	0
			1250	781	227	233	9		

- Molecule 4 is a protein called Very low-density lipoprotein receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	39	Total	C	N	O	S	0	0
			298	170	56	66	6		
4	N	39	Total	C	N	O	S	0	0
			298	170	56	66	6		
4	O	39	Total	C	N	O	S	0	0
			298	170	56	66	6		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	D	1	Total	C	N	O	0
			14	8	1	5	
5	D	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	H	1	Total	C	N	O	0
			14	8	1	5	
5	J	1	Total	C	N	O	0
			14	8	1	5	
5	J	1	Total	C	N	O	0
			14	8	1	5	
5	K	1	Total	C	N	O	0
			14	8	1	5	

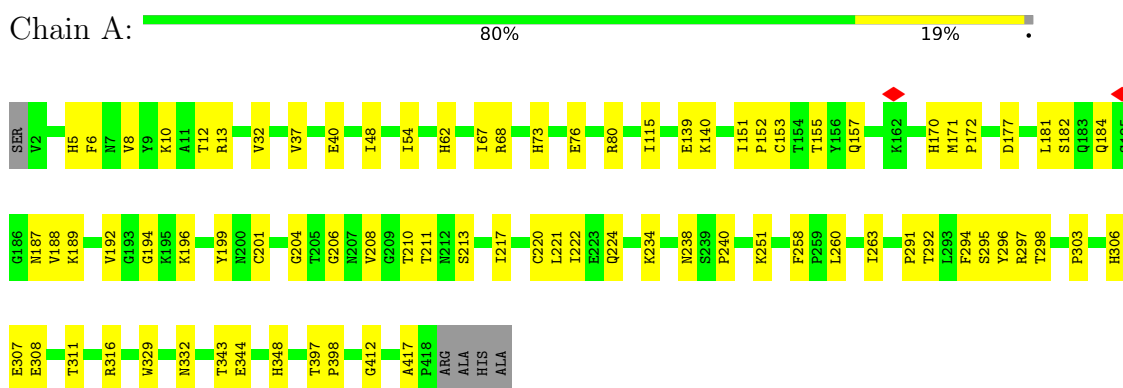
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	M	1	Total 1	Ca 1	0
6	N	1	Total 1	Ca 1	0
6	O	1	Total 1	Ca 1	0

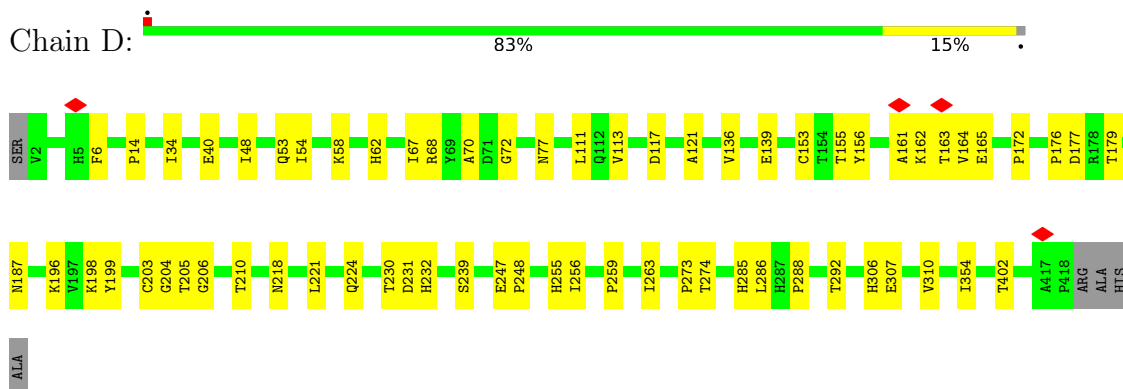
3 Residue-property plots

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.

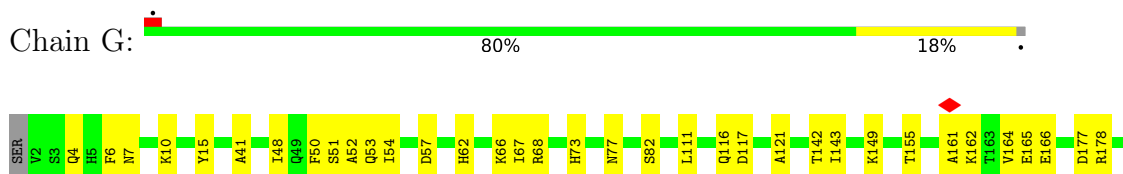
- Molecule 1: Spike glycoprotein E2

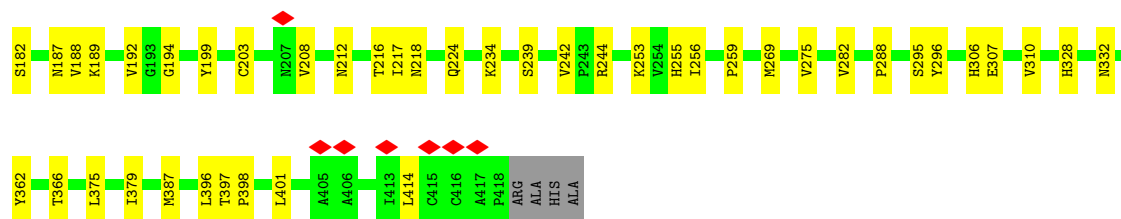


- Molecule 1: Spike glycoprotein E2



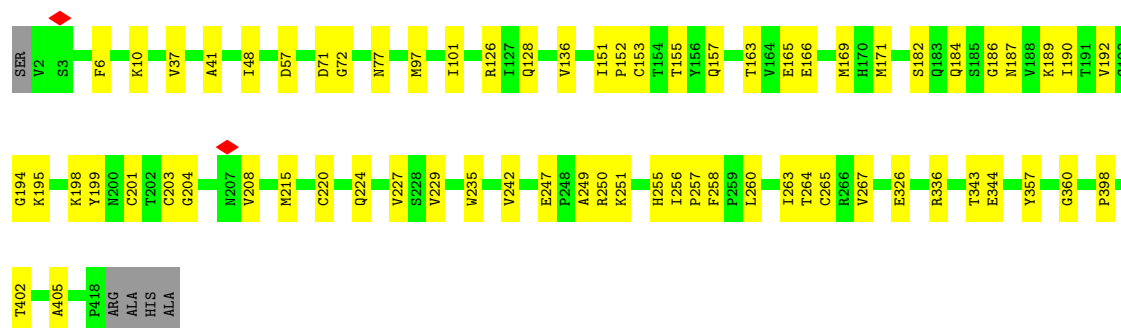
- Molecule 1: Spike glycoprotein E2





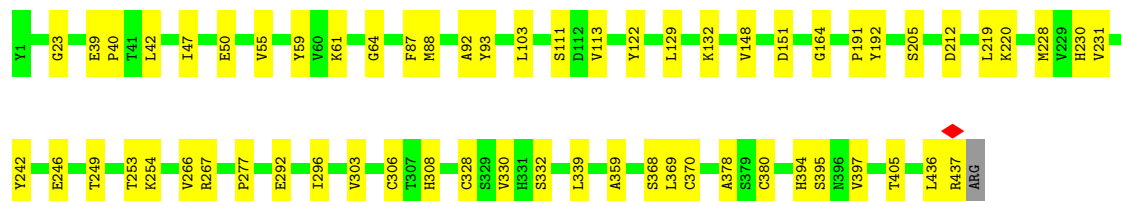
• Molecule 1: Spike glycoprotein E2

Chain J: 83% 16% .



