



Full wwPDB EM Validation Report ⓘ

Nov 4, 2025 – 07:05 PM EST

PDB ID : 9OCB / pdb_00009ocb
EMDB ID : EMD-70309
Title : Sf11 capsid Icosahedral Reconstruction
Authors : Subramanian, S.; Parent, K.N.
Deposited on : 2025-04-24
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.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

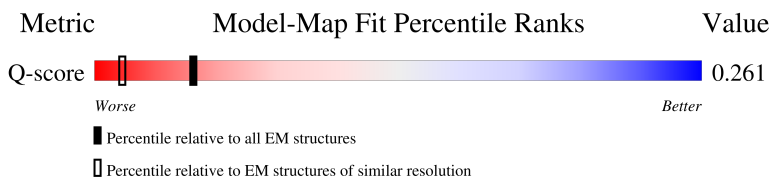
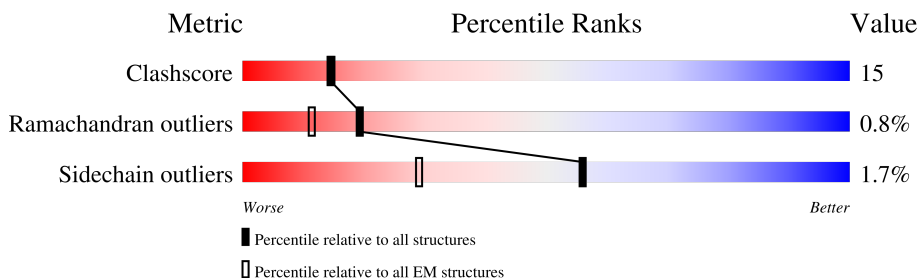
1 Overall quality at a glance

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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
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	356	
1	B	356	
1	C	356	
1	D	356	

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Mol	Chain	Length	Quality of chain
1	E	356	<div><div></div><div>16%62%24%13%</div></div>
1	F	356	<div><div></div><div>19%61%26%13%</div></div>
1	G	356	<div><div></div><div>19%58%24%15%</div></div>
2	H	155	<div><div></div><div>17%64%32%</div></div>
2	I	155	<div><div></div><div>8%57%36%</div></div>
2	J	155	<div><div></div><div>12%54%37%</div></div>
2	K	155	<div><div></div><div>9%59%34%</div></div>
2	L	155	<div><div></div><div>18%68%28%</div></div>
2	M	155	<div><div></div><div>5%73%25%</div></div>
2	N	155	<div><div></div><div>6%73%24%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24504 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 Major capsid protein gp39.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	310	Total	C	N	O	S	0	0
			2430	1532	425	465	8		
1	B	308	Total	C	N	O	S	0	0
			2411	1521	421	461	8		
1	C	309	Total	C	N	O	S	0	0
			2418	1525	423	462	8		
1	D	309	Total	C	N	O	S	0	0
			2422	1528	424	462	8		
1	E	308	Total	C	N	O	S	0	0
			2418	1525	423	462	8		
1	F	309	Total	C	N	O	S	0	0
			2425	1529	424	464	8		
1	G	301	Total	C	N	O	S	0	0
			2362	1491	412	451	8		

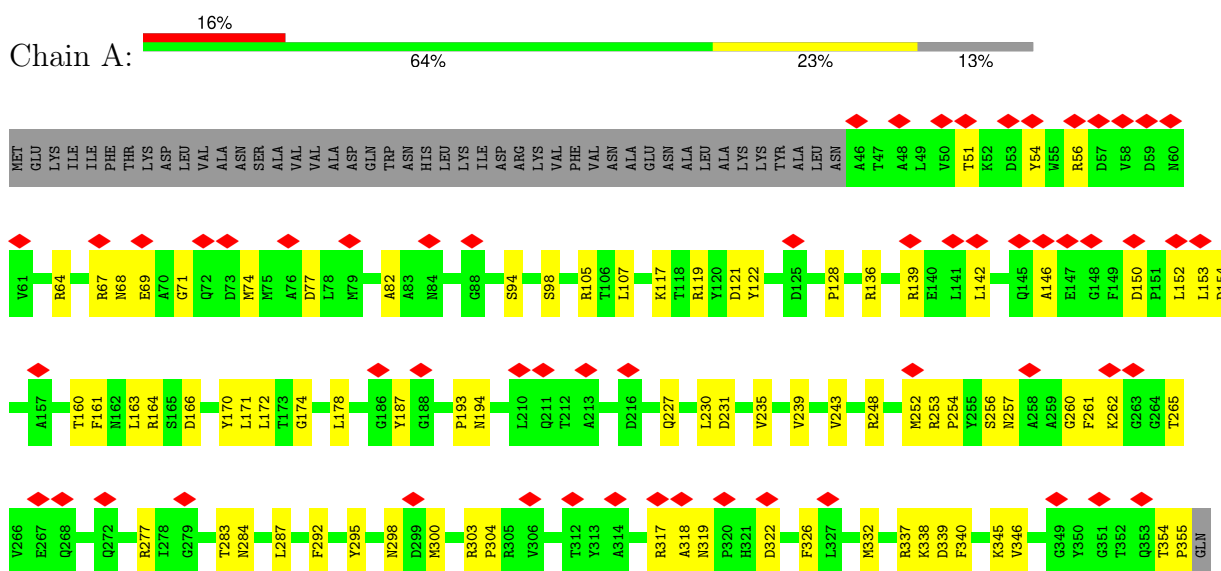
- Molecule 2 is a protein called Putative capsid decoration protein gp40.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	152	Total	C	N	O	S	0	0
			1097	686	192	215	4		
2	I	150	Total	C	N	O	S	0	0
			1085	679	190	212	4		
2	J	151	Total	C	N	O	S	0	0
			1083	680	191	208	4		
2	K	149	Total	C	N	O	S	0	0
			1076	673	189	210	4		
2	L	152	Total	C	N	O	S	0	0
			1094	685	192	213	4		
2	M	151	Total	C	N	O	S	0	0
			1092	683	191	214	4		
2	N	152	Total	C	N	O	S	0	0
			1091	683	189	215	4		

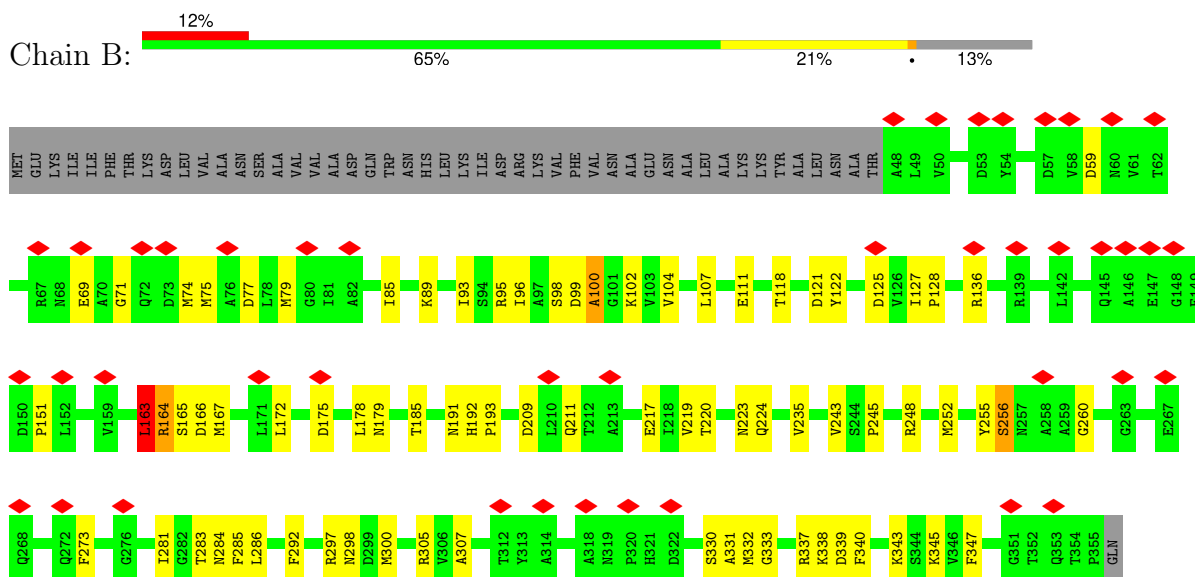
3 Residue-property plots

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: Major capsid protein gp39

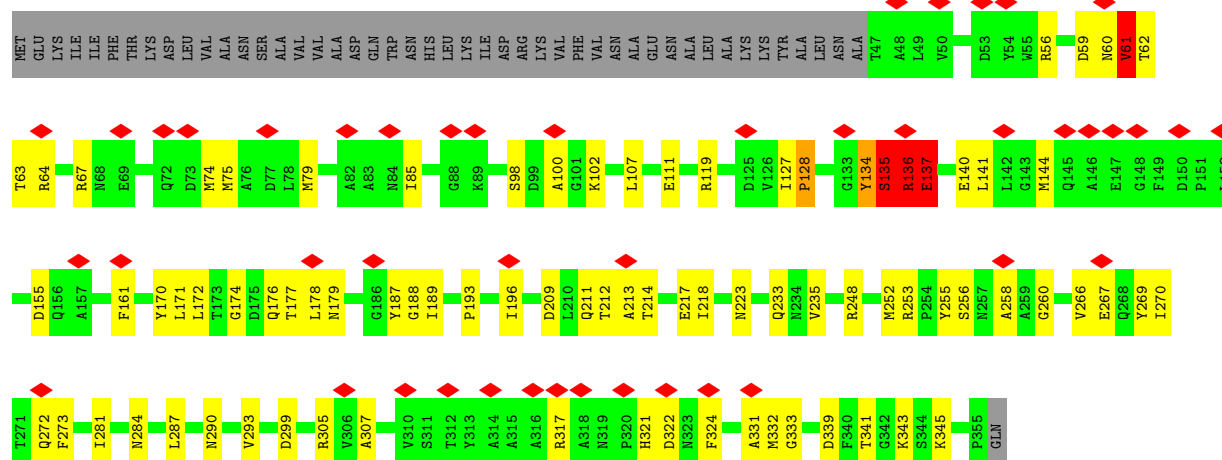


• Molecule 1: Major capsid protein gp39



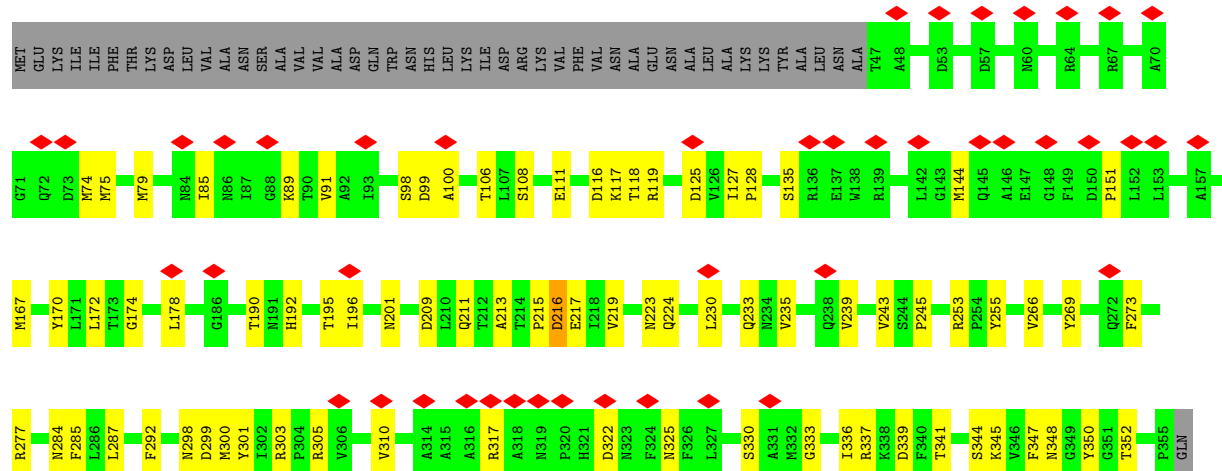
• Molecule 1: Major capsid protein gp39

Chain C: 



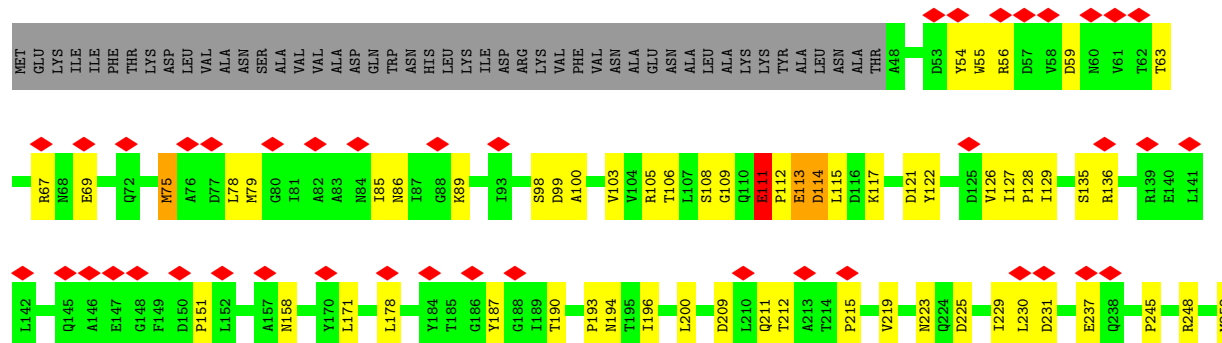
• Molecule 1: Major capsid protein gp39

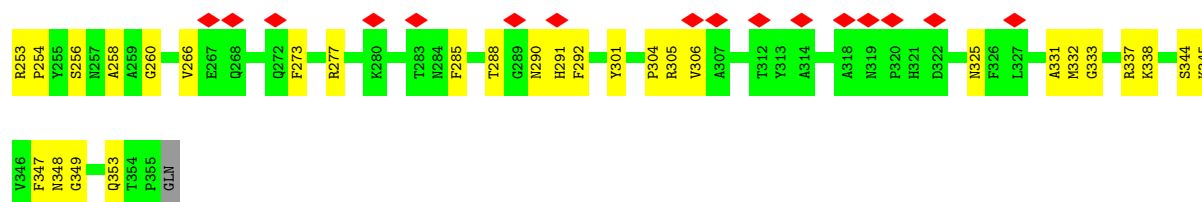
Chain D: 



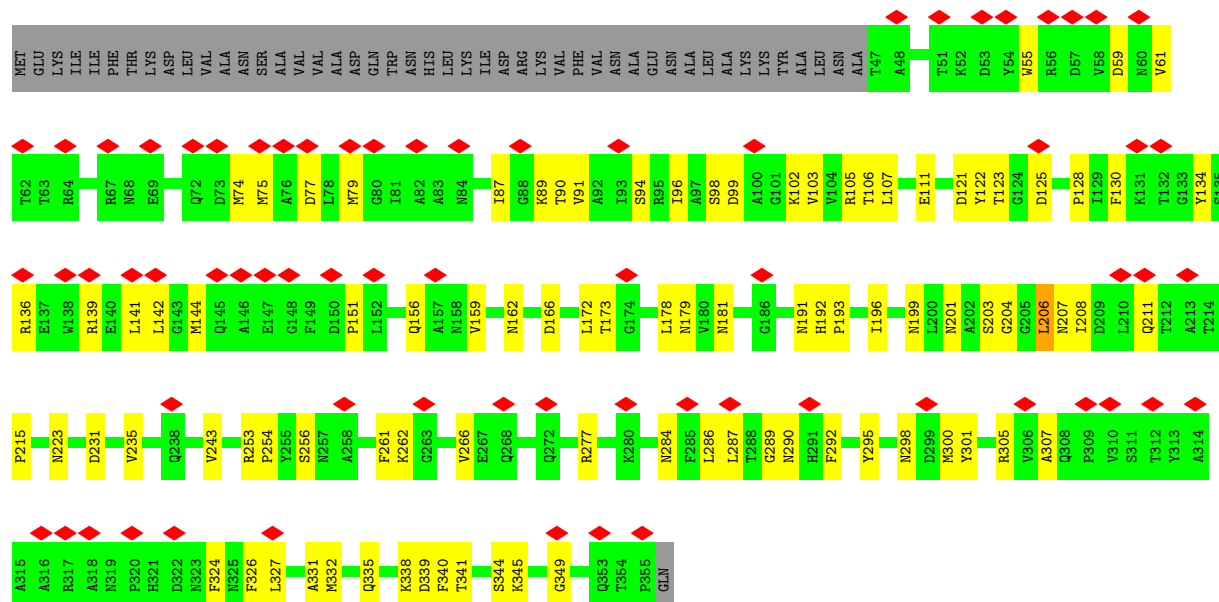
• Molecule 1: Major capsid protein gp39

Chain E: 

