



Full wwPDB EM Validation Report ⓘ

Mar 4, 2026 – 07:56 PM UTC

PDB ID : 6Q0B / pdb_00006q0b
EMDB ID : EMD-20546
Title : Poliovirus (Type 1 Mahoney), receptor-catalysed 135S particle incubated with anti-VP1 mAb at RT for 1 hr
Authors : Hogle, J.M.; Filman, D.J.; Shah, P.N.M.
Deposited on : 2019-08-01
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

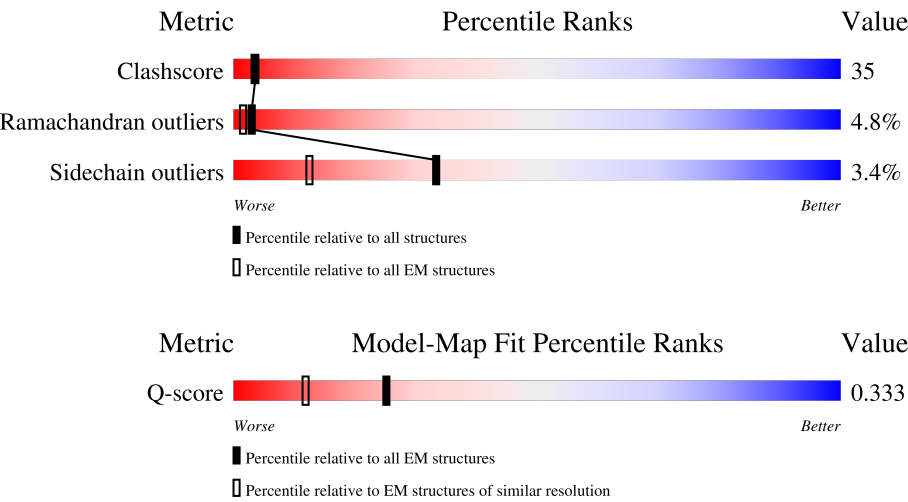
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
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	1	302	
2	2	272	
3	3	238	
4	4	70	

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Mol	Chain	Length	Quality of chain
5	7	520	40% 84% 16%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7856 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	1	191	Total	C	N	O	S	0	0
			1555	1005	264	281	5		

- Molecule 2 is a protein called Capsid protein VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	234	Total	C	N	O	S	0	0
			1818	1163	307	336	12		

- Molecule 3 is a protein called Capsid protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	228	Total	C	N	O	S	0	0
			1777	1134	290	336	17		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	123	SER	PHE	conflict	UNP P03300

- Molecule 4 is a protein called Capsid protein VP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	69	Total	C	N	O	S	0	0
			534	333	91	109	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	1	MYR	-	modified residue	UNP P03300

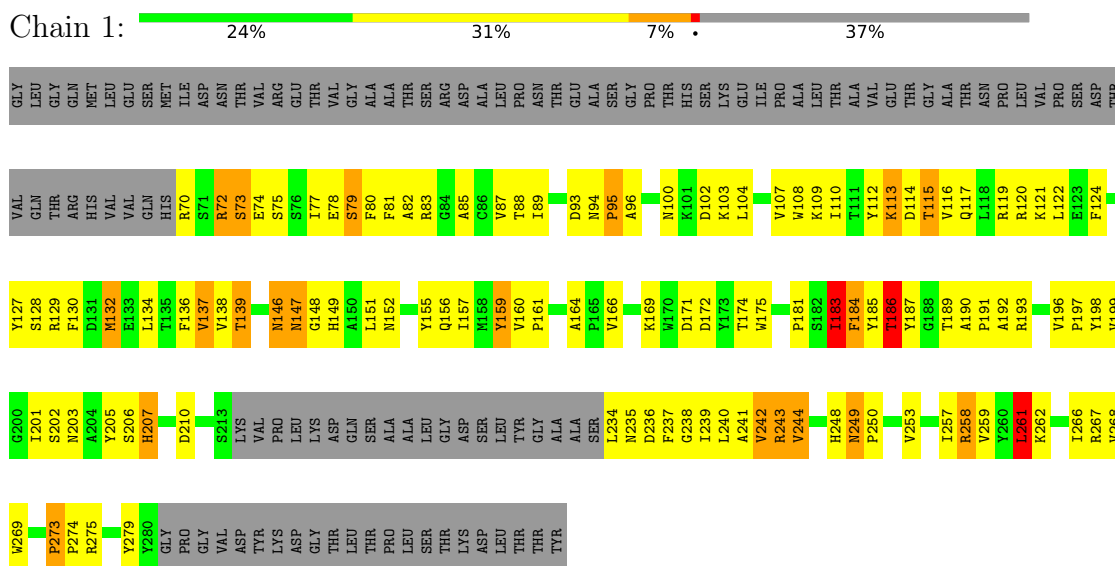
- Molecule 5 is a protein called anti-VP1 mAb.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	7	439	Total	C	N	O	S	0	0
			2172	1283	439	440	10		

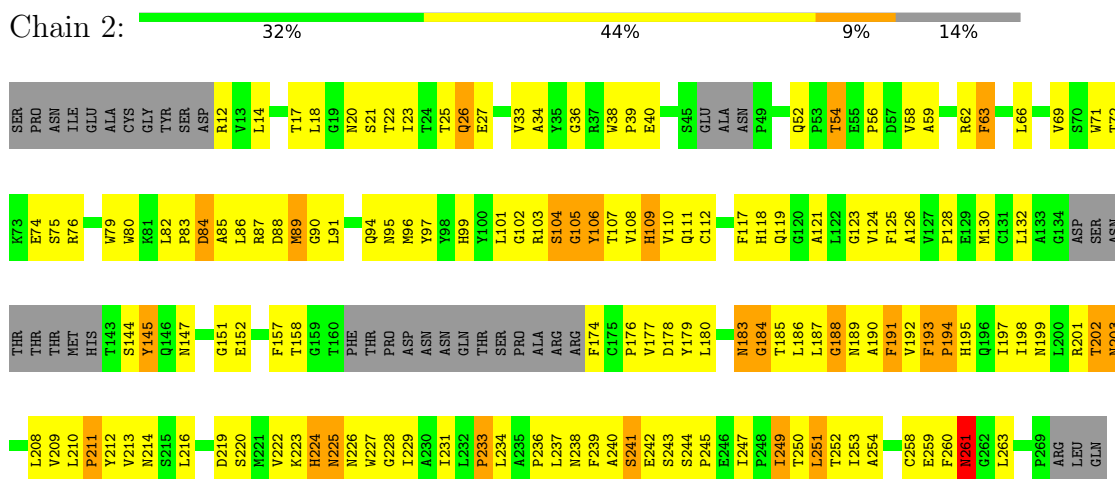
3 Residue-property plots

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.

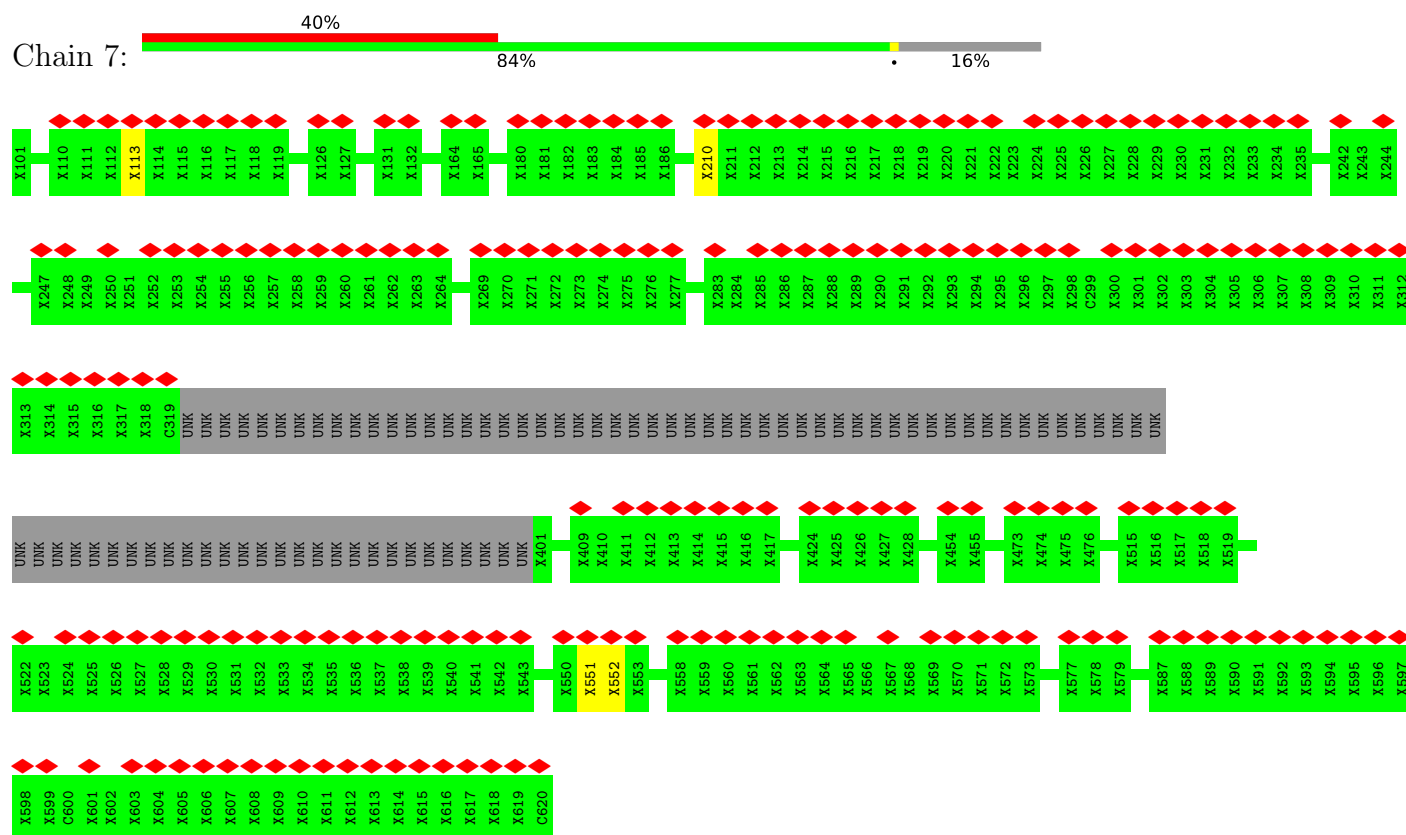
• Molecule 1: Capsid protein VP1



• Molecule 2: Capsid protein VP2



• Molecule 3: Capsid protein VP3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	17697	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.06	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	100.000	Depositor
Minimum map value	0.000	Depositor
Average map value	28.010	Depositor
Map value standard deviation	7.178	Depositor
Recommended contour level	32	Depositor
Map size (Å)	491.008, 491.008, 491.008	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.096, 1.096, 1.096	Depositor

5 Model quality

5.1 Standard geometry

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

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	1	0.70	0/1603	1.61	25/2186 (1.1%)
2	2	0.63	0/1867	1.51	21/2549 (0.8%)
3	3	0.65	0/1822	1.57	21/2482 (0.8%)
4	4	0.50	0/528	1.25	5/714 (0.7%)
5	7	0.17	0/51	0.38	0/50
All	All	0.65	0/5871	1.53	72/7981 (0.9%)

There are no bond length outliers.