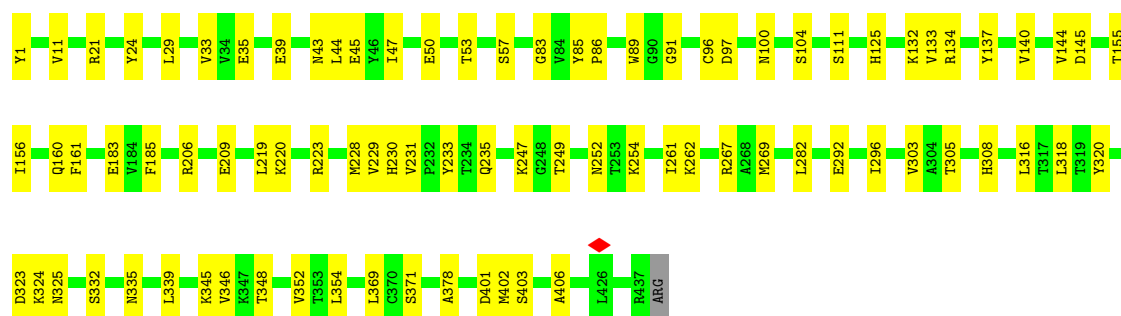
• Molecule 2: Spike glycoprotein E1

Chain B: 86% 14%



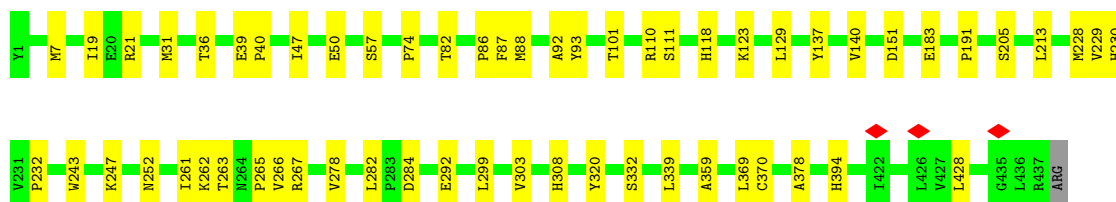
• Molecule 2: Spike glycoprotein E1

Chain E: 80% 19%



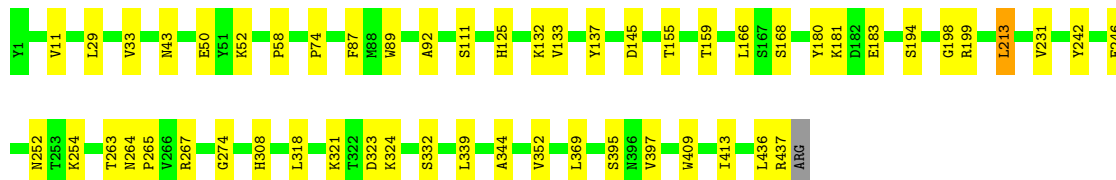
• Molecule 2: Spike glycoprotein E1

Chain H: 86% 13%



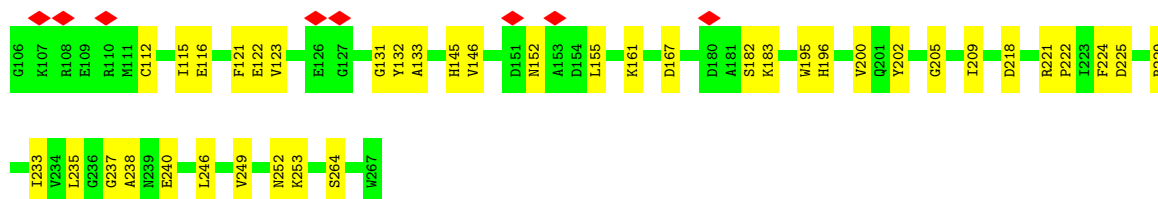
• Molecule 2: Spike glycoprotein E1

Chain K: 87% 12%



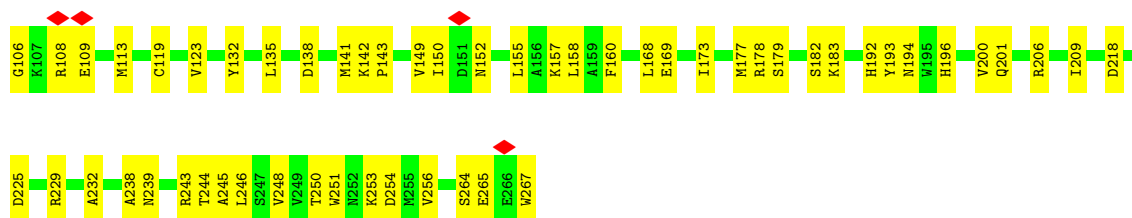
• Molecule 3: Capsid protein

Chain C: 5% 76% 24%



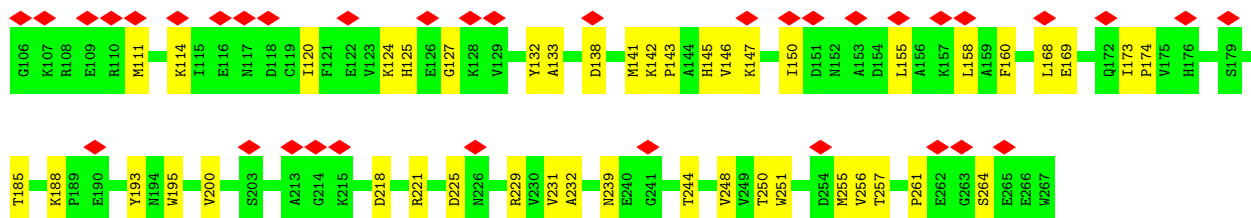
• Molecule 3: Capsid protein

Chain F: 67% 33%

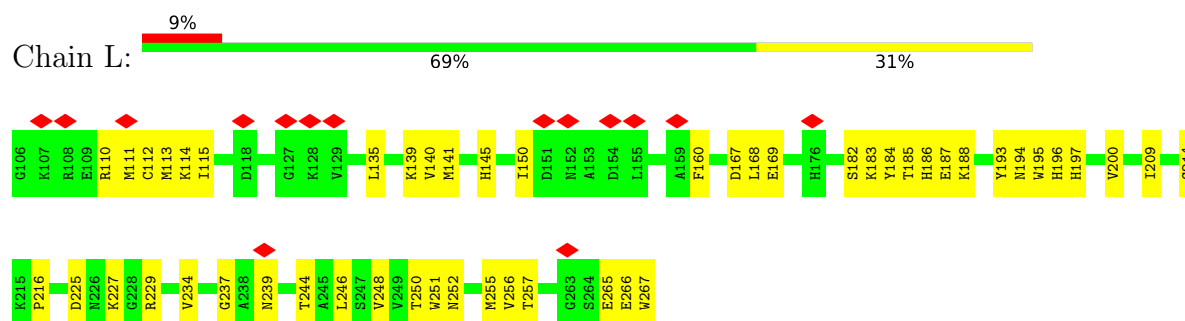


• Molecule 3: Capsid protein

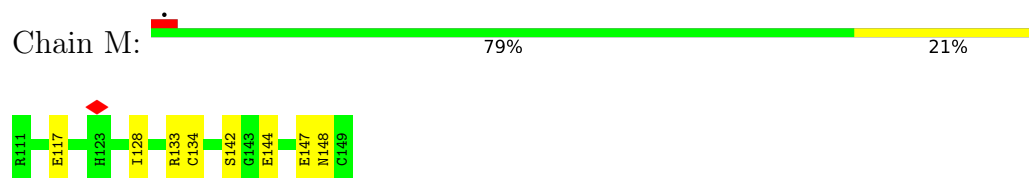
Chain I: 22% 73% 27%



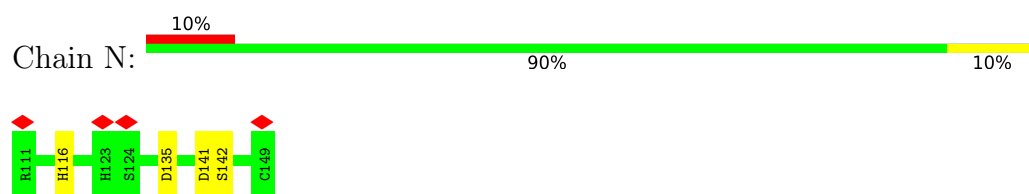
- Molecule 3: Capsid protein



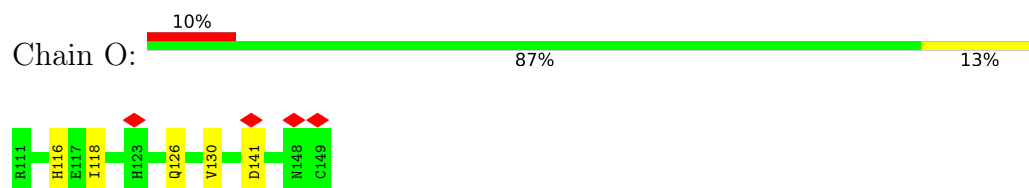
- Molecule 4: Very low-density lipoprotein receptor



- Molecule 4: Very low-density lipoprotein receptor



- Molecule 4: Very low-density lipoprotein receptor



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	651086	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.140	Depositor
Minimum map value	-0.084	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	407.03998, 407.03998, 407.03998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: CA, NAG

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	0/3343	0.42	0/4561
1	D	0.24	0/3343	0.41	0/4561
1	G	0.23	0/3343	0.39	0/4561
1	J	0.24	0/3343	0.44	0/4561
2	B	0.27	0/3404	0.40	0/4646
2	E	0.24	0/3404	0.38	0/4646
2	H	0.25	0/3404	0.39	0/4646
2	K	0.24	0/3404	0.40	1/4646 (0.0%)
3	C	0.15	0/1278	0.33	0/1719
3	F	0.16	0/1278	0.36	0/1719
3	I	0.13	0/1278	0.35	0/1719
3	L	0.14	0/1278	0.32	0/1719
4	M	0.19	0/302	0.47	0/407
4	N	0.14	0/302	0.34	0/407
4	O	0.17	0/302	0.52	0/407
All	All	0.23	0/33006	0.39	1/44925 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	213	LEU	N-CA-C	5.13	118.47	111.39

There are no chirality outliers.

There are no planarity outliers.

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	3250	0	3160	55	0
1	D	3250	0	3160	47	0
1	G	3250	0	3160	49	0
1	J	3250	0	3160	54	0
2	B	3318	0	3236	46	0
2	E	3318	0	3234	57	0
2	H	3318	0	3234	36	0
2	K	3318	0	3234	37	0
3	C	1250	0	1232	23	0
3	F	1250	0	1232	34	0
3	I	1250	0	1232	28	0
3	L	1250	0	1232	34	0
4	M	298	0	249	5	0
4	N	298	0	249	3	0
4	O	298	0	249	5	0
5	A	28	0	26	1	0
5	B	14	0	13	0	0
5	D	28	0	26	0	0
5	E	14	0	13	0	0
5	G	28	0	26	0	0
5	H	14	0	13	0	0
5	J	28	0	26	0	0
5	K	14	0	13	0	0
6	M	1	0	0	0	0
6	N	1	0	0	0	0
6	O	1	0	0	0	0
All	All	32337	0	31409	489	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 8.