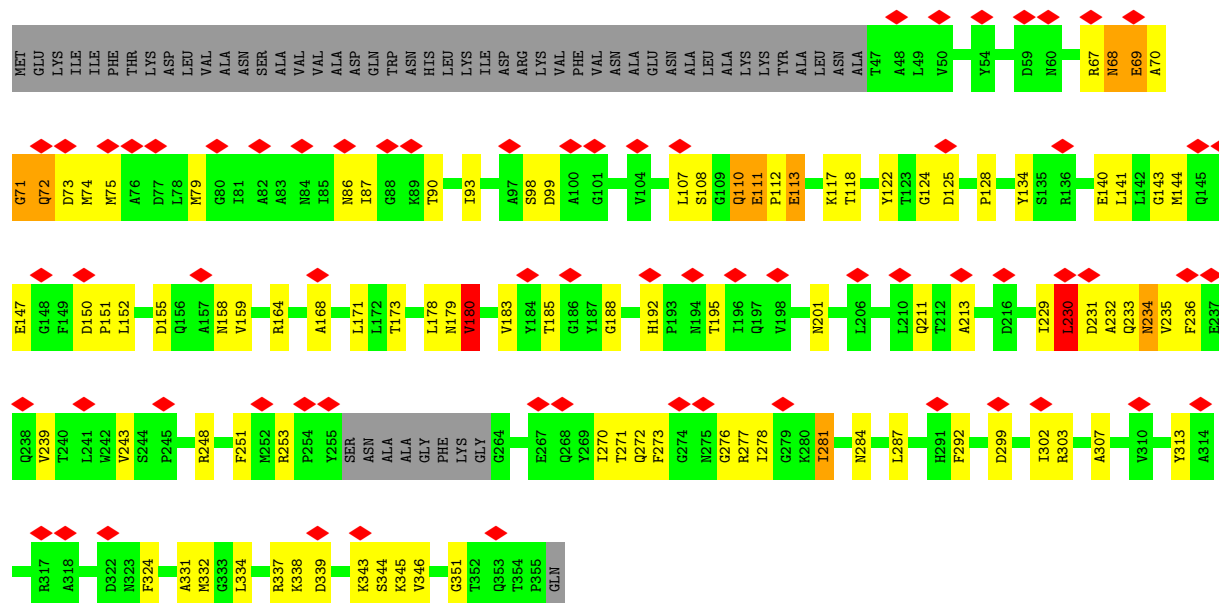




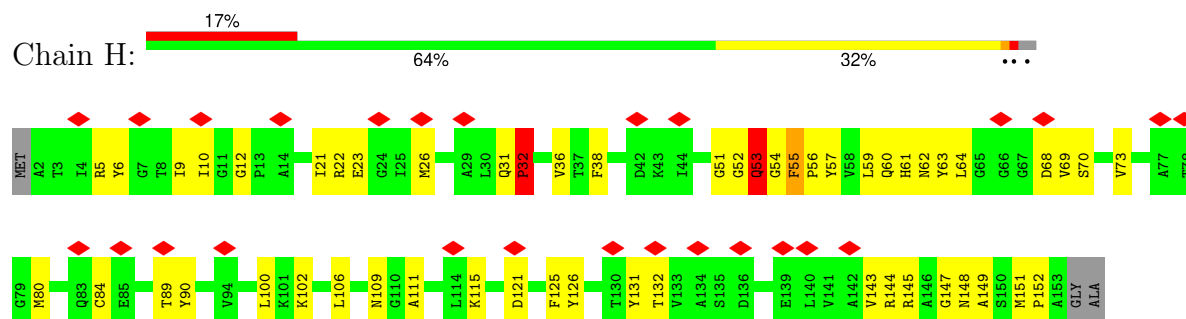
• Molecule 1: Major capsid protein gp39



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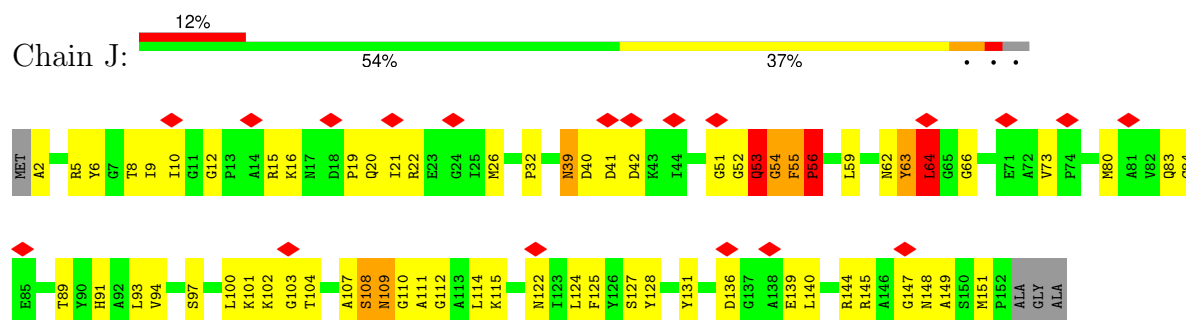
- Molecule 2: Putative capsid decoration protein gp40



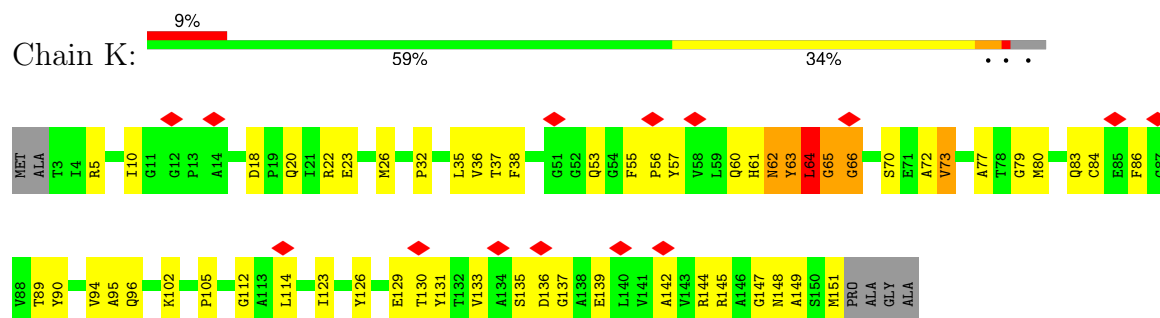
- Molecule 2: Putative capsid decoration protein gp40



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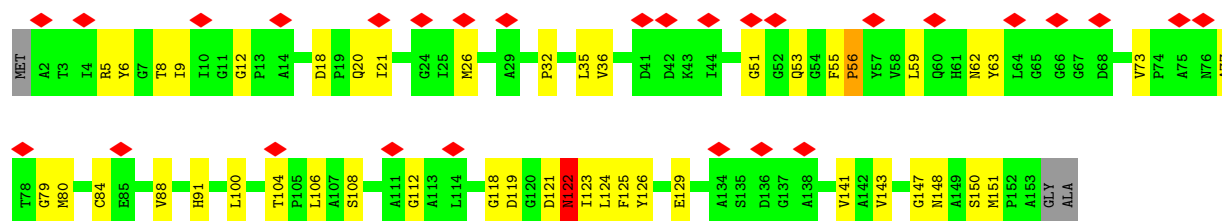


- Molecule 2: Putative capsid decoration protein gp40

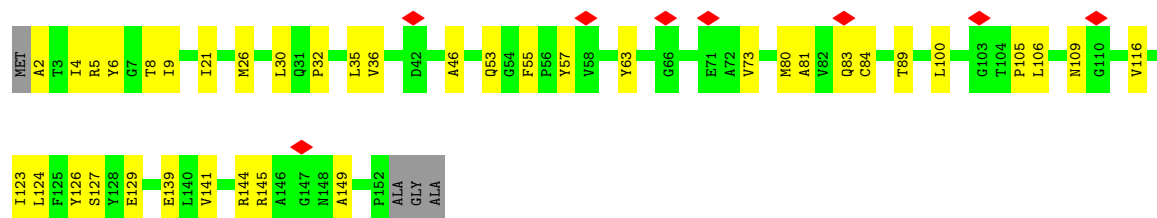
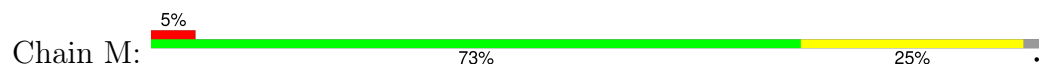


- Molecule 2: Putative capsid decoration protein gp40

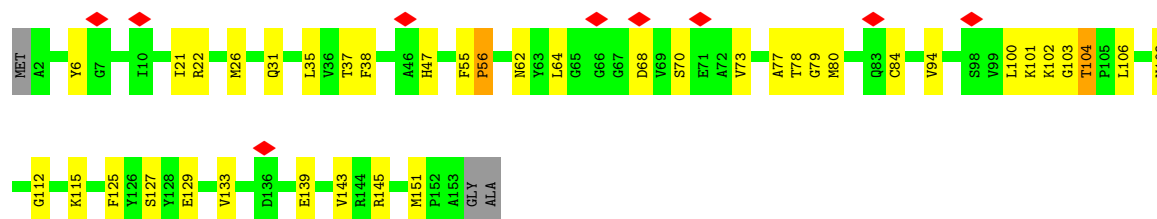
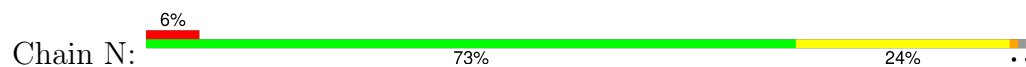




• Molecule 2: Putative capsid decoration protein gp40



• Molecule 2: Putative capsid decoration protein gp40



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	43242	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	3.757	Depositor
Minimum map value	-2.145	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.170	Depositor
Recommended contour level	0.47	Depositor
Map size (\AA)	1000.8, 1000.8, 1000.8	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.668, 1.668, 1.668	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/2481	0.41	0/3371
1	B	0.43	2/2462 (0.1%)	0.59	2/3346 (0.1%)
1	C	0.47	2/2469 (0.1%)	0.71	8/3356 (0.2%)
1	D	0.33	0/2473	0.46	1/3360 (0.0%)
1	E	0.32	0/2469	0.57	5/3354 (0.1%)
1	F	0.32	0/2476	0.50	2/3364 (0.1%)
1	G	0.47	1/2411 (0.0%)	0.70	3/3278 (0.1%)
2	H	0.47	1/1117 (0.1%)	0.72	4/1519 (0.3%)
2	I	0.36	1/1105 (0.1%)	0.63	1/1502 (0.1%)
2	J	0.62	1/1103 (0.1%)	1.33	18/1500 (1.2%)
2	K	0.45	0/1095	0.74	6/1488 (0.4%)
2	L	0.34	0/1114	0.62	3/1515 (0.2%)
2	M	0.28	0/1112	0.46	0/1512
2	N	0.37	0/1111	0.54	0/1512
All	All	0.39	8/24998 (0.0%)	0.64	53/33977 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	H	0	1
2	I	0	2
2	J	0	1
2	K	0	2
All	All	0	7

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	55	PHE	CA-C	-8.14	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	55	PHE	CA-C	-8.05	1.42	1.52
1	C	135	SER	CA-CB	-7.02	1.41	1.53
1	B	256	SER	CA-CB	-6.49	1.42	1.53
1	C	128	PRO	CA-CB	-5.90	1.46	1.53
1	B	100	ALA	CA-CB	-5.74	1.44	1.53
2	I	70	SER	CA-CB	-5.64	1.44	1.54
1	G	108	SER	CA-CB	-5.20	1.45	1.53

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	55	PHE	CB-CA-C	-22.67	95.10	111.20
2	J	55	PHE	N-CA-CB	13.10	126.20	111.66
2	H	55	PHE	CB-CA-C	-12.76	85.04	110.17
2	J	56	PRO	N-CA-CB	-10.46	92.26	103.25
1	E	115	LEU	N-CA-CB	-10.15	95.55	110.17
2	J	112	GLY	CA-C-N	-10.13	108.78	122.16
2	J	112	GLY	C-N-CA	-10.13	108.78	122.16
2	J	56	PRO	N-CD-CG	-9.87	88.40	103.20
2	J	56	PRO	CA-C-N	-9.14	109.30	122.19
2	J	56	PRO	C-N-CA	-9.14	109.30	122.19
2	J	109	ASN	N-CA-C	-8.84	103.05	113.21
1	E	112	PRO	N-CD-CG	-8.46	90.52	103.20
1	G	112	PRO	N-CA-CB	-8.24	96.52	103.36
2	H	55	PHE	CA-CB-CG	8.21	122.01	113.80
1	C	137	GLU	CB-CA-C	8.18	122.86	109.70
1	E	112	PRO	N-CA-CB	-8.06	94.79	103.25
2	H	32	PRO	N-CA-CB	-8.05	94.80	103.25
2	K	64	LEU	N-CA-C	-7.99	103.61	112.72
1	C	100	ALA	N-CA-CB	-7.76	97.79	110.59
1	B	163	LEU	N-CA-C	-7.69	101.59	112.13
1	C	137	GLU	N-CA-CB	-7.54	97.69	109.69
2	J	55	PHE	N-CA-C	-6.77	96.77	111.53
2	J	64	LEU	N-CA-C	-6.47	105.35	113.18
1	E	111	GLU	CB-CA-C	6.47	118.77	109.26
1	E	111	GLU	N-CA-CB	-6.39	101.13	110.14
2	J	66	GLY	CA-C-N	-6.25	115.80	122.67
2	J	66	GLY	C-N-CA	-6.25	115.80	122.67
1	C	137	GLU	CA-C-N	6.07	130.84	121.19
1	C	137	GLU	C-N-CA	6.07	130.84	121.19
1	C	134	TYR	CA-C-O	-6.03	114.75	121.51
1	B	100	ALA	N-CA-CB	-6.03	100.68	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	39	ASN	CB-CA-C	-5.97	99.23	110.51
1	G	180	VAL	CA-C-O	-5.93	114.50	120.31
2	K	64	LEU	N-CA-CB	5.89	119.48	110.70
2	J	63	TYR	CA-CB-CG	5.73	124.21	113.90
2	L	118	GLY	CA-C-N	-5.72	114.58	122.30
2	L	118	GLY	C-N-CA	-5.72	114.58	122.30
1	C	137	GLU	N-CA-C	5.70	118.28	110.24
2	K	66	GLY	N-CA-C	-5.65	99.78	113.18
2	L	118	GLY	O-C-N	-5.65	117.37	122.96
2	J	55	PHE	CA-CB-CG	5.62	119.42	113.80
2	H	55	PHE	N-CA-C	-5.51	97.63	109.81
2	K	73	VAL	CA-C-N	5.51	125.81	119.92
2	K	73	VAL	C-N-CA	5.51	125.81	119.92
2	K	63	TYR	CA-CB-CG	5.42	123.66	113.90
2	I	69	VAL	N-CA-CB	-5.40	102.32	111.23
1	G	278	ILE	N-CA-C	-5.23	102.76	109.30
1	C	135	SER	CA-C-O	-5.12	115.93	121.36
2	J	111	ALA	CA-C-N	-5.04	114.67	122.69
2	J	111	ALA	C-N-CA	-5.04	114.67	122.69
1	D	216	ASP	N-CA-C	-5.03	103.86	111.56
1	F	204	GLY	CA-C-N	-5.02	118.29	122.16
1	F	204	GLY	C-N-CA	-5.02	118.29	122.16

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	136	ARG	Sidechain
2	H	53	GLN	Peptide
2	I	55	PHE	Peptide
2	I	64	LEU	Mainchain
2	J	108	SER	Mainchain
2	K	62	ASN	Mainchain
2	K	65	GLY	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2430	0	2357	58	0
1	B	2411	0	2330	57	0
1	C	2418	0	2339	69	0
1	D	2422	0	2350	77	0
1	E	2418	0	2345	84	0
1	F	2425	0	2352	83	0
1	G	2362	0	2283	88	0
2	H	1097	0	1072	54	0
2	I	1085	0	1060	54	0
2	J	1083	0	1061	60	0
2	K	1076	0	1051	48	0
2	L	1094	0	1070	42	0
2	M	1092	0	1067	34	0
2	N	1091	0	1061	36	0
All	All	24504	0	23798	730	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 15.