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	107	THR	CA-CB-OG1	-11.12	92.92	109.60
3	3	7	THR	CA-CB-OG1	-10.90	93.25	109.60
1	1	273	PRO	CB-CA-C	-8.88	100.09	110.92
2	2	106	TYR	CB-CA-C	-8.48	93.54	110.42
2	2	63	PHE	CB-CA-C	-8.28	98.55	110.06
1	1	184	PHE	CA-CB-CG	-8.21	105.59	113.80
3	3	46	LEU	N-CA-C	-8.06	105.43	114.62
1	1	139	THR	CB-CA-C	7.72	123.16	109.65
2	2	111	GLN	CB-CA-C	-7.69	95.86	109.71
3	3	32	PRO	CB-CA-C	-7.68	101.55	110.92
3	3	220	PHE	CA-CB-CG	-7.63	106.17	113.80
3	3	6	ASN	CA-CB-CG	-7.44	105.16	112.60
3	3	220	PHE	CB-CA-C	-7.24	96.21	109.54
3	3	167	VAL	CB-CA-C	-7.22	103.43	111.23
3	3	31	THR	CB-CA-C	-7.20	97.79	109.67
2	2	193	PHE	CB-CA-C	-7.17	98.37	109.62
1	1	243	ARG	CB-CG-CD	-7.14	94.87	111.30
1	1	186	THR	CA-CB-OG1	-7.01	99.09	109.60
4	4	9	LYS	N-CA-C	-6.88	103.36	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	193	PHE	CA-C-N	-6.76	111.51	121.24
3	3	193	PHE	C-N-CA	-6.76	111.51	121.24
2	2	54	THR	CB-CA-C	6.64	119.29	110.06
3	3	226	ARG	CB-CA-C	-6.56	102.82	111.42
2	2	263	LEU	N-CA-C	-6.54	105.60	113.97
1	1	72	ARG	CG-CD-NE	-6.47	97.75	112.00
1	1	261	LEU	N-CA-CB	-6.34	100.65	109.97
3	3	47	ALA	N-CA-C	-6.33	104.82	112.54
2	2	249	ILE	CB-CA-C	-6.29	101.93	110.42
4	4	15	ASN	O-C-N	6.17	130.80	122.59
1	1	159	TYR	CA-C-N	-6.06	112.13	123.34
1	1	159	TYR	C-N-CA	-6.06	112.13	123.34
2	2	225	ASN	CA-CB-CG	-5.89	106.71	112.60
2	2	261	ASN	CB-CA-C	-5.78	98.91	110.42
1	1	253	VAL	CB-CA-C	-5.77	105.40	111.23
3	3	108	THR	CA-C-N	-5.77	114.56	122.93
3	3	108	THR	C-N-CA	-5.77	114.56	122.93
3	3	173	ASN	N-CA-C	-5.77	104.68	110.97
2	2	125	PHE	CA-CB-CG	-5.74	108.06	113.80
3	3	175	THR	CA-C-N	5.74	132.50	121.54
3	3	175	THR	C-N-CA	5.74	132.50	121.54
2	2	211	PRO	N-CA-C	-5.72	100.69	112.47
3	3	64	THR	CA-CB-OG1	-5.69	101.07	109.60
2	2	52	GLN	CB-CA-C	5.69	115.24	111.20
3	3	8	PRO	N-CA-C	-5.64	102.25	111.68
2	2	123	GLY	CA-C-N	-5.62	115.70	122.90
2	2	123	GLY	C-N-CA	-5.62	115.70	122.90
3	3	145	ARG	CB-CA-C	-5.62	101.46	110.79
2	2	109	HIS	N-CA-CB	-5.60	101.74	110.87
2	2	104	SER	CA-C-N	-5.59	115.60	122.75
2	2	104	SER	C-N-CA	-5.59	115.60	122.75
3	3	213	PHE	CA-CB-CG	-5.55	108.25	113.80
1	1	207	HIS	N-CA-C	-5.51	107.20	114.31
1	1	249	ASN	CB-CA-C	5.49	118.73	109.67
1	1	183	ILE	CA-C-N	-5.48	115.33	123.11
1	1	183	ILE	C-N-CA	-5.48	115.33	123.11
2	2	105	GLY	N-CA-C	-5.45	103.28	112.77
4	4	8	GLN	N-CA-C	5.34	118.42	110.14
2	2	193	PHE	CA-CB-CG	-5.28	108.52	113.80
1	1	132	MET	N-CA-CB	-5.24	101.89	110.43
1	1	198	TYR	CA-C-N	-5.20	112.62	121.97
1	1	198	TYR	C-N-CA	-5.20	112.62	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	244	VAL	N-CA-C	-5.19	104.34	110.21
4	4	15	ASN	CA-C-N	5.14	130.63	122.61
4	4	15	ASN	C-N-CA	5.14	130.63	122.61
2	2	233	PRO	CB-CA-C	5.12	116.06	111.40
1	1	258	ARG	CA-C-N	-5.11	116.85	123.19
1	1	258	ARG	C-N-CA	-5.11	116.85	123.19
1	1	174	THR	CA-CB-OG1	-5.08	101.98	109.60
1	1	159	TYR	CA-CB-CG	-5.07	104.77	113.90
1	1	207	HIS	N-CA-CB	5.05	117.61	110.90
1	1	241	ALA	CA-C-N	-5.05	115.93	122.94
1	1	241	ALA	C-N-CA	-5.05	115.93	122.94

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1555	0	1515	139	0
2	2	1818	0	1763	174	0
3	3	1777	0	1765	194	0
4	4	534	0	524	41	0
5	7	2172	0	514	2	0
All	All	7856	0	6081	493	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 35.

