



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:57 AM UTC

PDB ID : 5ZUF / pdb_00005zuf
EMDB ID : EMD-6964
Title : Fit R10 Fab coordinates into the cryo-EM of EV71 in complex with A9
Authors : Wang, X.; Zhu, L.; Wang, N.
Deposited on : 2018-05-07
Resolution : 6.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

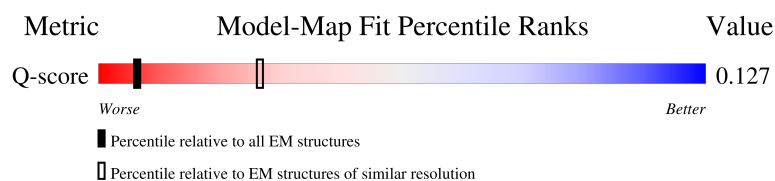
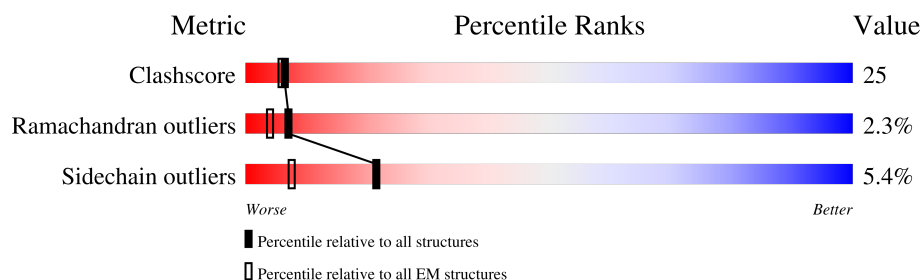
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 6.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	503 (6.30 - 7.30)

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	297	
2	B	245	
3	C	242	
4	D	212	

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Mol	Chain	Length	Quality of chain
5	E	220	43%70%25%..

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8629 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 Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	218	Total	C	N	O	S	0	0
			1724	1107	290	316	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	225	MET	CYS	conflict	UNP G5CUH3

- Molecule 2 is a protein called VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	237	Total	C	N	O	S	0	0
			1833	1179	301	345	8		

- Molecule 3 is a protein called VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	239	Total	C	N	O	S	0	0
			1830	1178	305	336	11		

- Molecule 4 is a protein called R10 ANTIBODY LIGHT CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	212	Total	C	N	O	S	0	0
			1614	1004	268	333	9		

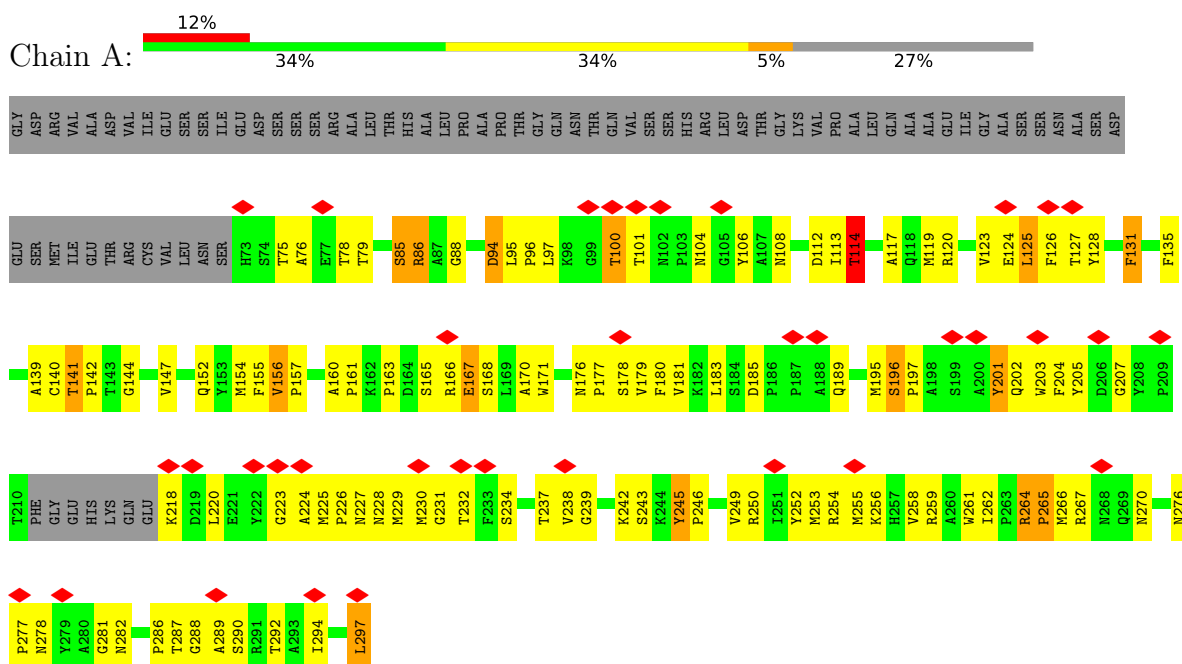
- Molecule 5 is a protein called R10 ANTIBODY HEAVY CHAIN.

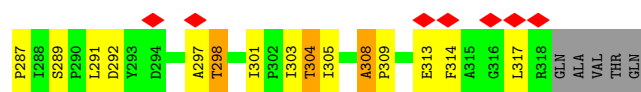
Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	217	Total	C	N	O	S	0	0
			1628	1037	265	318	8		

3 Residue-property plots [i](#)

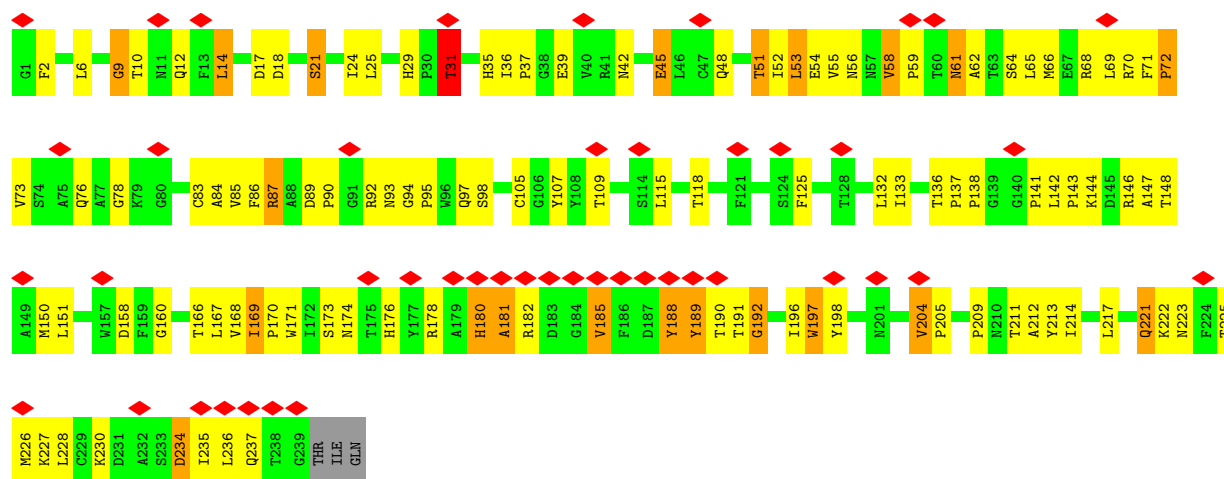
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Capsid protein VP1

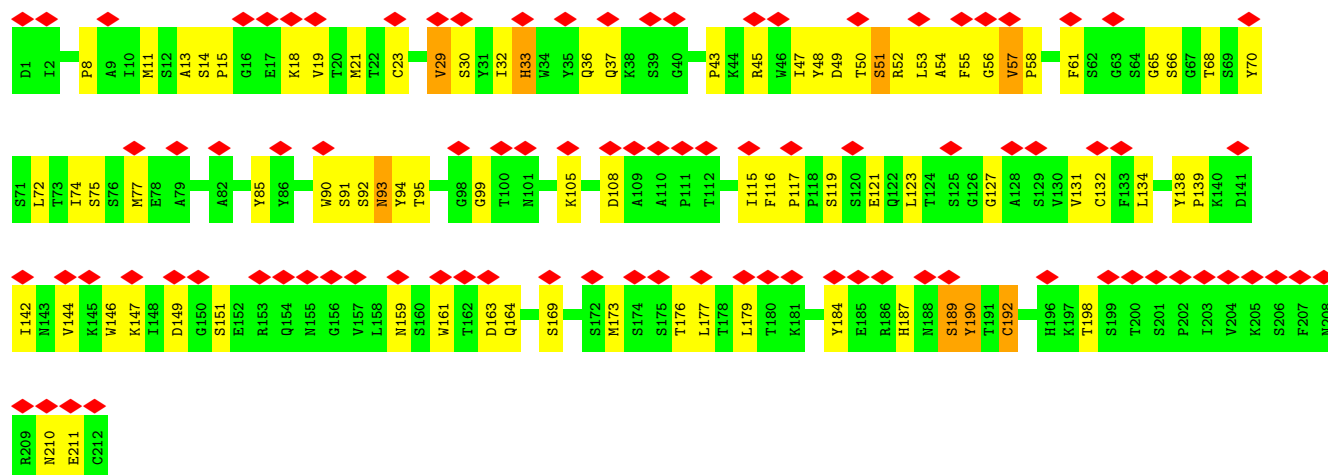




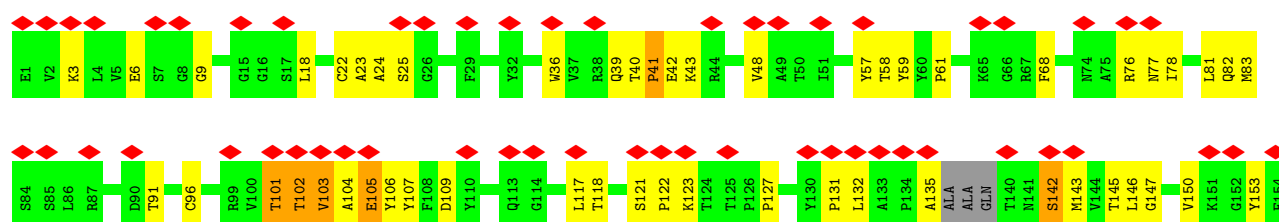
• Molecule 3: VP3



• Molecule 4: R10 ANTIBODY LIGHT CHAIN



• Molecule 5: R10 ANTIBODY HEAVY CHAIN



P155	E156	P157	V158	T159	V160	T161	S164	G165	S166	L167	S168	S169	V177	L178	Q179	S180	D181	L182	Y183	T184	L185	S186	S187	S188	V189	T190	V191	P192	S193	S194	T195	W196	P197	S198	E199	T200	V201	T202	C203	N204	V205	A206	H207	P208	A209	S210	S211	T212	K213	V214	D215	K216	K217	I218	R221
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1100	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.180	Depositor
Minimum map value	-0.129	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	648.0, 648.0, 648.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.35, 1.35, 1.35	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	0.55	0/1776	1.09	14/2419 (0.6%)
2	B	0.62	0/1888	1.08	18/2592 (0.7%)
3	C	0.60	0/1882	1.08	15/2576 (0.6%)
4	D	0.87	8/1653 (0.5%)	0.85	11/2248 (0.5%)
5	E	0.60	2/1672 (0.1%)	0.72	2/2285 (0.1%)
All	All	0.65	10/8871 (0.1%)	0.98	60/12120 (0.5%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	47	ILE	C-O	-7.74	1.16	1.24
4	D	94	TYR	CA-C	-6.83	1.43	1.52
4	D	190	TYR	C-O	-6.55	1.16	1.24
5	E	106	TYR	C-O	-6.19	1.15	1.23
5	E	145	THR	C-O	-6.16	1.16	1.24
4	D	29	VAL	C-O	-6.15	1.18	1.24
4	D	58	PRO	C-O	-5.41	1.17	1.23
4	D	95	THR	C-O	-5.29	1.17	1.23
4	D	33	HIS	C-O	-5.19	1.17	1.23
4	D	94	TYR	C-O	-5.04	1.17	1.23