All (730) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:ASN:OD1	1:D:300:MET:HE2	1.49	1.13
1:D:89:LYS:HE2	1:E:56:ARG:O	1.54	1.08
1:D:298:ASN:OD1	1:D:300:MET:CE	2.15	0.95
2:L:6:TYR:OH	2:L:129:GLU:OE2	1.84	0.93
1:C:196:ILE:HD11	1:C:233:GLN:OE1	1.70	0.92
2:L:26:MET:HE1	2:L:59:LEU:HD11	1.51	0.92
1:E:103:VAL:HG21	1:F:166:ASP:CG	1.97	0.90
1:E:103:VAL:HG21	1:F:166:ASP:OD2	1.72	0.89
2:L:26:MET:SD	2:L:79:GLY:HA3	2.13	0.88
2:J:64:LEU:HB3	2:J:80:MET:HE1	1.57	0.86
1:A:318:ALA:O	1:G:313:TYR:OH	1.94	0.85
1:D:117:LYS:HE3	1:E:136:ARG:HH11	1.43	0.83
1:C:256:SER:HB2	1:C:260:GLY:HA3	1.59	0.82
1:F:134:TYR:CD2	1:F:326:PHE:HB2	2.15	0.82
1:C:255:TYR:HE1	1:C:266:VAL:HA	1.43	0.82
2:I:131:TYR:HE2	2:I:133:VAL:HA	1.45	0.81
2:J:108:SER:C	2:J:110:GLY:H	1.89	0.80
2:I:131:TYR:OH	2:I:139:GLU:OE1	2.01	0.78
2:N:56:PRO:HG2	2:N:145:ARG:HE	1.47	0.78
1:E:67:ARG:NH2	1:E:158:ASN:OD1	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:106:THR:HA	1:F:111:GLU:OE2	1.83	0.77
1:G:231:ASP:OD2	1:G:277:ARG:CZ	2.33	0.77
1:B:136:ARG:HH21	1:B:151:PRO:HB2	1.50	0.75
1:C:213:ALA:O	1:C:253:ARG:NH2	2.17	0.75
2:K:96:GLN:NE2	2:K:135:SER:O	2.19	0.75
1:E:103:VAL:CG2	1:F:166:ASP:OD2	2.35	0.74
1:D:223:ASN:ND2	1:D:273:PHE:O	2.19	0.74
1:D:108:SER:OG	2:K:23:GLU:OE1	2.05	0.74
1:C:255:TYR:CE1	1:C:266:VAL:HA	2.23	0.74
2:I:55:PHE:HE2	2:I:83:GLN:HB3	1.54	0.73
2:I:131:TYR:CE2	2:I:133:VAL:HA	2.24	0.73
2:H:126:TYR:CE2	2:J:55:PHE:HB2	2.25	0.72
2:L:56:PRO:HB2	2:L:84:CYS:HB2	1.71	0.72
1:G:140:GLU:HG3	1:G:144:MET:HE3	1.69	0.72
2:H:12:GLY:HA2	2:H:89:THR:HG23	1.72	0.72
2:H:62:ASN:HB2	2:H:73:VAL:HG22	1.72	0.72
2:J:89:THR:HG22	2:J:144:ARG:HE	1.53	0.72
1:D:299:ASP:OD2	1:D:299:ASP:C	2.30	0.71
1:G:68:ASN:O	1:G:69:GLU:C	2.34	0.71
1:C:107:LEU:HB2	1:D:178:LEU:HD22	1.72	0.71
2:K:89:THR:OG1	2:K:144:ARG:NH1	2.24	0.71
1:G:70:ALA:O	1:G:72:GLN:N	2.24	0.70
2:H:89:THR:HG22	2:H:144:ARG:HE	1.56	0.70
2:I:62:ASN:HB3	2:I:67:GLY:HA3	1.72	0.70
1:D:75:MET:O	1:D:79:MET:HG2	1.91	0.70
1:C:255:TYR:CZ	1:C:269:TYR:HB2	2.26	0.70
2:J:131:TYR:OH	2:J:139:GLU:OE2	2.09	0.70
2:H:53:GLN:H	2:H:53:GLN:HE21	1.40	0.70
2:N:21:ILE:HG21	2:N:80:MET:HG2	1.73	0.69
1:F:134:TYR:HD2	1:F:326:PHE:HB2	1.54	0.69
2:J:100:LEU:HD22	2:J:104:THR:HB	1.75	0.69
2:K:144:ARG:NH2	2:L:20:GLN:OE1	2.25	0.69
2:N:101:LYS:O	2:N:104:THR:HG22	1.93	0.69
1:A:117:LYS:HD2	1:B:136:ARG:HD3	1.75	0.69
1:E:75:MET:O	1:E:79:MET:HG2	1.92	0.69
1:C:209:ASP:HA	1:C:290:ASN:HD21	1.56	0.68
1:D:74:MET:SD	1:D:284:ASN:ND2	2.66	0.68
2:I:21:ILE:HG22	2:I:82:VAL:HA	1.75	0.68
2:I:54:GLY:H	2:J:148:ASN:HD21	1.41	0.68
1:G:233:GLN:O	1:G:235:VAL:HG23	1.94	0.68
2:N:62:ASN:HB2	2:N:73:VAL:HG22	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:THR:OG1	1:E:129:ILE:O	2.11	0.68
1:B:179:ASN:OD1	1:B:185:THR:OG1	2.11	0.68
1:A:194:ASN:OD1	1:A:338:LYS:HE2	1.95	0.67
1:C:235:VAL:HG22	1:C:345:LYS:HG2	1.76	0.67
1:G:67:ARG:NH2	1:G:158:ASN:OD1	2.27	0.67
2:M:5:ARG:NH2	2:M:129:GLU:OE1	2.27	0.67
1:C:196:ILE:HD13	1:C:233:GLN:HG3	1.76	0.66
2:L:5:ARG:NH2	2:L:129:GLU:OE1	2.27	0.66
1:B:235:VAL:HG13	1:B:345:LYS:HD3	1.76	0.66
1:F:340:PHE:O	1:F:340:PHE:HD1	1.78	0.66
1:C:218:ILE:HG22	1:C:270:ILE:HD11	1.78	0.66
1:E:128:PRO:HB3	1:E:178:LEU:HD13	1.77	0.66
1:C:196:ILE:CD1	1:C:233:GLN:OE1	2.43	0.66
2:J:2:ALA:HB2	2:J:136:ASP:HB2	1.78	0.66
2:I:96:GLN:NE2	2:I:135:SER:O	2.28	0.66
1:C:176:GLN:NE2	1:C:187:TYR:HE1	1.92	0.66
2:H:84:CYS:O	2:H:145:ARG:NH1	2.29	0.66
2:K:84:CYS:O	2:K:145:ARG:NH1	2.28	0.66
1:A:172:LEU:HD11	1:A:287:LEU:HD21	1.78	0.65
2:I:61:HIS:CE1	2:I:63:TYR:HB3	2.31	0.65
1:A:139:ARG:NH1	1:G:87:ILE:O	2.29	0.65
1:E:117:LYS:HD2	1:F:136:ARG:HH11	1.61	0.65
1:F:121:ASP:OD2	1:F:122:TYR:N	2.28	0.65
2:J:64:LEU:HB3	2:J:80:MET:CE	2.25	0.65
2:K:149:ALA:O	2:L:122:ASN:HA	1.95	0.65
2:K:151:MET:SD	2:L:123:ILE:HD11	2.36	0.65
1:F:235:VAL:HG22	1:F:345:LYS:HG2	1.79	0.65
2:L:26:MET:HG2	2:L:77:ALA:O	1.97	0.65
1:D:273:PHE:HE1	1:E:254:PRO:HB3	1.61	0.65
1:F:134:TYR:CE1	1:F:156:GLN:HA	2.32	0.65
2:N:56:PRO:HG2	2:N:145:ARG:NE	2.11	0.64
2:L:147:GLY:O	2:L:148:ASN:ND2	2.30	0.64
1:B:298:ASN:ND2	1:B:300:MET:SD	2.70	0.64
2:M:6:TYR:OH	2:M:129:GLU:OE2	2.14	0.64
1:A:298:ASN:ND2	1:A:300:MET:SD	2.71	0.64
2:K:55:PHE:HB2	2:M:126:TYR:HE2	1.62	0.64
1:A:253:ARG:HA	1:F:223:ASN:HD21	1.63	0.64
1:A:339:ASP:OD1	1:A:340:PHE:N	2.30	0.64
1:B:98:SER:OG	1:B:99:ASP:N	2.31	0.64
1:G:107:LEU:CD2	2:H:64:LEU:HD13	2.27	0.64
2:I:68:ASP:C	2:I:70:SER:H	2.06	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:66:GLY:O	2:I:67:GLY:C	2.40	0.64
1:D:255:TYR:CE2	1:E:258:ALA:HA	2.33	0.63
1:B:167:MET:SD	1:B:330:SER:OG	2.56	0.63
1:D:339:ASP:OD1	1:D:341:THR:N	2.31	0.63
1:F:94:SER:OG	1:F:335:GLN:NE2	2.31	0.63
2:H:147:GLY:O	2:J:147:GLY:HA2	1.97	0.63
2:J:21:ILE:HG21	2:J:80:MET:HG2	1.80	0.63
1:D:119:ARG:HE	2:M:4:ILE:HD11	1.63	0.63
1:G:213:ALA:O	1:G:253:ARG:NH2	2.31	0.63
1:G:68:ASN:O	1:G:70:ALA:N	2.31	0.62
1:G:141:LEU:HD11	1:G:152:LEU:HD21	1.81	0.62
2:L:8:THR:O	2:L:91:HIS:ND1	2.32	0.62
2:N:26:MET:HE2	2:N:73:VAL:CG1	2.29	0.62
1:D:209:ASP:OD1	1:D:211:GLN:NE2	2.31	0.62
2:J:54:GLY:HA3	2:J:124:LEU:HD11	1.82	0.62
1:E:230:LEU:HD13	1:E:277:ARG:HD2	1.81	0.62
1:B:223:ASN:ND2	1:B:273:PHE:O	2.33	0.62
1:D:273:PHE:HD1	1:E:254:PRO:HG3	1.63	0.62
1:C:255:TYR:OH	1:C:269:TYR:HB2	1.98	0.62
2:J:108:SER:C	2:J:110:GLY:N	2.55	0.62
2:K:149:ALA:HB3	2:L:123:ILE:HB	1.82	0.62
1:E:79:MET:HE1	1:E:306:VAL:HG21	1.82	0.61
1:F:106:THR:OG1	1:F:111:GLU:OE2	2.19	0.61
1:G:272:GLN:HB2	1:G:276:GLY:HA3	1.82	0.61
2:H:149:ALA:HB2	2:J:148:ASN:H	1.65	0.61
1:E:136:ARG:HH21	1:E:151:PRO:HB2	1.65	0.61
1:D:89:LYS:HD2	1:E:56:ARG:N	2.14	0.61
2:L:121:ASP:O	2:L:122:ASN:C	2.41	0.61
2:I:54:GLY:H	2:J:148:ASN:ND2	1.98	0.61
1:E:223:ASN:ND2	1:F:253:ARG:HA	2.14	0.61
1:C:339:ASP:C	1:C:339:ASP:OD2	2.43	0.61
1:G:230:LEU:O	1:G:235:VAL:HB	2.00	0.61
2:M:2:ALA:N	2:M:139:GLU:OE2	2.33	0.61
1:C:74:MET:SD	1:C:284:ASN:ND2	2.73	0.60
1:F:134:TYR:CZ	1:F:156:GLN:HA	2.35	0.60
1:G:71:GLY:O	1:G:72:GLN:C	2.42	0.60
1:A:317:ARG:NH1	1:A:322:ASP:O	2.34	0.60
1:B:121:ASP:OD2	1:B:122:TYR:N	2.33	0.60
2:N:109:ASN:HB3	2:N:115:LYS:HB3	1.82	0.60
1:A:256:SER:HB2	1:A:260:GLY:HA3	1.82	0.60
1:A:150:ASP:OD1	1:A:153:LEU:HG	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:83:GLN:OE1	2:J:144:ARG:NH1	2.35	0.60
1:G:141:LEU:CD1	1:G:152:LEU:HD21	2.32	0.60
1:G:230:LEU:HD21	1:G:239:VAL:HG21	1.83	0.60
1:B:305:ARG:N	1:B:333:GLY:O	2.31	0.60
2:L:12:GLY:HA3	2:L:88:VAL:HG13	1.84	0.60
2:M:123:ILE:HG21	2:M:126:TYR:HE1	1.66	0.60
1:F:243:VAL:HG12	1:F:292:PHE:HB2	1.83	0.60
1:G:303:ARG:HE	1:G:337:ARG:HH22	1.48	0.60
1:E:211:GLN:HG2	1:E:212:THR:HG23	1.83	0.60
2:K:64:LEU:HG	2:K:80:MET:HE2	1.82	0.60
1:G:113:GLU:HG2	2:I:13:PRO:HA	1.84	0.59
2:J:22:ARG:HB2	2:J:83:GLN:HE21	1.66	0.59
2:K:55:PHE:HB2	2:M:126:TYR:CE2	2.37	0.59
2:L:62:ASN:HB2	2:L:73:VAL:HG22	1.83	0.59
1:D:98:SER:OG	1:D:99:ASP:N	2.35	0.59
1:D:216:ASP:O	1:D:217:GLU:C	2.45	0.59
2:N:31:GLN:NE2	2:N:70:SER:O	2.35	0.59
1:G:74:MET:SD	1:G:284:ASN:ND2	2.75	0.59
1:G:141:LEU:HD11	1:G:152:LEU:CD2	2.32	0.59
1:G:71:GLY:O	1:G:73:ASP:N	2.35	0.59
1:G:248:ARG:NH1	1:G:281:ILE:O	2.35	0.59
2:H:53:GLN:O	2:I:148:ASN:ND2	2.35	0.59
1:A:227:GLN:OE1	1:A:277:ARG:NH1	2.36	0.59
1:A:253:ARG:HG2	1:A:254:PRO:HD2	1.85	0.59
1:C:62:THR:O	1:C:64:ARG:HD3	2.03	0.59
1:G:107:LEU:HD22	2:H:64:LEU:HD13	1.84	0.59
2:N:6:TYR:OH	2:N:129:GLU:OE2	2.20	0.59
1:C:317:ARG:HE	1:C:322:ASP:HB2	1.68	0.58
1:F:231:ASP:OD1	1:F:277:ARG:NH2	2.33	0.58
1:G:234:ASN:O	1:G:345:LYS:HE2	2.03	0.58
2:J:97:SER:O	2:J:97:SER:OG	2.18	0.58
2:L:100:LEU:HD21	2:L:106:LEU:HD21	1.85	0.58
2:H:51:GLY:HA3	2:H:121:ASP:HB3	1.85	0.58
1:G:231:ASP:O	1:G:232:ALA:C	2.46	0.58
2:H:100:LEU:HD21	2:H:106:LEU:HD21	1.85	0.58
2:J:52:GLY:HA2	2:J:122:ASN:HD22	1.69	0.58
2:H:109:ASN:O	2:H:111:ALA:N	2.35	0.58
2:L:123:ILE:H	2:L:123:ILE:HD12	1.69	0.58
2:N:26:MET:HG2	2:N:77:ALA:O	2.04	0.58
1:A:82:ALA:HB2	1:A:304:PRO:HG2	1.85	0.58
1:B:337:ARG:HH22	1:C:61:VAL:HG21	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:59:ASP:OD1	1:E:59:ASP:N	2.35	0.58
2:L:121:ASP:O	2:L:123:ILE:N	2.37	0.58
1:G:107:LEU:HD23	2:H:64:LEU:HD22	1.86	0.58
1:E:86:ASN:HB3	1:E:89:LYS:HG2	1.86	0.57
1:G:299:ASP:HB2	1:G:303:ARG:HD3	1.85	0.57
2:H:52:GLY:O	2:H:54:GLY:N	2.37	0.57
1:B:245:PRO:HG3	1:B:285:PHE:HD1	1.68	0.57
1:C:341:THR:CG2	1:C:343:LYS:HE3	2.34	0.57
1:D:213:ALA:O	1:D:253:ARG:NH2	2.25	0.57
2:I:22:ARG:HD3	2:I:38:PHE:CE2	2.39	0.57
1:B:95:ARG:HD2	1:C:62:THR:HG23	1.87	0.57
1:C:75:MET:O	1:C:79:MET:HG2	2.05	0.57
1:D:317:ARG:HG2	1:D:322:ASP:HB2	1.85	0.57
2:M:123:ILE:HG21	2:M:126:TYR:CE1	2.39	0.57
1:C:85:ILE:HD13	1:C:127:ILE:HG13	1.86	0.57
1:G:233:GLN:O	1:G:234:ASN:C	2.47	0.57
1:D:273:PHE:CD1	1:E:254:PRO:HG3	2.40	0.57
1:D:170:TYR:CD1	1:D:174:GLY:HA2	2.40	0.56
2:H:54:GLY:O	2:H:55:PHE:C	2.45	0.56
2:K:126:TYR:OH	2:L:53:GLN:OE1	2.13	0.56
2:N:104:THR:HG23	2:N:127:SER:HB3	1.87	0.56
2:J:5:ARG:HD3	2:J:139:GLU:HG2	1.86	0.56
2:K:89:THR:HG22	2:K:142:ALA:HB1	1.87	0.56
1:A:128:PRO:HB3	1:A:178:LEU:HD13	1.88	0.56
1:G:141:LEU:HD21	1:G:152:LEU:HD21	1.87	0.56
2:I:123:ILE:HD11	2:J:151:MET:HG2	1.87	0.56
2:M:100:LEU:HD23	2:M:141:VAL:HG11	1.88	0.56
1:D:89:LYS:HD2	1:E:56:ARG:C	2.31	0.56
2:J:62:ASN:HB2	2:J:73:VAL:HG22	1.88	0.56
1:G:141:LEU:CD2	1:G:152:LEU:HD21	2.35	0.56
2:K:35:LEU:N	2:K:112:GLY:O	2.39	0.56
1:G:128:PRO:HB3	1:G:178:LEU:HD13	1.88	0.56
1:G:307:ALA:HB3	1:G:331:ALA:HB3	1.88	0.56
1:A:54:TYR:OH	2:I:63:TYR:O	2.23	0.55
2:N:56:PRO:HB3	2:N:125:PHE:CZ	2.42	0.55
1:C:128:PRO:HB3	1:C:178:LEU:HD13	1.88	0.55
1:B:245:PRO:HG3	1:B:285:PHE:CD1	2.42	0.55
2:J:101:LYS:O	2:J:104:THR:OG1	2.24	0.55
2:K:26:MET:HE2	2:K:73:VAL:HB	1.88	0.55
1:D:300:MET:HA	1:D:337:ARG:HH11	1.71	0.55
1:F:98:SER:OG	1:F:99:ASP:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:195:THR:HG23	1:G:346:VAL:HG12	1.87	0.55
2:K:133:VAL:HG13	2:K:139:GLU:HB2	1.88	0.55
1:A:98:SER:OG	1:A:119:ARG:O	2.19	0.55
1:B:127:ILE:HD13	1:B:333:GLY:HA3	1.88	0.55
1:D:172:LEU:HD21	1:D:287:LEU:HG	1.89	0.55
2:H:102:LYS:O	2:J:22:ARG:NH2	2.40	0.55
1:B:100:ALA:HB2	1:B:118:THR:HG22	1.89	0.55
1:E:194:ASN:O	1:E:344:SER:OG	2.23	0.55
1:E:245:PRO:HG3	1:E:285:PHE:CD2	2.41	0.55
1:D:128:PRO:HB3	1:D:178:LEU:HD13	1.89	0.55
2:H:5:ARG:NH2	2:H:6:TYR:OH	2.40	0.55
2:I:35:LEU:HD11	2:I:56:PRO:HB3	1.89	0.55
2:M:57:TYR:HB3	2:M:81:ALA:HB1	1.89	0.55
2:H:147:GLY:H	2:I:149:ALA:HB2	1.72	0.55
2:I:107:ALA:HA	2:I:124:LEU:HD12	1.88	0.55
1:E:117:LYS:HD2	1:F:136:ARG:NH1	2.21	0.54
1:G:155:ASP:O	1:G:159:VAL:HG22	2.07	0.54
2:K:57:TYR:HE1	2:K:83:GLN:HG2	1.71	0.54
1:B:128:PRO:HB3	1:B:178:LEU:HD13	1.88	0.54
1:C:171:LEU:HG	1:C:332:MET:HE1	1.89	0.54
1:E:103:VAL:CG2	1:F:166:ASP:CG	2.78	0.54
1:C:305:ARG:N	1:C:333:GLY:O	2.38	0.54
1:D:230:LEU:HD13	1:D:277:ARG:HD2	1.90	0.54
2:H:60:GLN:HE21	2:H:63:TYR:HE1	1.54	0.54
2:I:99:VAL:HA	2:I:132:THR:HG23	1.89	0.54
2:M:26:MET:HE2	2:M:73:VAL:HB	1.88	0.54
1:E:256:SER:HB2	1:E:260:GLY:HA3	1.88	0.54
1:G:229:ILE:C	1:G:231:ASP:H	2.14	0.54
1:G:230:LEU:HD22	1:G:235:VAL:HG11	1.89	0.54
2:I:5:ARG:HD3	2:I:140:LEU:O	2.07	0.54
1:A:121:ASP:OD2	1:A:122:TYR:N	2.41	0.54
1:C:341:THR:HG23	1:C:343:LYS:HE3	1.90	0.54
2:H:54:GLY:O	2:H:56:PRO:N	2.40	0.54
2:J:51:GLY:HA2	2:J:107:ALA:HB1	1.90	0.54
2:K:26:MET:SD	2:K:79:GLY:HA3	2.48	0.54
2:J:84:CYS:O	2:J:145:ARG:NH1	2.40	0.54
1:C:187:TYR:CD2	1:C:193:PRO:HD3	2.43	0.53
2:J:100:LEU:HD13	2:J:127:SER:HB2	1.90	0.53
2:M:89:THR:OG1	2:M:144:ARG:NH2	2.41	0.53
1:F:55:TRP:NE1	2:K:66:GLY:HA3	2.24	0.53
2:J:54:GLY:O	2:J:55:PHE:C	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:ILE:HB	1:B:305:ARG:HH11	1.73	0.53
1:D:223:ASN:ND2	1:D:273:PHE:HB3	2.23	0.53
1:F:307:ALA:HB3	1:F:331:ALA:HB3	1.89	0.53
2:I:133:VAL:HG13	2:I:139:GLU:HB2	1.90	0.53
1:A:94:SER:OG	1:A:337:ARG:NH1	2.41	0.53
1:F:173:THR:O	1:F:191:ASN:ND2	2.42	0.53
2:I:136:ASP:OD2	2:I:137:GLY:N	2.41	0.53
1:B:93:ILE:HD12	1:C:56:ARG:HD3	1.89	0.53
1:F:340:PHE:HD1	1:F:340:PHE:C	2.16	0.53
1:G:86:ASN:OD1	1:G:87:ILE:N	2.41	0.53
2:H:109:ASN:HB3	2:H:115:LYS:HD3	1.90	0.53
1:A:187:TYR:CD2	1:A:193:PRO:HD3	2.43	0.53
2:K:20:GLN:OE1	2:M:144:ARG:NH1	2.41	0.53
1:B:163:LEU:O	1:B:165:SER:N	2.41	0.53
2:I:32:PRO:HD3	2:I:72:ALA:HA	1.90	0.53
1:C:179:ASN:O	2:N:78:THR:HG23	2.09	0.53
2:I:68:ASP:O	2:I:70:SER:N	2.39	0.53
2:N:26:MET:SD	2:N:79:GLY:HA3	2.48	0.53
2:J:100:LEU:CD2	2:J:104:THR:HB	2.39	0.52
2:M:55:PHE:HE2	2:M:83:GLN:HG2	1.73	0.52
2:N:56:PRO:HB2	2:N:84:CYS:HB2	1.91	0.52
1:B:339:ASP:OD1	1:B:343:LYS:N	2.42	0.52
1:F:339:ASP:OD1	1:F:341:THR:N	2.43	0.52
2:I:89:THR:HG22	2:I:144:ARG:HG3	1.92	0.52
1:G:152:LEU:H	1:G:152:LEU:HD22	1.74	0.52
1:G:338:LYS:HG3	1:G:344:SER:HB3	1.90	0.52
1:D:117:LYS:HE3	1:E:136:ARG:NH1	2.18	0.52
2:H:144:ARG:NH1	2:J:20:GLN:OE1	2.41	0.52
1:C:172:LEU:HD21	1:C:287:LEU:HG	1.92	0.52
1:C:248:ARG:O	1:C:252:MET:HG2	2.10	0.52
1:G:90:THR:HG21	1:G:180:VAL:HG11	1.91	0.52
1:G:339:ASP:OD1	1:G:343:LYS:N	2.35	0.52
2:J:15:ARG:HG3	2:J:16:LYS:HD3	1.92	0.52
2:M:55:PHE:CE2	2:M:83:GLN:HG2	2.44	0.52
2:H:148:ASN:OD1	2:J:124:LEU:HA	2.09	0.52
2:I:68:ASP:C	2:I:70:SER:N	2.67	0.52
1:A:105:ARG:HD2	1:B:175:ASP:OD1	2.10	0.52
1:G:243:VAL:HG12	1:G:292:PHE:HB2	1.91	0.52
1:F:128:PRO:HB3	1:F:178:LEU:HD13	1.92	0.52
1:C:196:ILE:HG22	1:C:196:ILE:O	2.10	0.51
1:E:248:ARG:O	1:E:252:MET:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:340:PHE:C	1:F:340:PHE:CD1	2.88	0.51
1:G:93:ILE:HD13	1:G:124:GLY:HA3	1.91	0.51
1:G:79:MET:HE1	1:G:332:MET:HG3	1.92	0.51
1:A:64:ARG:NE	1:A:154:ASP:OD2	2.43	0.51
1:C:177:THR:HG22	1:C:177:THR:O	2.11	0.51
2:K:131:TYR:HE2	2:K:133:VAL:HA	1.76	0.51
2:N:106:LEU:HD11	2:N:127:SER:HB2	1.92	0.51
1:G:230:LEU:CD2	1:G:239:VAL:HG21	2.41	0.51
2:M:9:ILE:HD11	2:M:32:PRO:HB2	1.92	0.51
2:H:26:MET:HE2	2:H:73:VAL:CG1	2.41	0.51
2:I:26:MET:HG2	2:I:77:ALA:O	2.11	0.51
2:J:54:GLY:HA3	2:J:124:LEU:CD1	2.40	0.51
2:J:94:VAL:HG12	2:J:114:LEU:HB2	1.93	0.51
1:A:243:VAL:HG12	1:A:292:PHE:HB2	1.93	0.51
1:F:87:ILE:HD12	1:F:87:ILE:H	1.76	0.51
1:F:134:TYR:HE1	1:F:159:VAL:HB	1.75	0.51
2:J:100:LEU:HD13	2:J:127:SER:CB	2.40	0.51
1:C:107:LEU:HD12	1:C:107:LEU:O	2.11	0.51
1:D:299:ASP:HB2	1:D:303:ARG:HD3	1.93	0.51
1:D:310:VAL:HA	1:D:330:SER:OG	2.11	0.51
1:F:141:LEU:HD23	1:F:324:PHE:CG	2.46	0.51
1:D:243:VAL:HG12	1:D:292:PHE:HB2	1.92	0.51
2:I:56:PRO:HG3	2:I:124:LEU:HB3	1.93	0.51
2:I:101:LYS:O	2:I:104:THR:OG1	2.22	0.51
1:A:166:ASP:OD1	1:F:105:ARG:NH2	2.38	0.50
1:E:121:ASP:OD2	1:E:122:TYR:N	2.44	0.50
1:F:136:ARG:HH21	1:F:151:PRO:HB2	1.76	0.50
1:F:261:PHE:CD1	1:F:261:PHE:C	2.89	0.50
2:H:59:LEU:HD12	2:H:60:GLN:N	2.25	0.50
1:B:75:MET:O	1:B:79:MET:HG2	2.10	0.50
1:D:245:PRO:HG3	1:D:285:PHE:CD1	2.46	0.50
1:E:78:LEU:HB3	1:E:304:PRO:HG3	1.92	0.50
2:K:147:GLY:C	2:K:148:ASN:HD22	2.19	0.50
2:I:57:TYR:HB3	2:I:81:ALA:HB1	1.93	0.50
1:A:230:LEU:HD13	1:A:277:ARG:HD2	1.94	0.50
1:E:288:THR:O	1:E:288:THR:OG1	2.24	0.50
2:J:5:ARG:HD2	2:J:131:TYR:HE1	1.76	0.50
2:N:133:VAL:HG13	2:N:139:GLU:HB2	1.92	0.50
2:H:125:PHE:HB3	2:H:143:VAL:HB	1.92	0.50
2:L:126:TYR:OH	2:M:53:GLN:OE1	2.19	0.50
1:B:307:ALA:HB3	1:B:331:ALA:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:LYS:HD3	2:M:8:THR:CG2	2.42	0.50
2:I:118:GLY:N	2:I:121:ASP:OD2	2.34	0.50
2:K:5:ARG:HH22	2:K:129:GLU:CD	2.19	0.50
1:B:136:ARG:HE	1:B:151:PRO:HG2	1.75	0.50
2:K:126:TYR:CE2	2:L:55:PHE:HB2	2.47	0.50
1:E:103:VAL:HG21	1:F:166:ASP:CB	2.41	0.50
1:E:225:ASP:O	1:E:229:ILE:HG12	2.12	0.50
1:G:141:LEU:HD23	1:G:324:PHE:CG	2.47	0.50
2:L:51:GLY:N	2:L:108:SER:O	2.45	0.50
2:N:100:LEU:CD2	2:N:104:THR:HG21	2.42	0.50
1:E:79:MET:HE1	1:E:306:VAL:CG2	2.41	0.49
2:H:52:GLY:O	2:H:53:GLN:C	2.53	0.49
1:B:59:ASP:OD1	1:B:59:ASP:N	2.43	0.49
1:E:187:TYR:CD2	1:E:193:PRO:HD3	2.47	0.49
1:F:256:SER:OG	1:F:262:LYS:O	2.28	0.49
2:K:102:LYS:H	2:K:130:THR:HG22	1.78	0.49
1:B:243:VAL:HG12	1:B:292:PHE:HB2	1.94	0.49
2:M:35:LEU:HD21	2:M:124:LEU:HD12	1.93	0.49
1:E:100:ALA:O	1:F:162:ASN:ND2	2.45	0.49
2:H:148:ASN:H	2:I:149:ALA:HB2	1.78	0.49
2:I:26:MET:HE2	2:I:73:VAL:HB	1.95	0.49
1:B:163:LEU:O	1:B:166:ASP:N	2.46	0.49
1:C:141:LEU:HD23	1:C:324:PHE:CG	2.47	0.49
1:F:211:GLN:NE2	1:F:289:GLY:C	2.71	0.49
2:H:9:ILE:HD12	2:H:61:HIS:N	2.27	0.49
1:B:338:LYS:HG2	1:B:339:ASP:N	2.28	0.49