All (493) 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)
4:4:14:GLU:C	4:4:16:SER:H	1.26	1.20
2:2:124:VAL:HG12	2:2:231:ILE:CD1	1.76	1.14
2:2:124:VAL:CG1	2:2:231:ILE:HD12	1.79	1.10
3:3:110:TRP:HE1	3:3:179:THR:HG22	1.15	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:8:GLN:HE21	4:4:26:ASN:C	1.67	1.03
4:4:18:ARG:HD2	4:4:23:SER:HB3	1.41	1.02
3:3:170:TRP:CH2	3:3:177:ARG:HG3	1.94	1.02
3:3:44:MET:HA	3:3:44:MET:HE2	1.41	1.02
4:4:9:LYS:HB2	4:4:44:GLN:HE22	1.24	1.02
1:1:78:GLU:OE1	1:1:78:GLU:N	1.94	0.99
4:4:14:GLU:C	4:4:16:SER:N	2.04	0.98
1:1:261:LEU:HD23	1:1:262:LYS:N	1.78	0.98
2:2:124:VAL:HG12	2:2:231:ILE:HD12	0.94	0.94
3:3:45:GLU:O	3:3:46:LEU:HD12	1.69	0.93
4:4:14:GLU:O	4:4:16:SER:N	2.02	0.93
3:3:2:LEU:HD12	3:3:3:PRO:HD2	1.51	0.93
4:4:9:LYS:HB2	4:4:44:GLN:NE2	1.84	0.90
1:1:116:VAL:HG11	3:3:231:ILE:HD11	1.54	0.90
3:3:202:LEU:O	3:3:204:THR:N	2.06	0.88
3:3:170:TRP:CZ3	3:3:177:ARG:NE	2.41	0.88
3:3:110:TRP:NE1	3:3:179:THR:HG22	1.87	0.88
2:2:66:LEU:HD12	2:2:251:LEU:HD22	1.55	0.88
2:2:66:LEU:HD11	2:2:253:ILE:HD11	1.55	0.87
4:4:16:SER:O	4:4:17:ASN:HB3	1.73	0.87
3:3:44:MET:HA	3:3:44:MET:CE	2.07	0.85
2:2:39:PRO:HB3	2:2:211:PRO:HA	1.57	0.85
2:2:187:LEU:HD22	3:3:65:MET:CE	2.06	0.85
2:2:219:ASP:OD1	2:2:220:SER:N	2.10	0.84
2:2:17:THR:HG22	2:2:22:THR:HG22	1.58	0.84
1:1:205:TYR:HB3	1:1:235:ASN:HD21	1.41	0.84
1:1:249:ASN:OD1	1:1:250:PRO:HD2	1.78	0.84
2:2:103:ARG:O	2:2:103:ARG:HG3	1.75	0.83
3:3:170:TRP:CZ3	3:3:177:ARG:HG3	2.13	0.83
2:2:187:LEU:HD22	3:3:65:MET:HE1	1.60	0.82
4:4:18:ARG:CD	4:4:23:SER:HB3	2.11	0.81
3:3:170:TRP:HZ3	3:3:177:ARG:CD	1.93	0.81
1:1:261:LEU:C	1:1:261:LEU:CD2	2.55	0.79
2:2:128:PRO:HG3	2:2:227:TRP:CZ3	2.18	0.78
3:3:141:PRO:HD3	3:3:189:TYR:CE2	2.18	0.78
2:2:74:GLU:H	2:2:74:GLU:CD	1.91	0.78
1:1:137:VAL:HG23	1:1:258:ARG:HB2	1.64	0.78
2:2:110:VAL:HG11	2:2:124:VAL:HG11	1.66	0.78
2:2:71:TRP:CE3	2:2:247:ILE:HD11	2.19	0.77
1:1:78:GLU:H	1:1:78:GLU:CD	1.92	0.77
3:3:225:LEU:HD23	3:3:226:ARG:N	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:152:ASN:OD1	1:1:187:TYR:HB3	1.85	0.77
3:3:156:TRP:CD2	3:3:164:CYS:HB2	2.20	0.76
3:3:170:TRP:HH2	3:3:177:ARG:HG3	1.45	0.76
3:3:6:ASN:OD1	3:3:6:ASN:N	2.16	0.76
3:3:98:THR:HG23	3:3:101:GLY:H	1.51	0.76
1:1:127:TYR:HB2	1:1:269:TRP:HB2	1.67	0.76
2:2:210:LEU:HB3	2:2:227:TRP:NE1	2.01	0.76
3:3:109:HIS:HB3	3:3:176:TYR:HB3	1.67	0.75
4:4:15:ASN:O	4:4:18:ARG:N	2.20	0.75
1:1:191:PRO:HG2	3:3:13:TYR:HB2	1.69	0.75
1:1:261:LEU:HD23	1:1:261:LEU:C	2.11	0.75
1:1:79:SER:O	1:1:83:ARG:NH1	2.19	0.74
1:1:81:PHE:HE1	1:1:122:LEU:HD23	1.52	0.74
1:1:72:ARG:NH1	3:3:44:MET:HB3	2.02	0.73
1:1:157:ILE:HB	1:1:183:ILE:HB	1.68	0.73
3:3:27:GLU:CD	3:3:27:GLU:H	1.96	0.73
3:3:168:VAL:HG22	3:3:169:PRO:HD2	1.70	0.73
1:1:132:MET:HE1	1:1:237:PHE:HB3	1.70	0.73
1:1:116:VAL:CG1	3:3:231:ILE:HD11	2.19	0.72
1:1:193:ARG:NH2	3:3:13:TYR:HE1	1.86	0.72
2:2:74:GLU:OE2	2:2:74:GLU:N	2.19	0.72
3:3:80:ASP:HB2	3:3:81:PRO:HD2	1.72	0.72
1:1:81:PHE:CE1	1:1:122:LEU:HD23	2.23	0.72
3:3:170:TRP:CZ3	3:3:177:ARG:CD	2.73	0.72
3:3:49:ILE:O	3:3:51:THR:HG23	1.90	0.71
3:3:230:HIS:O	3:3:231:ILE:HG13	1.90	0.71
2:2:17:THR:HG22	2:2:22:THR:CG2	2.19	0.71
1:1:205:TYR:HB3	1:1:235:ASN:ND2	2.06	0.70
2:2:58:VAL:HG23	2:2:59:ALA:H	1.55	0.70
2:2:71:TRP:CE2	2:2:237:LEU:HB2	2.26	0.70
2:2:88:ASP:O	2:2:90:GLY:N	2.25	0.70
1:1:151:LEU:N	1:1:151:LEU:HD22	2.07	0.70
4:4:8:GLN:C	4:4:10:VAL:H	1.97	0.70
2:2:222:VAL:HG13	2:2:223:LYS:N	2.07	0.69
4:4:8:GLN:NE2	4:4:26:ASN:C	2.47	0.69
2:2:197:ILE:HD12	3:3:119:LEU:CD2	2.23	0.69
4:4:4:GLN:HB3	4:4:29:THR:O	1.92	0.69
4:4:8:GLN:NE2	4:4:26:ASN:O	2.26	0.68
2:2:234:LEU:O	3:3:69:ARG:NE	2.27	0.68
2:2:119:GLN:NE2	2:2:238:ASN:HB3	2.10	0.67
2:2:128:PRO:HG3	2:2:227:TRP:CH2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:261:LEU:CD2	1:1:262:LYS:N	2.55	0.67
3:3:110:TRP:HB3	3:3:222:VAL:HG12	1.77	0.67
3:3:115:LYS:HB3	3:3:167:VAL:HG22	1.75	0.67
3:3:208:MET:SD	3:3:208:MET:N	2.67	0.67
2:2:187:LEU:CD2	3:3:65:MET:HE3	2.25	0.66
1:1:77:ILE:HG12	3:3:41:LYS:O	1.96	0.66
4:4:9:LYS:CB	4:4:44:GLN:HE22	2.04	0.66
1:1:159:TYR:HB3	1:1:181:PRO:HG2	1.77	0.66
2:2:17:THR:O	2:2:18:LEU:HD23	1.96	0.66
2:2:33:VAL:HG12	2:2:209:VAL:HB	1.78	0.66
2:2:112:CYS:O	2:2:112:CYS:SG	2.53	0.65
2:2:187:LEU:CD2	3:3:65:MET:CE	2.74	0.65
3:3:112:GLY:HA3	3:3:220:PHE:HA	1.78	0.65
2:2:108:VAL:CG1	2:2:208:LEU:HB2	2.25	0.65
3:3:75:LYS:HB2	3:3:76:PRO:HD2	1.79	0.65
3:3:66:GLU:OE2	3:3:69:ARG:NH1	2.30	0.65
3:3:72:LEU:HB3	3:3:208:MET:HE2	1.77	0.65
2:2:191:PHE:CE1	3:3:52:MET:HE3	2.32	0.64
2:2:210:LEU:HB3	2:2:227:TRP:CE2	2.32	0.64
3:3:170:TRP:CZ3	3:3:177:ARG:CG	2.80	0.64
3:3:173:ASN:CG	3:3:174:THR:H	2.04	0.64
1:1:203:ASN:HD22	3:3:31:THR:HG21	1.62	0.64
2:2:183:ASN:O	2:2:185:THR:N	2.30	0.64
3:3:87:LEU:O	3:3:89:PRO:HD3	1.98	0.64
3:3:115:LYS:CB	3:3:167:VAL:HG22	2.28	0.64
3:3:230:HIS:C	3:3:231:ILE:HG13	2.22	0.64
3:3:24:ALA:O	3:3:25:LEU:HD23	1.97	0.64
2:2:191:PHE:CZ	3:3:52:MET:HE3	2.33	0.64
1:1:275:ARG:HB3	1:1:279:TYR:HE1	1.63	0.63
2:2:14:LEU:H	2:2:14:LEU:HD12	1.62	0.63
2:2:23:ILE:HG13	2:2:252:THR:HG21	1.80	0.63
2:2:188:GLY:O	3:3:51:THR:HB	1.97	0.63
1:1:193:ARG:NH2	3:3:13:TYR:CE1	2.66	0.63
3:3:125:MET:HA	3:3:125:MET:HE2	1.78	0.63
4:4:15:ASN:O	4:4:18:ARG:C	2.42	0.63
1:1:77:ILE:HG12	3:3:41:LYS:C	2.24	0.63
4:4:13:HIS:CB	4:4:16:SER:HA	2.28	0.63
2:2:187:LEU:O	2:2:189:ASN:N	2.32	0.62
3:3:110:TRP:CZ3	3:3:177:ARG:HD2	2.34	0.62
1:1:72:ARG:NH1	3:3:44:MET:CB	2.63	0.62
1:1:116:VAL:HG23	1:1:117:GLN:N	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:108:TRP:CH2	1:1:110:ILE:HA	2.33	0.62
2:2:118:HIS:CD2	2:2:239:PHE:HB3	2.35	0.62
3:3:88:SER:HB2	3:3:91:SER:HB3	1.81	0.62
2:2:190:ALA:O	2:2:192:VAL:N	2.34	0.61
1:1:197:PRO:O	1:1:199:VAL:HG13	2.01	0.61
1:1:261:LEU:HD23	1:1:262:LYS:H	1.65	0.61
1:1:112:TYR:O	1:1:114:ASP:N	2.29	0.61
1:1:275:ARG:HB3	1:1:279:TYR:CE1	2.36	0.61
2:2:119:GLN:HE21	2:2:238:ASN:HB3	1.65	0.61
1:1:107:VAL:HG13	1:1:107:VAL:O	2.01	0.60
3:3:20:GLN:OE1	3:3:20:GLN:N	2.32	0.60
3:3:111:ALA:HB1	3:3:170:TRP:CZ2	2.35	0.60
2:2:212:TYR:CE1	2:2:226:ASN:ND2	2.70	0.60
1:1:238:GLY:O	1:1:239:ILE:HD13	2.02	0.60
1:1:203:ASN:OD1	3:3:34:ILE:HG23	2.01	0.60
2:2:18:LEU:HG	2:2:63:PHE:CE2	2.37	0.60
3:3:201:PRO:O	3:3:202:LEU:O	2.20	0.59
1:1:273:PRO:HB2	2:2:185:THR:HG21	1.84	0.59
1:1:136:PHE:HB2	1:1:192:ALA:HB3	1.83	0.59
2:2:124:VAL:CG1	2:2:231:ILE:CD1	2.60	0.59
3:3:31:THR:HG22	3:3:32:PRO:O	2.02	0.59
1:1:134:LEU:HD13	1:1:240:LEU:HD11	1.85	0.59
2:2:71:TRP:HD1	2:2:72:THR:N	2.00	0.59
2:2:76:ARG:O	2:2:233:PRO:CD	2.51	0.59
3:3:45:GLU:C	3:3:46:LEU:HD12	2.27	0.59
1:1:273:PRO:HB2	2:2:185:THR:CG2	2.33	0.59
2:2:71:TRP:CD1	2:2:72:THR:N	2.71	0.58
3:3:83:LEU:HD12	3:3:83:LEU:O	2.02	0.58
3:3:225:LEU:HD23	3:3:225:LEU:C	2.28	0.58
2:2:220:SER:O	2:2:220:SER:OG	2.19	0.58
3:3:98:THR:CG2	3:3:101:GLY:H	2.15	0.58
2:2:71:TRP:CD1	2:2:71:TRP:C	2.79	0.58
2:2:85:ALA:HA	2:2:151:GLY:O	2.03	0.58
3:3:117:THR:HB	3:3:213:PHE:HB2	1.86	0.58
3:3:115:LYS:HA	3:3:167:VAL:HA	1.86	0.57
3:3:171:ILE:H	3:3:177:ARG:HH21	1.50	0.57
1:1:159:TYR:HE2	1:1:161:PRO:HG3	1.69	0.57
1:1:85:ALA:O	1:1:87:VAL:HG13	2.04	0.57
3:3:78:THR:HG22	3:3:79:ASP:H	1.70	0.57
2:2:38:TRP:CD1	2:2:39:PRO:HD2	2.40	0.56
4:4:10:VAL:C	4:4:12:ALA:H	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:159:TYR:CE2	1:1:161:PRO:HG3	2.41	0.56
2:2:210:LEU:N	2:2:210:LEU:HD23	2.20	0.56
2:2:104:SER:HB3	2:2:258:CYS:HB3	1.87	0.56
1:1:258:ARG:HG3	1:1:258:ARG:HH11	1.70	0.56
2:2:82:LEU:HD21	2:2:253:ILE:HD13	1.87	0.56
3:3:131:LEU:HD23	3:3:131:LEU:C	2.31	0.56
4:4:8:GLN:NE2	4:4:25:ILE:HG22	2.20	0.56
3:3:75:LYS:O	3:3:197:ARG:NH2	2.39	0.56
4:4:9:LYS:O	4:4:10:VAL:O	2.24	0.56
1:1:189:THR:HG22	1:1:190:ALA:H	1.71	0.55
1:1:94:ASN:O	1:1:96:ALA:N	2.40	0.55
1:1:273:PRO:HD2	2:2:193:PHE:CZ	2.42	0.55
2:2:54:THR:OG1	2:2:261:ASN:O	2.22	0.55
3:3:83:LEU:HD12	3:3:83:LEU:C	2.31	0.55
1:1:146:ASN:O	1:1:148:GLY:N	2.39	0.55
1:1:146:ASN:OD1	1:1:147:ASN:N	2.39	0.55
3:3:14:LEU:O	3:3:15:THR:C	2.50	0.55
3:3:112:GLY:O	3:3:170:TRP:HB2	2.07	0.55
3:3:202:LEU:C	3:3:204:THR:H	2.13	0.55
1:1:82:ALA:O	1:1:83:ARG:HD3	2.07	0.54
3:3:120:PHE:HA	3:3:210:ILE:HG22	1.89	0.54
3:3:128:GLY:HA3	3:3:198:ILE:HD13	1.89	0.54
1:1:95:PRO:HD3	1:1:244:VAL:HB	1.88	0.54
2:2:26:GLN:HG3	2:2:27:GLU:H	1.73	0.54
2:2:33:VAL:HG23	2:2:36:GLY:HA2	1.88	0.54
3:3:85:LEU:HA	3:3:94:ARG:NH2	2.22	0.54
2:2:66:LEU:CD1	2:2:251:LEU:HD22	2.30	0.54
3:3:114:LEU:HB3	3:3:116:PHE:HE1	1.71	0.54
1:1:175:TRP:CZ3	1:1:243:ARG:HG2	2.43	0.54
2:2:177:VAL:HB	2:2:180:LEU:HD12	1.89	0.54
3:3:111:ALA:HB1	3:3:170:TRP:CH2	2.43	0.54
3:3:134:TYR:CZ	3:3:136:PRO:HA	2.42	0.54
2:2:186:LEU:HD22	3:3:67:MET:HE1	1.90	0.54
2:2:210:LEU:HD13	2:2:227:TRP:CD2	2.43	0.54
3:3:131:LEU:HD12	3:3:155:ILE:HD11	1.89	0.54
1:1:72:ARG:O	1:1:73:SER:C	2.51	0.54
1:1:88:THR:OG1	1:1:89:ILE:N	2.40	0.53
1:1:138:VAL:HG11	1:1:155:TYR:CE1	2.42	0.53
1:1:108:TRP:CZ3	1:1:110:ILE:HA	2.43	0.53
1:1:136:PHE:CZ	1:1:240:LEU:HD13	2.43	0.53
2:2:54:THR:OG1	2:2:260:PHE:O	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:84:ASP:O	2:2:87:ARG:N	2.42	0.53
2:2:188:GLY:HA2	3:3:52:MET:HB3	1.90	0.53
2:2:236:PRO:HD2	3:3:209:ASP:OD2	2.08	0.53
2:2:71:TRP:NE1	2:2:237:LEU:HB2	2.23	0.53
4:4:16:SER:C	4:4:18:ARG:H	2.15	0.53
1:1:171:ASP:OD1	1:1:171:ASP:N	2.42	0.53
2:2:91:LEU:O	2:2:94:GLN:N	2.42	0.53
2:2:197:ILE:HD12	3:3:119:LEU:HD22	1.90	0.53
2:2:241:SER:OG	2:2:242:GLU:N	2.39	0.53
1:1:120:ARG:NH1	3:3:106:TYR:OH	2.41	0.53
2:2:222:VAL:HG13	2:2:223:LYS:H	1.74	0.53
3:3:135:ALA:HB2	3:3:142:PRO:HD3	1.90	0.53
1:1:159:TYR:CE1	1:1:196:VAL:HG11	2.44	0.52
3:3:99:MET:O	3:3:100:LEU:C	2.51	0.52
1:1:199:VAL:N	1:1:205:TYR:OH	2.32	0.52
1:1:160:VAL:HG12	1:1:164:ALA:HB3	1.89	0.52
1:1:258:ARG:HG3	1:1:258:ARG:NH1	2.23	0.52
2:2:102:GLY:HA2	2:2:259:GLU:O	2.10	0.52
3:3:195:GLN:HG3	3:3:196:THR:HG23	1.90	0.52
2:2:72:THR:N	2:2:75:SER:OG	2.33	0.52
4:4:8:GLN:HG2	4:4:27:TYR:HD1	1.75	0.52
2:2:80:TRP:CE3	2:2:251:LEU:HD21	2.45	0.52
1:1:102:ASP:C	1:1:104:LEU:H	2.16	0.52
1:1:157:ILE:HB	1:1:183:ILE:CB	2.39	0.52
2:2:130:MET:HE2	2:2:228:GLY:HA3	1.92	0.52
3:3:156:TRP:CG	3:3:164:CYS:HB2	2.44	0.52
3:3:173:ASN:CG	3:3:174:THR:N	2.68	0.51
1:1:129:ARG:CD	3:3:33:PRO:HB3	2.40	0.51
1:1:136:PHE:HZ	1:1:240:LEU:HD13	1.76	0.51
2:2:144:SER:O	2:2:145:TYR:C	2.54	0.51
3:3:114:LEU:O	3:3:168:VAL:HG12	2.10	0.51
3:3:129:LYS:O	3:3:195:GLN:HB3	2.10	0.51
1:1:75:SER:HB3	3:3:222:VAL:CG2	2.40	0.51
2:2:193:PHE:O	2:2:194:PRO:C	2.52	0.51
3:3:62:LYS:HA	3:3:67:MET:HB3	1.92	0.51
4:4:15:ASN:C	4:4:17:ASN:N	2.68	0.51
1:1:127:TYR:HE1	1:1:206:SER:HG	1.58	0.51
1:1:156:GLN:HG3	1:1:184:PHE:CE1	2.45	0.51
1:1:157:ILE:HG12	1:1:242:VAL:HG12	1.93	0.51
3:3:104:LEU:HD22	3:3:110:TRP:CG	2.45	0.51