All (489) 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:B:296:ILE:HG21	2:B:369:LEU:HD23	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296:ILE:HG13	2:B:369:LEU:HD23	1.58	0.85
1:D:155:THR:CG2	1:D:263:ILE:HD13	2.08	0.84
1:D:6:PHE:HA	1:D:62:HIS:HE1	1.43	0.82
1:J:402:THR:HB	1:J:405:ALA:HB2	1.63	0.80
2:B:296:ILE:CG1	2:B:369:LEU:HD23	2.15	0.76
1:J:151:ILE:CG2	1:J:152:PRO:HD2	2.16	0.75
1:J:136:VAL:HG21	1:J:265:CYS:SG	2.25	0.75
3:C:218:ASP:HB2	3:C:221:ARG:HE	1.51	0.74
1:G:295:SER:HB3	1:G:307:GLU:HG3	1.70	0.73
2:K:166:LEU:HD23	2:K:168:SER:H	1.52	0.73
3:L:112:CYS:SG	3:L:194:ASN:ND2	2.60	0.73
3:L:145:HIS:ND1	3:L:266:GLU:OE2	2.21	0.73
3:C:183:LYS:HB3	3:C:229:ARG:HG2	1.70	0.73
1:A:151:ILE:HG23	1:A:152:PRO:HD2	1.70	0.73
2:B:296:ILE:HG21	2:B:369:LEU:CD2	2.19	0.73
2:B:296:ILE:CG2	2:B:369:LEU:HD23	2.17	0.73
1:D:165:GLU:HB3	1:D:256:ILE:HB	1.71	0.73
3:F:138:ASP:HA	3:F:178:ARG:HH12	1.54	0.72
1:A:184:GLN:HB2	1:A:187:ASN:HB3	1.70	0.71
1:J:151:ILE:HG22	1:J:152:PRO:HD2	1.72	0.71
2:H:332:SER:HB2	2:H:339:LEU:HD13	1.72	0.71
1:J:136:VAL:CG2	1:J:265:CYS:SG	2.80	0.70
1:D:136:VAL:HG21	1:D:153:CYS:SG	2.31	0.70
1:G:66:LYS:HD3	1:G:77:ASN:HD22	1.56	0.69
1:D:155:THR:HB	1:D:263:ILE:CD1	2.21	0.69
2:K:74:PRO:HG2	2:K:213:LEU:HD23	1.72	0.69
1:D:155:THR:HB	1:D:263:ILE:HD13	1.76	0.68
1:G:164:VAL:HG12	1:G:165:GLU:H	1.57	0.68
1:D:203:CYS:SG	1:D:204:GLY:N	2.66	0.68
1:J:171:MET:HG2	1:J:250:ARG:HG2	1.74	0.68
1:G:192:VAL:HG22	1:G:194:GLY:H	1.60	0.67
1:G:50:PHE:HE2	1:G:52:ALA:HB3	1.60	0.67
3:I:150:ILE:HG21	3:I:155:LEU:HB2	1.76	0.67
1:D:139:GLU:HG2	1:D:292:THR:HG23	1.75	0.67
3:F:138:ASP:OD1	3:F:178:ARG:NH1	2.28	0.67
2:B:308:HIS:O	2:B:308:HIS:ND1	2.28	0.67
2:K:43:ASN:OD1	2:K:125:HIS:NE2	2.20	0.66
3:F:132:TYR:HE2	3:F:218:ASP:HA	1.61	0.66
3:I:142:LYS:NZ	3:I:146:VAL:O	2.26	0.66
1:D:163:THR:HG23	1:D:164:VAL:H	1.61	0.66
3:L:111:MET:HG2	3:L:114:LYS:HE3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:402:THR:HG22	3:F:256:VAL:HB	1.79	0.65
2:E:43:ASN:OD1	2:E:125:HIS:NE2	2.22	0.65
3:I:141:MET:HE1	3:I:251:TRP:HE1	1.60	0.65
1:G:165:GLU:O	1:G:256:ILE:HG12	1.96	0.64
2:B:332:SER:HB2	2:B:339:LEU:HD13	1.79	0.64
3:C:200:VAL:HG12	3:C:209:ILE:HG22	1.78	0.64
2:K:308:HIS:O	2:K:308:HIS:ND1	2.31	0.64
1:A:37:VAL:HG13	1:A:48:ILE:HG22	1.80	0.64
3:C:112:CYS:HA	3:C:115:ILE:HD12	1.80	0.64
1:J:151:ILE:HD11	1:J:267:VAL:HG21	1.78	0.64
1:D:58:LYS:H	1:D:77:ASN:HD21	1.45	0.64
1:G:166:GLU:HG3	1:G:253:LYS:HG2	1.80	0.63
2:K:436:LEU:HD23	2:K:437:ARG:HE	1.64	0.63
1:D:155:THR:CB	1:D:263:ILE:HD13	2.27	0.63
2:E:308:HIS:O	2:E:308:HIS:ND1	2.31	0.63
2:H:88:MET:HB2	2:H:93:TYR:HB2	1.79	0.63
1:A:13:ARG:HH22	1:A:172:PRO:HG3	1.64	0.63
2:E:401:ASP:OD1	2:E:402:MET:N	2.32	0.63
1:A:155:THR:CG2	1:A:263:ILE:HD13	2.28	0.62
2:E:1:TYR:N	2:E:282:LEU:O	2.27	0.62
3:I:239:ASN:HA	3:I:244:THR:HG22	1.80	0.62
1:G:10:LYS:O	1:G:234:LYS:NZ	2.32	0.62
1:J:192:VAL:HG12	1:J:194:GLY:H	1.65	0.62
2:K:332:SER:HB2	2:K:339:LEU:HD13	1.82	0.62
1:G:4:GLN:HA	1:G:7:ASN:HB2	1.82	0.61
2:E:183:GLU:HA	2:E:252:ASN:HD21	1.65	0.61
2:B:88:MET:HB2	2:B:93:TYR:HB2	1.82	0.61
1:G:57:ASP:OD1	1:G:77:ASN:ND2	2.32	0.61
1:J:37:VAL:HG13	1:J:48:ILE:HG22	1.82	0.61
1:J:247:GLU:OE2	1:J:250:ARG:NH1	2.34	0.61
2:E:262:LYS:HG3	2:E:269:MET:SD	2.41	0.60
2:E:228:MET:HE2	2:E:230:HIS:CD2	2.36	0.60
1:D:161:ALA:HB3	1:D:259:PRO:HG3	1.83	0.60
3:L:239:ASN:HA	3:L:244:THR:HG22	1.83	0.60
1:A:295:SER:HB3	1:A:307:GLU:HG3	1.84	0.59
2:E:323:ASP:OD1	2:E:324:LYS:N	2.36	0.59
3:F:135:LEU:HD11	3:F:155:LEU:HD21	1.84	0.59
1:G:187:ASN:HD22	1:G:216:THR:HG23	1.67	0.59
2:E:45:GLU:O	2:E:206:ARG:NH1	2.34	0.58
3:I:145:HIS:CE1	3:I:146:VAL:HG13	2.38	0.58
2:H:82:THR:HA	2:H:101:THR:HG22	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:72:GLY:HA2	2:K:89:TRP:HH2	1.69	0.58
2:E:29:LEU:HD23	2:E:137:TYR:HB3	1.84	0.58
2:B:87:PHE:HA	2:B:92:ALA:HA	1.86	0.58
2:E:33:VAL:HG12	2:E:133:VAL:HG22	1.83	0.58
3:I:125:HIS:ND1	3:I:147:LYS:O	2.35	0.58
1:J:153:CYS:HB2	1:J:263:ILE:HG23	1.85	0.58
2:E:303:VAL:HG21	2:E:378:ALA:HB2	1.86	0.58
3:C:225:ASP:OD2	3:C:229:ARG:NH2	2.35	0.57
2:K:213:LEU:O	2:K:213:LEU:HG	2.04	0.57
3:L:160:PHE:HD1	3:L:169:GLU:HB3	1.69	0.57
3:I:160:PHE:HB3	3:I:169:GLU:HG3	1.84	0.57
3:I:255:MET:HG3	3:I:256:VAL:H	1.68	0.57
2:B:328:CYS:HG	2:B:370:CYS:CB	2.16	0.57
1:G:53:GLN:OE1	1:G:68:ARG:NH2	2.29	0.57
2:B:359:ALA:HB2	2:B:394:HIS:CE1	2.40	0.57
3:F:251:TRP:HD1	3:F:256:VAL:HG23	1.69	0.57
1:J:57:ASP:OD1	1:J:77:ASN:ND2	2.34	0.57
1:D:54:ILE:HG23	1:D:67:ILE:HG12	1.86	0.57
2:E:1:TYR:O	2:E:282:LEU:N	2.37	0.56
2:E:219:LEU:HA	2:E:235:GLN:HB3	1.87	0.56
2:H:262:LYS:HG3	2:H:263:THR:H	1.70	0.56
1:A:13:ARG:NH2	1:A:172:PRO:HG3	2.20	0.56
1:J:153:CYS:N	1:J:263:ILE:O	2.27	0.56
1:A:151:ILE:CG2	1:A:152:PRO:HD2	2.35	0.56
5:A:501:NAG:H3	5:A:501:NAG:H83	1.87	0.56
3:L:195:TRP:CD1	3:L:196:HIS:H	2.24	0.56
2:B:59:TYR:HB3	2:B:103:LEU:HB3	1.86	0.56
2:B:192:TYR:OH	2:B:212:ASP:OD2	2.21	0.56
2:B:436:LEU:HD23	2:B:437:ARG:HG3	1.87	0.56
4:N:141:ASP:OD1	4:N:142:SER:N	2.39	0.56
1:A:199:TYR:OH	1:A:201:CYS:SG	2.61	0.56
2:B:296:ILE:HG13	2:B:369:LEU:CD2	2.34	0.56
3:L:209:ILE:O	3:L:244:THR:N	2.29	0.56
3:F:253:LYS:HD2	3:F:254:ASP:HB2	1.87	0.56
1:A:73:HIS:NE2	1:A:177:ASP:OD2	2.35	0.56
3:C:195:TRP:CD1	3:C:196:HIS:H	2.24	0.56
1:J:97:MET:HE2	1:J:257:PRO:HB3	1.88	0.55
1:D:136:VAL:CG2	1:D:153:CYS:SG	2.93	0.55
1:G:182:SER:HB2	1:G:189:LYS:HB3	1.88	0.55
1:D:153:CYS:O	1:D:263:ILE:O	2.24	0.55
1:D:155:THR:HG22	1:D:263:ILE:HD13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:161:ALA:HB3	1:G:259:PRO:HG3	1.88	0.55
4:M:133:ARG:NH2	4:M:134:CYS:HB2	2.21	0.55
1:D:117:ASP:OD2	1:D:121:ALA:N	2.39	0.55
1:J:208:VAL:HG11	1:J:215:MET:HE1	1.89	0.55
1:G:199:TYR:CD2	1:G:208:VAL:HG12	2.42	0.55
1:A:308:GLU:OE2	1:A:316:ARG:NH2	2.36	0.55
1:J:165:GLU:HB2	1:J:256:ILE:HG12	1.87	0.55
4:O:126:GLN:NE2	4:O:126:GLN:HA	2.22	0.55
2:E:11:VAL:HA	2:E:33:VAL:HG23	1.88	0.55
3:L:141:MET:HB3	3:L:168:LEU:HD11	1.88	0.55
3:F:238:ALA:HB2	3:F:264:SER:HA	1.89	0.54
2:H:19:ILE:HD13	2:H:282:LEU:HD11	1.88	0.54
2:K:132:LYS:NZ	2:K:145:ASP:OD1	2.39	0.54
2:E:50:GLU:O	2:E:111:SER:HB2	2.06	0.54
3:F:106:GLY:N	3:F:109:GLU:OE2	2.41	0.54
1:G:188:VAL:N	1:G:217:ILE:O	2.40	0.54
3:F:201:GLN:HE22	3:F:243:ARG:NH2	2.06	0.54
4:M:133:ARG:HH21	4:M:134:CYS:HB2	1.73	0.54
1:A:348:HIS:HA	2:B:405:THR:HG21	1.90	0.53
1:G:117:ASP:OD2	1:G:121:ALA:N	2.41	0.53
3:I:158:LEU:HD11	3:I:174:PRO:HD3	1.90	0.53
4:O:126:GLN:HA	4:O:126:GLN:HE21	1.74	0.53
2:B:50:GLU:O	2:B:111:SER:HB2	2.09	0.53
2:H:359:ALA:HB2	2:H:394:HIS:CE1	2.44	0.53
1:A:139:GLU:HG2	1:A:292:THR:HG23	1.91	0.53
1:G:401:LEU:HD12	3:I:168:LEU:HD23	1.90	0.53
3:I:185:THR:O	3:I:188:LYS:NZ	2.39	0.53
2:K:183:GLU:HA	2:K:252:ASN:HD21	1.74	0.53
2:B:328:CYS:HG	2:B:370:CYS:HB3	1.74	0.52
1:D:176:PRO:HB2	2:E:91:GLY:HA3	1.91	0.52
1:J:249:ALA:HB1	1:J:251:LYS:HG2	1.90	0.52
2:H:50:GLU:O	2:H:111:SER:HB2	2.09	0.52
2:K:198:GLY:O	2:K:199:ARG:NH1	2.42	0.52
2:B:328:CYS:HG	2:B:370:CYS:HG	1.43	0.52
1:D:196:LYS:HG2	1:D:231:ASP:HB2	1.92	0.52
1:A:329:TRP:O	1:A:332:ASN:ND2	2.41	0.52
2:B:328:CYS:SG	2:B:370:CYS:HB3	2.49	0.52
3:F:142:LYS:NZ	3:F:143:PRO:O	2.35	0.52
1:G:328:HIS:NE2	1:G:332:ASN:O	2.42	0.52
2:E:155:THR:HA	2:E:160:GLN:HA	1.91	0.52
1:J:203:CYS:SG	1:J:204:GLY:N	2.83	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:395:SER:O	2:K:397:VAL:N	2.41	0.52
1:A:188:VAL:HB	1:A:217:ILE:HB	1.91	0.52
3:F:113:MET:HE1	3:F:196:HIS:HA	1.89	0.52
2:H:110:ARG:NH2	2:H:205:SER:OG	2.42	0.52
2:E:156:ILE:HB	2:E:161:PHE:HE1	1.74	0.52
1:D:6:PHE:HA	1:D:62:HIS:CE1	2.35	0.52
2:H:183:GLU:HA	2:H:252:ASN:HD21	1.74	0.52
3:I:120:ILE:HG23	3:I:132:TYR:HB3	1.91	0.52
1:J:220:CYS:SG	1:J:224:GLN:HB2	2.50	0.52
1:G:54:ILE:HG23	1:G:67:ILE:HG22	1.90	0.52
1:J:182:SER:HB2	1:J:189:LYS:HB3	1.92	0.52
3:L:225:ASP:OD2	3:L:229:ARG:NH2	2.37	0.52
2:E:325:ASN:OD1	2:E:348:THR:OG1	2.20	0.52
2:H:31:MET:HE1	2:H:278:VAL:HG11	1.90	0.52
3:I:132:TYR:HE1	3:I:218:ASP:HA	1.74	0.52
1:D:273:PRO:HB3	1:D:286:LEU:HD23	1.92	0.51
2:H:36:THR:HG23	2:H:129:LEU:HD11	1.93	0.51
1:J:169:MET:HB3	1:J:235:TRP:HB3	1.92	0.51
1:A:54:ILE:HG23	1:A:67:ILE:HG12	1.91	0.51
1:J:6:PHE:O	1:J:10:LYS:HG2	2.10	0.51
1:A:32:VAL:HG11	1:A:115:ILE:HG12	1.92	0.51
1:J:357:TYR:OH	2:K:308:HIS:NE2	2.44	0.51
3:L:227:LYS:HE3	3:L:229:ARG:HD3	1.93	0.51
1:J:199:TYR:HD1	1:J:227:VAL:HG12	1.75	0.51
2:B:61:LYS:HG2	2:B:64:GLY:HA3	1.93	0.51
3:I:232:ALA:HB1	3:I:248:VAL:HB	1.93	0.51
2:K:74:PRO:HG2	2:K:213:LEU:CD2	2.41	0.51
1:A:40:GLU:HG2	2:B:113:VAL:HG21	1.92	0.51
1:D:155:THR:HB	1:D:263:ILE:HD11	1.92	0.51
1:G:82:SER:HB2	1:G:116:GLN:HG2	1.92	0.51
2:K:11:VAL:HA	2:K:33:VAL:HG23	1.93	0.51
3:L:209:ILE:HD12	3:L:246:LEU:HD11	1.92	0.51
1:A:155:THR:HB	1:A:263:ILE:HD13	1.93	0.51
2:E:83:GLY:O	2:E:223:ARG:NH2	2.43	0.51
2:H:228:MET:HE3	2:H:230:HIS:CD2	2.46	0.50
1:G:73:HIS:NE2	1:G:177:ASP:OD2	2.43	0.50
1:A:221:LEU:HB2	1:A:224:GLN:HG3	1.93	0.50
1:J:184:GLN:HB3	1:J:187:ASN:O	2.11	0.50
2:K:50:GLU:O	2:K:111:SER:HB2	2.12	0.50
1:D:198:LYS:HB2	1:D:230:THR:HB	1.94	0.50
2:E:86:PRO:HB3	2:E:229:VAL:HG22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:15:TYR:O	1:G:51:SER:OG	2.30	0.50
2:K:29:LEU:HD13	2:K:137:TYR:HB3	1.93	0.50
1:A:155:THR:HB	1:A:263:ILE:CD1	2.41	0.50
2:K:194:SER:OG	2:K:194:SER:O	2.23	0.50
3:C:145:HIS:ND1	3:C:167:ASP:OD2	2.36	0.50
2:E:252:ASN:OD1	2:E:261:ILE:HB	2.12	0.50
1:J:263:ILE:HG12	1:J:264:THR:N	2.27	0.50
3:L:184:TYR:HB2	3:L:251:TRP:CZ3	2.47	0.50
1:A:296:TYR:CE1	1:A:306:HIS:HB3	2.47	0.50
3:F:265:GLU:OE2	3:F:267:TRP:NE1	2.34	0.49
2:H:303:VAL:HG21	2:H:378:ALA:HB2	1.94	0.49
1:J:153:CYS:O	1:J:263:ILE:HG22	2.11	0.49
1:J:190:ILE:HD11	1:J:199:TYR:CE1	2.47	0.49
1:G:162:LYS:HD2	1:G:255:HIS:HB3	1.93	0.49
3:C:252:ASN:ND2	3:C:253:LYS:H	2.10	0.49
2:E:318:LEU:HB2	2:E:352:VAL:HG12	1.95	0.49
1:D:53:GLN:OE1	1:D:68:ARG:NH2	2.27	0.49
1:G:187:ASN:HA	1:G:218:ASN:HA	1.93	0.49
1:A:196:LYS:HE2	1:A:211:THR:HG23	1.94	0.49
1:G:288:PRO:HG3	1:G:310:VAL:HG12	1.95	0.49
3:C:235:LEU:HD11	3:C:249:VAL:HB	1.93	0.49
3:F:108:ARG:NH1	3:F:194:ASN:OD1	2.44	0.49
3:I:188:LYS:HE3	3:I:231:VAL:HG23	1.95	0.49
2:K:87:PHE:HA	2:K:92:ALA:HA	1.93	0.49
4:O:141:ASP:OD1	4:O:141:ASP:N	2.45	0.49
1:J:151:ILE:HG23	1:J:152:PRO:HD2	1.93	0.49
2:K:263:THR:HG22	2:K:267:ARG:HH22	1.78	0.49
3:C:252:ASN:CG	3:C:253:LYS:H	2.20	0.49
2:H:86:PRO:HB3	2:H:229:VAL:HG22	1.95	0.49
1:J:326:GLU:HB3	1:J:336:ARG:HG2	1.95	0.49
3:F:152:ASN:HB3	3:F:155:LEU:HB2	1.94	0.48
2:E:249:THR:HG23	2:E:254:LYS:NZ	2.28	0.48
1:J:190:ILE:HD11	1:J:199:TYR:CZ	2.48	0.48
1:J:198:LYS:HG2	1:J:199:TYR:H	1.77	0.48
2:H:87:PHE:HA	2:H:92:ALA:HA	1.96	0.48
2:H:137:TYR:O	2:H:140:VAL:HG12	2.13	0.48
3:L:182:SER:OG	3:L:183:LYS:N	2.47	0.48
2:B:23:GLY:HA2	2:E:305:THR:HG21	1.96	0.48