1:F:125:ASP:CG	1:F:192:HIS:HE2	2.21	0.49
2:L:56:PRO:HD3	2:L:124:LEU:HD12	1.93	0.49
1:G:125:ASP:CG	1:G:192:HIS:HE2	2.20	0.49
2:L:56:PRO:HB3	2:L:125:PHE:CZ	2.47	0.49
1:E:113:GLU:CD	1:F:327:LEU:HD13	2.38	0.49
1:G:231:ASP:O	1:G:234:ASN:N	2.46	0.49
2:K:26:MET:HG2	2:K:77:ALA:O	2.12	0.49
1:C:267:GLU:HG3	1:C:281:ILE:HD12	1.95	0.48
1:F:206:LEU:O	1:F:207:ASN:C	2.56	0.48
2:K:136:ASP:OD2	2:K:137:GLY:N	2.46	0.48
1:B:136:ARG:HH21	1:B:151:PRO:CB	2.20	0.48
1:E:129:ILE:HG12	1:E:331:ALA:HB2	1.95	0.48
1:E:273:PHE:HE1	1:F:254:PRO:HB3	1.78	0.48
1:F:211:GLN:HE21	1:F:290:ASN:N	2.10	0.48
1:B:163:LEU:O	1:B:164:ARG:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:199:ASN:OD1	1:F:201:ASN:ND2	2.47	0.48
2:H:144:ARG:NH1	2:J:83:GLN:OE1	2.46	0.48
2:L:63:TYR:CE1	2:L:80:MET:HE1	2.48	0.48
1:G:231:ASP:OD2	1:G:277:ARG:NH1	2.47	0.48
2:J:114:LEU:HD21	2:J:125:PHE:HD2	1.78	0.48
1:D:305:ARG:N	1:D:333:GLY:O	2.45	0.48
1:E:290:ASN:ND2	1:E:353:GLN:OE1	2.47	0.48
1:E:105:ARG:HD3	1:F:130:PHE:HE1	1.79	0.48
2:J:103:GLY:N	2:J:127:SER:O	2.41	0.48
1:D:224:GLN:HG3	1:E:253:ARG:HH21	1.78	0.48
2:N:68:ASP:N	2:N:68:ASP:OD1	2.41	0.48
1:A:171:LEU:HD12	1:A:332:MET:HE1	1.95	0.48
1:F:123:THR:HG21	1:F:338:LYS:HE2	1.95	0.48
2:I:11:GLY:O	2:I:88:VAL:HG13	2.14	0.48
2:L:18:ASP:OD1	2:L:18:ASP:O	2.32	0.48
2:N:64:LEU:HG	2:N:80:MET:HE1	1.96	0.48
1:D:298:ASN:OD1	1:D:300:MET:HE3	2.08	0.48
1:F:172:LEU:HD12	1:F:286:LEU:HB2	1.96	0.48
1:G:150:ASP:OD1	1:G:152:LEU:HD23	2.14	0.48
2:H:131:TYR:CD2	2:H:132:THR:N	2.82	0.48
1:A:262:LYS:NZ	1:B:260:GLY:O	2.46	0.48
1:G:144:MET:SD	1:G:151:PRO:HG3	2.54	0.48
2:H:59:LEU:HD12	2:H:60:GLN:H	1.78	0.48
2:H:151:MET:SD	2:H:152:PRO:HD2	2.53	0.47
2:J:109:ASN:HA	2:J:115:LYS:HD3	1.96	0.47
1:D:85:ILE:HB	1:D:305:ARG:HH11	1.79	0.47
1:D:144:MET:SD	1:D:151:PRO:HG3	2.54	0.47
1:F:134:TYR:OH	1:F:156:GLN:HG3	2.14	0.47
1:F:339:ASP:OD1	1:F:339:ASP:C	2.57	0.47
1:A:77:ASP:OD2	1:A:295:TYR:OH	2.30	0.47
1:E:75:MET:HG3	1:E:171:LEU:HD22	1.96	0.47
1:G:111:GLU:OE1	2:H:23:GLU:HG3	2.15	0.47
2:I:87:GLY:HA2	2:I:144:ARG:HH12	1.79	0.47
2:M:21:ILE:HG21	2:M:80:MET:HB3	1.96	0.47
1:A:107:LEU:HB2	1:B:178:LEU:HD22	1.96	0.47
1:D:89:LYS:HD2	1:E:56:ARG:CA	2.44	0.47
1:E:126:VAL:C	1:E:127:ILE:HD13	2.39	0.47
1:G:134:TYR:HD1	1:G:159:VAL:HG21	1.80	0.47
1:G:236:PHE:H	1:G:236:PHE:HD2	1.62	0.47
2:I:148:ASN:HB2	2:J:149:ALA:HB2	1.96	0.47
1:A:74:MET:SD	1:A:284:ASN:ND2	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ARG:HA	1:F:223:ASN:ND2	2.27	0.47
1:G:302:ILE:HD11	1:G:334:LEU:HD11	1.96	0.47
2:H:68:ASP:OD2	2:H:68:ASP:N	2.37	0.47
2:M:109:ASN:OD1	2:M:109:ASN:N	2.38	0.47
2:N:125:PHE:HB3	2:N:143:VAL:HB	1.97	0.47
1:A:56:ARG:C	1:F:89:LYS:HD2	2.39	0.47
1:B:235:VAL:HG21	1:B:347:PHE:HZ	1.80	0.47
2:J:6:TYR:CD1	2:J:91:HIS:ND1	2.82	0.47
2:J:102:LYS:HG3	2:J:128:TYR:C	2.40	0.47
2:N:35:LEU:N	2:N:112:GLY:O	2.42	0.47
1:F:300:MET:HE2	1:F:300:MET:HB3	1.83	0.47
1:C:176:GLN:NE2	1:C:187:TYR:CE1	2.80	0.47
2:M:63:TYR:CZ	2:M:80:MET:HE1	2.50	0.47
2:H:31:GLN:NE2	2:H:70:SER:O	2.48	0.47
2:I:22:ARG:HE	2:J:102:LYS:NZ	2.13	0.47
1:C:223:ASN:ND2	1:C:273:PHE:O	2.33	0.46
1:G:75:MET:HE2	1:G:168:ALA:HB2	1.96	0.46
2:J:9:ILE:HD13	2:J:9:ILE:N	2.29	0.46
2:K:86:PHE:CE1	2:K:145:ARG:HG2	2.50	0.46
2:L:26:MET:HE1	2:L:59:LEU:CD1	2.36	0.46
1:B:111:GLU:HG2	2:N:21:ILE:O	2.15	0.46
1:C:299:ASP:C	1:C:299:ASP:OD2	2.57	0.46
2:J:10:ILE:CD1	2:J:19:PRO:HB3	2.45	0.46
2:K:131:TYR:CE2	2:K:133:VAL:HA	2.49	0.46
1:D:255:TYR:CD2	1:D:269:TYR:CE2	3.03	0.46
1:E:237:GLU:N	1:E:237:GLU:OE2	2.49	0.46
2:L:21:ILE:HG21	2:L:80:MET:HB3	1.96	0.46
1:F:211:GLN:HE21	1:F:289:GLY:C	2.24	0.46
2:H:6:TYR:O	2:H:69:VAL:HG21	2.15	0.46
2:I:65:GLY:O	2:I:67:GLY:N	2.48	0.46
2:M:63:TYR:CE1	2:M:80:MET:HE1	2.49	0.46
1:A:56:ARG:HA	1:F:91:VAL:O	2.15	0.46
2:J:55:PHE:O	2:J:56:PRO:C	2.57	0.46
1:G:231:ASP:OD2	1:G:277:ARG:NH2	2.48	0.46
2:M:84:CYS:O	2:M:145:ARG:NH1	2.48	0.46
1:A:170:TYR:CD1	1:A:174:GLY:HA2	2.51	0.46
1:C:179:ASN:HB3	2:N:77:ALA:HA	1.97	0.46
1:F:74:MET:SD	1:F:284:ASN:ND2	2.88	0.46
1:C:135:SER:OG	1:C:136:ARG:N	2.48	0.46
1:E:219:VAL:O	1:E:223:ASN:HB2	2.15	0.46
2:N:151:MET:HE3	2:N:151:MET:HB3	1.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:63:TYR:CD1	2:K:80:MET:HE1	2.51	0.46
1:D:192:HIS:O	1:D:195:THR:HG22	2.16	0.46
1:D:216:ASP:O	1:D:219:VAL:N	2.49	0.46
1:D:350:TYR:CD1	1:D:350:TYR:C	2.94	0.46
1:F:215:PRO:HB3	1:F:266:VAL:HG22	1.98	0.46
1:A:146:ALA:HB2	1:G:86:ASN:ND2	2.31	0.45
1:B:128:PRO:HD2	1:B:332:MET:O	2.16	0.45
1:B:172:LEU:HD12	1:B:286:LEU:HB2	1.98	0.45
1:G:134:TYR:CD1	1:G:159:VAL:HG21	2.51	0.45
1:G:243:VAL:HG11	1:G:251:PHE:HE2	1.81	0.45
1:C:272:GLN:NE2	1:C:273:PHE:CE1	2.85	0.45
2:L:151:MET:SD	2:M:123:ILE:HD11	2.57	0.45
1:D:339:ASP:OD1	1:D:339:ASP:C	2.59	0.45
1:E:196:ILE:HD12	1:E:347:PHE:CE1	2.50	0.45
1:F:79:MET:HE1	1:F:332:MET:HE1	1.98	0.45
2:J:100:LEU:HD13	2:J:127:SER:OG	2.16	0.45
1:A:252:MET:HA	1:A:265:THR:HB	1.98	0.45
1:B:338:LYS:HG2	1:B:339:ASP:O	2.17	0.45
2:N:26:MET:HE2	2:N:73:VAL:HG11	1.97	0.45
2:H:53:GLN:H	2:H:53:GLN:NE2	2.12	0.45
2:L:122:ASN:O	2:L:124:LEU:HD22	2.16	0.45
1:A:303:ARG:HH21	1:A:337:ARG:HH22	1.65	0.45
1:B:96:ILE:HD11	1:B:121:ASP:HB3	1.99	0.45
1:G:143:GLY:O	1:G:147:GLU:HG2	2.16	0.45
2:I:126:TYR:N	2:I:144:ARG:O	2.31	0.45
1:A:67:ARG:HD3	1:A:161:PHE:CE2	2.52	0.45
1:D:119:ARG:NE	2:M:4:ILE:HD11	2.30	0.45
1:D:125:ASP:CG	1:D:192:HIS:HE2	2.24	0.45
1:D:196:ILE:HG12	1:D:233:GLN:CD	2.41	0.45
1:D:273:PHE:CE1	1:E:254:PRO:HB3	2.47	0.45
1:E:209:ASP:OD1	1:E:211:GLN:NE2	2.49	0.45
1:G:270:ILE:C	1:G:272:GLN:H	2.25	0.45
2:H:31:GLN:O	2:H:32:PRO:C	2.58	0.45
2:I:148:ASN:HB2	2:J:149:ALA:CB	2.47	0.45
1:C:179:ASN:H	2:N:78:THR:CG2	2.30	0.45
1:D:298:ASN:HB3	1:D:301:TYR:CD2	2.52	0.45
1:F:305:ARG:HD2	1:F:305:ARG:HA	1.76	0.45
2:H:9:ILE:HD12	2:H:61:HIS:H	1.81	0.45
2:I:26:MET:SD	2:I:79:GLY:HA3	2.56	0.45
1:B:77:ASP:OD1	1:B:297:ARG:NE	2.50	0.44
1:B:163:LEU:C	1:B:165:SER:N	2.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:171:LEU:HG	1:G:332:MET:HE1	1.99	0.44
1:G:303:ARG:HE	1:G:337:ARG:NH2	2.12	0.44
1:C:196:ILE:HD13	1:C:233:GLN:CG	2.45	0.44
1:F:55:TRP:HE1	2:K:66:GLY:HA3	1.82	0.44
1:F:75:MET:O	1:F:79:MET:HG2	2.18	0.44
1:E:106:THR:HG23	1:E:109:GLY:H	1.81	0.44
1:E:108:SER:OG	2:I:21:ILE:HD11	2.17	0.44
2:I:125:PHE:HB3	2:I:143:VAL:HB	2.00	0.44
2:J:12:GLY:HA2	2:J:89:THR:HG23	2.00	0.44
1:B:69:GLU:O	1:B:71:GLY:N	2.48	0.44
1:B:75:MET:HE1	1:B:167:MET:CE	2.48	0.44
1:D:235:VAL:HG21	1:D:347:PHE:HZ	1.83	0.44
1:E:301:TYR:HB3	1:E:345:LYS:HB2	1.99	0.44
1:F:77:ASP:OD2	1:F:295:TYR:OH	2.32	0.44
1:F:172:LEU:HD22	1:F:287:LEU:HD21	2.00	0.44
2:H:9:ILE:HD11	2:H:32:PRO:HB3	1.98	0.44
1:A:152:LEU:HD13	1:A:326:PHE:CE2	2.52	0.44
1:A:194:ASN:OD1	1:A:338:LYS:CE	2.64	0.44
2:K:62:ASN:HB2	2:K:73:VAL:HG22	2.00	0.44
1:F:292:PHE:CE1	1:F:349:GLY:HA3	2.53	0.44
1:B:107:LEU:HG	1:C:178:LEU:HD22	2.00	0.44
1:C:128:PRO:HG3	1:C:170:TYR:CZ	2.52	0.44
1:D:301:TYR:CD1	1:D:345:LYS:HD2	2.52	0.44
1:D:344:SER:OG	1:D:345:LYS:N	2.50	0.44
2:K:123:ILE:HB	2:M:149:ALA:HB3	1.98	0.44
2:M:30:LEU:HD11	2:M:46:ALA:HB2	2.00	0.44
1:B:248:ARG:NH1	1:B:283:THR:OG1	2.50	0.44
1:G:98:SER:OG	1:G:99:ASP:N	2.50	0.44
2:H:22:ARG:HG2	2:H:38:PHE:CE1	2.53	0.44
2:K:36:VAL:O	2:K:57:TYR:HB2	2.18	0.44
2:M:100:LEU:HG	2:M:127:SER:OG	2.18	0.44
1:D:190:THR:O	1:D:348:ASN:ND2	2.51	0.44
1:E:136:ARG:HH21	1:E:151:PRO:CB	2.29	0.44
1:G:70:ALA:C	1:G:72:GLN:H	2.20	0.44
2:K:60:GLN:HG3	2:K:61:HIS:N	2.32	0.44
2:K:94:VAL:HG22	2:K:114:LEU:HB2	2.00	0.44
1:F:90:THR:HG22	1:F:91:VAL:HG23	2.00	0.43
2:H:52:GLY:C	2:H:54:GLY:N	2.74	0.43
2:K:5:ARG:NH2	2:K:129:GLU:OE2	2.43	0.43
1:A:163:LEU:HA	1:F:103:VAL:HG21	1.99	0.43
1:E:63:THR:HG23	1:E:63:THR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:106:THR:OG1	1:F:111:GLU:HG3	2.18	0.43
1:G:271:THR:O	1:G:272:GLN:C	2.61	0.43
1:G:284:ASN:HB3	1:G:287:LEU:HD12	1.99	0.43
1:A:71:GLY:HA2	1:A:284:ASN:OD1	2.19	0.43
1:C:196:ILE:CD1	1:C:233:GLN:HG3	2.44	0.43
1:G:75:MET:HE1	1:G:164:ARG:O	2.18	0.43
1:G:272:GLN:O	1:G:273:PHE:HB2	2.19	0.43
2:K:56:PRO:HG2	2:K:84:CYS:HB2	1.99	0.43
1:D:300:MET:HA	1:D:337:ARG:NH1	2.32	0.43
2:H:10:ILE:HG13	2:H:90:TYR:CE1	2.53	0.43
2:J:109:ASN:O	2:J:110:GLY:C	2.59	0.43
1:B:255:TYR:O	1:C:258:ALA:HB1	2.18	0.43
1:E:190:THR:HG23	1:E:348:ASN:ND2	2.33	0.43
1:C:136:ARG:NH2	1:C:155:ASP:OD1	2.52	0.43
1:D:230:LEU:HD21	1:D:239:VAL:HG21	2.00	0.43
1:G:188:GLY:O	1:G:192:HIS:HB2	2.19	0.43
2:I:9:ILE:HG13	2:I:69:VAL:HG12	2.01	0.43
2:K:5:ARG:HE	2:K:5:ARG:HB3	1.41	0.43
2:M:105:PRO:HB3	2:M:123:ILE:HD13	2.00	0.43
1:C:307:ALA:HB3	1:C:331:ALA:HB3	2.01	0.43
1:D:201:ASN:OD1	1:D:352:THR:HG23	2.19	0.43
1:E:117:LYS:HG2	2:J:8:THR:HG23	1.99	0.43
1:F:96:ILE:HD11	1:F:123:THR:HG23	2.01	0.43
1:F:106:THR:CA	1:F:111:GLU:OE2	2.61	0.43
2:M:100:LEU:HD21	2:M:127:SER:HB2	2.00	0.43
2:N:101:LYS:O	2:N:103:GLY:N	2.52	0.43
1:A:257:ASN:OD1	1:A:257:ASN:N	2.49	0.43
1:E:190:THR:HG23	1:E:348:ASN:HD21	1.83	0.43
1:A:136:ARG:HD3	1:A:136:ARG:HA	1.66	0.43
1:A:295:TYR:HB3	1:A:346:VAL:HG13	2.00	0.43
2:L:63:TYR:CZ	2:L:80:MET:HE1	2.54	0.43
1:B:209:ASP:OD1	1:B:211:GLN:NE2	2.37	0.43
1:D:273:PHE:HE1	1:E:254:PRO:CB	2.28	0.43
2:N:37:THR:HB	2:N:47:HIS:HD2	1.84	0.43
1:E:194:ASN:OD1	1:E:338:LYS:HD3	2.19	0.42
2:H:12:GLY:HA2	2:H:89:THR:H	1.84	0.42
2:K:53:GLN:HB3	2:L:150:SER:O	2.19	0.42
1:C:255:TYR:CE2	1:C:269:TYR:HD2	2.35	0.42
1:E:135:SER:HB2	1:E:325:ASN:OD1	2.19	0.42
1:E:231:ASP:OD1	1:E:277:ARG:NH1	2.47	0.42
1:B:191:ASN:OD1	1:B:191:ASN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:THR:HG23	1:C:217:GLU:H	1.85	0.42
1:E:69:GLU:HG3	1:E:285:PHE:HD1	1.84	0.42
1:G:70:ALA:C	1:G:72:GLN:N	2.75	0.42
1:A:160:THR:HG22	1:A:164:ARG:HE	1.84	0.42
1:A:231:ASP:OD1	1:A:277:ARG:NH2	2.52	0.42
1:F:179:ASN:H	2:I:78:THR:CG2	2.32	0.42
1:G:230:LEU:HA	1:G:230:LEU:HD23	1.70	0.42
2:L:9:ILE:HD11	2:L:32:PRO:HB2	2.01	0.42
2:N:100:LEU:HD22	2:N:104:THR:CG2	2.49	0.42
1:C:179:ASN:H	2:N:78:THR:HG23	1.85	0.42
1:D:301:TYR:CE1	1:D:345:LYS:HE3	2.54	0.42
1:E:305:ARG:N	1:E:333:GLY:O	2.47	0.42
1:E:337:ARG:NH2	1:F:61:VAL:HG11	2.34	0.42
1:F:298:ASN:HB3	1:F:301:TYR:CD2	2.55	0.42
2:I:100:LEU:HD23	2:I:127:SER:HB2	2.01	0.42
2:J:93:LEU:O	2:J:114:LEU:HD12	2.20	0.42
1:A:142:LEU:HD23	1:A:142:LEU:HA	1.84	0.42
1:B:192:HIS:ND1	1:B:193:PRO:HD2	2.34	0.42
1:D:215:PRO:HB3	1:D:266:VAL:HG22	2.00	0.42
1:E:291:HIS:HA	1:E:349:GLY:O	2.20	0.42
1:F:139:ARG:HB2	2:J:63:TYR:HE2	1.84	0.42
1:G:141:LEU:CD1	1:G:152:LEU:CD2	2.97	0.42
1:G:211:GLN:H	1:G:211:GLN:HG2	1.73	0.42
2:H:36:VAL:O	2:H:57:TYR:HB2	2.19	0.42
2:L:59:LEU:HD21	2:L:73:VAL:HG21	2.02	0.42
2:N:94:VAL:HG11	2:N:100:LEU:HD11	2.01	0.42
1:A:303:ARG:NH2	1:A:337:ARG:HH22	2.17	0.42
1:D:106:THR:HG22	1:D:111:GLU:HB2	2.01	0.42
2:J:53:GLN:HE21	2:J:54:GLY:N	2.17	0.42
2:L:100:LEU:HD22	2:L:104:THR:HB	2.01	0.42
1:A:51:THR:OG1	1:G:122:TYR:OH	2.15	0.42
1:B:98:SER:HB2	1:B:340:PHE:CD2	2.54	0.42
1:B:224:GLN:HE22	1:C:253:ARG:HG2	1.84	0.42
1:D:167:MET:HE3	1:D:330:SER:HB2	2.01	0.42
1:E:171:LEU:CD1	1:E:332:MET:HE1	2.50	0.42
2:H:126:TYR:CD2	2:J:55:PHE:HB2	2.55	0.42
2:J:5:ARG:NE	2:J:140:LEU:O	2.47	0.42
1:B:217:GLU:O	1:B:220:THR:HG22	2.20	0.42
1:C:98:SER:HG	1:C:119:ARG:H	1.67	0.42
1:D:89:LYS:HD2	1:E:55:TRP:C	2.44	0.42
2:N:22:ARG:CZ	2:N:38:PHE:CG	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:55:PHE:O	2:N:55:PHE:CG	2.73	0.42
2:N:100:LEU:HD22	2:N:104:THR:HG21	2.01	0.42
1:E:111:GLU:HG2	2:I:21:ILE:O	2.20	0.42
2:H:126:TYR:N	2:H:144:ARG:O	2.44	0.42
2:K:18:ASP:OD1	2:K:18:ASP:N	2.52	0.42
2:K:37:THR:OG1	2:K:38:PHE:N	2.53	0.42
2:K:105:PRO:HB3	2:K:126:TYR:HE1	1.85	0.42
1:C:140:GLU:O	1:C:144:MET:HG3	2.20	0.41
1:D:196:ILE:HD11	1:D:344:SER:H	1.85	0.41
1:D:298:ASN:HB3	1:D:301:TYR:HD2	1.84	0.41
1:G:313:TYR:CD2	1:G:313:TYR:C	2.98	0.41
2:K:95:ALA:N	2:K:114:LEU:O	2.47	0.41
1:D:89:LYS:HE3	1:E:54:TYR:O	2.20	0.41
1:D:118:THR:HG21	1:E:158:ASN:HD22	1.85	0.41
1:F:172:LEU:HD23	1:F:172:LEU:HA	1.90	0.41
1:G:229:ILE:C	1:G:231:ASP:N	2.77	0.41
2:H:64:LEU:HD11	2:H:80:MET:SD	2.60	0.41
2:H:145:ARG:HH21	2:I:147:GLY:HA3	1.84	0.41
2:L:35:LEU:N	2:L:112:GLY:O	2.51	0.41
1:E:79:MET:HE3	1:E:79:MET:HB3	1.84	0.41
1:E:85:ILE:HB	1:E:305:ARG:HH11	1.85	0.41
1:F:144:MET:SD	1:F:151:PRO:HG3	2.61	0.41
1:F:181:ASN:HD21	2:I:65:GLY:HA3	1.85	0.41
1:G:337:ARG:HG3	1:G:337:ARG:HH11	1.85	0.41
1:C:174:GLY:H	1:C:188:GLY:HA3	1.85	0.41
1:C:341:THR:HG21	1:C:343:LYS:HE3	2.02	0.41
1:E:223:ASN:HD21	1:F:253:ARG:HA	1.81	0.41
1:F:142:LEU:HD23	1:F:142:LEU:HA	1.85	0.41
2:J:26:MET:HE3	2:J:73:VAL:HB	2.01	0.41
2:L:151:MET:HE3	2:L:151:MET:HB3	1.98	0.41
1:C:67:ARG:HD2	1:C:161:PHE:CE2	2.55	0.41
1:C:211:GLN:HG2	1:C:212:THR:HG23	2.01	0.41
1:C:284:ASN:HB3	1:C:287:LEU:HD12	2.02	0.41
1:A:68:ASN:OD1	1:A:68:ASN:N	2.53	0.41
1:A:69:GLU:O	1:A:71:GLY:N	2.53	0.41
1:C:128:PRO:HD2	1:C:332:MET:O	2.20	0.41
1:D:85:ILE:HD13	1:D:127:ILE:HG13	2.02	0.41
1:F:59:ASP:OD1	1:F:59:ASP:N	2.37	0.41
1:G:110:GLN:HB2	2:H:21:ILE:HD12	2.01	0.41
1:G:171:LEU:HD22	1:G:334:LEU:HD13	2.03	0.41
1:G:201:ASN:OD1	1:G:351:GLY:HA2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:26:MET:CE	2:L:59:LEU:HD11	2.33	0.41
2:N:55:PHE:O	2:N:56:PRO:C	2.63	0.41
1:A:319:ASN:HB2	1:A:322:ASP:CG	2.45	0.41
1:F:196:ILE:HD11	1:F:344:SER:HB3	2.02	0.41
1:A:230:LEU:HD21	1:A:239:VAL:HG21	2.02	0.41
1:A:235:VAL:HG22	1:A:345:LYS:HE2	2.03	0.41
1:A:261:PHE:HD2	1:F:261:PHE:CD2	2.38	0.41
1:B:74:MET:SD	1:B:284:ASN:ND2	2.94	0.41
1:B:89:LYS:HD2	1:C:56:ARG:O	2.21	0.41
1:B:125:ASP:OD2	1:B:192:HIS:NE2	2.32	0.41
1:B:219:VAL:HG21	1:B:255:TYR:HE1	1.85	0.41
1:C:79:MET:HE3	1:C:79:MET:HB3	1.87	0.41
1:D:91:VAL:O	1:E:56:ARG:HA	2.21	0.41
1:D:100:ALA:HB1	1:D:116:ASP:HB3	2.02	0.41
1:E:215:PRO:HB3	1:E:266:VAL:HG22	2.03	0.41
1:G:90:THR:HG22	1:G:180:VAL:HG21	2.03	0.41
1:G:230:LEU:HD13	1:G:277:ARG:HD2	2.02	0.41
2:I:61:HIS:HE1	2:I:63:TYR:HB3	1.82	0.41
2:K:32:PRO:HD3	2:K:72:ALA:HA	2.03	0.41
1:C:137:GLU:H	1:C:137:GLU:HG2	1.31	0.41
1:D:192:HIS:CD2	1:D:336:ILE:HD12	2.55	0.41
1:E:200:LEU:HD11	1:E:292:PHE:HE1	1.86	0.41
2:J:32:PRO:HA	2:J:59:LEU:HD23	2.03	0.41
2:J:39:ASN:O	2:J:40:ASP:C	2.61	0.41
1:B:337:ARG:NH2	1:C:61:VAL:HG21	2.35	0.40
1:E:98:SER:OG	1:E:99:ASP:N	2.54	0.40
1:G:179:ASN:HB3	1:G:185:THR:HG22	2.02	0.40
2:L:55:PHE:O	2:L:55:PHE:CG	2.72	0.40
2:L:55:PHE:O	2:L:56:PRO:C	2.62	0.40
2:M:36:VAL:O	2:M:57:TYR:HB2	2.22	0.40
2:M:106:LEU:HD23	2:M:116:VAL:HA	2.02	0.40
1:E:230:LEU:HD23	1:E:230:LEU:HA	1.88	0.40
2:L:141:VAL:O	2:L:143:VAL:HG13	2.22	0.40
1:A:248:ARG:HG2	1:A:283:THR:OG1	2.21	0.40
1:D:119:ARG:H	1:D:119:ARG:HG2	1.78	0.40
1:D:135:SER:HB2	1:D:325:ASN:OD1	2.22	0.40
1:F:107:LEU:HD12	1:F:107:LEU:HA	1.90	0.40
1:F:206:LEU:O	1:F:208:ILE:N	2.54	0.40
1:G:273:PHE:HD2	1:G:273:PHE:HA	1.71	0.40
2:K:10:ILE:HG12	2:K:90:TYR:HE1	1.85	0.40
2:K:22:ARG:HB2	2:K:83:GLN:HE21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:105:PRO:HB3	2:K:123:ILE:HD13	2.03	0.40
1:C:189:ILE:HG21	1:C:293:VAL:HG13	2.03	0.40
1:E:301:TYR:CD2	1:E:345:LYS:HG3	2.57	0.40
1:G:110:GLN:O	2:H:21:ILE:HB	2.21	0.40
2:I:55:PHE:CE2	2:I:83:GLN:HB3	2.44	0.40
2:L:36:VAL:HG11	2:L:59:LEU:HD12	2.04	0.40
2:M:26:MET:HE1	2:M:30:LEU:HB2	2.02	0.40
1:A:354:THR:HA	1:A:355:PRO:HD3	1.95	0.40
1:C:196:ILE:CD1	1:C:233:GLN:CD	2.94	0.40
1:D:89:LYS:CE	1:E:56:ARG:O	2.45	0.40
1:D:192:HIS:CG	1:D:336:ILE:HD12	2.57	0.40
1:E:79:MET:CE	1:E:306:VAL:HG21	2.51	0.40
1:F:192:HIS:ND1	1:F:193:PRO:HD2	2.37	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	308/356 (86%)	299 (97%)	9 (3%)	0	100	100
1	B	306/356 (86%)	292 (95%)	12 (4%)	2 (1%)	19	47
1	C	307/356 (86%)	294 (96%)	10 (3%)	3 (1%)	13	39
1	D	307/356 (86%)	295 (96%)	12 (4%)	0	100	100
1	E	306/356 (86%)	293 (96%)	12 (4%)	1 (0%)	37	66
1	F	307/356 (86%)	293 (95%)	13 (4%)	1 (0%)	37	66
1	G	297/356 (83%)	277 (93%)	15 (5%)	5 (2%)	7	28
2	H	150/155 (97%)	136 (91%)	13 (9%)	1 (1%)	19	47
2	I	148/155 (96%)	132 (89%)	13 (9%)	3 (2%)	6	25
2	J	149/155 (96%)	135 (91%)	11 (7%)	3 (2%)	6	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	147/155 (95%)	139 (95%)	7 (5%)	1 (1%)	19	47
2	L	150/155 (97%)	142 (95%)	6 (4%)	2 (1%)	10	33
2	M	149/155 (96%)	144 (97%)	5 (3%)	0	100	100
2	N	150/155 (97%)	146 (97%)	2 (1%)	2 (1%)	10	33
All	All	3181/3577 (89%)	3017 (95%)	140 (4%)	24 (1%)	19	44