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	91	SER	N-CA-C	10.21	122.49	111.36
4	D	30	SER	N-CA-C	8.07	120.16	111.36
5	E	142	SER	N-CA-C	7.82	121.63	112.72
4	D	57	VAL	N-CA-C	7.66	117.30	108.96
4	D	51	SER	N-CA-C	7.62	122.70	112.88
3	C	192	GLY	N-CA-C	-7.54	103.25	111.93
4	D	93	ASN	N-CA-C	-7.37	96.88	108.90
3	C	94	GLY	CA-C-N	7.02	128.61	119.84
3	C	94	GLY	C-N-CA	7.02	128.61	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	45	GLU	N-CA-C	-7.01	103.57	111.14
3	C	9	GLY	N-CA-C	-6.97	104.96	115.00
3	C	31	THR	CA-C-N	6.77	126.81	119.90
3	C	31	THR	C-N-CA	6.77	126.81	119.90
4	D	189	SER	N-CA-C	6.63	119.33	108.52
1	A	125	LEU	N-CA-C	-6.35	105.36	113.23
3	C	234	ASP	N-CA-C	-6.26	105.77	113.41
1	A	264	ARG	N-CA-C	6.21	115.45	108.25
2	B	225	ASP	N-CA-C	-6.15	105.60	113.23
1	A	201	TYR	N-CA-C	-6.05	101.32	110.28
2	B	175	PHE	N-CA-C	6.00	119.26	109.06
4	D	56	GLY	N-CA-C	6.00	120.45	112.77
1	A	225	MET	CA-C-N	5.91	125.46	119.19
1	A	225	MET	C-N-CA	5.91	125.46	119.19
1	A	119	MET	N-CA-C	5.91	118.22	111.02
2	B	298	THR	CA-C-N	5.88	126.39	120.04
2	B	298	THR	C-N-CA	5.88	126.39	120.04
2	B	241	ILE	N-CA-C	-5.83	103.63	111.44
2	B	132	PHE	N-CA-C	5.83	117.79	108.41
2	B	221	GLN	CA-C-N	5.83	127.13	119.84
2	B	221	GLN	C-N-CA	5.83	127.13	119.84
5	E	103	VAL	CB-CA-C	-5.83	104.51	111.97
3	C	29	HIS	CA-C-N	5.82	125.75	119.76
3	C	29	HIS	C-N-CA	5.82	125.75	119.76
2	B	162	GLY	N-CA-C	-5.80	107.14	114.16
1	A	282	ASN	N-CA-C	-5.71	105.33	112.93
1	A	141	THR	N-CA-C	-5.67	102.76	110.36
4	D	14	SER	N-CA-C	5.59	120.35	112.75
3	C	169	ILE	CA-C-N	5.55	126.78	119.84
3	C	169	ILE	C-N-CA	5.55	126.78	119.84
1	A	100	THR	N-CA-C	-5.51	105.68	112.90
1	A	114	THR	N-CA-C	-5.50	106.52	113.18
2	B	169	TYR	N-CA-C	5.48	117.33	111.36
2	B	161	PHE	N-CA-C	-5.46	104.86	112.45
3	C	185	VAL	N-CA-C	5.45	115.95	107.28
2	B	289	SER	N-CA-C	-5.45	100.06	109.15
4	D	14	SER	CA-C-N	5.42	140.01	127.00
4	D	14	SER	C-N-CA	5.42	140.01	127.00
3	C	2	PHE	CA-C-N	5.34	125.60	119.83
3	C	2	PHE	C-N-CA	5.34	125.60	119.83
1	A	258	VAL	N-CA-C	5.30	116.92	108.87
1	A	288	GLY	N-CA-C	5.29	118.83	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	308	ALA	CA-C-N	5.27	125.43	119.90
2	B	308	ALA	C-N-CA	5.27	125.43	119.90
2	B	135	LEU	N-CA-C	5.25	117.49	110.35
4	D	54	ALA	N-CA-C	-5.24	103.62	110.53
1	A	147	VAL	N-CA-C	5.22	113.47	109.19
2	B	113	ASP	N-CA-C	5.12	117.76	111.82
2	B	262	ILE	N-CA-C	5.06	115.55	108.17
2	B	192	LEU	N-CA-C	-5.05	101.47	109.96
1	A	131	PHE	N-CA-C	5.01	115.79	107.73

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	1724	0	1688	117	0
2	B	1833	0	1774	120	0
3	C	1830	0	1804	119	0
4	D	1614	0	1511	68	0
5	E	1628	0	1586	77	0
All	All	8629	0	8363	429	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 25.