2:K:242:TYR:CZ	2:K:246:GLU:HG3	2.48	0.48
3:F:183:LYS:HB2	3:F:229:ARG:HG2	1.94	0.48
1:G:362:TYR:O	1:G:366:THR:OG1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:209:ILE:HD12	3:F:246:LEU:HD21	1.96	0.48
3:C:222:PRO:HB3	3:C:233:ILE:HD13	1.96	0.48
1:G:164:VAL:HG12	1:G:165:GLU:N	2.29	0.48
1:G:188:VAL:HB	1:G:217:ILE:HG12	1.95	0.48
2:H:47:ILE:HD12	2:H:118:HIS:CD2	2.49	0.47
1:A:397:THR:N	1:A:398:PRO:HD2	2.30	0.47
2:B:40:PRO:HD2	2:B:266:VAL:O	2.15	0.47
1:J:166:GLU:OE2	1:J:255:HIS:NE2	2.48	0.47
2:K:318:LEU:HD13	2:K:369:LEU:HD21	1.95	0.47
3:C:152:ASN:HB3	3:C:155:LEU:HB2	1.95	0.47
2:E:39:GLU:HG3	2:E:267:ARG:HB3	1.95	0.47
1:A:153:CYS:N	1:A:263:ILE:O	2.43	0.47
1:A:170:HIS:ND1	1:A:171:MET:O	2.45	0.47
1:J:151:ILE:CD1	1:J:267:VAL:HG21	2.44	0.47
2:K:33:VAL:HG12	2:K:133:VAL:HG22	1.96	0.47
2:B:151:ASP:O	2:H:191:PRO:HB3	2.15	0.47
3:F:250:THR:OG1	3:F:251:TRP:N	2.48	0.47
2:K:166:LEU:HD21	2:K:274:GLY:HA3	1.95	0.47
2:K:180:TYR:CE2	2:K:181:LYS:HG3	2.49	0.47
2:B:296:ILE:HG12	2:B:370:CYS:SG	2.55	0.47
1:D:288:PRO:HG3	1:D:310:VAL:HG12	1.96	0.47
2:E:89:TRP:O	2:E:89:TRP:CD1	2.68	0.47
2:E:185:PHE:CZ	2:E:247:LYS:HD3	2.50	0.47
2:B:231:VAL:O	2:B:231:VAL:HG13	2.15	0.47
1:A:182:SER:O	1:A:189:LYS:N	2.43	0.47
1:G:192:VAL:HG21	1:G:212:ASN:HA	1.97	0.47
3:I:195:TRP:HE1	3:I:221:ARG:HB3	1.79	0.47
3:I:255:MET:HG3	3:I:256:VAL:N	2.30	0.47
3:L:110:ARG:HA	3:L:113:MET:HE1	1.97	0.47
1:D:172:PRO:HG2	1:D:232:HIS:CG	2.50	0.47
1:G:239:SER:HB3	1:G:242:VAL:HG22	1.97	0.47
1:G:244:ARG:HG3	2:H:57:SER:HB2	1.96	0.47
3:L:195:TRP:CZ3	3:L:197:HIS:HB2	2.50	0.47
1:G:48:ILE:HG12	1:G:111:LEU:HD21	1.97	0.46
3:I:261:PRO:HG2	3:I:264:SER:HB3	1.97	0.46
3:L:135:LEU:HD23	3:L:140:VAL:HG12	1.97	0.46
4:M:142:SER:O	4:M:144:GLU:N	2.46	0.46
2:E:249:THR:HG23	2:E:254:LYS:HZ3	1.79	0.46
3:F:239:ASN:HA	3:F:244:THR:HG22	1.97	0.46
1:J:343:THR:HG23	1:J:360:GLY:HA3	1.96	0.46
1:A:6:PHE:CD1	1:A:62:HIS:HD2	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ARG:HB3	1:A:234:LYS:HD3	1.97	0.46
3:C:131:GLY:HA3	3:C:146:VAL:HG21	1.97	0.46
2:E:96:CYS:O	2:E:100:ASN:ND2	2.37	0.46
1:G:375:LEU:O	1:G:379:ILE:HG12	2.15	0.46
1:D:354:ILE:HG21	2:E:406:ALA:HB2	1.98	0.46
1:J:151:ILE:HG22	1:J:152:PRO:CD	2.42	0.46
3:F:160:PHE:HB3	3:F:169:GLU:HG2	1.96	0.46
2:H:39:GLU:HG2	2:H:267:ARG:HB3	1.97	0.46
1:J:163:THR:HG21	1:J:256:ILE:O	2.15	0.46
2:E:316:LEU:HD11	2:E:354:LEU:HD12	1.98	0.46
3:I:111:MET:O	3:I:114:LYS:HG2	2.14	0.46
2:K:323:ASP:OD2	2:K:324:LYS:HG2	2.16	0.46
1:J:199:TYR:CD1	1:J:227:VAL:HG12	2.51	0.46
1:A:204:GLY:N	1:A:220:CYS:SG	2.88	0.46
1:G:50:PHE:CE2	1:G:52:ALA:HB3	2.47	0.46
3:L:193:TYR:HB2	3:L:200:VAL:HG13	1.97	0.46
1:A:5:HIS:HA	1:A:8:VAL:HG12	1.98	0.46
3:F:206:ARG:HH21	3:F:245:ALA:HB2	1.81	0.46
1:D:199:TYR:HH	1:D:205:THR:HG1	1.59	0.45
1:G:142:THR:OG1	1:J:128:GLN:OE1	2.28	0.45
1:G:396:LEU:HD21	1:G:414:LEU:HB2	1.97	0.45
3:I:250:THR:HB	3:I:257:THR:HB	1.97	0.45
3:L:186:HIS:O	3:L:188:LYS:NZ	2.38	0.45
2:B:164:GLY:N	2:B:277:PRO:O	2.36	0.45
1:G:149:LYS:HB2	1:G:269:MET:SD	2.56	0.45
3:I:225:ASP:OD1	3:I:229:ARG:N	2.48	0.45
1:A:76:GLU:N	1:A:76:GLU:OE1	2.50	0.45
1:D:239:SER:O	2:E:57:SER:OG	2.20	0.45
1:J:398:PRO:HB2	3:L:255:MET:SD	2.57	0.45
1:A:199:TYR:CD2	1:A:208:VAL:HG12	2.52	0.45
2:E:296:ILE:HD11	2:E:346:VAL:HG21	1.98	0.45
3:F:141:MET:HB2	3:F:168:LEU:HD11	1.97	0.45
2:H:21:ARG:NH1	2:H:284:ASP:OD1	2.42	0.45
4:M:147:GLU:OE1	4:M:148:ASN:ND2	2.49	0.45
1:A:199:TYR:CE2	1:A:206:GLY:HA2	2.52	0.45
1:A:6:PHE:O	1:A:10:LYS:HB3	2.16	0.45
3:C:238:ALA:HB2	3:C:264:SER:HB3	1.98	0.45
2:E:104:SER:HB3	2:E:231:VAL:HG13	1.98	0.45
2:H:299:LEU:HD12	2:H:320:TYR:HB3	1.97	0.45
1:J:71:ASP:N	1:J:71:ASP:OD1	2.50	0.45
2:B:129:LEU:HB3	2:B:148:VAL:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:53:THR:HB	2:E:235:GLN:HE22	1.81	0.45
3:L:185:THR:HG21	3:L:229:ARG:CZ	2.46	0.45
1:A:12:THR:O	1:A:68:ARG:NH2	2.50	0.45
2:E:332:SER:HB2	2:E:339:LEU:HD13	1.99	0.45
2:H:40:PRO:HD2	2:H:266:VAL:O	2.17	0.45
1:A:170:HIS:HD2	1:A:238:ASN:HB3	1.81	0.44
3:C:240:GLU:OE1	3:F:179:SER:N	2.50	0.44
1:G:296:TYR:CE1	1:G:306:HIS:HB3	2.52	0.44
1:G:387:MET:HG3	2:H:428:LEU:HD13	1.99	0.44
3:L:200:VAL:HG23	3:L:209:ILE:HG13	1.99	0.44
4:O:116:HIS:O	4:O:130:VAL:HG23	2.17	0.44
2:B:292:GLU:O	2:B:292:GLU:HG3	2.17	0.44
2:B:191:PRO:HB3	2:H:151:ASP:O	2.17	0.44
2:K:231:VAL:O	2:K:231:VAL:HG13	2.18	0.44
2:B:242:TYR:CZ	2:B:246:GLU:HG3	2.52	0.44
3:I:138:ASP:HA	3:I:173:ILE:HD11	2.00	0.44
1:A:297:ARG:HD3	2:B:253:THR:O	2.18	0.44
3:F:119:CYS:SG	3:F:182:SER:HB3	2.58	0.44
1:G:6:PHE:CD1	1:G:62:HIS:HB2	2.53	0.44
3:C:122:GLU:HA	3:C:132:TYR:HA	2.00	0.44
1:G:7:ASN:O	1:G:10:LYS:HG2	2.18	0.44
3:L:237:GLY:HA2	3:L:246:LEU:HA	2.00	0.44
2:B:395:SER:O	2:B:397:VAL:N	2.49	0.43
1:D:196:LYS:HD2	1:D:210:THR:O	2.18	0.43
2:E:21:ARG:HD3	2:E:24:TYR:CD1	2.53	0.43
2:E:44:LEU:HD11	2:E:47:ILE:HD11	2.00	0.43
2:E:137:TYR:O	2:E:140:VAL:HG22	2.18	0.43
3:F:193:TYR:HE2	3:F:225:ASP:HB3	1.82	0.43
1:A:181:LEU:HB3	1:A:222:ILE:HG13	2.00	0.43
1:D:48:ILE:HG12	1:D:111:LEU:HD21	2.00	0.43
3:L:150:ILE:HD12	3:L:150:ILE:H	1.83	0.43
3:C:116:GLU:HB3	3:C:224:PHE:HZ	1.83	0.43
1:J:343:THR:HG21	1:J:357:TYR:O	2.18	0.43
1:A:294:PHE:HB2	1:A:329:TRP:HE3	1.83	0.43
2:E:97:ASP:OD1	2:E:97:ASP:N	2.46	0.43
2:E:345:LYS:NZ	4:N:135:ASP:OD2	2.43	0.43
1:J:343:THR:HG22	1:J:344:GLU:N	2.33	0.43
2:E:320:TYR:CE2	2:E:346:VAL:HG23	2.54	0.43
1:G:275:VAL:HG13	1:G:282:VAL:HG13	1.99	0.43
2:E:369:LEU:O	2:E:371:SER:N	2.52	0.43
2:H:308:HIS:O	2:H:308:HIS:ND1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:369:LEU:O	2:H:370:CYS:C	2.61	0.43
3:C:182:SER:OG	3:C:183:LYS:N	2.52	0.43
2:K:52:LYS:HB3	2:K:52:LYS:HE2	1.84	0.43
1:A:192:VAL:HG12	1:A:194:GLY:H	1.84	0.43
1:A:298:THR:OG1	1:A:303:PRO:O	2.29	0.43
2:E:35:GLU:OE2	2:E:269:MET:HE3	2.19	0.43
1:A:155:THR:CB	1:A:263:ILE:HD13	2.49	0.43
1:D:274:THR:HB	1:D:285:HIS:HB2	2.01	0.43
1:A:157:GLN:O	1:A:258:PHE:HA	2.19	0.43
2:E:144:VAL:HG21	2:E:156:ILE:HD11	2.00	0.43
2:H:74:PRO:HG2	2:H:213:LEU:HD23	1.99	0.43
3:L:252:ASN:N	3:L:255:MET:O	2.48	0.43
2:E:209:GLU:OE2	2:E:209:GLU:N	2.52	0.42
1:G:143:ILE:HD13	1:J:126:ARG:HG2	2.01	0.42
3:C:161:LYS:HB3	3:C:161:LYS:HE3	1.72	0.42
3:F:150:ILE:HG22	3:F:152:ASN:H	1.84	0.42
3:I:142:LYS:HE2	3:I:146:VAL:HG23	2.00	0.42
3:I:193:TYR:HD1	3:I:225:ASP:HA	1.84	0.42
2:B:249:THR:HG23	2:B:254:LYS:NZ	2.35	0.42
2:H:265:PRO:O	2:H:267:ARG:HD3	2.20	0.42
1:J:184:GLN:O	1:J:186:GLY:N	2.52	0.42
2:B:39:GLU:HG3	2:B:267:ARG:HB3	2.02	0.42
2:E:220:LYS:O	2:E:233:TYR:HB2	2.20	0.42
1:G:397:THR:OG1	1:G:398:PRO:HD3	2.19	0.42
3:I:120:ILE:HA	3:I:133:ALA:O	2.20	0.42
1:J:402:THR:OG1	3:L:256:VAL:HG13	2.19	0.42
2:K:409:TRP:O	2:K:413:ILE:HD12	2.18	0.42
1:A:155:THR:HG21	1:A:263:ILE:HD13	2.00	0.42
1:A:291:PRO:HG3	1:A:311:THR:HG22	2.02	0.42
1:D:14:PRO:HG2	1:D:70:ALA:HB2	2.00	0.42
3:F:173:ILE:HD11	3:F:177:MET:HG3	2.01	0.42
3:I:124:LYS:HE2	3:I:127:GLY:C	2.44	0.42
3:L:197:HIS:HD1	3:L:214:GLY:HA2	1.85	0.42
1:A:140:LYS:HD2	1:A:291:PRO:HB2	2.02	0.42
1:G:41:ALA:HB1	1:G:155:THR:HA	2.01	0.42
2:H:243:TRP:O	2:H:247:LYS:HB3	2.20	0.42
1:A:155:THR:O	1:A:260:LEU:HD12	2.19	0.42
2:B:303:VAL:HG21	2:B:378:ALA:HB2	2.02	0.42
1:D:34:ILE:HD11	1:D:113:VAL:HG12	2.02	0.42
2:K:254:LYS:O	2:K:254:LYS:HG3	2.19	0.42
3:L:111:MET:SD	3:L:115:ILE:HD11	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:THR:OG1	1:A:344:GLU:N	2.53	0.42
1:D:155:THR:HG22	1:D:263:ILE:HG21	2.01	0.42
1:D:177:ASP:OD1	1:D:179:THR:HG22	2.20	0.42
1:D:221:LEU:H	1:D:224:GLN:HE21	1.68	0.42
3:F:193:TYR:CE2	3:F:225:ASP:HB3	2.54	0.42
3:F:200:VAL:HG12	3:F:209:ILE:HG12	2.02	0.42
3:F:232:ALA:HB1	3:F:248:VAL:CG2	2.50	0.42
3:I:143:PRO:HG2	3:I:146:VAL:HG22	2.02	0.42
3:L:145:HIS:HD2	3:L:167:ASP:OD2	2.03	0.42
2:B:330:VAL:HA	2:B:368:SER:O	2.19	0.42
3:C:123:VAL:O	3:C:123:VAL:HG13	2.20	0.42
1:D:221:LEU:HD23	1:D:221:LEU:HA	1.85	0.42
2:H:123:LYS:HZ2	2:H:123:LYS:HG2	1.69	0.42
2:K:155:THR:HA	2:K:159:THR:O	2.19	0.42
3:L:139:LYS:HE2	3:L:139:LYS:HB3	1.74	0.41
1:A:6:PHE:CD1	1:A:62:HIS:CD2	3.08	0.41
2:E:134:ARG:HG3	2:E:134:ARG:HH11	1.85	0.41
3:F:157:LYS:C	3:F:158:LEU:HD12	2.45	0.41
1:J:48:ILE:HD11	1:J:101:ILE:HD12	2.02	0.41
1:J:199:TYR:CZ	1:J:201:CYS:SG	3.13	0.41
2:E:132:LYS:NZ	2:E:145:ASP:HB3	2.35	0.41
2:E:402:MET:O	2:E:403:SER:HB2	2.20	0.41
2:H:213:LEU:HA	2:H:213:LEU:HD12	1.83	0.41
1:J:41:ALA:HB1	1:J:155:THR:HA	2.02	0.41
4:M:117:GLU:HB3	4:M:128:ILE:O	2.21	0.41
2:B:47:ILE:N	2:B:205:SER:O	2.47	0.41
1:D:155:THR:HG21	1:D:263:ILE:HD13	1.98	0.41
3:F:192:HIS:HA	3:F:201:GLN:HA	2.02	0.41
2:H:252:ASN:OD1	2:H:261:ILE:HB	2.20	0.41
2:K:264:ASN:HB2	2:K:265:PRO:HD3	2.02	0.41
3:L:216:PRO:HA	3:L:267:TRP:HB3	2.02	0.41
2:B:228:MET:HG3	2:B:230:HIS:CD2	2.56	0.41
4:O:118:ILE:HG23	4:O:130:VAL:HG22	2.02	0.41
2:B:219:LEU:HD12	2:B:220:LYS:H	1.85	0.41
1:D:187:ASN:CG	1:D:218:ASN:HA	2.46	0.41
2:K:263:THR:OG1	2:K:264:ASN:N	2.49	0.41
1:A:210:THR:HB	1:A:213:SER:OG	2.20	0.41
3:C:121:PHE:O	3:C:133:ALA:N	2.54	0.41
2:E:292:GLU:OE1	2:E:292:GLU:HA	2.20	0.41
2:E:292:GLU:OE2	4:N:116:HIS:CD2	2.74	0.41
2:K:199:ARG:HA	2:K:199:ARG:HD3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:178:ARG:HD3	1:G:178:ARG:HA	1.78	0.41
1:A:251:LYS:HA	1:A:251:LYS:HD3	1.83	0.41
2:B:42:LEU:HB3	2:B:122:TYR:CD2	2.56	0.41
2:B:132:LYS:HB2	2:B:132:LYS:HE2	1.89	0.41
2:B:306:CYS:HB3	2:B:380:CYS:HA	2.03	0.41
3:C:202:TYR:CZ	3:C:205:GLY:HA2	2.56	0.41
1:J:242:VAL:O	2:K:58:PRO:HD2	2.21	0.41
2:K:344:ALA:HB1	2:K:352:VAL:HG21	2.02	0.41
1:A:80:ARG:O	1:A:80:ARG:NH2	2.47	0.41
3:F:251:TRP:CD1	3:F:256:VAL:HG23	2.52	0.41
2:H:292:GLU:OE2	2:H:292:GLU:HA	2.21	0.41
1:J:195:LYS:HD2	1:J:229:VAL:HG11	2.02	0.41
3:L:185:THR:HB	3:L:187:GLU:OE2	2.21	0.41
3:L:234:VAL:HA	3:L:248:VAL:HG23	2.03	0.41
1:A:240:PRO:HB3	2:B:55:VAL:HG12	2.04	0.40
1:D:72:GLY:HA2	2:E:89:TRP:CH2	2.56	0.40
2:H:230:HIS:CE1	2:H:232:PRO:HG3	2.56	0.40
1:G:203:CYS:HB3	1:G:224:GLN:OE1	2.22	0.40
2:H:7:MET:HE1	2:H:31:MET:HG3	2.03	0.40
1:J:155:THR:O	1:J:260:LEU:HD12	2.21	0.40
1:D:162:LYS:HB2	1:D:255:HIS:CG	2.57	0.40
1:J:157:GLN:O	1:J:258:PHE:HA	2.22	0.40
3:L:265:GLU:OE2	3:L:266:GLU:N	2.55	0.40
1:A:412:GLY:HA2	1:A:417:ALA:HB3	2.02	0.40
2:B:296:ILE:CB	2:B:369:LEU:HD23	2.52	0.40
3:C:237:GLY:HA2	3:C:246:LEU:HA	2.04	0.40
1:D:199:TYR:CE2	1:D:206:GLY:HA2	2.57	0.40
1:D:247:GLU:HB3	1:D:248:PRO:HD3	2.03	0.40
3:F:123:VAL:HG23	3:F:149:VAL:C	2.46	0.40
1:G:199:TYR:OH	1:G:217:ILE:HG21	2.20	0.40
2:K:321:LYS:HE3	2:K:321:LYS:HB2	1.90	0.40
1:D:40:GLU:HG2	1:D:156:TYR:OH	2.21	0.40
1:D:306:HIS:CG	1:D:307:GLU:H	2.39	0.40
2:E:85:TYR:CE1	2:E:97:ASP:HA	2.57	0.40
2:E:335:ASN:OD1	2:E:335:ASN:N	2.53	0.40
3:I:193:TYR:HB2	3:I:200:VAL:HG23	2.04	0.40
3:L:250:THR:N	3:L:257:THR:O	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