1:1:236:ASP:OD1	1:1:237:PHE:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:94:ASN:O	1:1:100:ASN:ND2	2.44	0.51
2:2:236:PRO:HD3	3:3:69:ARG:CD	2.40	0.51
2:2:240:ALA:O	2:2:241:SER:C	2.54	0.51
2:2:201:ARG:HD3	3:3:120:PHE:HD2	1.76	0.51
2:2:199:ASN:HD22	3:3:119:LEU:HD11	1.77	0.50
1:1:136:PHE:CE2	1:1:259:VAL:HG22	2.47	0.50
2:2:144:SER:O	2:2:147:ASN:N	2.37	0.50
3:3:104:LEU:HD22	3:3:110:TRP:CD1	2.45	0.50
2:2:201:ARG:CD	3:3:120:PHE:HD2	2.25	0.50
1:1:249:ASN:OD1	1:1:250:PRO:CD	2.56	0.50
2:2:40:GLU:N	2:2:40:GLU:OE1	2.45	0.50
2:2:76:ARG:O	2:2:233:PRO:HD2	2.11	0.50
3:3:25:LEU:HB3	3:3:28:PHE:HB3	1.93	0.49
4:4:13:HIS:C	4:4:16:SER:HA	2.37	0.49
1:1:261:LEU:C	1:1:261:LEU:HD22	2.36	0.49
2:2:238:ASN:OD1	2:2:239:PHE:N	2.46	0.49
2:2:121:ALA:HA	2:2:198:ILE:O	2.12	0.49
1:1:87:VAL:HG23	1:1:88:THR:HG22	1.93	0.49
3:3:73:SER:HB2	3:3:75:LYS:HE3	1.94	0.49
1:1:203:ASN:ND2	3:3:31:THR:HG21	2.27	0.49
1:1:115:THR:O	1:1:116:VAL:C	2.56	0.49
1:1:128:SER:HB3	1:1:268:VAL:HG12	1.95	0.49
1:1:205:TYR:CB	1:1:235:ASN:ND2	2.74	0.49
3:3:44:MET:SD	3:3:220:PHE:HD1	2.36	0.49
3:3:178:GLN:HG2	3:3:180:ILE:HG12	1.94	0.49
2:2:71:TRP:CZ2	2:2:237:LEU:HB2	2.48	0.49
2:2:108:VAL:HG13	2:2:208:LEU:HB2	1.93	0.49
2:2:180:LEU:HD22	2:2:184:GLY:HA2	1.93	0.49
3:3:12:GLN:O	3:3:12:GLN:HG3	2.13	0.49
1:1:89:ILE:HG12	1:1:258:ARG:HG2	1.94	0.49
1:1:120:ARG:O	1:1:121:LYS:C	2.53	0.49
2:2:83:PRO:HA	2:2:106:TYR:OH	2.12	0.49
2:2:213:VAL:O	2:2:214:ASN:HB2	2.11	0.49
3:3:181:ASP:OD1	3:3:185:THR:OG1	2.22	0.49
1:1:78:GLU:O	1:1:80:PHE:N	2.46	0.48
1:1:201:ILE:HG13	1:1:202:SER:N	2.27	0.48
2:2:126:ALA:O	2:2:193:PHE:HB3	2.14	0.48
2:2:213:VAL:HG22	3:3:37:PRO:HG2	1.94	0.48
2:2:132:LEU:HD13	2:2:176:PRO:HG3	1.96	0.48
3:3:45:GLU:OE1	3:3:45:GLU:N	2.47	0.48
3:3:171:ILE:O	3:3:172:SER:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:175:TRP:CE2	1:1:243:ARG:HD3	2.49	0.48
2:2:213:VAL:HG22	3:3:37:PRO:CG	2.43	0.48
3:3:54:PRO:HA	3:3:67:MET:O	2.14	0.48
3:3:141:PRO:HD3	3:3:189:TYR:CZ	2.48	0.48
2:2:104:SER:CB	2:2:258:CYS:HB3	2.44	0.48
1:1:129:ARG:O	1:1:130:PHE:HB3	2.14	0.48
2:2:223:LYS:O	2:2:224:HIS:HB2	2.14	0.48
4:4:13:HIS:HB2	4:4:16:SER:OG	2.14	0.48
1:1:93:ASP:CG	1:1:103:LYS:HG2	2.39	0.48
3:3:131:LEU:CD1	3:3:153:HIS:HD2	2.26	0.48
2:2:128:PRO:CG	2:2:227:TRP:CZ3	2.94	0.48
3:3:2:LEU:HD12	3:3:3:PRO:CD	2.34	0.48
3:3:168:VAL:CG2	3:3:169:PRO:HD2	2.41	0.48
2:2:33:VAL:HG12	2:2:209:VAL:CB	2.42	0.47
4:4:54:THR:C	4:4:56:PRO:HD3	2.39	0.47
1:1:151:LEU:O	1:1:152:ASN:C	2.57	0.47
3:3:50:ASP:HA	3:3:215:SER:HB3	1.96	0.47
3:3:202:LEU:C	3:3:204:THR:N	2.71	0.47
2:2:109:HIS:HB3	2:2:252:THR:HB	1.97	0.47
3:3:116:PHE:CD1	3:3:116:PHE:N	2.82	0.47
1:1:147:ASN:OD1	1:1:149:HIS:ND1	2.44	0.47
4:4:17:ASN:O	4:4:18:ARG:NE	2.39	0.47
2:2:236:PRO:HD3	3:3:69:ARG:NE	2.29	0.47
2:2:59:ALA:HB3	2:2:91:LEU:HD22	1.95	0.47
3:3:9:GLY:O	3:3:12:GLN:HG2	2.15	0.47
1:1:273:PRO:CB	2:2:185:THR:HG21	2.44	0.47
2:2:187:LEU:CD2	3:3:65:MET:HE1	2.40	0.47
2:2:89:MET:HE1	2:2:152:GLU:OE1	2.15	0.47
2:2:82:LEU:HB3	2:2:106:TYR:CZ	2.50	0.47
2:2:83:PRO:O	2:2:84:ASP:C	2.58	0.47
3:3:52:MET:HE3	3:3:52:MET:HB2	1.81	0.47
4:4:8:GLN:HE21	4:4:26:ASN:CA	2.24	0.47
1:1:242:VAL:HG21	1:1:257:ILE:CD1	2.46	0.46
2:2:101:LEU:HB2	2:2:261:ASN:HB3	1.97	0.46
2:2:95:ASN:HB3	2:2:260:PHE:CZ	2.50	0.46
3:3:11:ASN:OD1	3:3:11:ASN:N	2.45	0.46
1:1:275:ARG:HD2	1:1:279:TYR:CE1	2.50	0.46
2:2:157:PHE:HB3	2:2:178:ASP:HB3	1.98	0.46
1:1:74:GLU:CD	3:3:224:LEU:H	2.24	0.46
3:3:73:SER:O	3:3:74:ASP:OD2	2.34	0.46
1:1:203:ASN:ND2	3:3:31:THR:CG2	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:12:ARG:HG3	2:2:27:GLU:OE2	2.15	0.46
2:2:222:VAL:CG1	2:2:223:LYS:N	2.77	0.46
3:3:132:VAL:HG12	3:3:192:VAL:HG13	1.98	0.46
1:1:77:ILE:HD11	3:3:40:VAL:HG12	1.96	0.46
2:2:117:PHE:CE2	3:3:125:MET:HG3	2.51	0.46
3:3:158:ILE:HD13	3:3:158:ILE:HA	1.62	0.46
4:4:8:GLN:C	4:4:10:VAL:N	2.67	0.46
1:1:102:ASP:C	1:1:104:LEU:N	2.73	0.46
2:2:34:ALA:HB1	2:2:194:PRO:HG3	1.98	0.46
4:4:15:ASN:C	4:4:17:ASN:H	2.23	0.46
1:1:124:PHE:CZ	1:1:274:PRO:HB3	2.51	0.46
3:3:64:THR:OG1	3:3:65:MET:N	2.49	0.46
1:1:78:GLU:N	1:1:78:GLU:CD	2.61	0.46
1:1:159:TYR:CE2	1:1:161:PRO:HA	2.51	0.46
2:2:211:PRO:HD2	2:2:227:TRP:HZ2	1.80	0.46
2:2:216:LEU:HD23	2:2:216:LEU:HA	1.66	0.46
3:3:132:VAL:O	3:3:132:VAL:HG23	2.16	0.46
2:2:14:LEU:HD12	2:2:14:LEU:N	2.31	0.45
2:2:243:SER:O	2:2:244:SER:C	2.59	0.45
3:3:1:GLY:O	3:3:2:LEU:C	2.58	0.45
2:2:83:PRO:CA	2:2:106:TYR:OH	2.64	0.45
4:4:13:HIS:HB3	4:4:16:SER:HA	1.97	0.45
2:2:187:LEU:HB3	3:3:68:TYR:HE2	1.81	0.45
3:3:84:CYS:O	3:3:94:ARG:NH1	2.43	0.45
3:3:171:ILE:CG2	3:3:172:SER:N	2.79	0.45
2:2:84:ASP:O	2:2:85:ALA:C	2.59	0.45
2:2:96:MET:O	2:2:97:TYR:CG	2.70	0.45
2:2:203:ASN:C	2:2:203:ASN:HD22	2.25	0.45
4:4:15:ASN:O	4:4:18:ARG:CA	2.64	0.45
3:3:171:ILE:HG22	3:3:172:SER:N	2.30	0.45
1:1:134:LEU:CD1	1:1:240:LEU:HD11	2.46	0.45
1:1:160:VAL:HB	1:1:239:ILE:HB	1.97	0.45
2:2:180:LEU:HD23	2:2:185:THR:O	2.17	0.45
2:2:251:LEU:HD12	2:2:251:LEU:N	2.31	0.45
1:1:234:LEU:C	1:1:234:LEU:HD23	2.42	0.45
2:2:20:ASN:OD1	2:2:20:ASN:N	2.49	0.45
2:2:86:LEU:HD23	2:2:86:LEU:N	2.31	0.45
3:3:71:ARG:O	3:3:72:LEU:C	2.58	0.45
4:4:9:LYS:O	4:4:10:VAL:C	2.59	0.45
1:1:116:VAL:CG2	1:1:117:GLN:N	2.79	0.45
1:1:183:ILE:HD13	1:1:183:ILE:HA	1.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:44:MET:C	3:3:46:LEU:H	2.24	0.45
2:2:74:GLU:CD	2:2:74:GLU:N	2.66	0.45
3:3:60:THR:HG23	3:3:61:LYS:H	1.82	0.45
2:2:18:LEU:CB	2:2:62:ARG:HA	2.47	0.45
4:4:45:ASP:O	4:4:46:PHE:C	2.59	0.45
3:3:227:ASP:OD1	3:3:228:THR:N	2.50	0.44
1:1:70:ARG:HD2	3:3:219:ASP:O	2.17	0.44
1:1:109:LYS:HG3	1:1:239:ILE:CD1	2.47	0.44
2:2:174:PHE:CE2	2:2:176:PRO:HD3	2.53	0.44
3:3:52:MET:HG2	3:3:68:TYR:CD1	2.52	0.44
3:3:170:TRP:CE3	3:3:177:ARG:NE	2.85	0.44
3:3:224:LEU:C	3:3:224:LEU:HD12	2.41	0.44
1:1:205:TYR:HA	1:1:235:ASN:HD22	1.82	0.44
1:1:193:ARG:HH22	3:3:13:TYR:HE1	1.63	0.44
4:4:55:GLU:N	4:4:56:PRO:HD3	2.33	0.44
1:1:129:ARG:HD2	3:3:33:PRO:HB3	1.99	0.44
2:2:210:LEU:HD13	2:2:227:TRP:CG	2.52	0.44
3:3:58:SER:O	3:3:59:ALA:C	2.60	0.44
2:2:99:HIS:ND1	2:2:260:PHE:HB3	2.32	0.44
3:3:170:TRP:HZ3	3:3:177:ARG:HD2	1.80	0.44
4:4:1:MYR:H52	4:4:30:ILE:HD13	2.00	0.44
1:1:78:GLU:O	1:1:79:SER:C	2.61	0.44
1:1:262:LYS:NZ	3:3:17:ASP:O	2.51	0.44
2:2:66:LEU:HD12	2:2:251:LEU:HB2	1.99	0.44
3:3:7:THR:HB	3:3:8:PRO:CD	2.47	0.44
3:3:131:LEU:HD11	3:3:153:HIS:CD2	2.53	0.44
4:4:22:GLY:O	4:4:23:SER:HB2	2.18	0.44
3:3:44:MET:HE2	3:3:47:ALA:HB3	2.00	0.44
3:3:112:GLY:HA3	3:3:220:PHE:HD2	1.81	0.44
1:1:78:GLU:C	1:1:80:PHE:N	2.73	0.44
3:3:218:ASN:OD1	3:3:218:ASN:N	2.50	0.44
2:2:79:TRP:HA	2:2:229:ILE:O	2.19	0.43
3:3:58:SER:O	3:3:60:THR:N	2.51	0.43
2:2:234:LEU:HB3	3:3:211:LEU:HD11	2.00	0.43
3:3:115:LYS:HB3	3:3:217:CYS:SG	2.58	0.43
4:4:9:LYS:CB	4:4:44:GLN:NE2	2.69	0.43
1:1:156:GLN:CG	1:1:184:PHE:CE1	3.00	0.43
1:1:203:ASN:HD22	3:3:31:THR:CG2	2.30	0.43
1:1:266:ILE:HG22	1:1:267:ARG:N	2.33	0.43
2:2:219:ASP:CG	2:2:220:SER:N	2.74	0.43
3:3:131:LEU:HD11	3:3:153:HIS:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:204:THR:HG23	3:3:205:PRO:HD2	2.00	0.43
1:1:128:SER:OG	1:1:207:HIS:NE2	2.52	0.43
1:1:186:THR:O	1:1:187:TYR:C	2.60	0.43
2:2:71:TRP:HB2	2:2:249:ILE:HD11	2.00	0.43
3:3:72:LEU:HD22	3:3:194:TYR:CE1	2.53	0.43
3:3:176:TYR:CZ	3:3:223:ARG:NE	2.86	0.43
1:1:127:TYR:O	1:1:269:TRP:N	2.49	0.43
2:2:59:ALA:HB3	2:2:91:LEU:CD2	2.48	0.43
2:2:179:TYR:HB3	3:3:65:MET:SD	2.58	0.43
2:2:210:LEU:HD11	2:2:229:ILE:HD11	2.01	0.43
3:3:125:MET:HB3	3:3:201:PRO:HG3	2.00	0.43
1:1:151:LEU:N	1:1:151:LEU:CD2	2.79	0.43
2:2:187:LEU:C	2:2:189:ASN:H	2.26	0.43
3:3:75:LYS:O	3:3:76:PRO:C	2.62	0.43
4:4:16:SER:O	4:4:17:ASN:CB	2.53	0.43
1:1:128:SER:HA	1:1:267:ARG:O	2.18	0.43
2:2:99:HIS:CG	2:2:260:PHE:HB3	2.54	0.43
3:3:65:MET:N	3:3:65:MET:SD	2.92	0.43
3:3:145:ARG:HD2	3:3:195:GLN:OE1	2.18	0.43
1:1:157:ILE:HB	1:1:183:ILE:CG2	2.49	0.43
1:1:279:TYR:O	1:1:279:TYR:CG	2.71	0.43
2:2:105:GLY:O	2:2:106:TYR:CG	2.72	0.43
3:3:207:GLU:OE2	3:3:207:GLU:HA	2.19	0.43
2:2:23:ILE:HG22	2:2:25:THR:HG23	1.99	0.42
2:2:178:ASP:C	2:2:180:LEU:H	2.27	0.42
2:2:82:LEU:HD13	2:2:106:TYR:CD2	2.54	0.42
2:2:110:VAL:HG13	2:2:198:ILE:HD11	2.01	0.42
3:3:176:TYR:CE2	3:3:223:ARG:HD3	2.53	0.42
1:1:185:TYR:CD1	1:1:192:ALA:HB2	2.54	0.42
3:3:116:PHE:N	3:3:116:PHE:HD1	2.16	0.42
2:2:86:LEU:C	2:2:88:ASP:H	2.27	0.42
3:3:110:TRP:CD1	3:3:179:THR:HG22	2.51	0.42
3:3:111:ALA:HB2	3:3:176:TYR:HA	2.00	0.42
1:1:210:ASP:O	2:2:224:HIS:HA	2.20	0.42
2:2:191:PHE:HD2	2:2:195:HIS:ND1	2.17	0.42
5:7:113:UNK:N	5:7:210:UNK:O	2.53	0.42
1:1:122:LEU:HD23	1:1:122:LEU:HA	1.92	0.42
1:1:205:TYR:CB	1:1:235:ASN:HD21	2.23	0.42
3:3:203:SER:O	3:3:204:THR:C	2.63	0.42
1:1:116:VAL:HG23	1:1:117:GLN:H	1.81	0.42
1:1:274:PRO:HD3	3:3:99:MET:SD	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:23:ILE:HD13	2:2:23:ILE:HA	1.77	0.42
2:2:71:TRP:CZ3	2:2:247:ILE:HD11	2.54	0.41
2:2:126:ALA:HA	2:2:229:ILE:HD13	2.02	0.41
5:7:551:UNK:O	5:7:552:UNK:C	2.68	0.41
2:2:83:PRO:HD2	2:2:225:ASN:HA	2.01	0.41
1:1:113:LYS:HA	1:1:119:ARG:HD2	2.02	0.41
1:1:169:LYS:H	1:1:172:ASP:HB2	1.85	0.41
1:1:189:THR:HG22	1:1:190:ALA:N	2.33	0.41
3:3:95:LEU:O	3:3:98:THR:HG22	2.20	0.41
4:4:57:ILE:HG13	4:4:59:ASP:O	2.20	0.41
2:2:211:PRO:O	2:2:211:PRO:CD	2.68	0.41
2:2:247:ILE:O	2:2:247:ILE:HG13	2.20	0.41
3:3:152:THR:HG22	3:3:153:HIS:N	2.35	0.41
1:1:159:TYR:CD2	1:1:159:TYR:C	2.97	0.41
2:2:63:PHE:HA	2:2:254:ALA:HB2	2.02	0.41
2:2:82:LEU:HD23	2:2:82:LEU:HA	1.92	0.41
1:1:75:SER:HA	3:3:107:TYR:OH	2.20	0.41
2:2:21:SER:HB3	2:2:62:ARG:NH2	2.36	0.41
2:2:33:VAL:HG12	2:2:209:VAL:CG1	2.51	0.41
2:2:191:PHE:CZ	3:3:52:MET:CE	3.03	0.41
3:3:74:ASP:HB2	3:3:206:ARG:HB3	2.03	0.41
3:3:226:ARG:O	3:3:226:ARG:HG2	2.18	0.41
1:1:169:LYS:HB2	1:1:172:ASP:N	2.36	0.41
2:2:18:LEU:HB3	2:2:62:ARG:HA	2.03	0.41
2:2:190:ALA:C	2:2:192:VAL:N	2.79	0.41
3:3:89:PRO:HG3	3:3:114:LEU:HD11	2.03	0.41
3:3:115:LYS:HB2	3:3:167:VAL:HG22	2.00	0.41
3:3:132:VAL:HG12	3:3:192:VAL:HG22	2.03	0.41
2:2:97:TYR:C	2:2:99:HIS:N	2.75	0.40
2:2:239:PHE:CE2	2:2:245:PRO:HA	2.56	0.40
3:3:80:ASP:HB2	3:3:81:PRO:CD	2.47	0.40
2:2:124:VAL:O	2:2:195:HIS:HA	2.21	0.40
2:2:126:ALA:HB2	2:2:208:LEU:HD13	2.04	0.40
2:2:201:ARG:O	2:2:202:THR:OG1	2.32	0.40
2:2:110:VAL:HG13	2:2:110:VAL:O	2.21	0.40
3:3:118:PHE:HA	3:3:211:LEU:O	2.21	0.40
1:1:120:ARG:HD3	3:3:229:THR:HG21	2.04	0.40
4:4:52:LYS:HG3	4:4:53:PHE:CD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1	187/302 (62%)	150 (80%)	30 (16%)	7 (4%)	2	16
2	2	226/272 (83%)	167 (74%)	46 (20%)	13 (6%)	1	8
3	3	224/238 (94%)	173 (77%)	43 (19%)	8 (4%)	2	16
4	4	66/70 (94%)	46 (70%)	14 (21%)	6 (9%)	0	3
5	7	8/520 (2%)	7 (88%)	1 (12%)	0	100	100
All	All	711/1402 (51%)	543 (76%)	134 (19%)	34 (5%)	3	11