All (429) 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)
4:D:132:CYS:SG	4:D:146:TRP:CH2	2.22	1.33
5:E:22:CYS:SG	5:E:96:CYS:SG	1.38	1.27
5:E:36:TRP:CZ3	5:E:96:CYS:SG	2.45	1.10
5:E:36:TRP:CH2	5:E:96:CYS:SG	2.45	1.09
5:E:22:CYS:SG	5:E:36:TRP:CH2	2.46	1.08
1:A:229:MET:HE2	1:A:231:GLY:H	1.12	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:76:GLN:O	5:E:103:VAL:HA	1.56	1.05
1:A:281:GLY:HA3	2:B:204:VAL:HG13	1.35	1.04
4:D:52:ARG:HH12	5:E:103:VAL:HG13	1.23	1.03
3:C:105:CYS:HA	3:C:226:MET:HE1	1.40	1.01
2:B:124:ARG:HG2	2:B:313:GLU:HG2	1.48	0.94
2:B:233:TYR:HA	3:C:66:MET:HE3	1.49	0.93
1:A:104:ASN:O	1:A:166:ARG:HD2	1.76	0.85
4:D:132:CYS:SG	4:D:146:TRP:CZ2	2.70	0.84
4:D:117:PRO:HG2	5:E:135:ALA:HB2	1.59	0.84
3:C:76:GLN:O	5:E:102:THR:C	2.20	0.83
1:A:229:MET:HE2	1:A:231:GLY:N	1.94	0.82
3:C:76:GLN:O	5:E:102:THR:O	1.97	0.81
3:C:76:GLN:O	5:E:103:VAL:CA	2.29	0.80
2:B:85:LEU:HD21	2:B:94:THR:CG2	2.12	0.80
3:C:6:LEU:HD13	3:C:10:THR:HG21	1.65	0.79
3:C:144:LYS:HD3	3:C:148:THR:HG21	1.63	0.79
4:D:132:CYS:SG	4:D:146:TRP:HH2	1.98	0.79
1:A:281:GLY:CA	2:B:204:VAL:HG13	2.10	0.78
2:B:243:GLN:HA	3:C:51:THR:HG22	1.66	0.78
1:A:156:VAL:HG22	1:A:232:THR:HB	1.66	0.77
2:B:241:ILE:HG21	3:C:66:MET:HE1	1.67	0.77
3:C:9:GLY:O	3:C:12:GLN:HG2	1.86	0.76
3:C:78:GLY:HA3	5:E:103:VAL:HB	1.66	0.76
1:A:197:PRO:HA	3:C:31:THR:HG21	1.68	0.75
2:B:252:ILE:HA	2:B:257:ASN:HD21	1.51	0.75
2:B:138:LYS:HE3	2:B:225:ASP:O	1.87	0.73
3:C:58:VAL:HG23	3:C:59:PRO:HD3	1.69	0.73
2:B:128:SER:O	2:B:131:ARG:HG2	1.89	0.73
2:B:188:GLN:NE2	3:C:209:PRO:HB2	2.04	0.73
3:C:42:ASN:O	3:C:45:GLU:HG3	1.88	0.72
3:C:105:CYS:CA	3:C:226:MET:HE1	2.20	0.72
4:D:134:LEU:HD11	4:D:144:VAL:HG11	1.71	0.72
3:C:167:LEU:HD12	3:C:168:VAL:H	1.55	0.72
4:D:52:ARG:HH22	5:E:103:VAL:HG11	1.55	0.72
2:B:90:SER:HB2	2:B:132:PHE:HB2	1.72	0.72
4:D:32:ILE:CG2	4:D:70:TYR:HD2	2.03	0.71
2:B:85:LEU:HD21	2:B:94:THR:HG22	1.72	0.71
5:E:24:ALA:HB3	5:E:77:ASN:HB3	1.71	0.71
5:E:6:GLU:HB3	5:E:22:CYS:SG	2.31	0.71
4:D:18:LYS:HB3	4:D:75:SER:HB2	1.74	0.70
1:A:297:LEU:HD12	1:A:297:LEU:H	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:TYR:CA	3:C:66:MET:HE3	2.21	0.70
4:D:21:MET:HE2	4:D:72:LEU:HD22	1.73	0.70
2:B:240:PRO:HG3	2:B:243:GLN:NE2	2.07	0.69
3:C:188:TYR:O	3:C:189:TYR:HD2	1.74	0.69
5:E:103:VAL:HG23	5:E:104:ALA:N	2.07	0.68
3:C:235:ILE:C	3:C:236:LEU:HD12	2.19	0.67
1:A:226:PRO:C	1:A:228:ASN:H	2.02	0.66
4:D:159:ASN:HB3	4:D:173:MET:HE3	1.76	0.66
3:C:188:TYR:O	3:C:189:TYR:CD2	2.48	0.66
3:C:105:CYS:HA	3:C:226:MET:CE	2.19	0.66
3:C:73:VAL:HA	3:C:198:TYR:OH	1.95	0.66
1:A:75:THR:HG22	3:C:225:THR:HG22	1.77	0.66
1:A:76:ALA:O	1:A:79:THR:HG23	1.95	0.66
1:A:112:ASP:OD1	1:A:114:THR:HG22	1.96	0.66
3:C:142:LEU:HD23	3:C:143:PRO:O	1.95	0.66
5:E:91:THR:HG23	5:E:118:THR:HA	1.77	0.65
5:E:131:PRO:O	5:E:132:LEU:HD23	1.96	0.65
4:D:52:ARG:NH1	5:E:103:VAL:HG13	2.03	0.65
1:A:141:THR:HB	1:A:142:PRO:HD2	1.78	0.65
5:E:23:ALA:HA	5:E:78:ILE:HG22	1.79	0.65
5:E:203:CYS:SG	5:E:218:ILE:HD11	2.37	0.64
5:E:102:THR:OG1	5:E:103:VAL:N	2.27	0.64
2:B:82:VAL:N	2:B:96:GLU:HG3	2.13	0.63
3:C:76:GLN:CB	5:E:101:THR:HG22	2.29	0.63
4:D:149:ASP:OD2	4:D:187:HIS:HB3	1.99	0.63
5:E:41:PRO:HB2	5:E:43:LYS:HE3	1.81	0.63
1:A:294:ILE:HD11	3:C:55:VAL:HG12	1.80	0.63
4:D:32:ILE:H	4:D:50:THR:HG22	1.63	0.63
4:D:45:ARG:NH2	5:E:109:ASP:OD1	2.31	0.63
4:D:90:TRP:HB2	5:E:105:GLU:OE1	1.98	0.63
1:A:152:GLN:HG3	1:A:180:PHE:CE2	2.34	0.62
1:A:229:MET:CE	1:A:231:GLY:H	2.01	0.62
1:A:117:ALA:HB1	3:C:236:LEU:HD23	1.80	0.62
3:C:204:VAL:HG22	3:C:205:PRO:HD2	1.82	0.61
3:C:180:HIS:CD2	3:C:181:ALA:H	2.18	0.61
4:D:32:ILE:HB	4:D:70:TYR:CD2	2.35	0.61
5:E:22:CYS:SG	5:E:96:CYS:CB	2.79	0.61
5:E:40:THR:O	5:E:42:GLU:N	2.33	0.61
2:B:267:ILE:HG12	3:C:37:PRO:HG2	1.82	0.61
4:D:8:PRO:HD2	4:D:11:MET:HE3	1.81	0.61
1:A:112:ASP:CG	1:A:114:THR:HG22	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:MET:HE3	1:A:230:MET:H	1.66	0.60
3:C:190:THR:O	3:C:192:GLY:N	2.33	0.60
5:E:9:GLY:HA2	5:E:18:LEU:HD21	1.82	0.60
2:B:187:HIS:CD2	2:B:301:ILE:HD11	2.37	0.60
1:A:276:ASN:HB2	1:A:277:PRO:HD2	1.83	0.60
2:B:85:LEU:HD23	2:B:85:LEU:H	1.67	0.60
1:A:254:ARG:NH2	1:A:256:LYS:HD3	2.16	0.60
3:C:167:LEU:HD12	3:C:168:VAL:N	2.16	0.60
1:A:267:ARG:HD2	2:B:238:GLY:O	2.02	0.59
1:A:292:THR:HG22	5:E:57:TYR:HD2	1.66	0.59
3:C:54:GLU:HG2	3:C:69:LEU:HD23	1.82	0.59
2:B:191:LEU:HD23	2:B:287:PRO:HA	1.83	0.59
4:D:52:ARG:HH12	5:E:103:VAL:CG1	2.07	0.59
1:A:254:ARG:NH1	3:C:18:ASP:HA	2.18	0.59
3:C:138:PRO:HB3	3:C:190:THR:HA	1.83	0.59
4:D:32:ILE:HB	4:D:70:TYR:HD2	1.67	0.59
3:C:58:VAL:H	3:C:59:PRO:HD2	1.68	0.59
2:B:268:ASN:OD1	2:B:278:HIS:HE1	1.85	0.58
1:A:254:ARG:HH21	1:A:256:LYS:HD3	1.68	0.58
2:B:204:VAL:HG22	2:B:231:HIS:HE1	1.67	0.58
4:D:184:TYR:O	4:D:190:TYR:OH	2.21	0.58
3:C:133:ILE:HG12	3:C:196:ILE:HG12	1.86	0.58
4:D:116:PHE:CE2	5:E:132:LEU:O	2.57	0.58
1:A:97:LEU:HD11	1:A:246:PRO:HD3	1.86	0.58
3:C:65:LEU:O	3:C:68:ARG:HG3	2.03	0.58
3:C:185:VAL:O	3:C:185:VAL:HG23	2.04	0.58
1:A:125:LEU:HD23	1:A:126:PHE:CE2	2.39	0.57
5:E:83:MET:HE1	5:E:117:LEU:HD22	1.86	0.57
4:D:142:ILE:HG22	4:D:161:TRP:HZ2	1.69	0.57
1:A:294:ILE:HD12	3:C:56:ASN:HA	1.87	0.57
1:A:154:MET:HE2	1:A:176:ASN:HB2	1.86	0.57
2:B:164:ASN:O	2:B:168:HIS:HB2	2.04	0.57
2:B:203:THR:HG23	2:B:219:GLN:HE22	1.68	0.57
3:C:144:LYS:CD	3:C:148:THR:HG21	2.34	0.57
4:D:61:PHE:CE1	4:D:74:ILE:HG12	2.40	0.57
1:A:270:ASN:HA	3:C:235:ILE:HG23	1.86	0.57
2:B:117:THR:CG2	2:B:120:ASP:HB3	2.35	0.56
3:C:76:GLN:O	5:E:103:VAL:N	2.37	0.56
2:B:85:LEU:HD23	2:B:85:LEU:N	2.20	0.56
2:B:148:TYR:HB3	2:B:284:LEU:HD12	1.86	0.56
3:C:66:MET:HE2	3:C:66:MET:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:135:LEU:HD23	2:B:135:LEU:N	2.21	0.56
4:D:32:ILE:CB	4:D:70:TYR:HD2	2.19	0.56
1:A:104:ASN:HA	1:A:242:LYS:NZ	2.21	0.56
2:B:125:PRO:HB3	2:B:129:VAL:HG21	1.88	0.56
1:A:171:TRP:CH2	1:A:234:SER:HB3	2.42	0.55
4:D:23:CYS:SG	4:D:32:ILE:HD11	2.46	0.55
1:A:229:MET:CE	1:A:230:MET:H	2.20	0.55
3:C:180:HIS:CG	3:C:181:ALA:H	2.24	0.55
4:D:33:HIS:CD2	4:D:90:TRP:HD1	2.24	0.55
1:A:94:ASP:C	1:A:96:PRO:HD3	2.31	0.55
2:B:185:LYS:HD3	3:C:125:PHE:CE1	2.42	0.55
2:B:148:TYR:CB	2:B:284:LEU:HD12	2.37	0.54
1:A:166:ARG:NH2	1:A:237:THR:OG1	2.39	0.54
1:A:112:ASP:OD2	1:A:114:THR:HG22	2.08	0.54
1:A:156:VAL:HG23	1:A:156:VAL:O	2.08	0.54