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](#)

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	J	500	1	14,14,15	0.16	0	17,19,21	0.46	0
5	NAG	D	501	1	14,14,15	0.38	0	17,19,21	0.58	0
5	NAG	E	500	2	14,14,15	0.38	0	17,19,21	0.36	0
5	NAG	K	500	2	14,14,15	0.17	0	17,19,21	0.51	0
5	NAG	G	500	1	14,14,15	0.25	0	17,19,21	0.44	0
5	NAG	G	501	1	14,14,15	0.27	0	17,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	J	501	1	14,14,15	0.24	0	17,19,21	0.61	0
5	NAG	D	500	1	14,14,15	0.22	0	17,19,21	0.47	0
5	NAG	B	500	2	14,14,15	0.20	0	17,19,21	0.48	0
5	NAG	H	500	2	14,14,15	0.47	0	17,19,21	0.38	0
5	NAG	A	500	1	14,14,15	0.21	0	17,19,21	0.46	0
5	NAG	A	501	1	14,14,15	0.40	0	17,19,21	1.34	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	J	500	1	-	2/6/23/26	0/1/1/1
5	NAG	D	501	1	-	0/6/23/26	0/1/1/1
5	NAG	E	500	2	-	0/6/23/26	0/1/1/1
5	NAG	K	500	2	-	2/6/23/26	0/1/1/1
5	NAG	G	500	1	-	2/6/23/26	0/1/1/1
5	NAG	G	501	1	-	2/6/23/26	0/1/1/1
5	NAG	J	501	1	-	4/6/23/26	0/1/1/1
5	NAG	D	500	1	-	1/6/23/26	0/1/1/1
5	NAG	B	500	2	-	2/6/23/26	0/1/1/1
5	NAG	H	500	2	-	0/6/23/26	0/1/1/1
5	NAG	A	500	1	-	2/6/23/26	0/1/1/1
5	NAG	A	501	1	-	6/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	NAG	C2-N2-C7	4.57	129.03	122.90
5	A	501	NAG	C1-C2-N2	2.13	113.80	110.43

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	500	NAG	C4-C5-C6-O6
5	G	500	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	K	500	NAG	O5-C5-C6-O6
5	A	500	NAG	O5-C5-C6-O6
5	B	500	NAG	O5-C5-C6-O6
5	J	500	NAG	O5-C5-C6-O6
5	J	501	NAG	O5-C5-C6-O6
5	A	501	NAG	C4-C5-C6-O6
5	G	500	NAG	C4-C5-C6-O6
5	J	501	NAG	C4-C5-C6-O6
5	A	501	NAG	O5-C5-C6-O6
5	A	500	NAG	C4-C5-C6-O6
5	K	500	NAG	C4-C5-C6-O6
5	A	501	NAG	C8-C7-N2-C2
5	A	501	NAG	O7-C7-N2-C2
5	D	500	NAG	O5-C5-C6-O6
5	G	501	NAG	C4-C5-C6-O6
5	G	501	NAG	O5-C5-C6-O6
5	J	500	NAG	C4-C5-C6-O6
5	J	501	NAG	C3-C2-N2-C7
5	A	501	NAG	C1-C2-N2-C7
5	J	501	NAG	C1-C2-N2-C7
5	A	501	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	NAG	1	0

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.

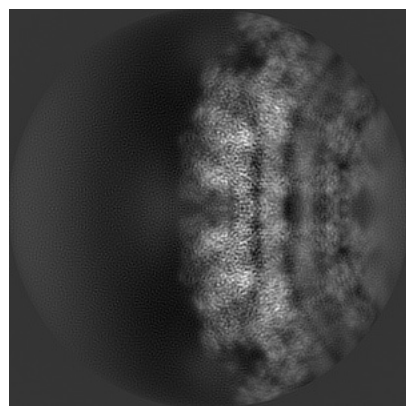
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35451. These allow visual inspection of the internal detail of the map and identification of artifacts.