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	113	LYS
1	1	146	ASN
2	2	89	MET
2	2	145	TYR
2	2	188	GLY
2	2	191	PHE
2	2	241	SER
3	3	172	SER
3	3	175	THR
3	3	202	LEU
3	3	203	SER
4	4	10	VAL
4	4	15	ASN
4	4	44	GLN
4	4	47	SER
2	2	84	ASP
2	2	184	GLY
2	2	202	THR
2	2	224	HIS
4	4	23	SER
4	4	45	ASP

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Mol	Chain	Res	Type
1	1	73	SER
2	2	26	GLN
2	2	56	PRO
3	3	59	ALA
2	2	261	ASN
3	3	162	SER
3	3	166	MET
1	1	79	SER
1	1	95	PRO
1	1	147	ASN
1	1	248	HIS
3	3	16	ALA
2	2	194	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	1	171/261 (66%)	163 (95%)	8 (5%)	23	50
2	2	198/232 (85%)	192 (97%)	6 (3%)	36	59
3	3	204/212 (96%)	196 (96%)	8 (4%)	28	53
4	4	57/58 (98%)	57 (100%)	0	100	100
5	7	10/10 (100%)	10 (100%)	0	100	100
All	All	640/773 (83%)	618 (97%)	22 (3%)	33	57