1:A:123:VAL:C	1:A:125:LEU:H	2.16	0.54
2:B:235:LEU:O	2:B:236:ASP:C	2.51	0.54
3:C:227:LYS:O	3:C:228:LEU:HB2	2.07	0.54
4:D:131:VAL:HG22	4:D:176:THR:HG23	1.88	0.54
2:B:156:THR:HG22	2:B:165:ALA:HB1	1.90	0.54
1:A:290:SER:OG	3:C:68:ARG:NH2	2.41	0.53
2:B:168:HIS:CD2	2:B:314:PHE:HB3	2.43	0.53
2:B:184:SER:C	2:B:186:PHE:H	2.13	0.53
1:A:238:VAL:HG12	1:A:239:GLY:N	2.24	0.53
4:D:45:ARG:HD2	5:E:109:ASP:HA	1.90	0.53
1:A:154:MET:HE2	1:A:176:ASN:CB	2.39	0.53
3:C:56:ASN:O	3:C:68:ARG:HA	2.09	0.53
3:C:221:GLN:HB3	3:C:223:ASN:OD1	2.09	0.53
1:A:253:MET:HE3	1:A:255:MET:HG3	1.91	0.52
1:A:117:ALA:CB	3:C:236:LEU:HD23	2.40	0.52
2:B:137:THR:OG1	2:B:304:THR:HG23	2.09	0.52
3:C:52:ILE:HA	3:C:217:LEU:HD23	1.91	0.52
2:B:154:VAL:HG23	2:B:224:ALA:HA	1.91	0.52
2:B:222:PRO:HB3	2:B:227:PHE:HB2	1.90	0.52
1:A:127:THR:HG23	1:A:264:ARG:NH2	2.24	0.52
5:E:127:PRO:HB3	5:E:153:TYR:HB3	1.91	0.52
1:A:156:VAL:O	1:A:156:VAL:CG2	2.57	0.52
2:B:137:THR:HG23	2:B:303:ILE:O	2.10	0.52
1:A:237:THR:HG21	1:A:243:SER:HB2	1.92	0.52
4:D:115:ILE:HG13	4:D:192:CYS:SG	2.50	0.52
4:D:45:ARG:HH21	5:E:109:ASP:HA	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:22:CYS:SG	5:E:36:TRP:HH2	2.24	0.52
1:A:205:TYR:O	1:A:223:GLY:HA2	2.10	0.52
1:A:292:THR:HG23	5:E:57:TYR:HB3	1.90	0.51
4:D:121:GLU:OE1	5:E:216:LYS:HE3	2.10	0.51
1:A:262:ILE:HG21	2:B:197:PRO:HG2	1.92	0.51
2:B:203:THR:CG2	2:B:219:GLN:HE22	2.22	0.51
3:C:58:VAL:HG23	3:C:59:PRO:CD	2.39	0.51
5:E:142:SER:O	5:E:142:SER:OG	2.26	0.51
2:B:126:ASP:O	2:B:127:VAL:O	2.28	0.51
1:A:226:PRO:C	1:A:228:ASN:N	2.69	0.51
2:B:140:TRP:CE2	2:B:291:LEU:HB2	2.46	0.51
2:B:140:TRP:HD1	2:B:141:GLU:N	2.09	0.51
1:A:265:PRO:HB2	2:B:239:ILE:HB	1.92	0.51
3:C:71:PHE:HE1	3:C:214:ILE:HD12	1.75	0.51
5:E:36:TRP:CZ2	5:E:96:CYS:SG	3.02	0.51
2:B:117:THR:HG21	2:B:120:ASP:HB3	1.93	0.51
4:D:13:ALA:HB3	4:D:77:MET:HG2	1.92	0.51
5:E:22:CYS:SG	5:E:36:TRP:CZ3	3.02	0.51
1:A:181:VAL:HG23	1:A:185:ASP:HB2	1.93	0.50
1:A:297:LEU:HD12	1:A:297:LEU:N	2.26	0.50
5:E:103:VAL:CG2	5:E:104:ALA:N	2.72	0.50
5:E:58:THR:O	5:E:59:TYR:HD1	1.94	0.50
2:B:145:LYS:NZ	2:B:145:LYS:HB3	2.27	0.50
3:C:109:THR:HB	3:C:228:LEU:HB2	1.94	0.50
3:C:197:TRP:N	3:C:197:TRP:CD1	2.80	0.50
4:D:11:MET:SD	4:D:19:VAL:HG13	2.52	0.50
1:A:224:ALA:O	1:A:226:PRO:HD3	2.11	0.50
2:B:156:THR:HG22	2:B:165:ALA:CB	2.42	0.50
3:C:147:ALA:O	3:C:150:MET:HB3	2.11	0.50
4:D:36:GLN:O	4:D:43:PRO:HA	2.12	0.50
1:A:165:SER:HB2	1:A:167:GLU:OE2	2.11	0.49
3:C:109:THR:HB	3:C:228:LEU:CB	2.42	0.49
4:D:138:TYR:CG	4:D:139:PRO:HA	2.48	0.49
1:A:152:GLN:HG3	1:A:180:PHE:CZ	2.47	0.49
1:A:104:ASN:HB2	1:A:106:TYR:CD1	2.48	0.49
3:C:142:LEU:HD23	3:C:142:LEU:C	2.37	0.49
4:D:105:LYS:HD2	4:D:138:TYR:OH	2.11	0.49
2:B:172:ARG:HD2	2:B:272:PHE:CZ	2.48	0.49
2:B:241:ILE:C	2:B:243:GLN:H	2.20	0.49
1:A:195:MET:O	1:A:196:SER:C	2.55	0.49
3:C:14:LEU:HB3	3:C:17:ASP:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:TYR:CD1	1:A:245:TYR:N	2.81	0.49
2:B:119:VAL:O	2:B:121:LYS:HG2	2.13	0.49
5:E:36:TRP:CE3	5:E:96:CYS:SG	3.03	0.49
1:A:226:PRO:O	1:A:228:ASN:N	2.44	0.48
3:C:174:ASN:OD1	3:C:174:ASN:O	2.31	0.48
1:A:195:MET:O	1:A:196:SER:O	2.31	0.48
3:C:78:GLY:CA	5:E:103:VAL:HB	2.39	0.48
3:C:132:LEU:HD23	3:C:132:LEU:C	2.39	0.48
4:D:138:TYR:CD1	4:D:139:PRO:HA	2.47	0.48
2:B:149:TRP:HZ3	2:B:285:VAL:CG1	2.25	0.48
2:B:108:PRO:HB3	2:B:174:GLY:HA3	1.96	0.48
3:C:66:MET:CE	3:C:69:LEU:HD11	2.44	0.48
5:E:210:SER:OG	5:E:212:THR:OG1	2.27	0.48
3:C:90:PRO:HD2	3:C:188:TYR:OH	2.13	0.48
3:C:171:TRP:HE1	3:C:173:SER:HB2	1.77	0.48
4:D:147:LYS:HA	4:D:151:SER:O	2.14	0.48
3:C:141:PRO:O	3:C:142:LEU:C	2.57	0.48
5:E:150:VAL:HG13	5:E:185:LEU:CD2	2.44	0.48
1:A:289:ALA:HB3	3:C:93:ASN:HB3	1.96	0.47
2:B:145:LYS:HB3	2:B:145:LYS:HZ2	1.79	0.47
2:B:184:SER:C	2:B:186:PHE:N	2.72	0.47
3:C:70:ARG:HG2	3:C:213:TYR:CD2	2.48	0.47
1:A:180:PHE:CD1	1:A:180:PHE:N	2.83	0.47
1:A:201:TYR:HA	1:A:228:ASN:HD21	1.79	0.47
2:B:230:GLN:O	2:B:231:HIS:CD2	2.66	0.47
5:E:127:PRO:HB2	5:E:150:VAL:CG2	2.45	0.47
1:A:95:LEU:N	1:A:96:PRO:HD3	2.28	0.47
4:D:108:ASP:HB3	4:D:198:THR:HG22	1.95	0.47
1:A:204:PHE:CE1	1:A:264:ARG:HD3	2.50	0.47
2:B:151:PHE:O	2:B:279:CYS:HA	2.15	0.47
5:E:68:PHE:CE2	5:E:83:MET:HB3	2.49	0.47
1:A:139:ALA:HB2	1:A:249:VAL:HG22	1.96	0.47
1:A:156:VAL:CG2	1:A:232:THR:HB	2.41	0.47
4:D:65:GLY:HA3	4:D:70:TYR:HA	1.96	0.47
4:D:163:ASP:OD1	4:D:163:ASP:N	2.47	0.47
1:A:163:PRO:HB3	1:A:168:SER:HB3	1.97	0.47
4:D:55:PHE:C	4:D:55:PHE:CD2	2.90	0.47
1:A:238:VAL:CG1	1:A:239:GLY:N	2.78	0.47
2:B:155:LEU:HD23	2:B:158:THR:HB	1.96	0.47
2:B:235:LEU:HD21	2:B:241:ILE:HG13	1.97	0.47
3:C:176:HIS:HB2	3:C:189:TYR:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:48:VAL:HA	5:E:61:PRO:HG3	1.97	0.47
3:C:90:PRO:CG	3:C:115:LEU:HD11	2.45	0.46
4:D:177:LEU:HG	4:D:179:LEU:HD21	1.97	0.46
5:E:22:CYS:O	5:E:78:ILE:HA	2.15	0.46
2:B:241:ILE:C	2:B:243:GLN:N	2.72	0.46
1:A:85:SER:O	1:A:86:ARG:O	2.34	0.46
1:A:292:THR:CG2	5:E:57:TYR:HB3	2.46	0.46
2:B:195:VAL:HG13	2:B:281:PHE:CD2	2.51	0.46
4:D:53:LEU:HD12	4:D:53:LEU:N	2.30	0.46
5:E:127:PRO:HB2	5:E:150:VAL:HG23	1.97	0.46
1:A:104:ASN:HA	1:A:242:LYS:HZ2	1.80	0.46
1:A:201:TYR:HA	1:A:228:ASN:ND2	2.30	0.46
1:A:266:MET:HE1	3:C:107:TYR:HE2	1.81	0.46
3:C:66:MET:HE1	3:C:69:LEU:HD11	1.96	0.46
1:A:177:PRO:HB2	3:C:24:ILE:HD11	1.98	0.45
2:B:218:LYS:HD2	2:B:218:LYS:N	2.30	0.45
2:B:222:PRO:HB2	2:B:226:GLY:O	2.16	0.45
2:B:233:TYR:HA	3:C:66:MET:CE	2.34	0.45
5:E:40:THR:O	5:E:41:PRO:C	2.59	0.45
5:E:41:PRO:O	5:E:43:LYS:HE3	2.15	0.45
1:A:250:ARG:HH21	1:A:250:ARG:HG3	1.82	0.45
1:A:281:GLY:HA3	2:B:204:VAL:CG1	2.24	0.45
3:C:58:VAL:CG2	3:C:59:PRO:HD3	2.42	0.45
1:A:108:ASN:ND2	1:A:234:SER:OG	2.49	0.45
1:A:189:GLN:HG2	3:C:21:SER:HB3	1.97	0.45
5:E:131:PRO:HG3	5:E:216:LYS:HD2	1.98	0.45
2:B:220:THR:HG22	2:B:221:GLN:NE2	2.31	0.45
2:B:243:GLN:O	2:B:246:VAL:HG12	2.16	0.45
3:C:71:PHE:CE1	3:C:214:ILE:HB	2.51	0.45
1:A:197:PRO:CA	3:C:31:THR:HG21	2.42	0.45
1:A:276:ASN:OD1	1:A:278:ASN:HB2	2.16	0.45
2:B:218:LYS:HD2	2:B:218:LYS:H	1.81	0.45
2:B:305:ILE:N	2:B:305:ILE:HD12	2.30	0.45
3:C:109:THR:HG21	3:C:228:LEU:HD12	1.99	0.45
2:B:125:PRO:HB3	2:B:129:VAL:CG2	2.47	0.45
1:A:113:ILE:HB	1:A:253:MET:HE1	1.98	0.44
1:A:135:PHE:O	1:A:189:GLN:HA	2.18	0.44
2:B:140:TRP:NE1	2:B:291:LEU:HB2	2.32	0.44
2:B:148:TYR:HA	2:B:283:LEU:O	2.17	0.44