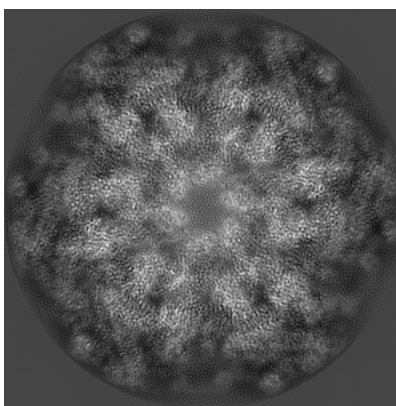
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

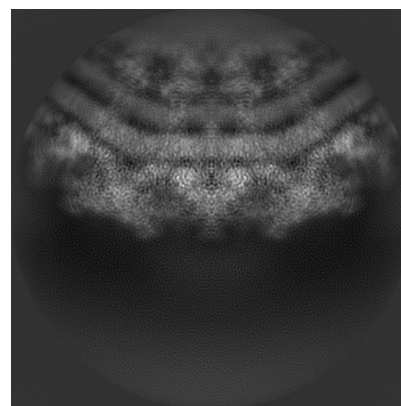
6.1.1 Primary map



X

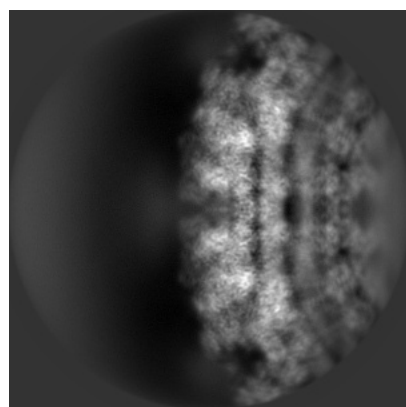


Y

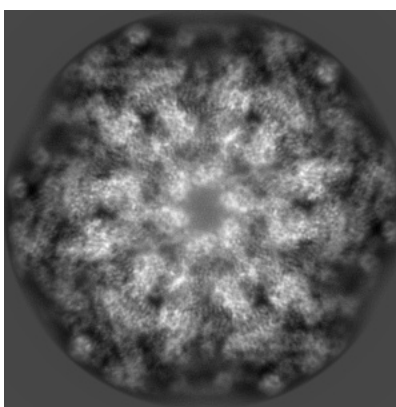


Z

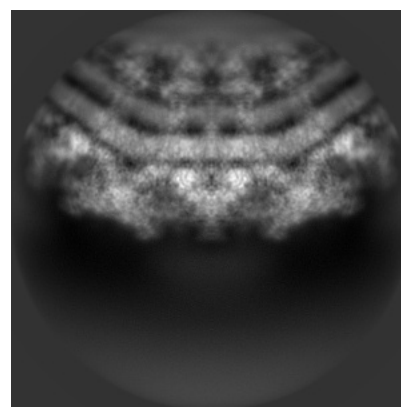
6.1.2 Raw map



X



Y

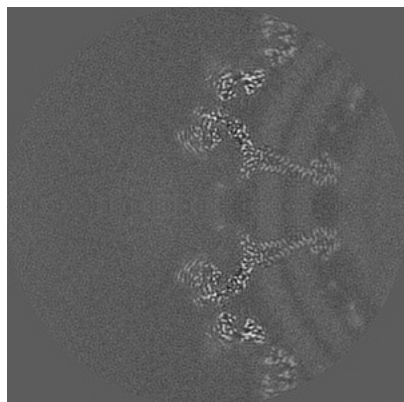


Z

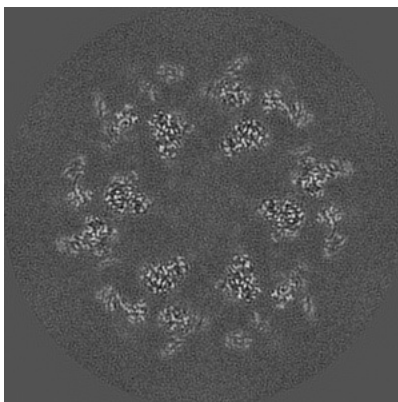
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

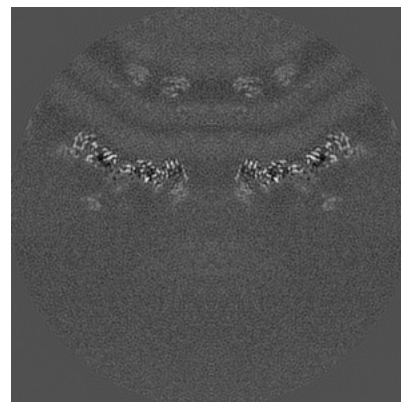
6.2.1 Primary map



X Index: 192

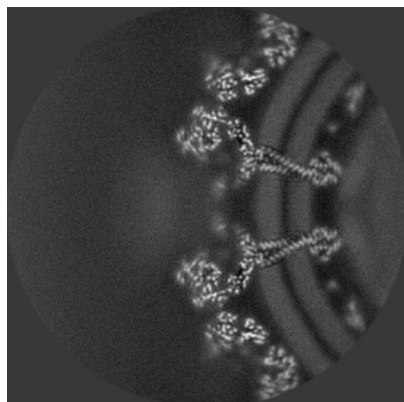


Y Index: 192

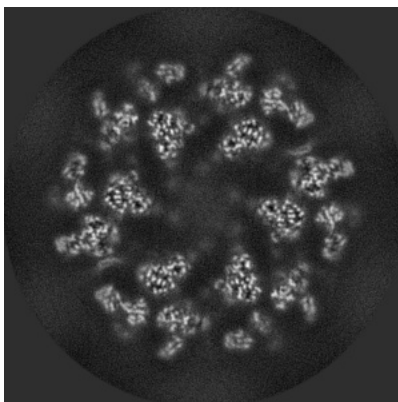


Z Index: 192

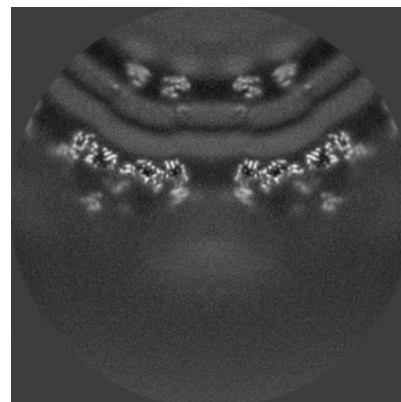
6.2.2 Raw map



X Index: 192



Y Index: 192

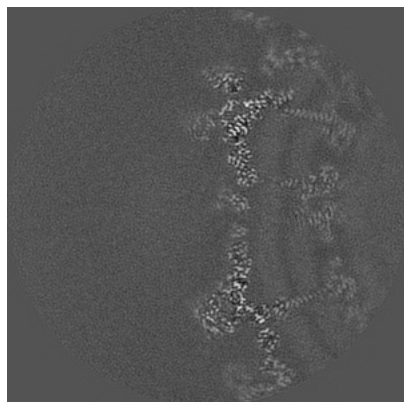


Z Index: 192

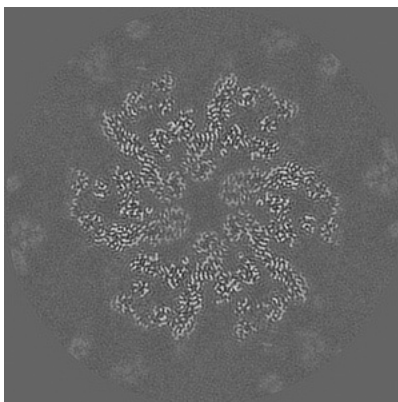
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

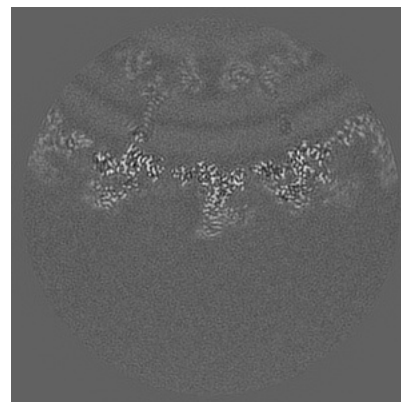
6.3.1 Primary map



X Index: 165

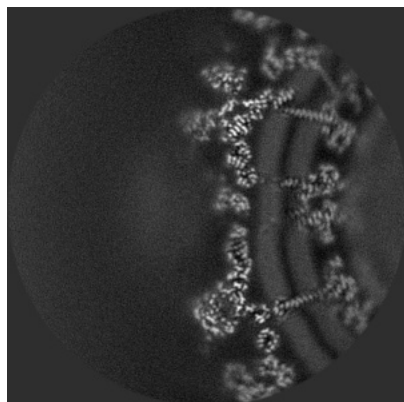


Y Index: 222

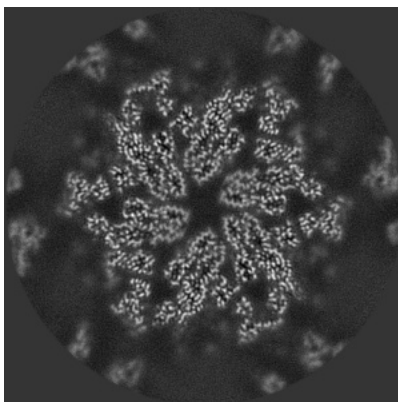


Z Index: 124

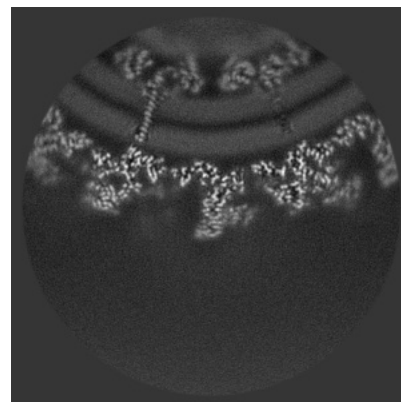
6.3.2 Raw map



X Index: 165



Y Index: 226

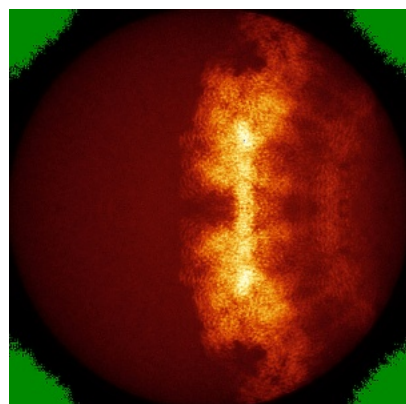


Z Index: 125

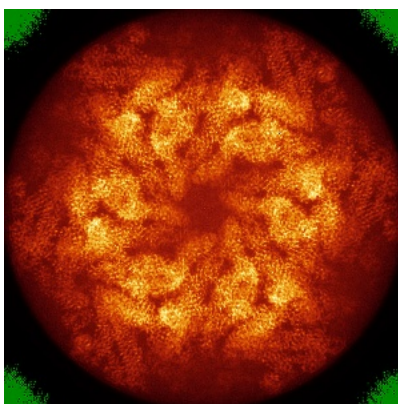
The images above show the largest variance slices of the map in three orthogonal directions.

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

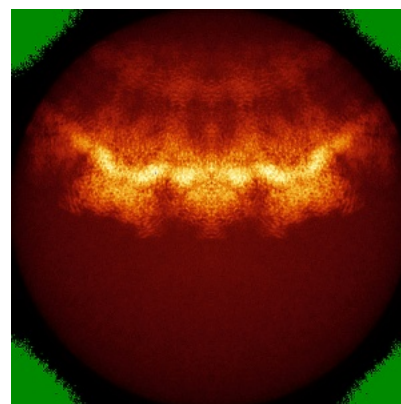
6.4.1 Primary map



X

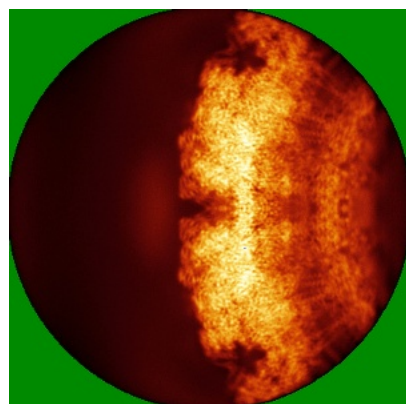


Y

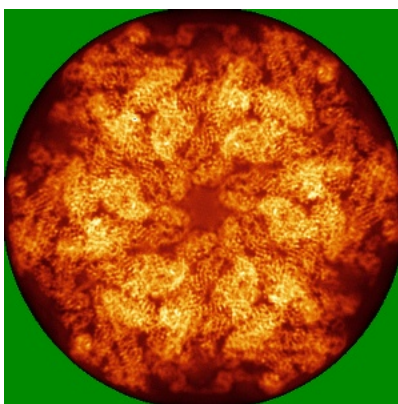


Z

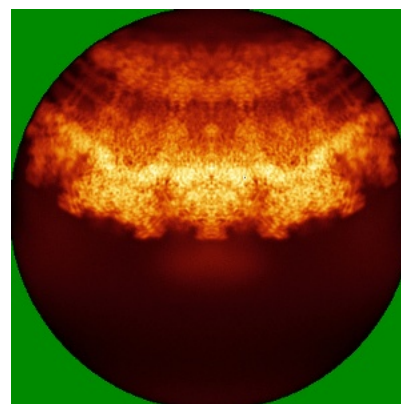
6.4.2 Raw map



X



Y

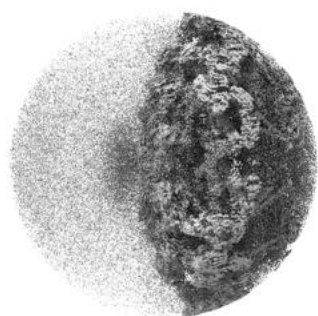


Z

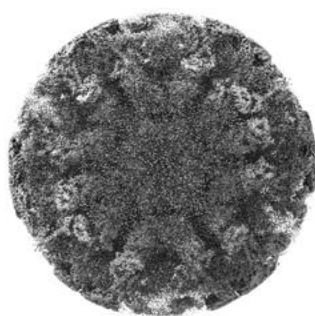
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