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	115	THR
1	1	137	VAL
1	1	139	THR
1	1	166	VAL
1	1	183	ILE
1	1	186	THR

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Mol	Chain	Res	Type
1	1	242	VAL
1	1	261	LEU
2	2	69	VAL
2	2	158	THR
2	2	183	ASN
2	2	203	ASN
2	2	250	THR
2	2	251	LEU
3	3	6	ASN
3	3	17	ASP
3	3	44	MET
3	3	70	VAL
3	3	83	LEU
3	3	158	ILE
3	3	214	VAL
3	3	218	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	235	ASN
2	2	183	ASN
2	2	199	ASN
3	3	153	HIS
4	4	4	GLN
4	4	8	GLN
4	4	26	ASN
4	4	44	GLN
4	4	48	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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.

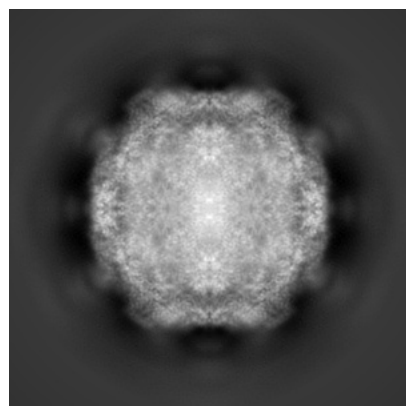
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20546. These allow visual inspection of the internal detail of the map and identification of artifacts.

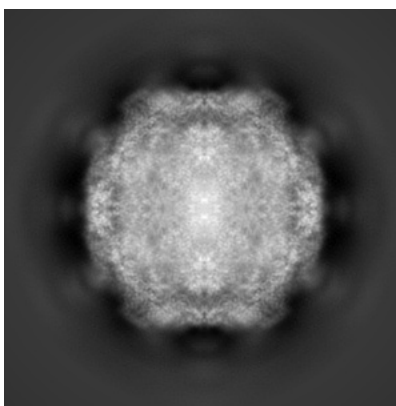
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

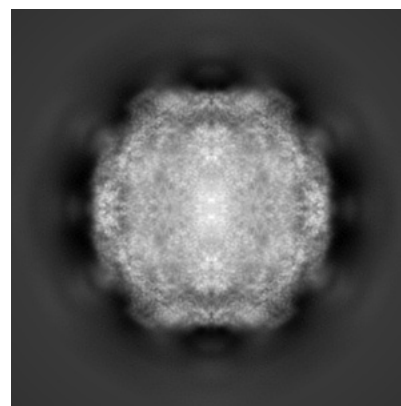
6.1.1 Primary map



X

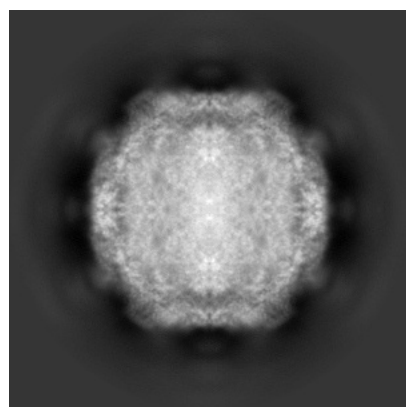


Y

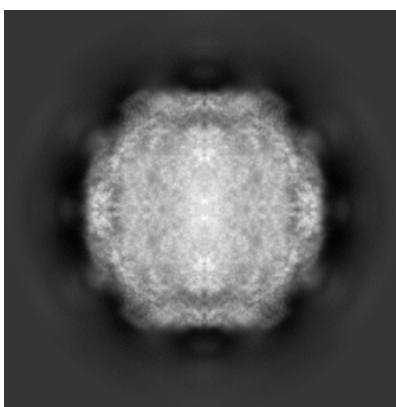


Z

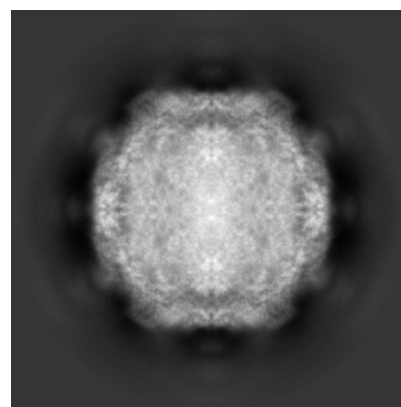
6.1.2 Raw map



X



Y

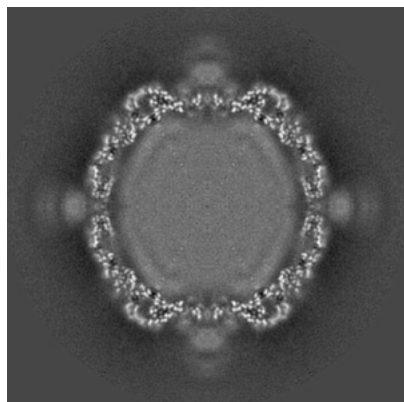


Z

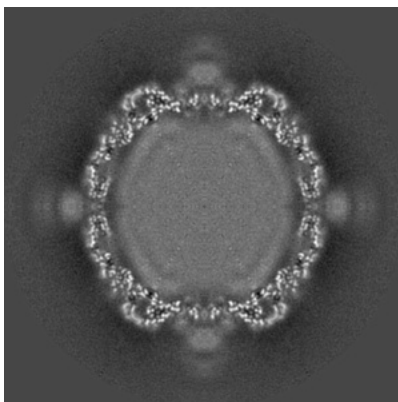
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