2:B:171:TYR:CE2	2:B:173:SER:HB3	2.52	0.44
4:D:15:PRO:HB3	4:D:77:MET:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:132:CYS:SG	4:D:146:TRP:CZ3	3.02	0.44
2:B:115:ASP:CG	2:B:116:ALA:H	2.24	0.44
3:C:56:ASN:OD1	3:C:58:VAL:HG22	2.17	0.44
4:D:92:SER:OG	4:D:93:ASN:N	2.45	0.44
2:B:185:LYS:HB3	3:C:125:PHE:HD1	1.82	0.44
5:E:76:ARG:HD2	5:E:78:ILE:HD11	1.99	0.44
1:A:97:LEU:HD21	1:A:245:TYR:C	2.41	0.44
3:C:93:ASN:N	3:C:93:ASN:HD22	2.13	0.44
4:D:15:PRO:CB	4:D:77:MET:HG3	2.46	0.44
4:D:55:PHE:CD2	4:D:55:PHE:O	2.71	0.44
5:E:121:SER:N	5:E:122:PRO:CD	2.81	0.44
1:A:266:MET:O	2:B:240:PRO:HD3	2.17	0.44
3:C:188:TYR:O	3:C:189:TYR:HB3	2.16	0.44
5:E:103:VAL:HG23	5:E:104:ALA:H	1.82	0.44
1:A:135:PHE:CE1	1:A:253:MET:HB2	2.53	0.44
1:A:140:CYS:SG	1:A:144:GLY:HA2	2.57	0.44
1:A:218:LYS:CA	2:B:216:PRO:HA	2.47	0.44
1:A:286:PRO:O	1:A:287:THR:C	2.61	0.44
2:B:96:GLU:O	2:B:97:ALA:HB2	2.17	0.44
2:B:117:THR:HG22	2:B:117:THR:O	2.18	0.44
3:C:158:ASP:C	3:C:160:GLY:H	2.26	0.44
5:E:131:PRO:HG3	5:E:216:LYS:CD	2.47	0.44
4:D:85:TYR:O	4:D:99:GLY:HA2	2.18	0.44
4:D:210:ASN:O	4:D:211:GLU:HG3	2.17	0.44
5:E:158:VAL:HG11	5:E:185:LEU:HD21	2.00	0.44
1:A:88:GLY:O	1:A:252:TYR:HA	2.18	0.44
1:A:154:MET:HE3	1:A:178:SER:OG	2.18	0.44
5:E:3:LYS:HB2	5:E:25:SER:HB2	1.99	0.44
1:A:181:VAL:CG2	1:A:185:ASP:HB2	2.47	0.43
1:A:220:LEU:HD23	2:B:214:HIS:HD2	1.82	0.43
1:A:281:GLY:N	2:B:204:VAL:HG13	2.33	0.43
2:B:268:ASN:OD1	2:B:278:HIS:CE1	2.67	0.43
1:A:120:ARG:HH11	3:C:237:GLN:HE22	1.64	0.43
1:A:261:TRP:CD1	3:C:36:ILE:HB	2.54	0.43
2:B:198:GLU:OE2	2:B:278:HIS:NE2	2.51	0.43
3:C:148:THR:HA	3:C:151:LEU:HD12	1.99	0.43
2:B:92:ILE:HG13	2:B:92:ILE:O	2.18	0.43
3:C:83:CYS:HB3	3:C:196:ILE:HG22	2.00	0.43
2:B:156:THR:HA	2:B:162:GLY:HA2	2.00	0.43
2:B:234:VAL:HA	2:B:239:ILE:O	2.19	0.43
3:C:188:TYR:O	3:C:189:TYR:CB	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:37:GLN:NE2	5:E:39:GLN:OE1	2.42	0.43
5:E:36:TRP:NE1	5:E:81:LEU:HB2	2.33	0.43
2:B:148:TYR:HB3	2:B:284:LEU:CD1	2.49	0.43
2:B:286:VAL:HA	2:B:287:PRO:HD3	1.86	0.43
3:C:53:LEU:CD2	3:C:95:PRO:HB3	2.49	0.43
4:D:32:ILE:CG2	4:D:70:TYR:CD2	2.94	0.43
2:B:185:LYS:HB3	3:C:125:PHE:CD1	2.53	0.43
3:C:54:GLU:HG3	3:C:98:SER:CB	2.49	0.43
3:C:144:LYS:CG	3:C:148:THR:HG21	2.49	0.43
4:D:19:VAL:HB	4:D:74:ILE:HB	2.00	0.43
4:D:21:MET:HE1	4:D:85:TYR:CB	2.49	0.43
4:D:123:LEU:HD23	4:D:127:GLY:O	2.19	0.43
2:B:148:TYR:C	2:B:148:TYR:CD1	2.96	0.43
2:B:168:HIS:CE1	2:B:317:LEU:HD13	2.54	0.43
1:A:117:ALA:HB1	3:C:236:LEU:HB3	2.01	0.43
2:B:170:LEU:HB3	2:B:272:PHE:HB3	2.01	0.43
2:B:252:ILE:HD11	2:B:260:ALA:HB3	2.01	0.43
3:C:211:THR:HG22	3:C:212:ALA:N	2.33	0.43
5:E:82:GLN:HG3	5:E:83:MET:N	2.33	0.43
1:A:128:TYR:HD1	1:A:202:GLN:HB3	1.84	0.43
3:C:89:ASP:HA	3:C:188:TYR:CE1	2.54	0.43
1:A:218:LYS:HA	2:B:216:PRO:HA	2.00	0.42
1:A:131:PHE:CD1	1:A:131:PHE:C	2.97	0.42
2:B:241:ILE:CG2	3:C:66:MET:HE1	2.44	0.42
3:C:169:ILE:HA	3:C:170:PRO:HD2	1.82	0.42
4:D:66:SER:C	4:D:70:TYR:HE1	2.27	0.42
5:E:123:LYS:HD2	5:E:123:LYS:N	2.34	0.42
1:A:266:MET:O	1:A:267:ARG:C	2.61	0.42
2:B:188:GLN:HG3	2:B:292:ASP:HB3	2.00	0.42
2:B:241:ILE:O	2:B:243:GLN:N	2.52	0.42
5:E:131:PRO:C	5:E:132:LEU:HD23	2.44	0.42
1:A:123:VAL:HB	1:A:203:TRP:NE1	2.33	0.42
3:C:118:THR:HG23	3:C:166:THR:OG1	2.19	0.42
4:D:32:ILE:HG21	4:D:32:ILE:HD13	1.84	0.42
1:A:163:PRO:HG3	1:A:170:ALA:HB3	2.00	0.42
1:A:207:GLY:HA3	2:B:277:ASN:O	2.19	0.42
2:B:86:THR:HG23	2:B:90:SER:O	2.18	0.42
2:B:270:LEU:HB3	2:B:271:PRO:HD2	2.02	0.42
4:D:13:ALA:CB	4:D:77:MET:HG2	2.49	0.42
2:B:89:ASN:HD21	2:B:131:ARG:NH1	2.16	0.42
2:B:90:SER:CB	2:B:132:PHE:HB2	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:180:HIS:O	3:C:181:ALA:C	2.62	0.42
5:E:196:TRP:CD1	5:E:197:PRO:HA	2.55	0.42
2:B:85:LEU:HD21	2:B:94:THR:HG21	1.95	0.42
2:B:222:PRO:HB2	2:B:226:GLY:C	2.45	0.42
3:C:85:VAL:HG22	3:C:86:PHE:N	2.34	0.42
4:D:33:HIS:NE2	4:D:90:TRP:HD1	2.18	0.42
3:C:35:HIS:O	3:C:36:ILE:HD13	2.20	0.42
5:E:58:THR:C	5:E:59:TYR:HD1	2.28	0.42
1:A:104:ASN:HB2	1:A:106:TYR:CE1	2.55	0.41
1:A:114:THR:HG23	3:C:237:GLN:HG2	2.01	0.41
1:A:155:PHE:O	1:A:177:PRO:HD2	2.21	0.41
1:A:157:PRO:HD2	1:A:176:ASN:OD1	2.19	0.41
1:A:292:THR:CG2	5:E:57:TYR:HD2	2.31	0.41
2:B:171:TYR:CD1	2:B:171:TYR:C	2.96	0.41
2:B:308:ALA:HA	2:B:309:PRO:HD3	1.84	0.41
3:C:71:PHE:CE1	3:C:214:ILE:HD12	2.53	0.41
3:C:90:PRO:CD	3:C:188:TYR:OH	2.68	0.41
5:E:181:ASP:O	5:E:182:LEU:HD23	2.19	0.41
4:D:53:LEU:N	4:D:53:LEU:CD1	2.83	0.41
2:B:196:LEU:HD12	2:B:196:LEU:C	2.45	0.41
3:C:61:ASN:ND2	3:C:64:SER:OG	2.53	0.41
3:C:48:GLN:OE1	3:C:222:LYS:HA	2.21	0.41
3:C:53:LEU:HD21	3:C:95:PRO:CB	2.51	0.41
4:D:52:ARG:NH2	5:E:103:VAL:HG11	2.28	0.41
2:B:203:THR:HG23	2:B:219:GLN:NE2	2.34	0.41
3:C:92:ARG:HD3	3:C:188:TYR:CD2	2.55	0.41
4:D:48:TYR:HB3	5:E:107:TYR:CD2	2.55	0.41
2:B:297:ALA:O	2:B:298:THR:C	2.63	0.41
3:C:90:PRO:HG2	3:C:115:LEU:HD11	2.02	0.41
1:A:294:ILE:HG12	3:C:84:ALA:HB1	2.03	0.41
5:E:146:LEU:HD22	5:E:218:ILE:HG21	2.03	0.41
1:A:261:TRP:CD1	3:C:39:GLU:HB2	2.56	0.41
2:B:197:PRO:O	2:B:198:GLU:C	2.63	0.41
4:D:18:LYS:HE3	4:D:18:LYS:HB2	1.75	0.41
5:E:102:THR:HG23	5:E:105:GLU:O	2.20	0.41
2:B:102:VAL:HA	2:B:263:ILE:HB	2.03	0.41
2:B:172:ARG:HD3	2:B:313:GLU:OE2	2.20	0.41
2:B:246:VAL:HG22	2:B:246:VAL:O	2.21	0.41
2:B:252:ILE:HD11	2:B:260:ALA:CB	2.51	0.41
3:C:87:ARG:HG3	3:C:89:ASP:OD2	2.20	0.41
4:D:49:ASP:C	4:D:50:THR:HG23	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LEU:HD23	1:A:95:LEU:HA	1.91	0.41
1:A:286:PRO:HA	2:B:233:TYR:HE2	1.86	0.41
2:B:140:TRP:CD1	2:B:141:GLU:N	2.87	0.41
4:D:119:SER:C	4:D:121:GLU:H	2.29	0.41
1:A:259:ARG:HG2	3:C:39:GLU:OE1	2.21	0.40
1:A:289:ALA:N	3:C:97:GLN:OE1	2.54	0.40
2:B:201:ILE:HG21	2:B:219:GLN:HE21	1.86	0.40
3:C:58:VAL:H	3:C:59:PRO:CD	2.32	0.40
4:D:164:GLN:NE2	4:D:169:SER:HB3	2.36	0.40
5:E:132:LEU:HB2	5:E:147:GLY:C	2.46	0.40
2:B:283:LEU:HD12	2:B:284:LEU:N	2.36	0.40
1:A:160:ALA:HA	1:A:161:PRO:HD3	1.83	0.40
2:B:85:LEU:CD2	2:B:94:THR:HG22	2.44	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	214/297 (72%)	185 (86%)	24 (11%)	5 (2%)	5	28
2	B	235/245 (96%)	195 (83%)	31 (13%)	9 (4%)	2	19
3	C	237/242 (98%)	208 (88%)	19 (8%)	10 (4%)	2	17
4	D	210/212 (99%)	196 (93%)	14 (7%)	0	100	100
5	E	213/220 (97%)	186 (87%)	26 (12%)	1 (0%)	24	63
All	All	1109/1216 (91%)	970 (88%)	114 (10%)	25 (2%)	7	28