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	72	GLN
2	L	56	PRO
2	N	56	PRO
1	C	61	VAL
1	G	69	GLU
1	G	230	LEU
1	G	234	ASN
2	H	53	GLN
2	I	69	VAL
2	N	102	LYS
1	B	164	ARG
1	C	136	ARG
1	F	203	SER
2	J	53	GLN
2	J	56	PRO
2	K	65	GLY
2	L	122	ASN
1	B	256	SER
1	C	63	THR
1	E	114	ASP
2	I	56	PRO
2	I	55	PHE
2	J	54	GLY
1	G	71	GLY

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	257/296 (87%)	257 (100%)	0	100	100
1	B	254/296 (86%)	249 (98%)	5 (2%)	50	70
1	C	255/296 (86%)	245 (96%)	10 (4%)	27	53
1	D	256/296 (86%)	256 (100%)	0	100	100
1	E	256/296 (86%)	252 (98%)	4 (2%)	58	75
1	F	257/296 (87%)	255 (99%)	2 (1%)	79	87
1	G	250/296 (84%)	239 (96%)	11 (4%)	24	50
2	H	108/109 (99%)	106 (98%)	2 (2%)	52	71
2	I	107/109 (98%)	106 (99%)	1 (1%)	75	86
2	J	105/109 (96%)	101 (96%)	4 (4%)	28	54
2	K	106/109 (97%)	104 (98%)	2 (2%)	52	71
2	L	107/109 (98%)	105 (98%)	2 (2%)	52	71
2	M	108/109 (99%)	108 (100%)	0	100	100
2	N	107/109 (98%)	106 (99%)	1 (1%)	75	86
All	All	2533/2835 (89%)	2489 (98%)	44 (2%)	56	74