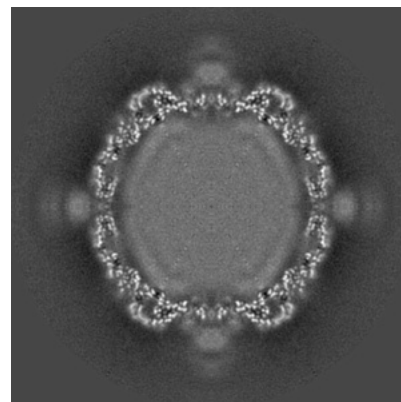
6.2.1 Primary map



X Index: 224

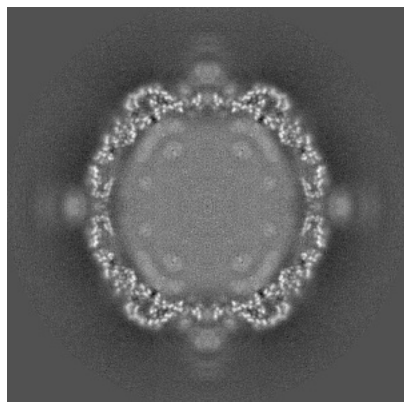


Y Index: 224

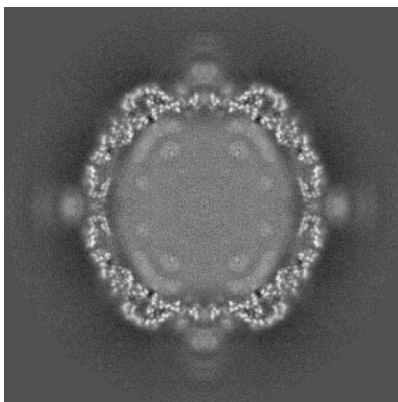


Z Index: 224

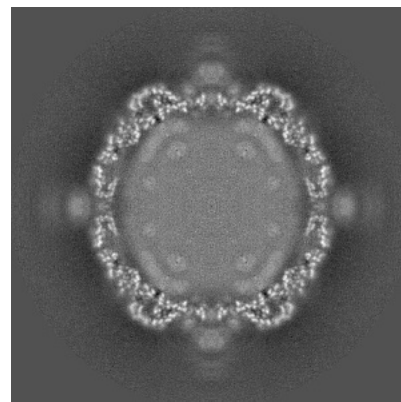
6.2.2 Raw map



X Index: 224



Y Index: 224

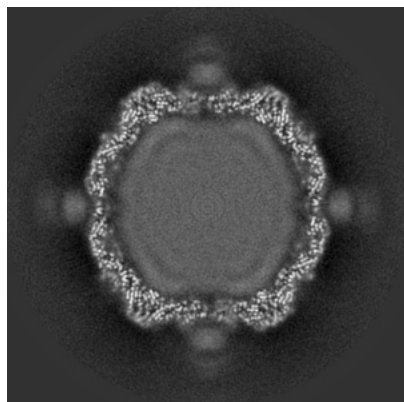


Z Index: 224

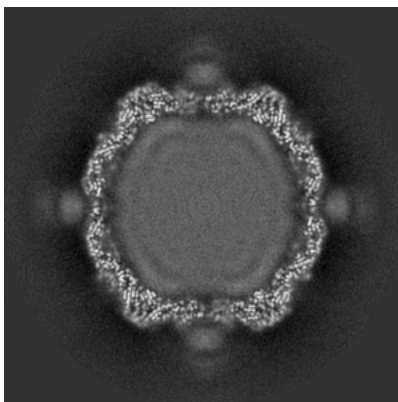
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

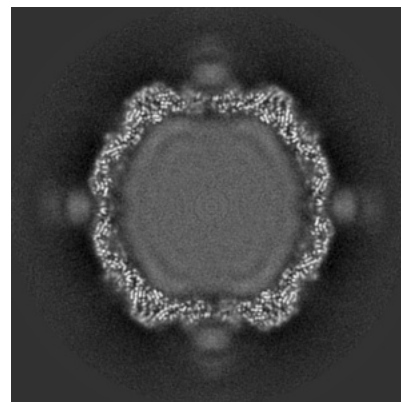
6.3.1 Primary map



X Index: 218

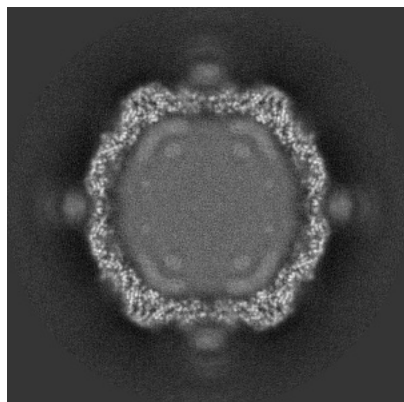


Y Index: 218

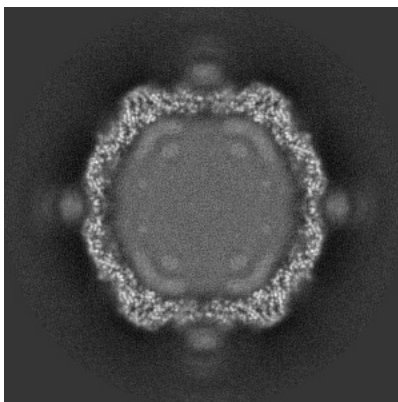


Z Index: 218

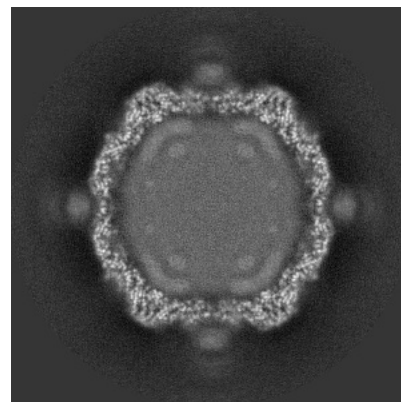
6.3.2 Raw map



X Index: 218



Y Index: 230

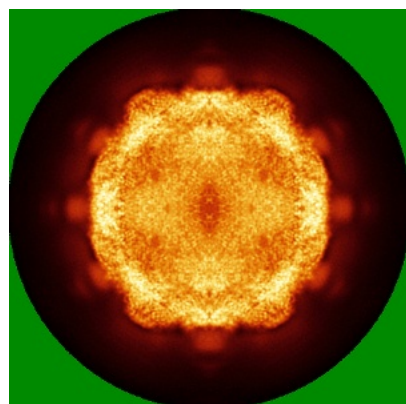


Z Index: 218

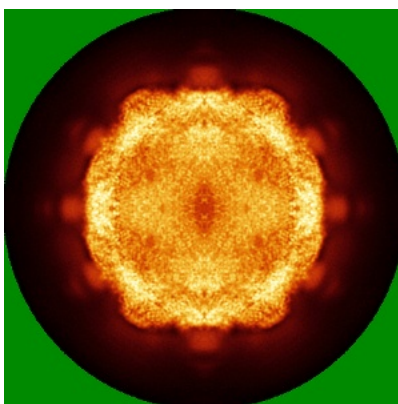
The images above show the largest variance slices of the map in three orthogonal directions.

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

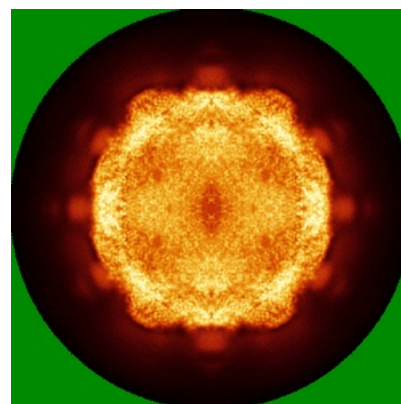
6.4.1 Primary map



X

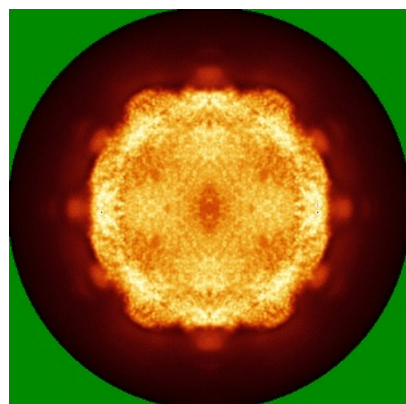


Y

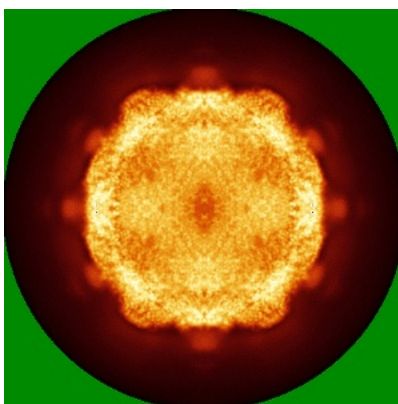


Z

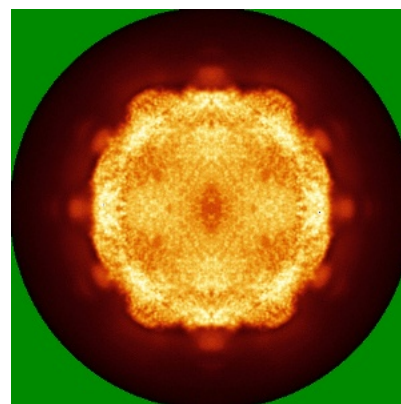
6.4.2 Raw map



X



Y

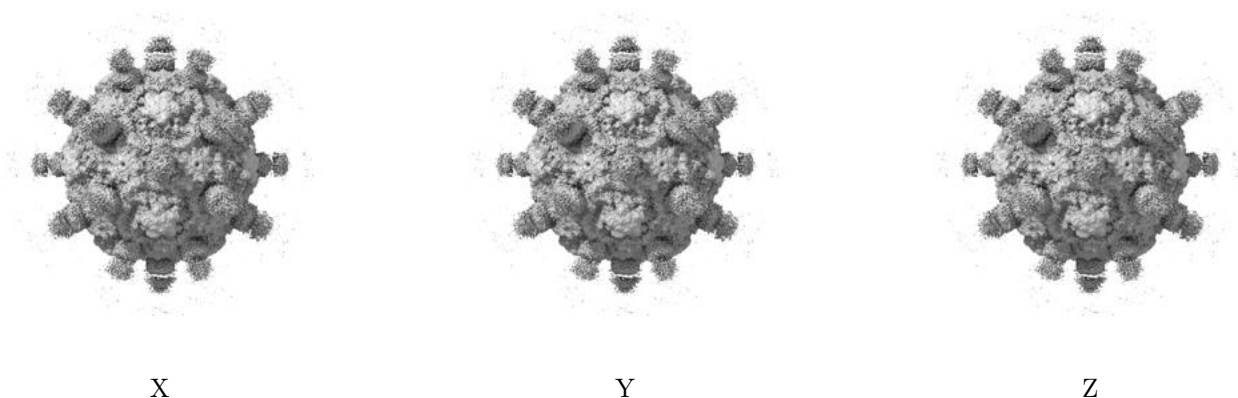


Z

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

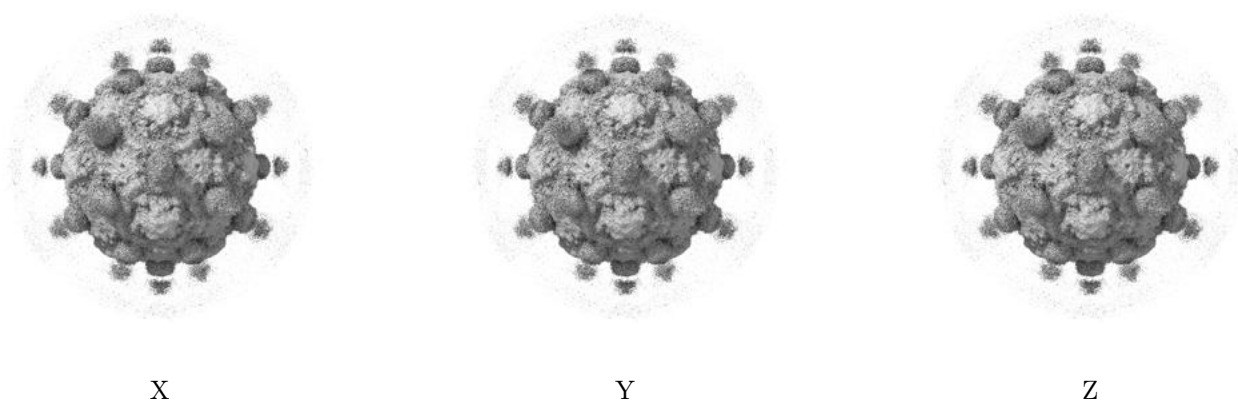
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 32.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