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	SER

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Mol	Chain	Res	Type
1	A	196	SER
2	B	127	VAL
2	B	159	GLY
3	C	180	HIS
3	C	188	TYR
5	E	41	PRO
1	A	86	ARG
1	A	124	GLU
2	B	97	ALA
2	B	237	ALA
3	C	62	ALA
3	C	182	ARG
3	C	189	TYR
3	C	191	THR
1	A	227	ASN
2	B	98	ALA
2	B	216	PRO
3	C	72	PRO
2	B	108	PRO
2	B	242	SER
3	C	181	ALA
2	B	112	SER
3	C	58	VAL
3	C	137	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	187/252 (74%)	175 (94%)	12 (6%)	16	37
2	B	201/208 (97%)	190 (94%)	11 (6%)	19	41
3	C	197/202 (98%)	180 (91%)	17 (9%)	10	29
4	D	181/186 (97%)	175 (97%)	6 (3%)	33	55
5	E	182/187 (97%)	177 (97%)	5 (3%)	39	61
All	All	948/1035 (92%)	897 (95%)	51 (5%)	21	41

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	THR
1	A	94	ASP
1	A	100	THR
1	A	101	THR
1	A	114	THR
1	A	156	VAL
1	A	167	GLU
1	A	179	VAL
1	A	183	LEU
1	A	245	TYR
1	A	265	PRO
1	A	297	LEU
2	B	85	LEU
2	B	119	VAL
2	B	121	LYS
2	B	135	LEU
2	B	145	LYS
2	B	171	TYR
2	B	180	GLN
2	B	203	THR
2	B	239	ILE
2	B	285	VAL
2	B	304	THR
3	C	14	LEU
3	C	21	SER
3	C	25	LEU
3	C	31	THR
3	C	51	THR
3	C	53	LEU
3	C	61	ASN
3	C	72	PRO
3	C	87	ARG
3	C	136	THR
3	C	146	ARG
3	C	178	ARG
3	C	197	TRP
3	C	204	VAL
3	C	221	GLN
3	C	230	LYS
3	C	234	ASP
4	D	29	VAL
4	D	51	SER

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Mol	Chain	Res	Type
4	D	57	VAL
4	D	68	THR
4	D	189	SER
4	D	192	CYS
5	E	101	THR
5	E	102	THR
5	E	105	GLU
5	E	143	MET
5	E	203	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	189	GLN
1	A	202	GLN
1	A	228	ASN
2	B	168	HIS
2	B	188	GLN
2	B	214	HIS
2	B	219	GLN
2	B	257	ASN
2	B	258	ASN
2	B	277	ASN
3	C	11	ASN
3	C	48	GLN
3	C	61	ASN
3	C	93	ASN
3	C	162	GLN
3	C	174	ASN
3	C	176	HIS
3	C	221	GLN
3	C	237	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

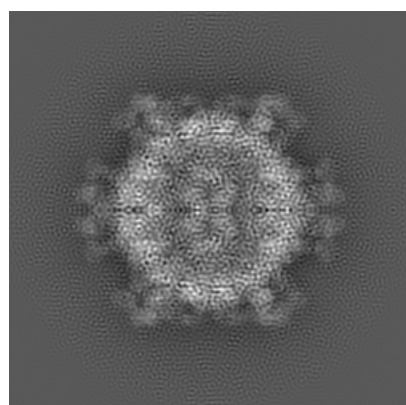
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6964. These allow visual inspection of the internal detail of the map and identification of artifacts.

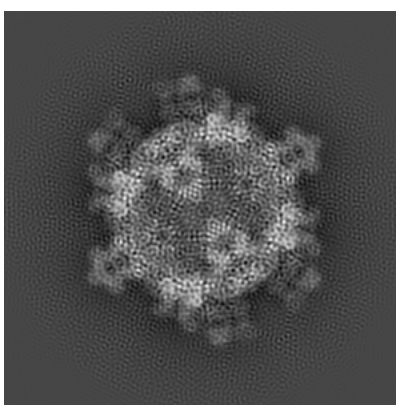
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

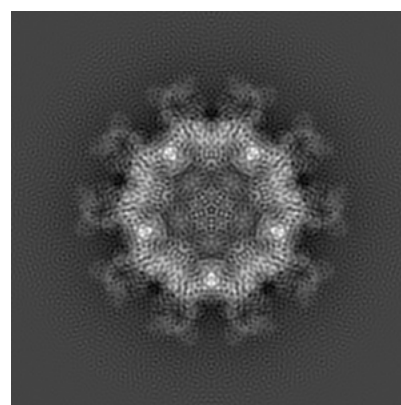
6.1.1 Primary map



X



Y

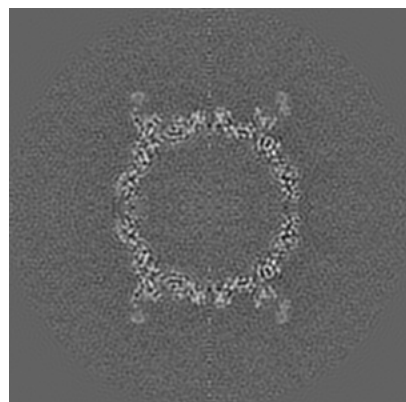


Z

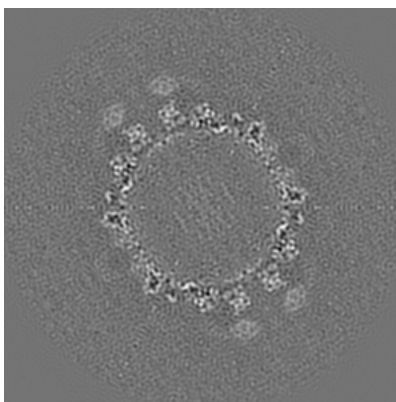
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

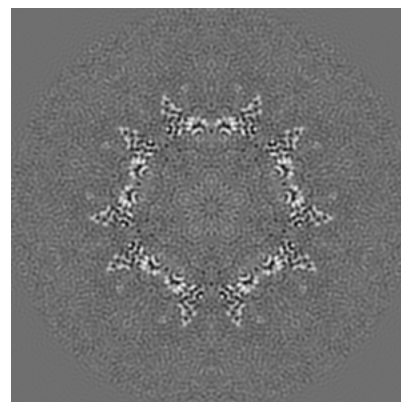
6.2.1 Primary map



X Index: 240



Y Index: 240

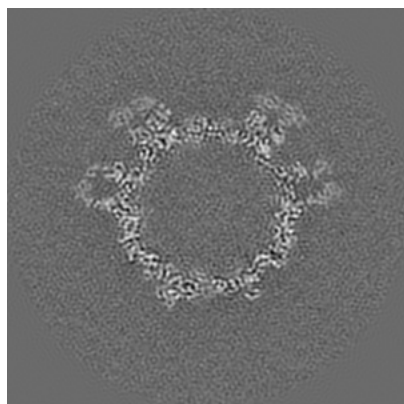


Z Index: 240

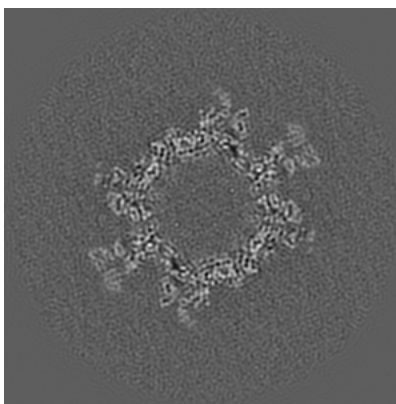
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

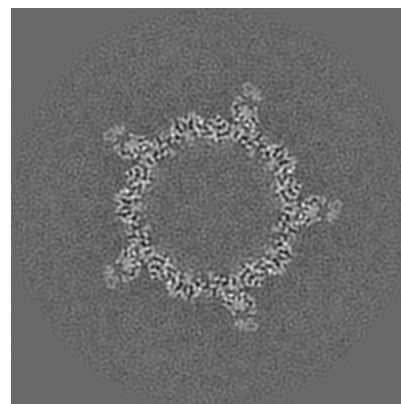
6.3.1 Primary map



X Index: 204



Y Index: 177

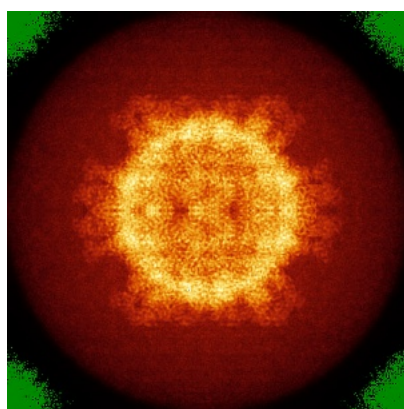


Z Index: 201

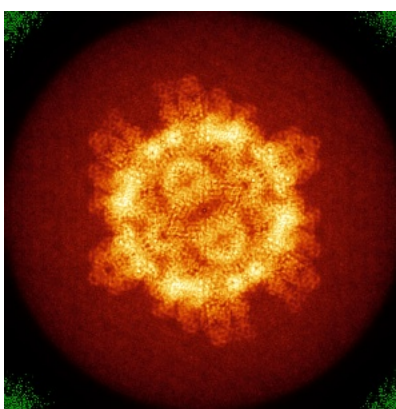
The images above show the largest variance slices of the map in three orthogonal directions.