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	102	LYS
1	B	104	VAL
1	B	163	LEU
1	B	252	MET
1	B	281	ILE
1	C	59	ASP
1	C	60	ASN
1	C	61	VAL
1	C	102	LYS
1	C	111	GLU
1	C	134	TYR
1	C	135	SER
1	C	136	ARG
1	C	137	GLU
1	C	321	HIS
1	E	75	MET
1	E	111	GLU

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Mol	Chain	Res	Type
1	E	113	GLU
1	E	114	ASP
1	F	102	LYS
1	F	206	LEU
1	G	68	ASN
1	G	110	GLN
1	G	111	GLU
1	G	113	GLU
1	G	117	LYS
1	G	118	THR
1	G	173	THR
1	G	180	VAL
1	G	183	VAL
1	G	230	LEU
1	G	281	ILE
2	H	32	PRO
2	H	53	GLN
2	I	68	ASP
2	J	41	ASP
2	J	42	ASP
2	J	53	GLN
2	J	64	LEU
2	K	64	LEU
2	K	70	SER
2	L	119	ASP
2	L	122	ASN
2	N	104	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	238	GLN
1	A	298	ASN
1	B	176	GLN
1	B	224	GLN
1	C	272	GLN
1	D	223	ASN
1	D	272	GLN
1	D	291	HIS
1	D	319	ASN
1	E	290	ASN
1	E	319	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	348	ASN
1	F	60	ASN
1	F	207	ASN
1	F	211	GLN
1	F	223	ASN
1	F	291	HIS
1	F	321	HIS
1	G	110	GLN
1	G	321	HIS
2	H	53	GLN
2	H	83	GLN
2	I	61	HIS
2	J	53	GLN
2	J	83	GLN
2	J	122	ASN
2	J	148	ASN
2	K	148	ASN
2	L	148	ASN
2	M	61	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

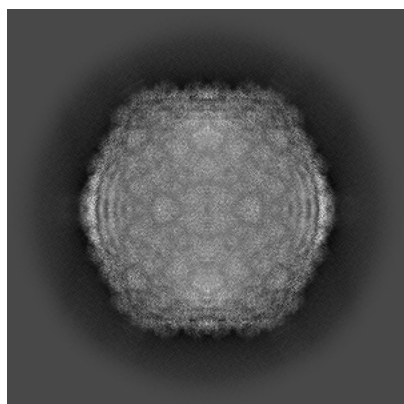
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70309. These allow visual inspection of the internal detail of the map and identification of artifacts.

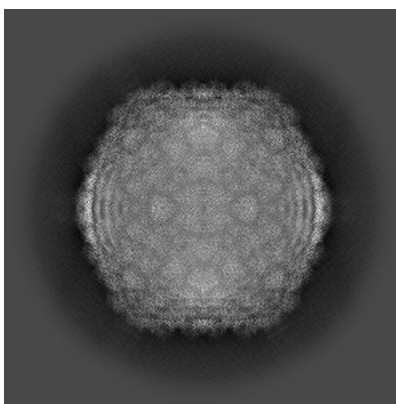
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

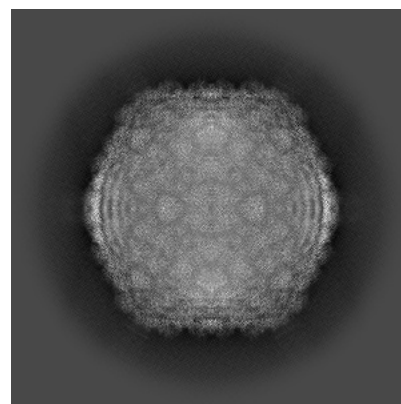
6.1.1 Primary map



X

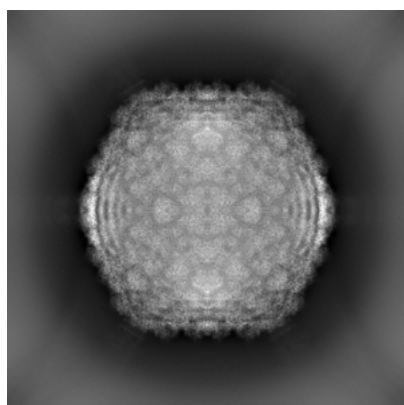


Y

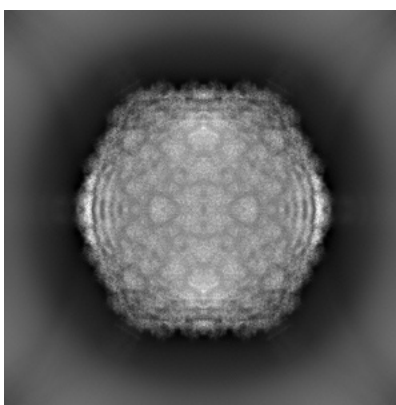


Z

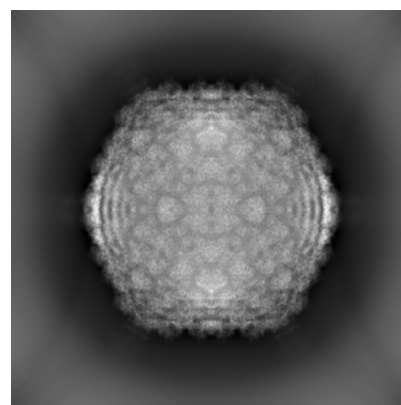
6.1.2 Raw map



X



Y

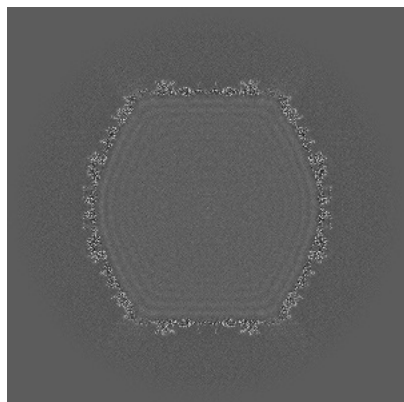


Z

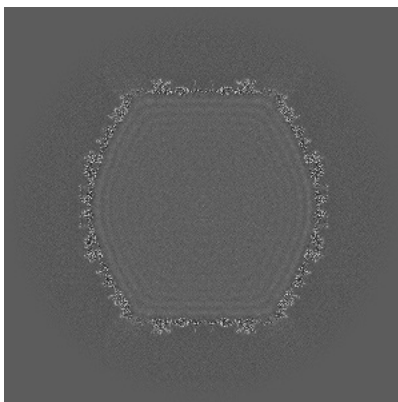
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

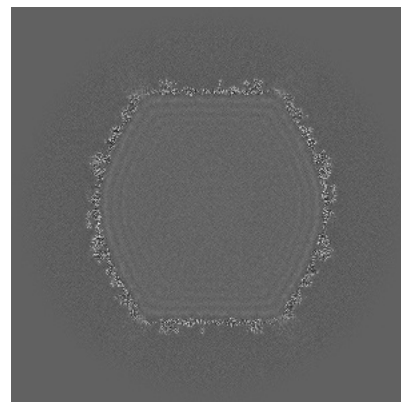
6.2.1 Primary map



X Index: 300

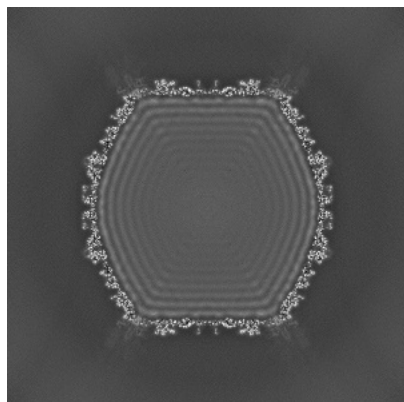


Y Index: 300

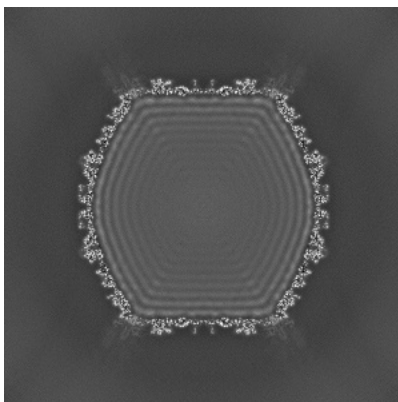


Z Index: 300

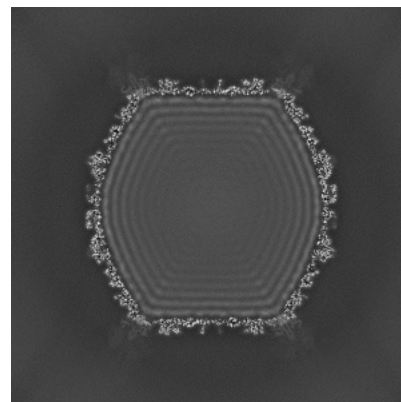
6.2.2 Raw map



X Index: 300



Y Index: 300

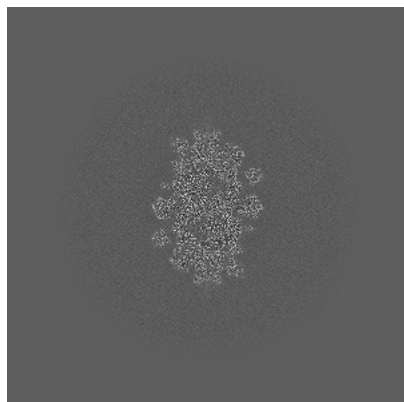


Z Index: 300

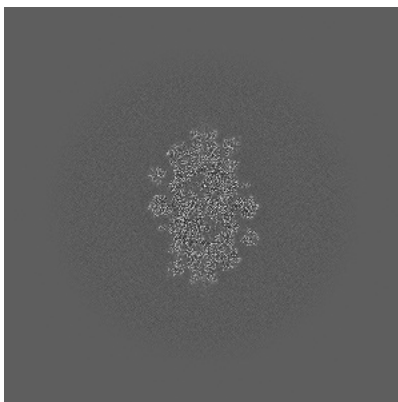
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