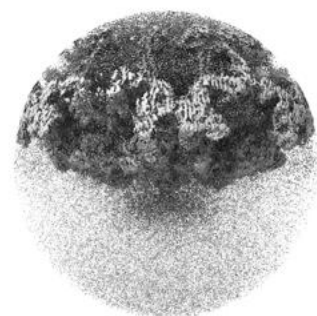
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

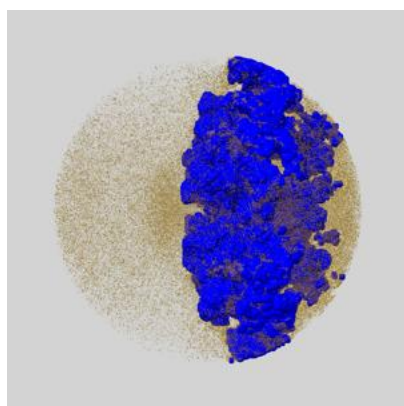
6.6 Mask visualisation [i](#)

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

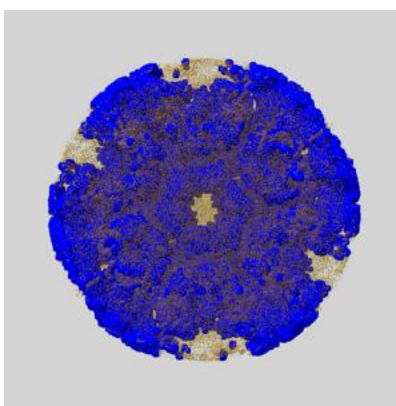
A mask typically either:

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

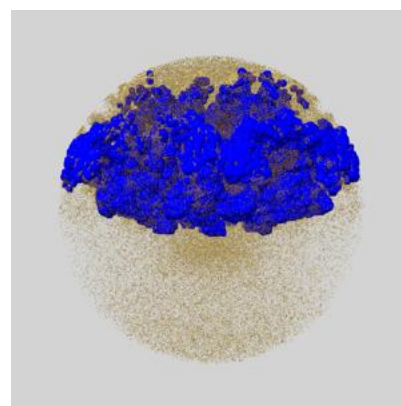
6.6.1 emd_35451_msk_1.map [i](#)



X



Y

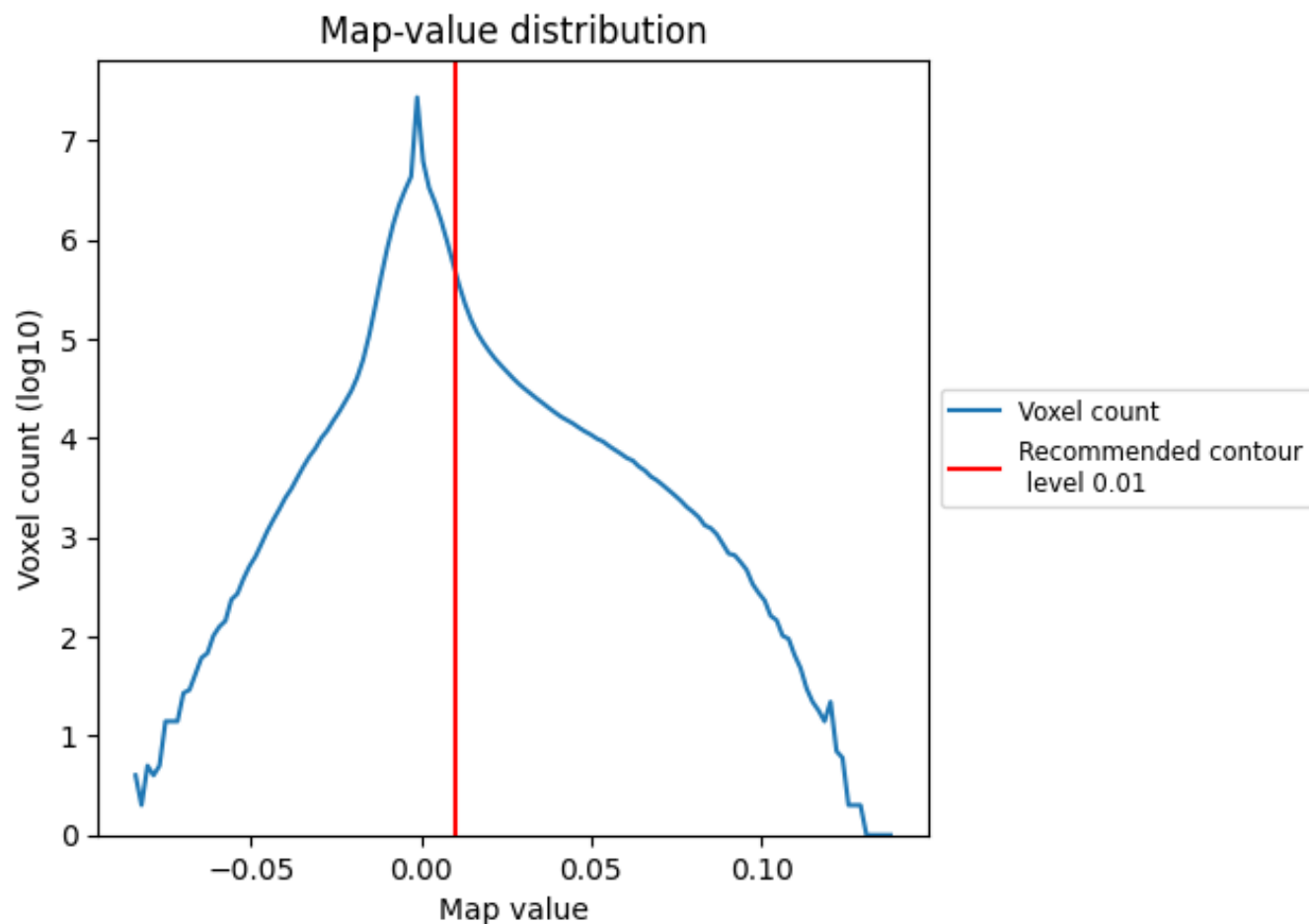


Z

7 Map analysis [i](#)

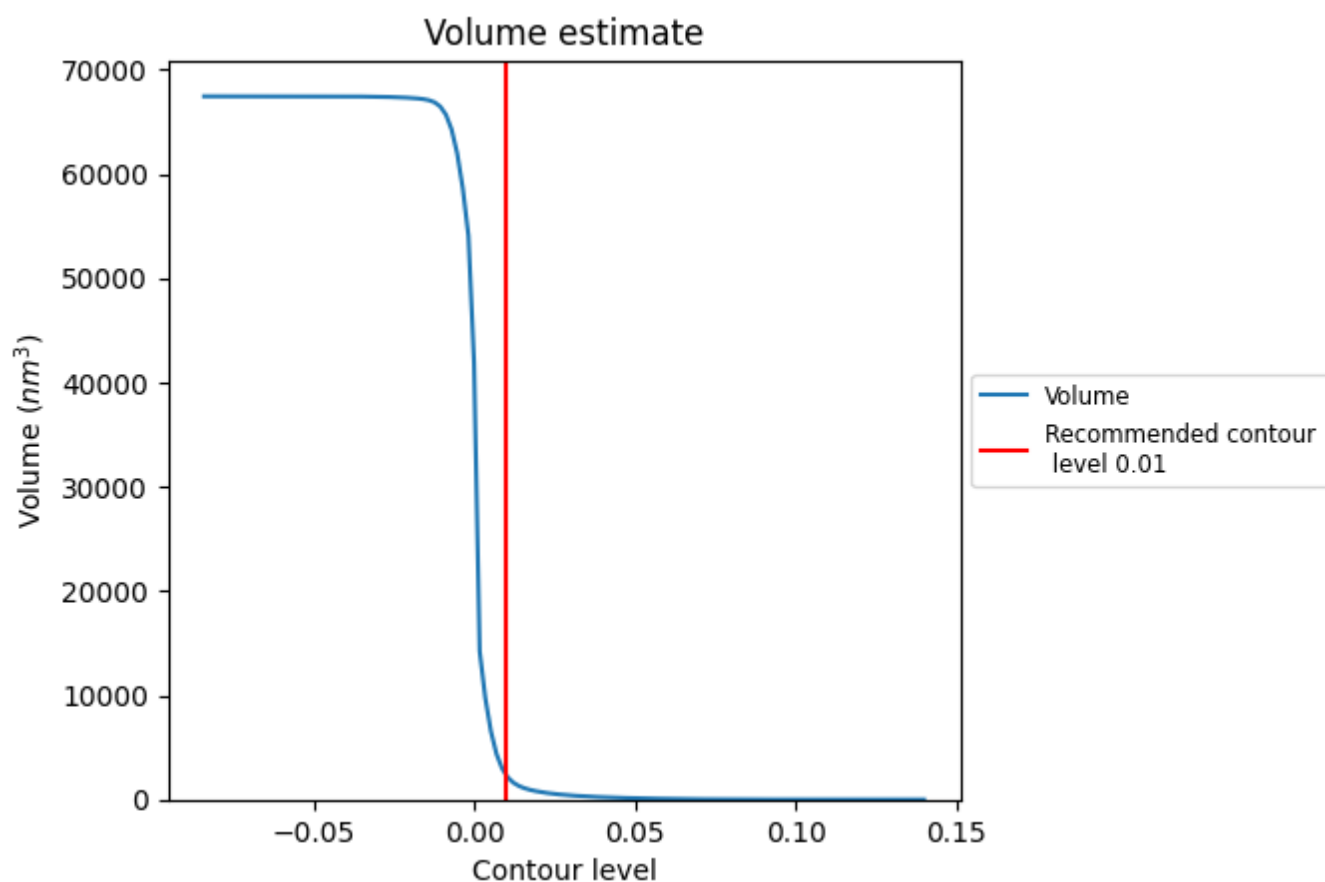
This section contains the results of statistical analysis of the map.

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.

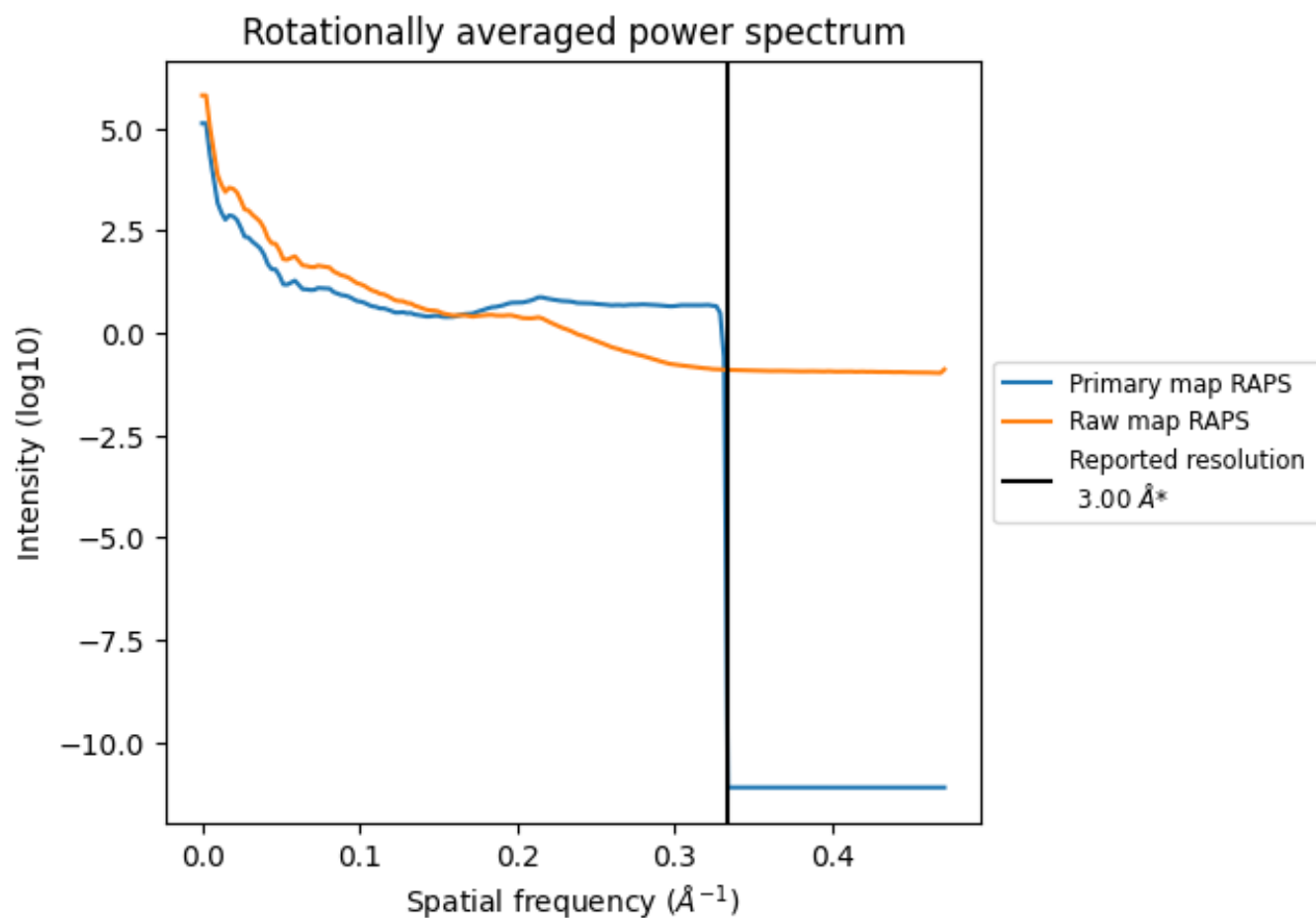
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2337 nm³; this corresponds to an approximate mass of 2111 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 ⓘ