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

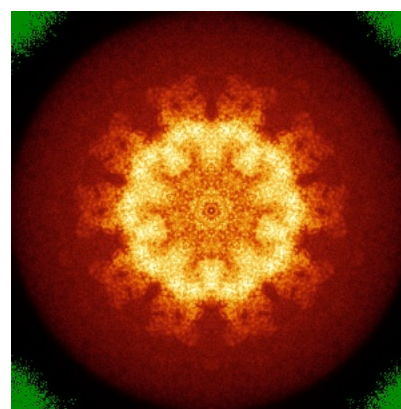
6.4.1 Primary map



X



Y

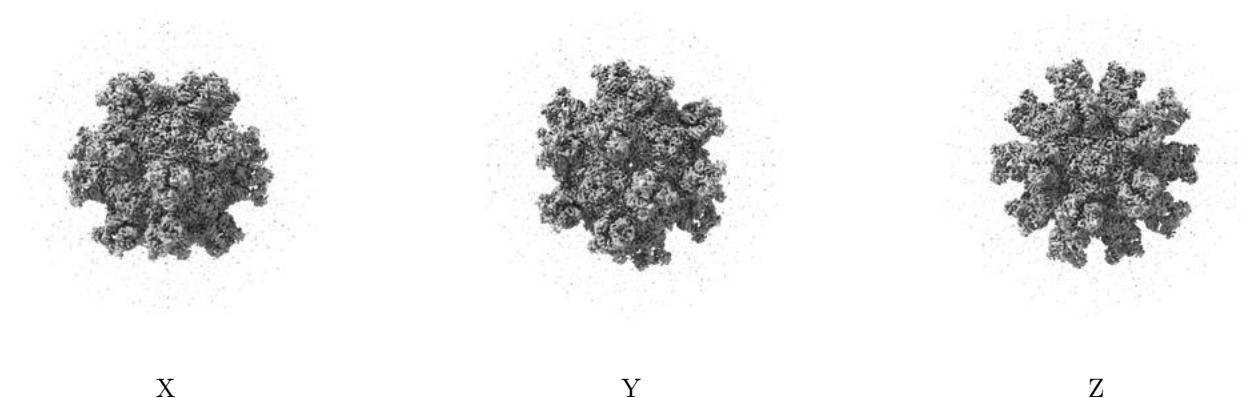


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

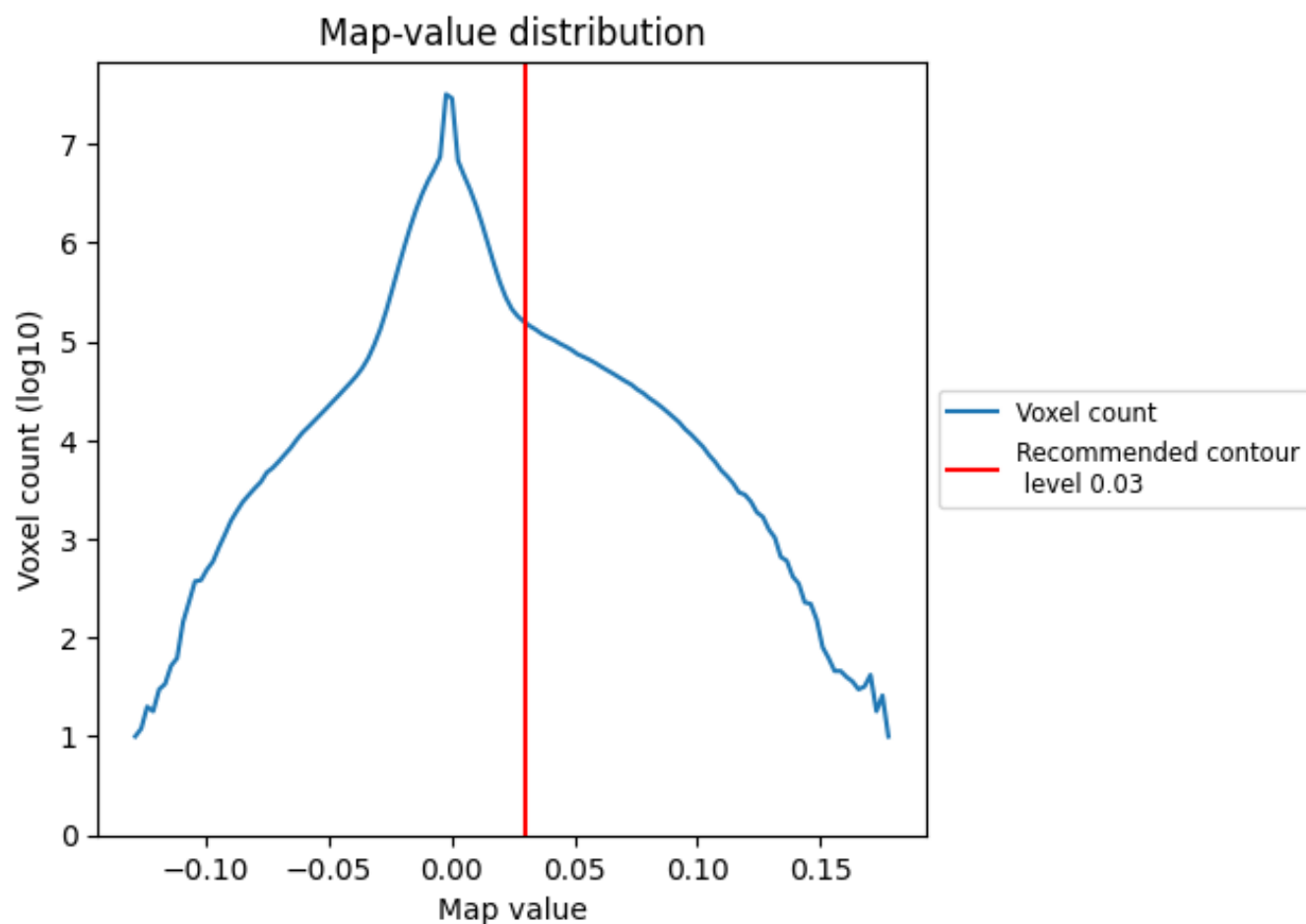
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

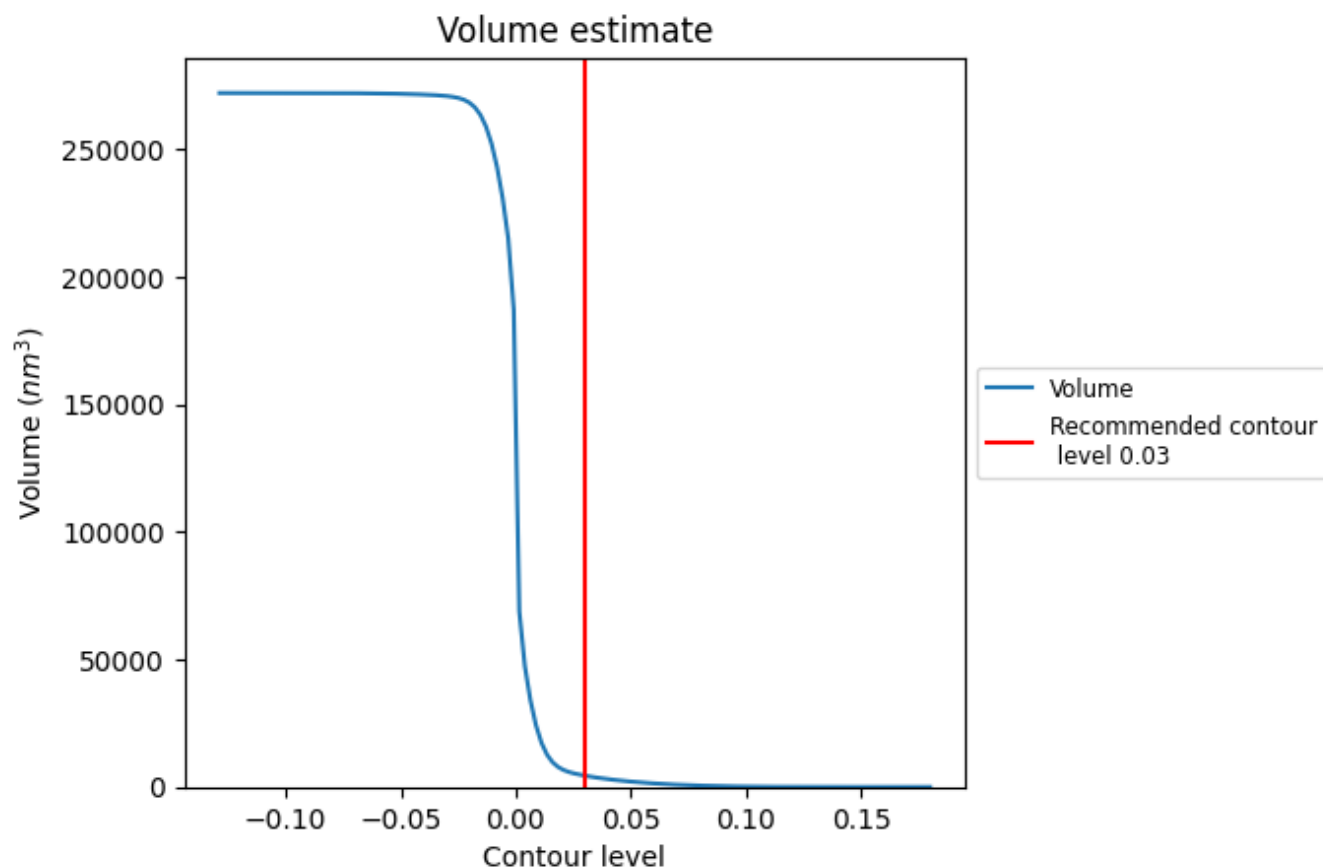
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

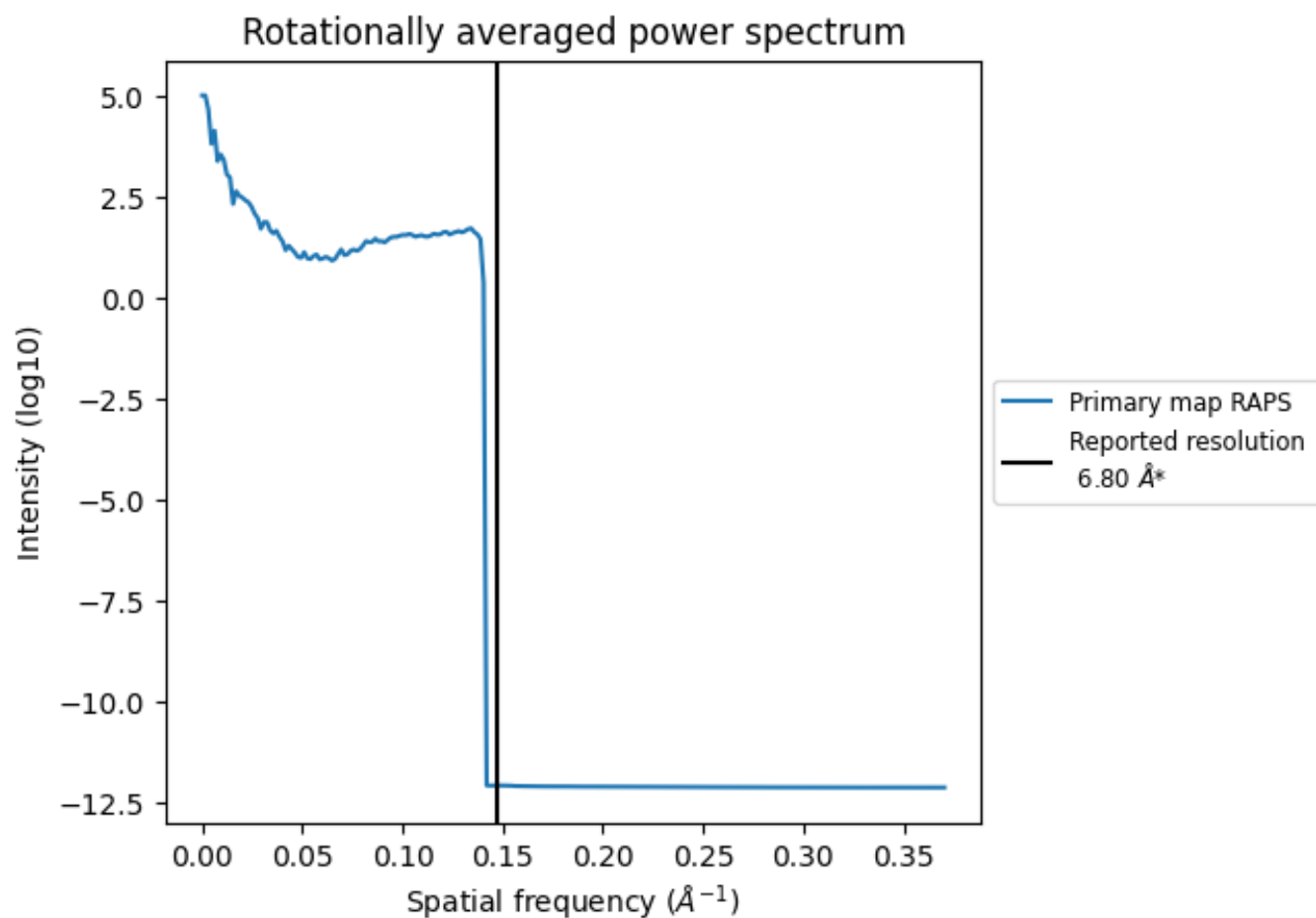
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4436 nm^3 ; this corresponds to an approximate mass of 4007 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 0.147 $\text{\AA}^{-1}$