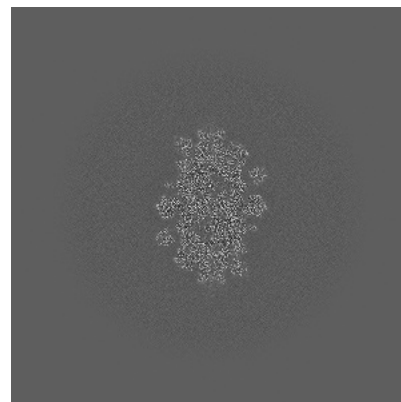
6.3.1 Primary map



X Index: 130

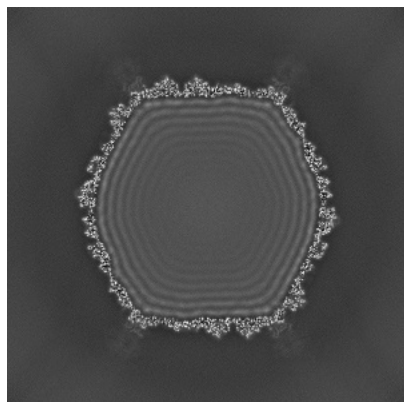


Y Index: 470

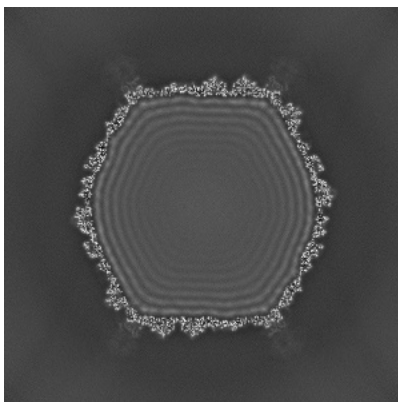


Z Index: 129

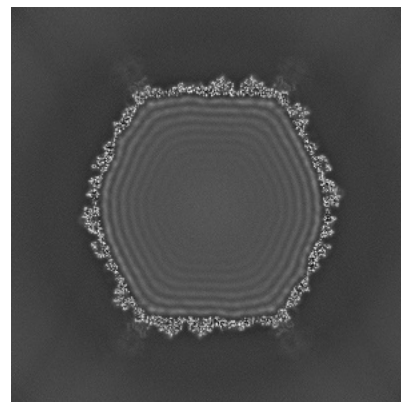
6.3.2 Raw map



X Index: 285



Y Index: 315

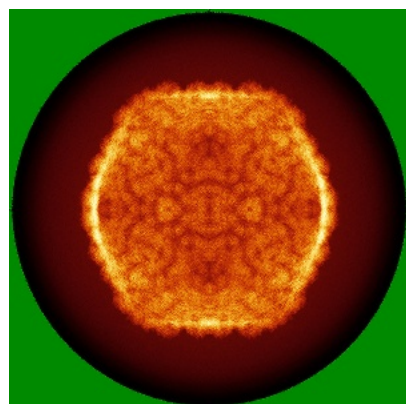


Z Index: 314

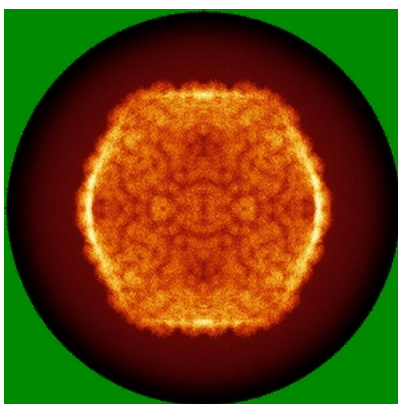
The images above show the largest variance slices of the map in three orthogonal directions.

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

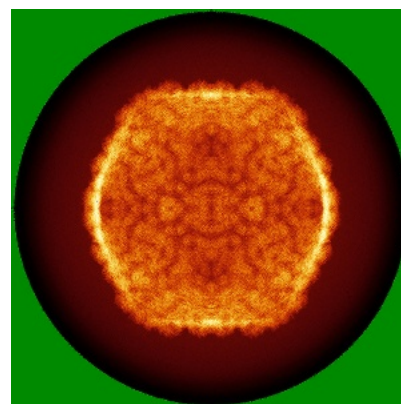
6.4.1 Primary map



X

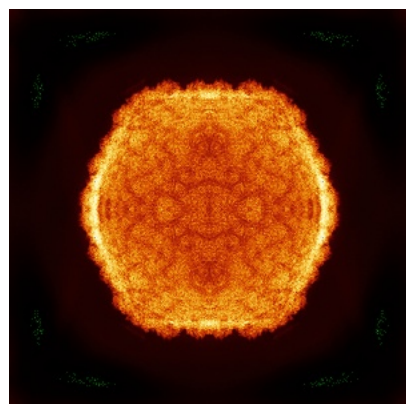


Y

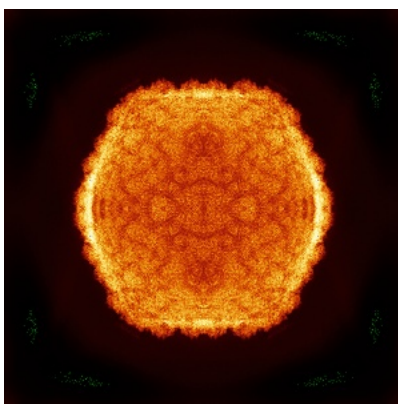


Z

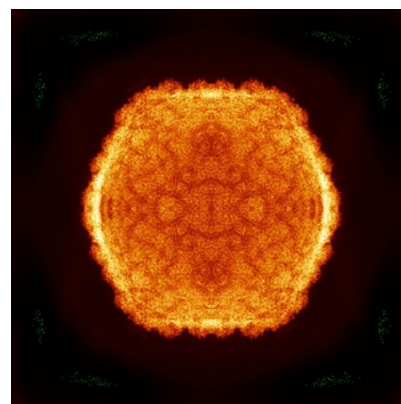
6.4.2 Raw map



X



Y

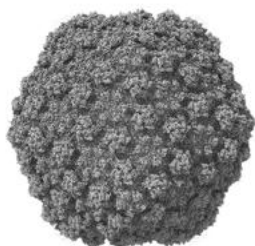


Z

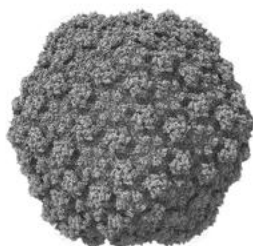
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

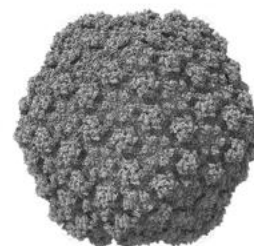
6.5.1 Primary map



X



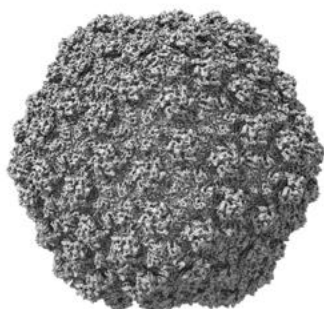
Y



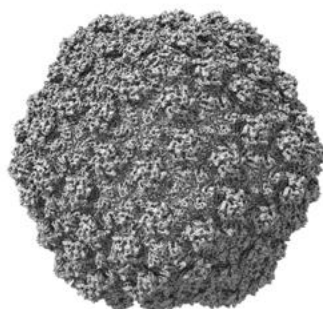
Z

The images above show the 3D surface view of the map at the recommended contour level 0.47. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

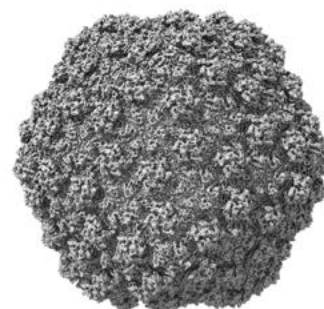
6.5.2 Raw map



X



Y



Z

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

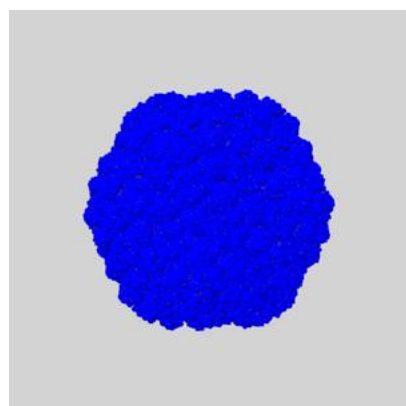
6.6 Mask visualisation [i](#)

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

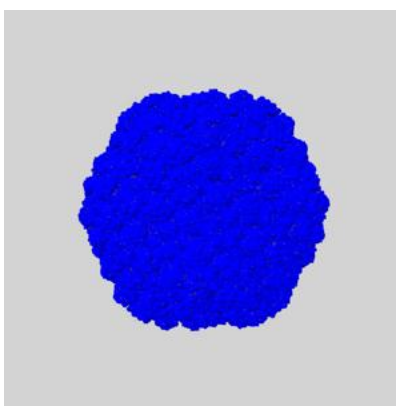
A mask typically either:

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

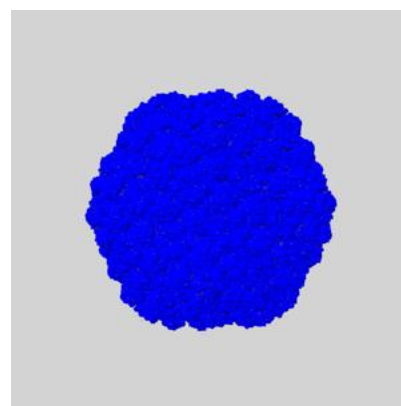
6.6.1 emd_70309_msk_1.map [i](#)



X



Y

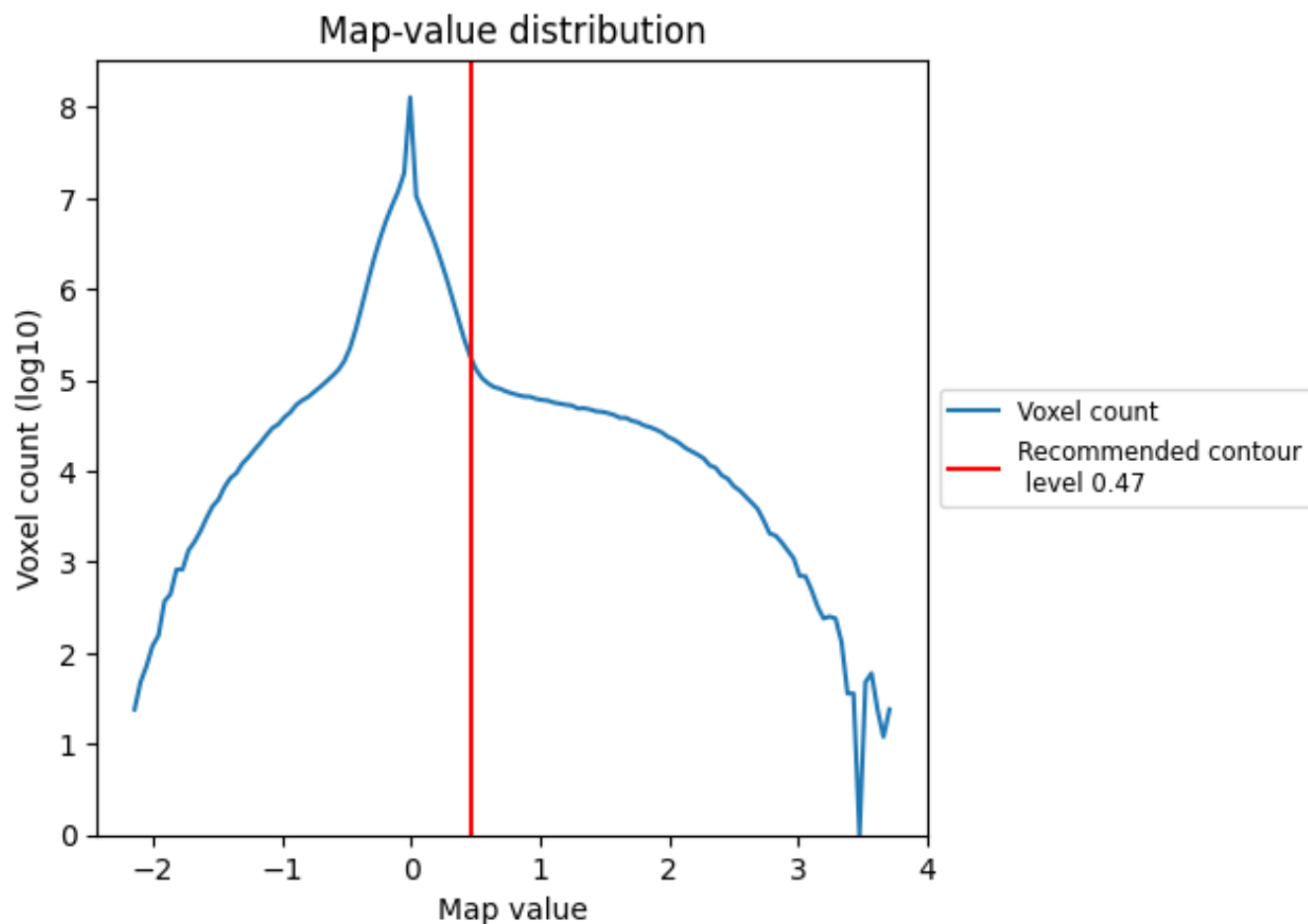


Z

7 Map analysis [i](#)

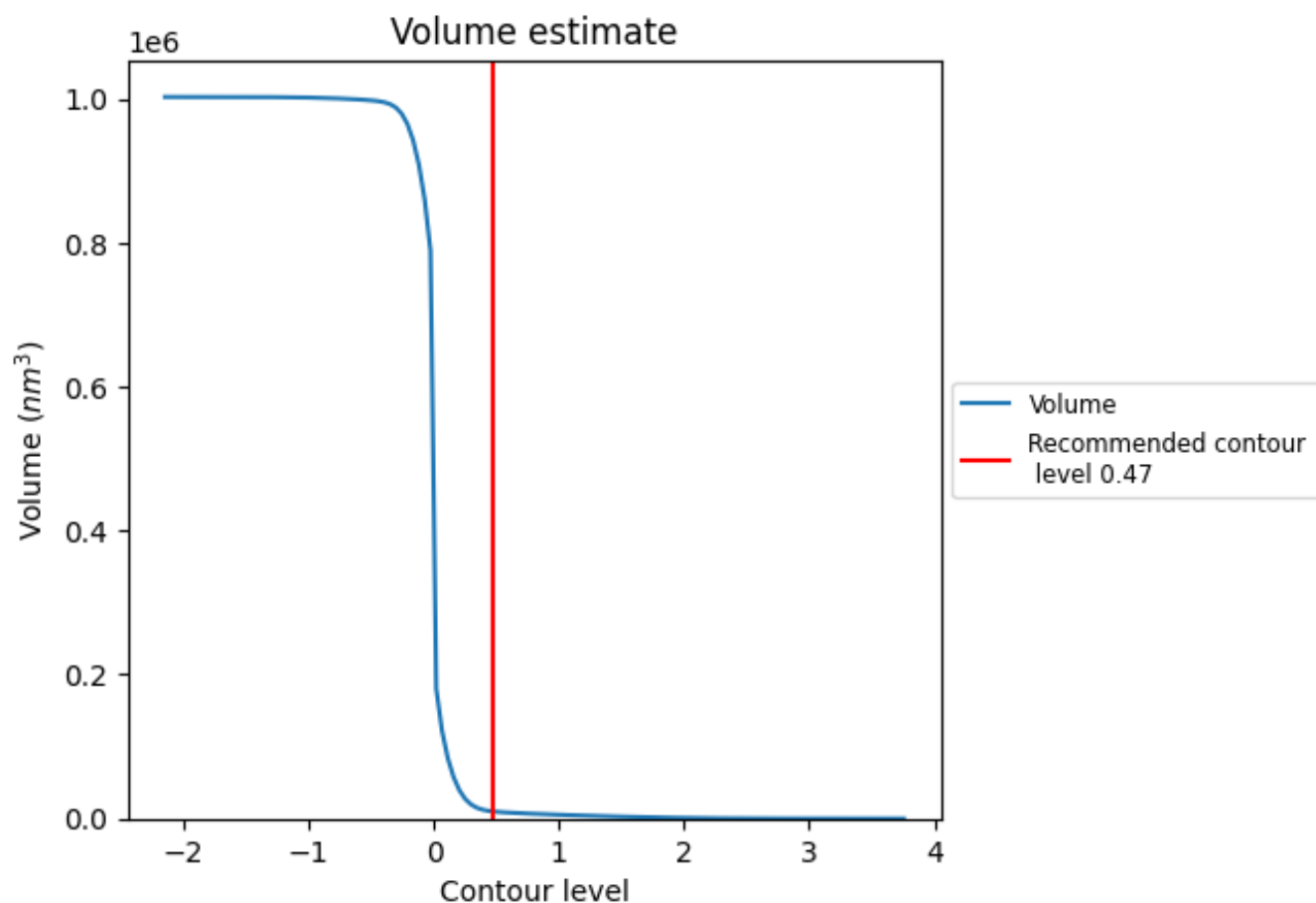
This section contains the results of statistical analysis of the map.

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.