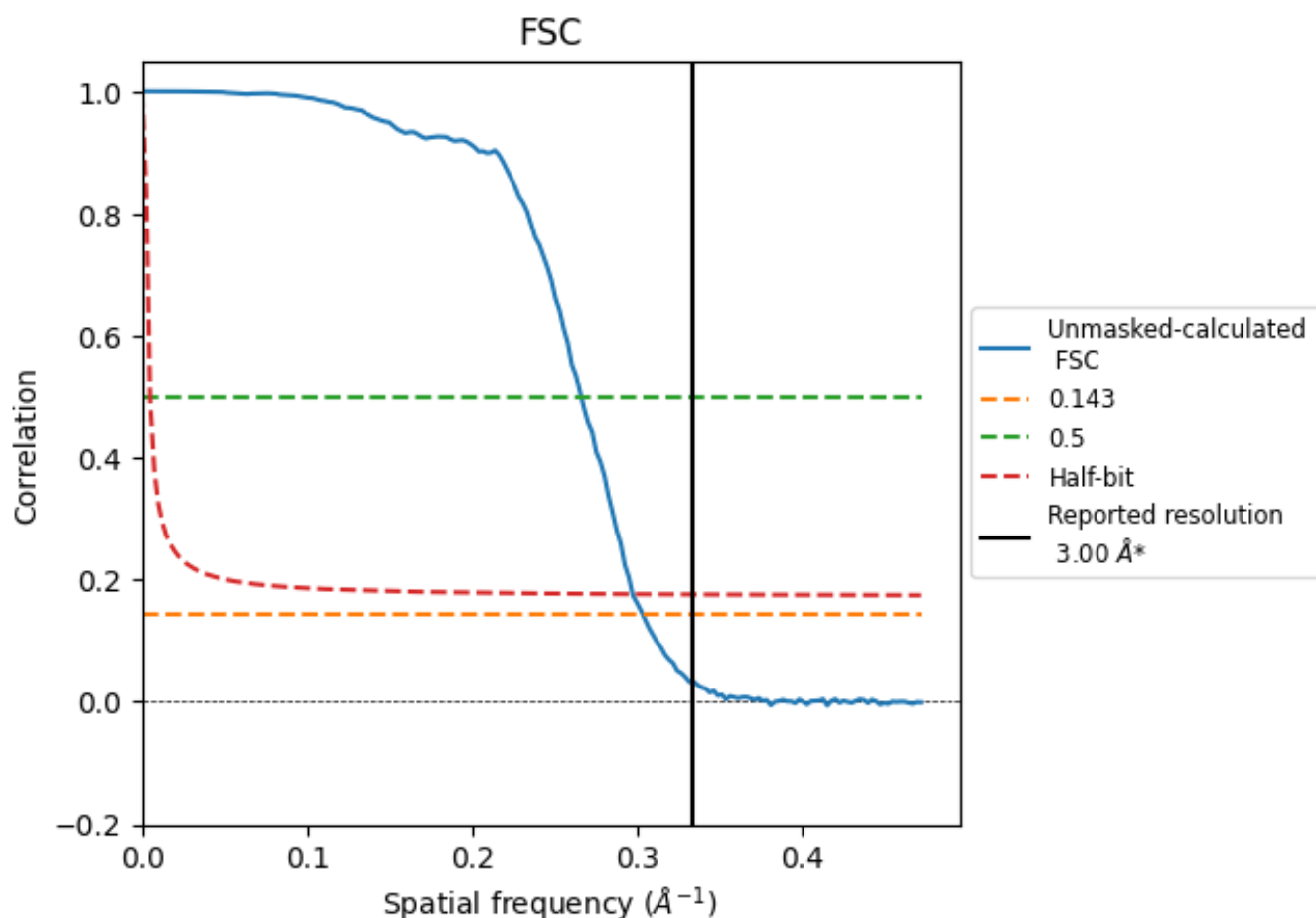


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

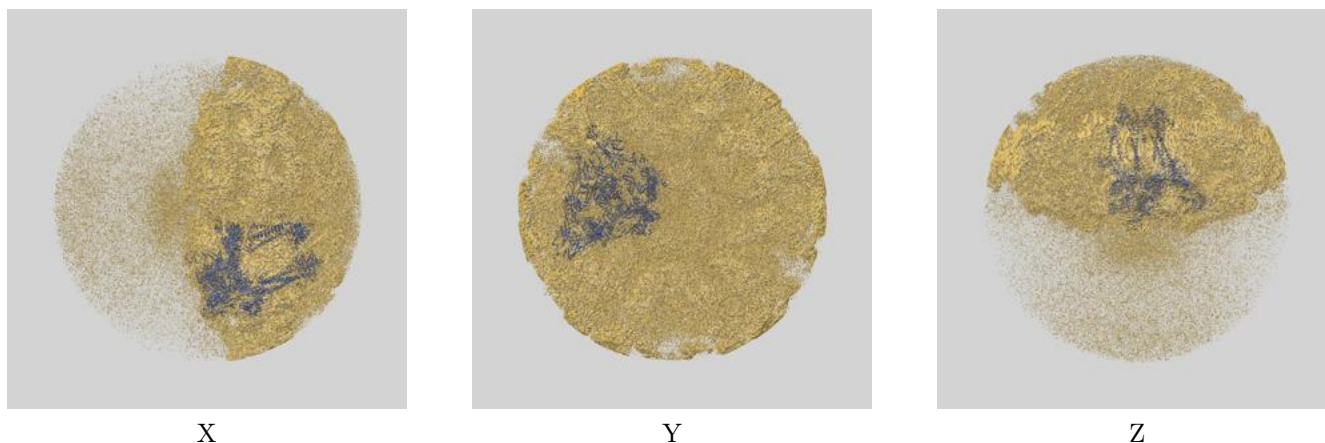
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.30	3.76	3.37

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

9 Map-model fit [i](#)

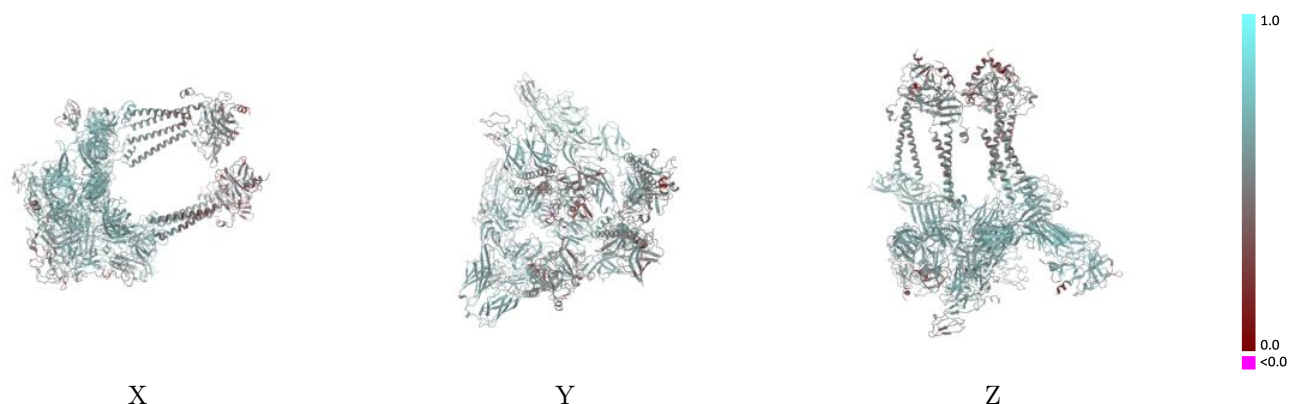
This section contains information regarding the fit between EMDB map EMD-35451 and PDB model 8IHP. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

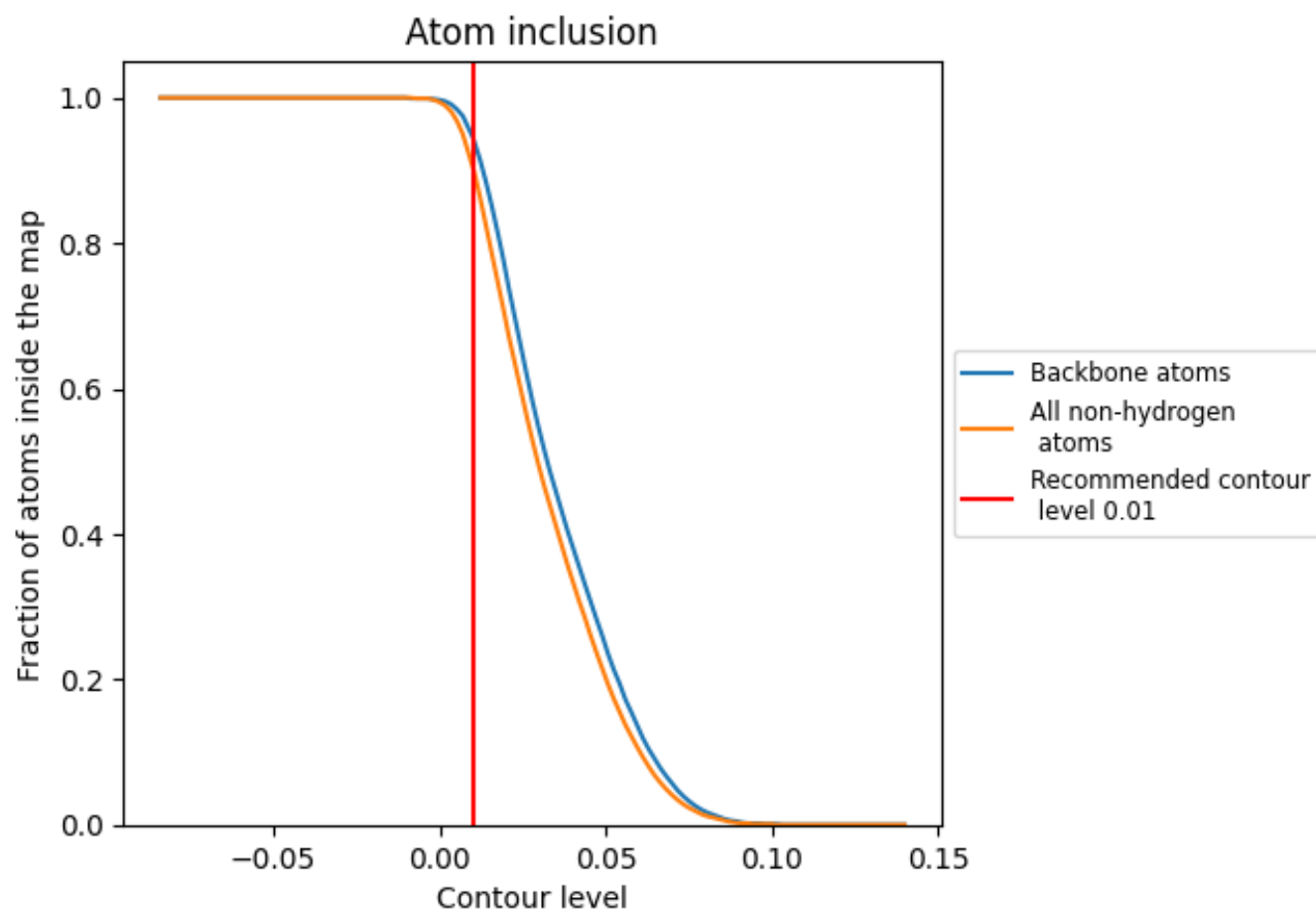


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 90% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9040	 0.5560
A	 0.9390	 0.5710
B	 0.9550	 0.6000
C	 0.8030	 0.4830
D	 0.9310	 0.5640
E	 0.9530	 0.5900
F	 0.7940	 0.4800
G	 0.9190	 0.5620
H	 0.9510	 0.5960
I	 0.6260	 0.3970
J	 0.9300	 0.5650
K	 0.9490	 0.5910
L	 0.7160	 0.4660
M	 0.8320	 0.4800
N	 0.7300	 0.3570
O	 0.7120	 0.3660