8 Fourier-Shell correlation

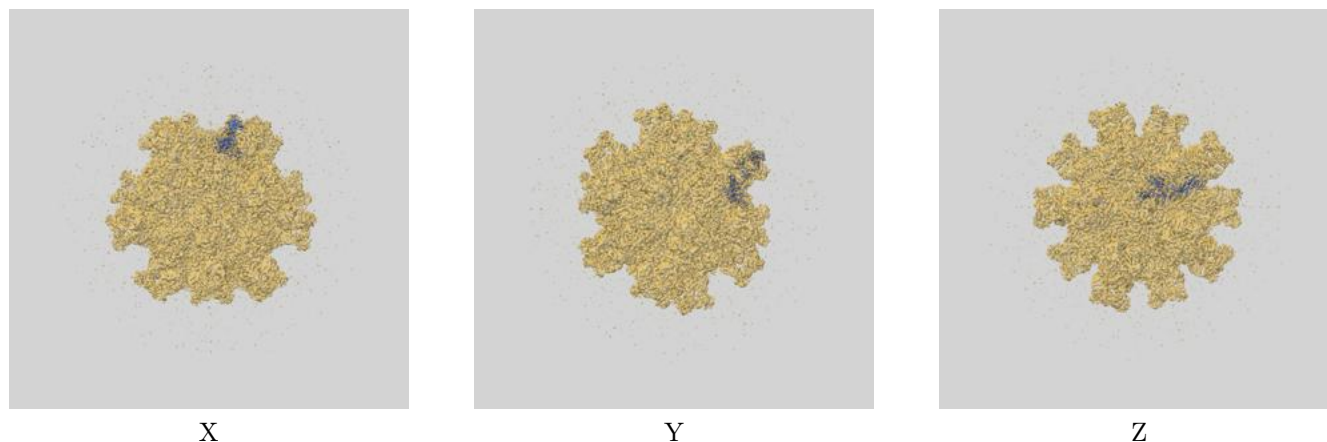
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

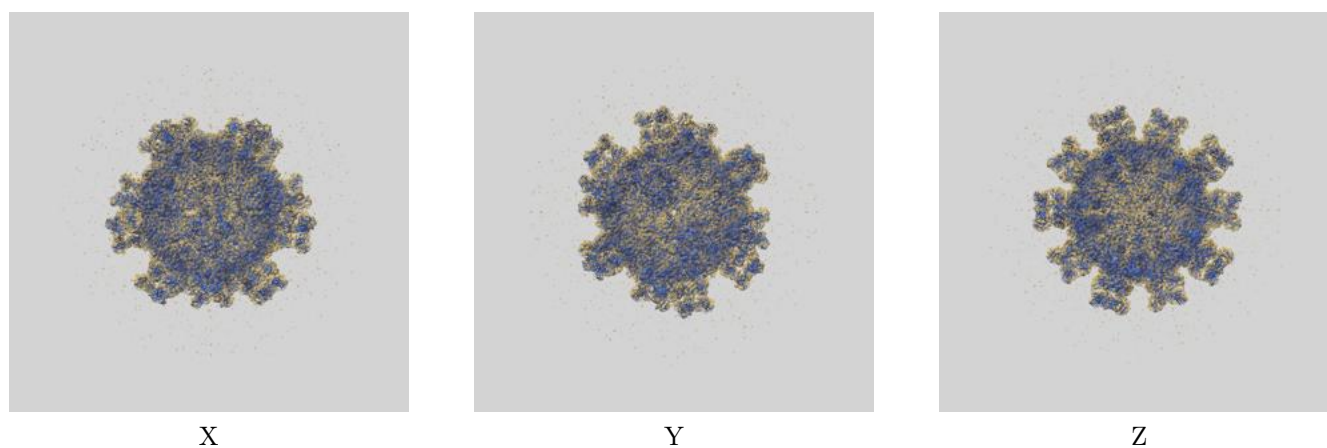
This section contains information regarding the fit between EMDB map EMD-6964 and PDB model 5ZUF. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

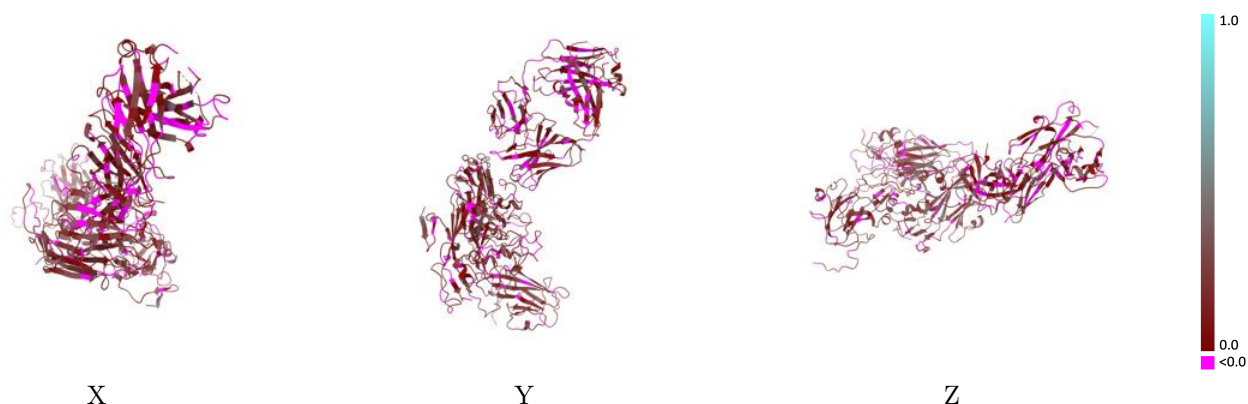


9.1.2 Map-model assembly overlay [i](#)



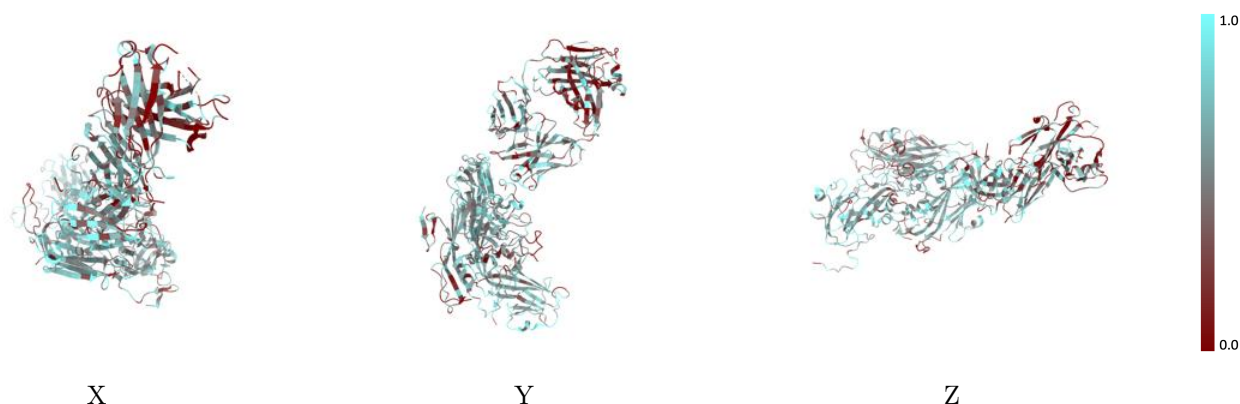
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



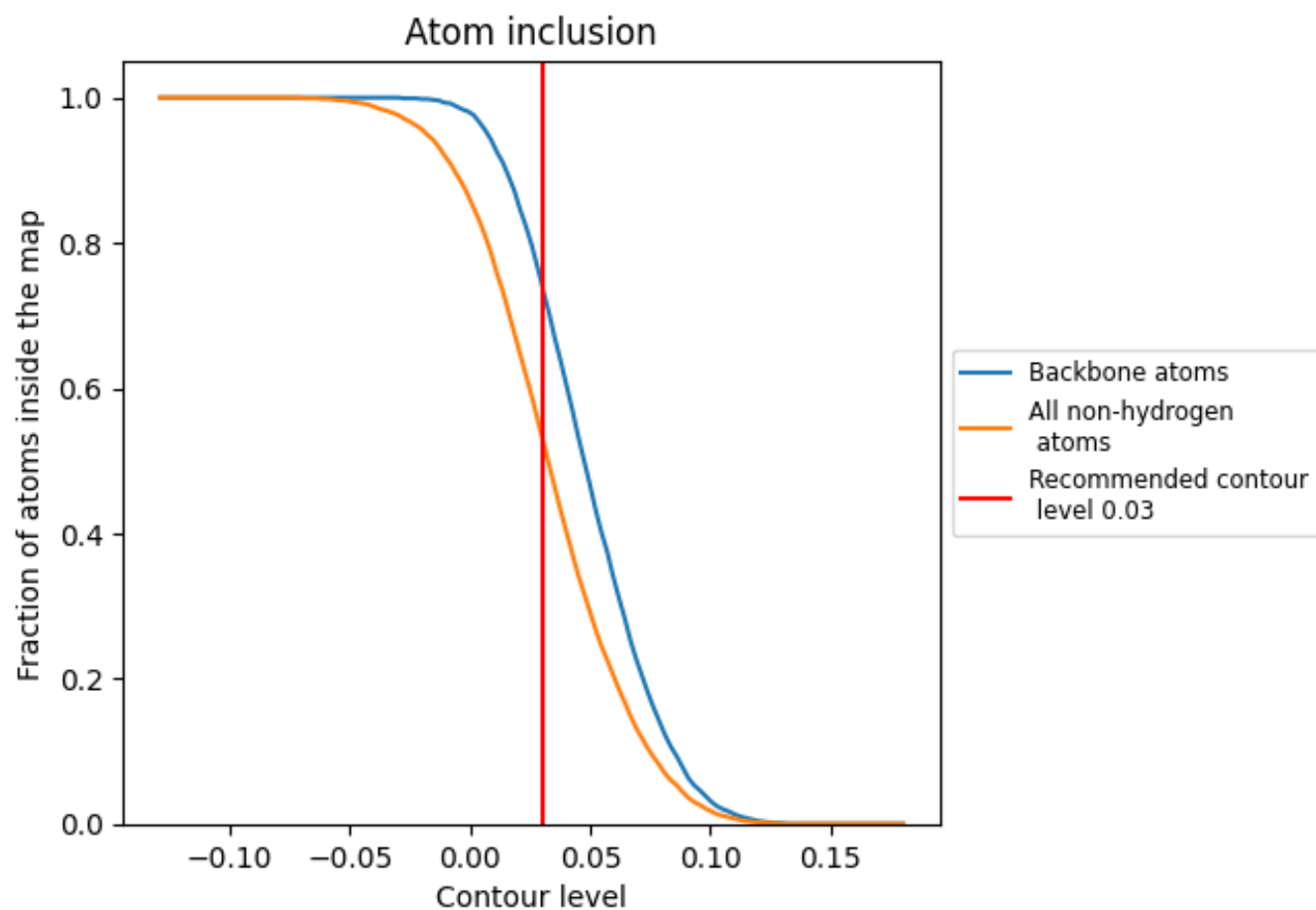
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 53% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5320	0.1270
A	0.6110	0.1620
B	0.5210	0.1380
C	0.5990	0.1430
D	0.4710	0.1000
E	0.4460	0.0860