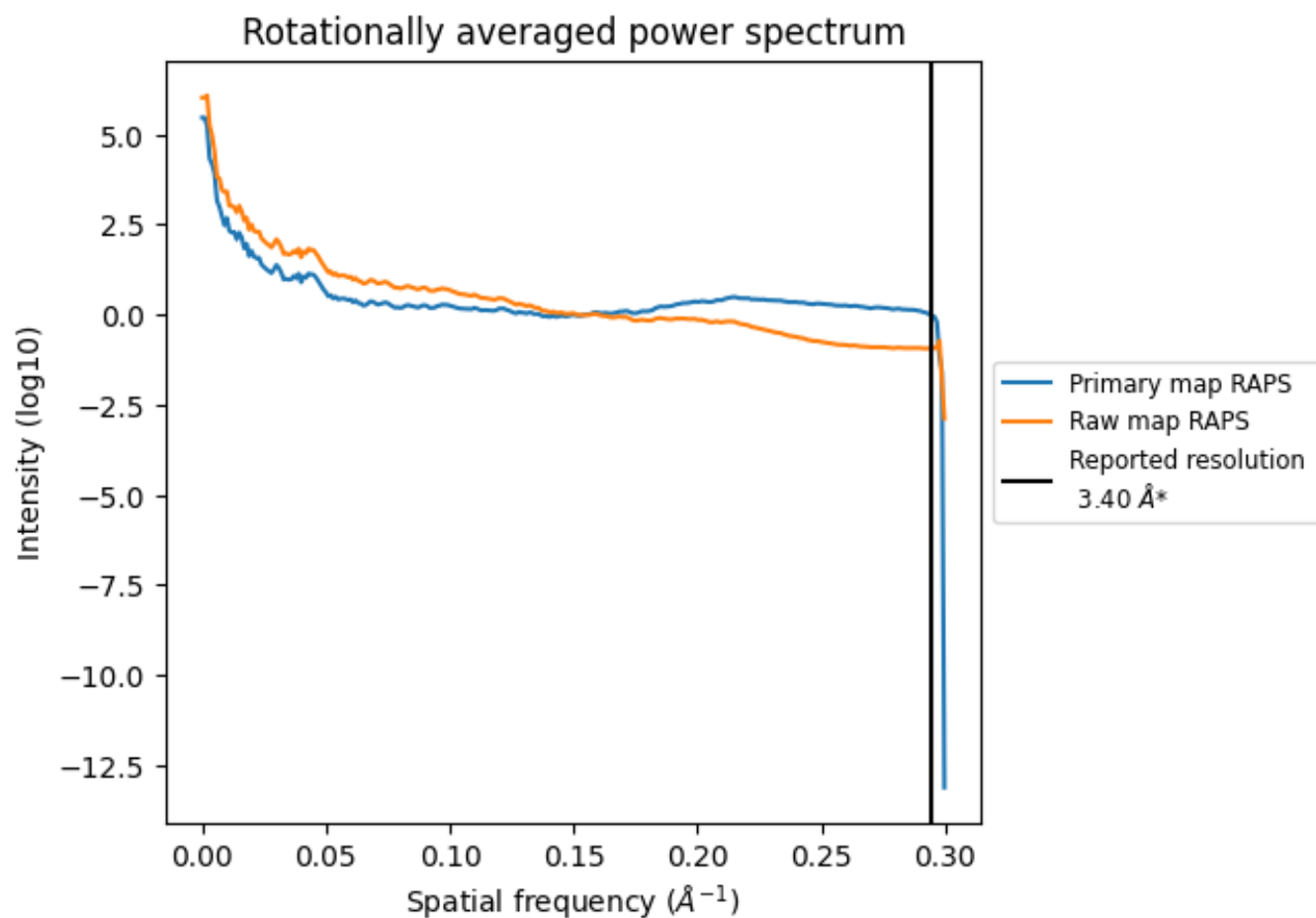
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 10065 nm³; this corresponds to an approximate mass of 9092 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 ⓘ

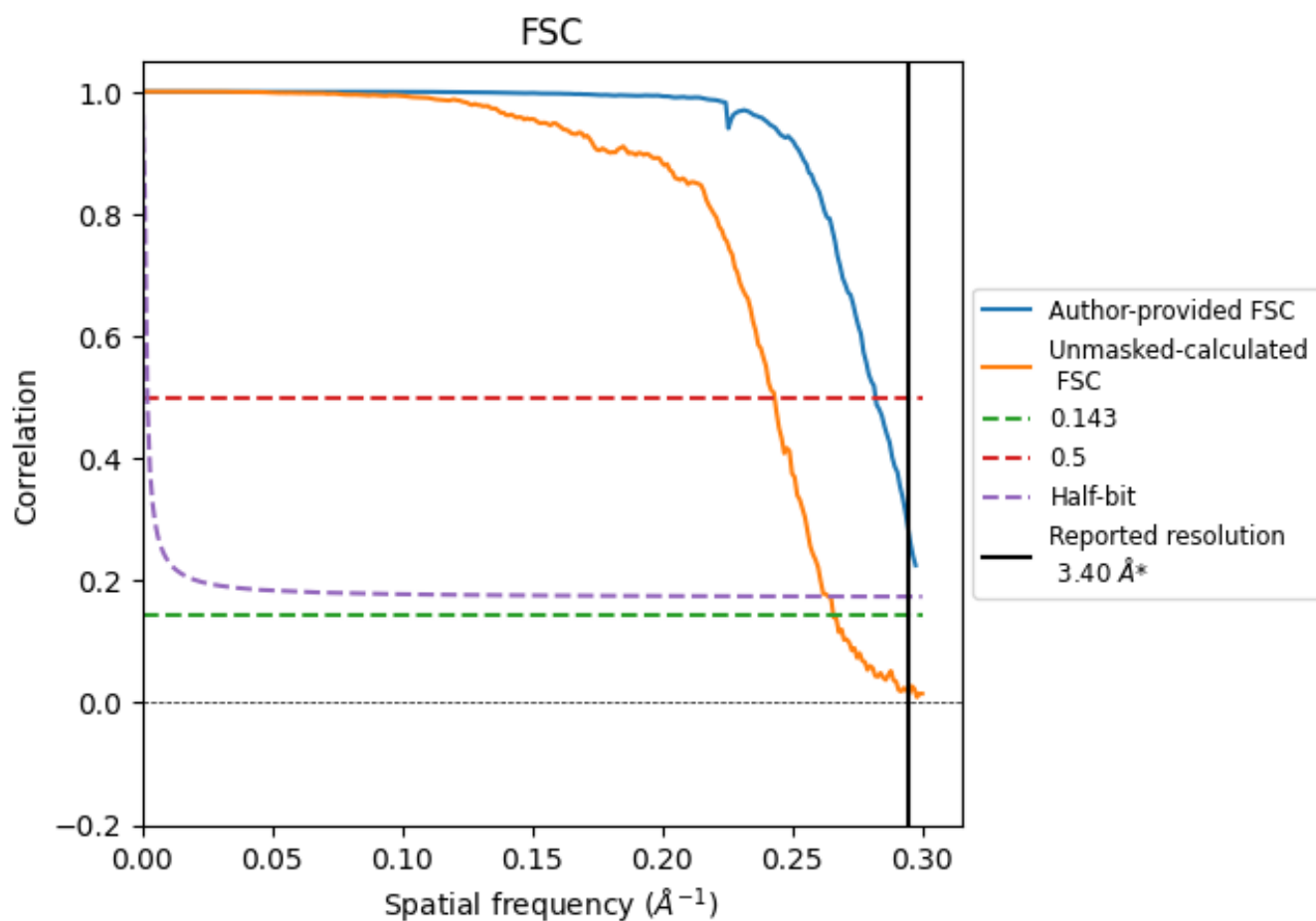


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	3.55	-
Unmasked-calculated*	3.76	4.12	3.79

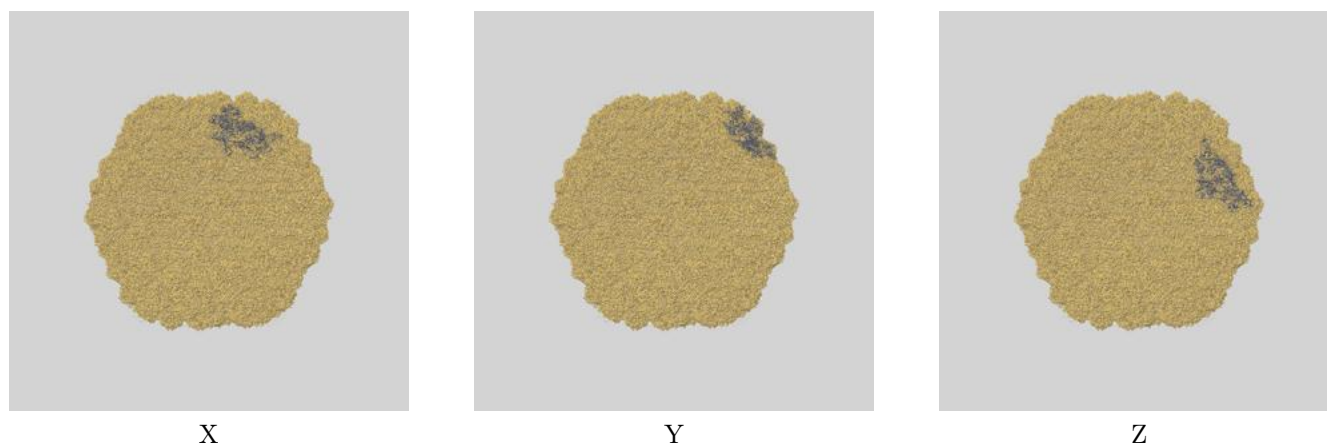
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.76 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

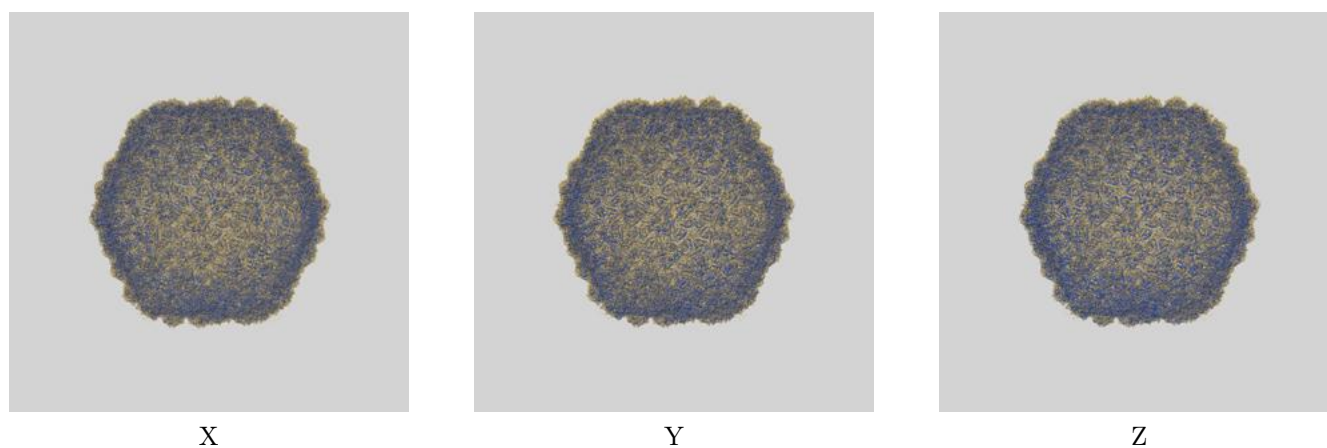
This section contains information regarding the fit between EMDB map EMD-70309 and PDB model 9OCB. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)



9.1.2 Map-model assembly overlay [i](#)



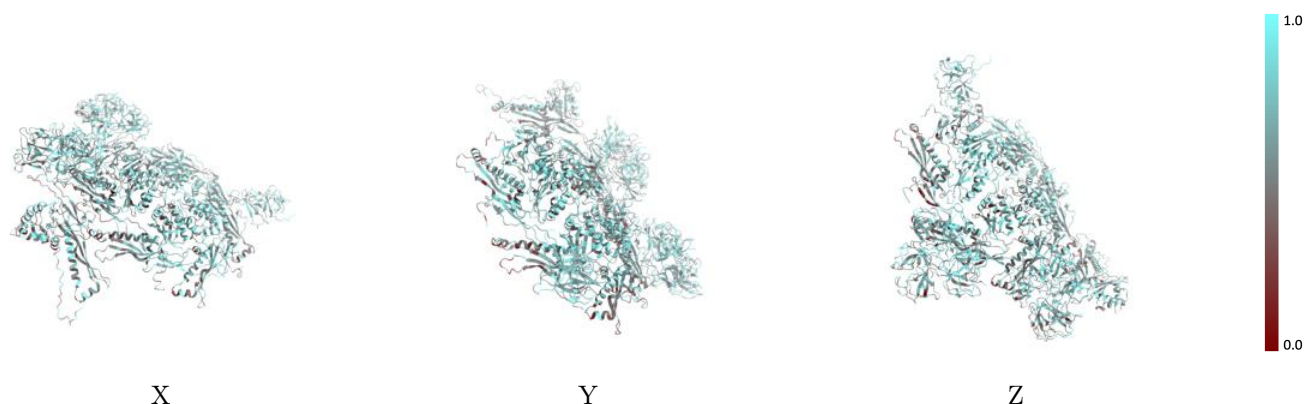
The images above show the 3D surface view of the map at the recommended contour level 0.47 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



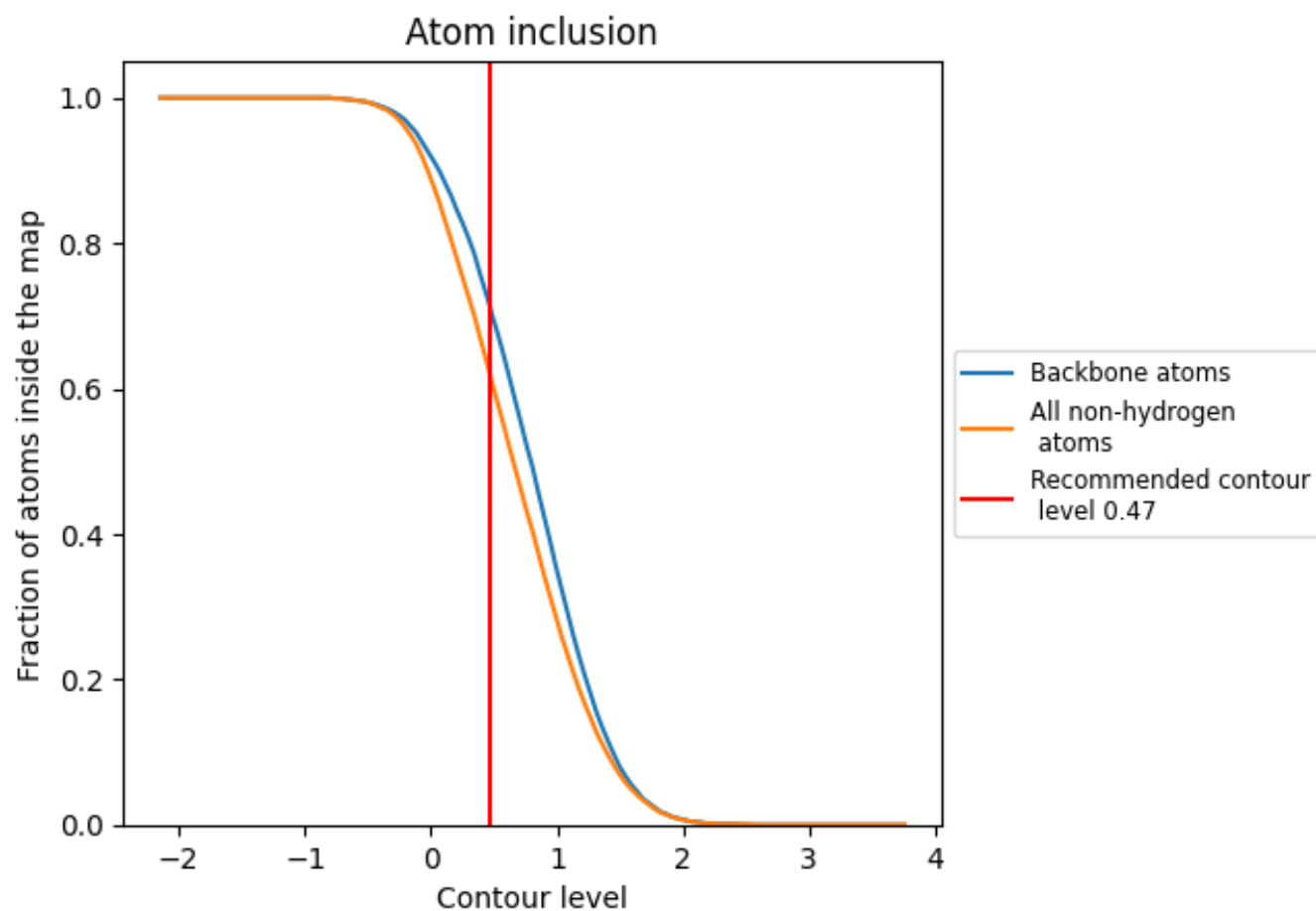
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.47).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 62% 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 (0.47) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6190	<div></div> 0.2610
A	<div></div> 0.6100	<div></div> 0.2570
B	<div></div> 0.6230	<div></div> 0.2650
C	<div></div> 0.6290	<div></div> 0.2640
D	<div></div> 0.6210	<div></div> 0.2650
E	<div></div> 0.5890	<div></div> 0.2340
F	<div></div> 0.5940	<div></div> 0.2420
G	<div></div> 0.5700	<div></div> 0.2450
H	<div></div> 0.5930	<div></div> 0.2430
I	<div></div> 0.6830	<div></div> 0.3150
J	<div></div> 0.6300	<div></div> 0.2590
K	<div></div> 0.6860	<div></div> 0.3200
L	<div></div> 0.6050	<div></div> 0.2370
M	<div></div> 0.6900	<div></div> 0.2980
N	<div></div> 0.6540	<div></div> 0.2900