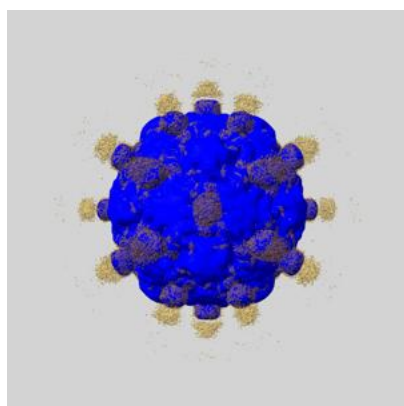
6.6 Mask visualisation [i](#)

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

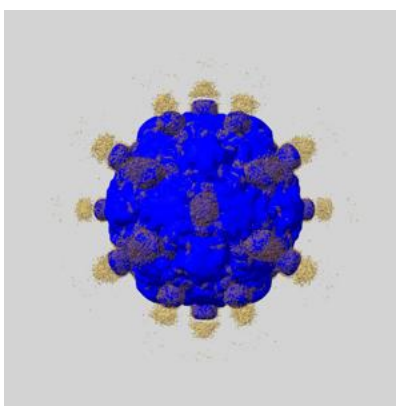
A mask typically either:

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

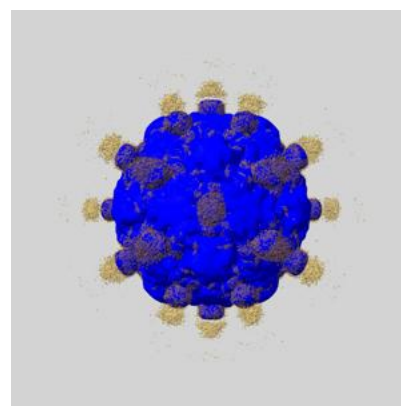
6.6.1 emd_20546_msk_1.map [i](#)



X



Y

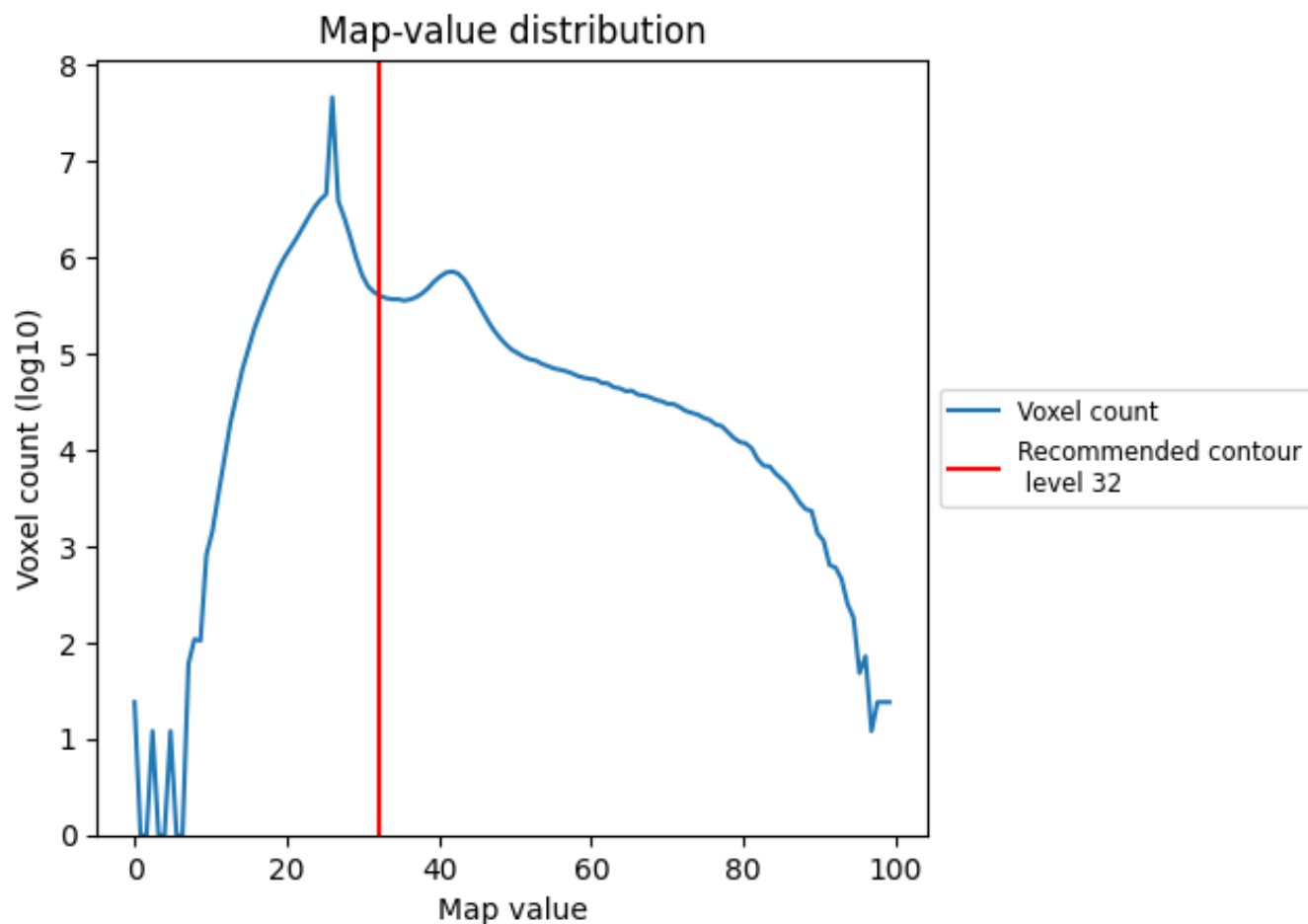


Z

7 Map analysis [i](#)

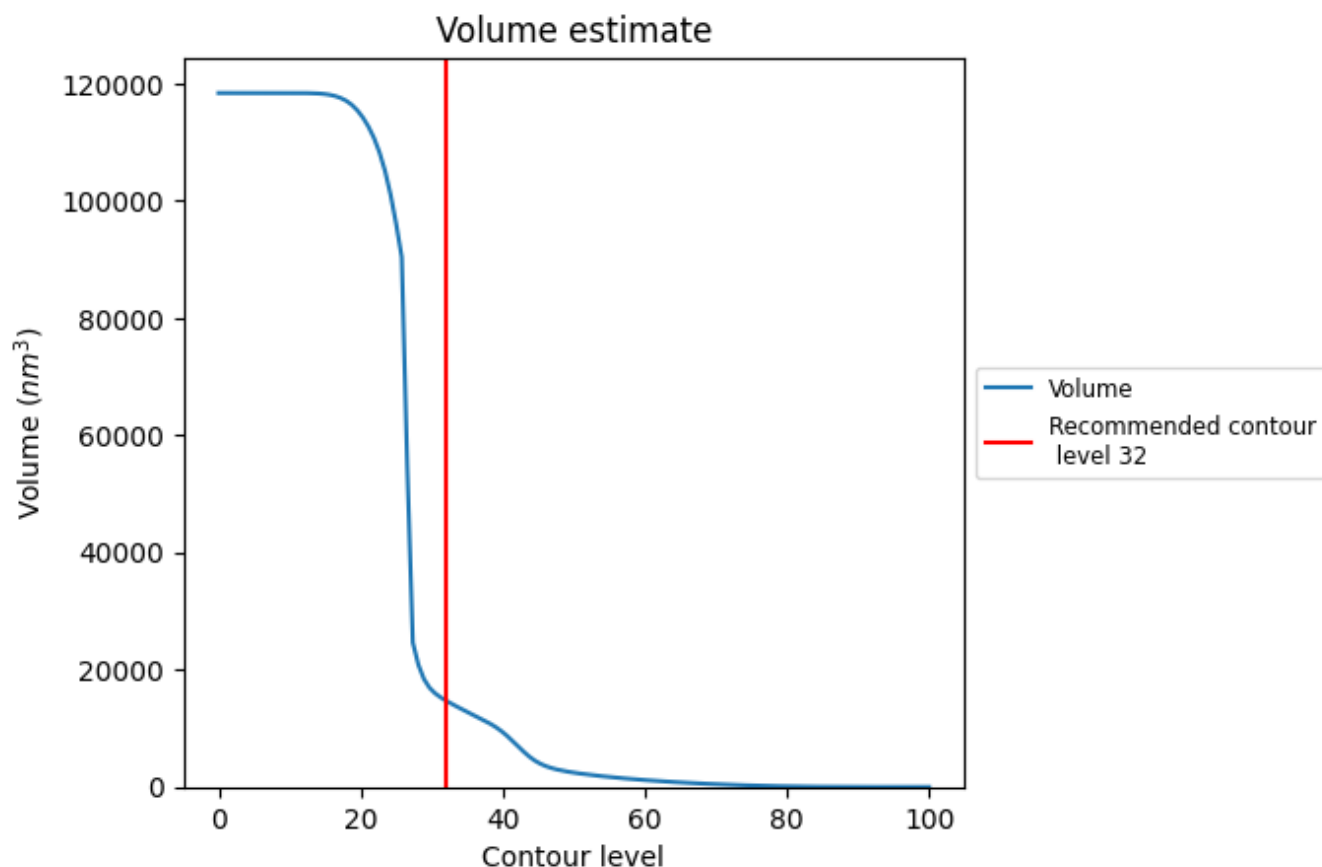
This section contains the results of statistical analysis of the map.

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.

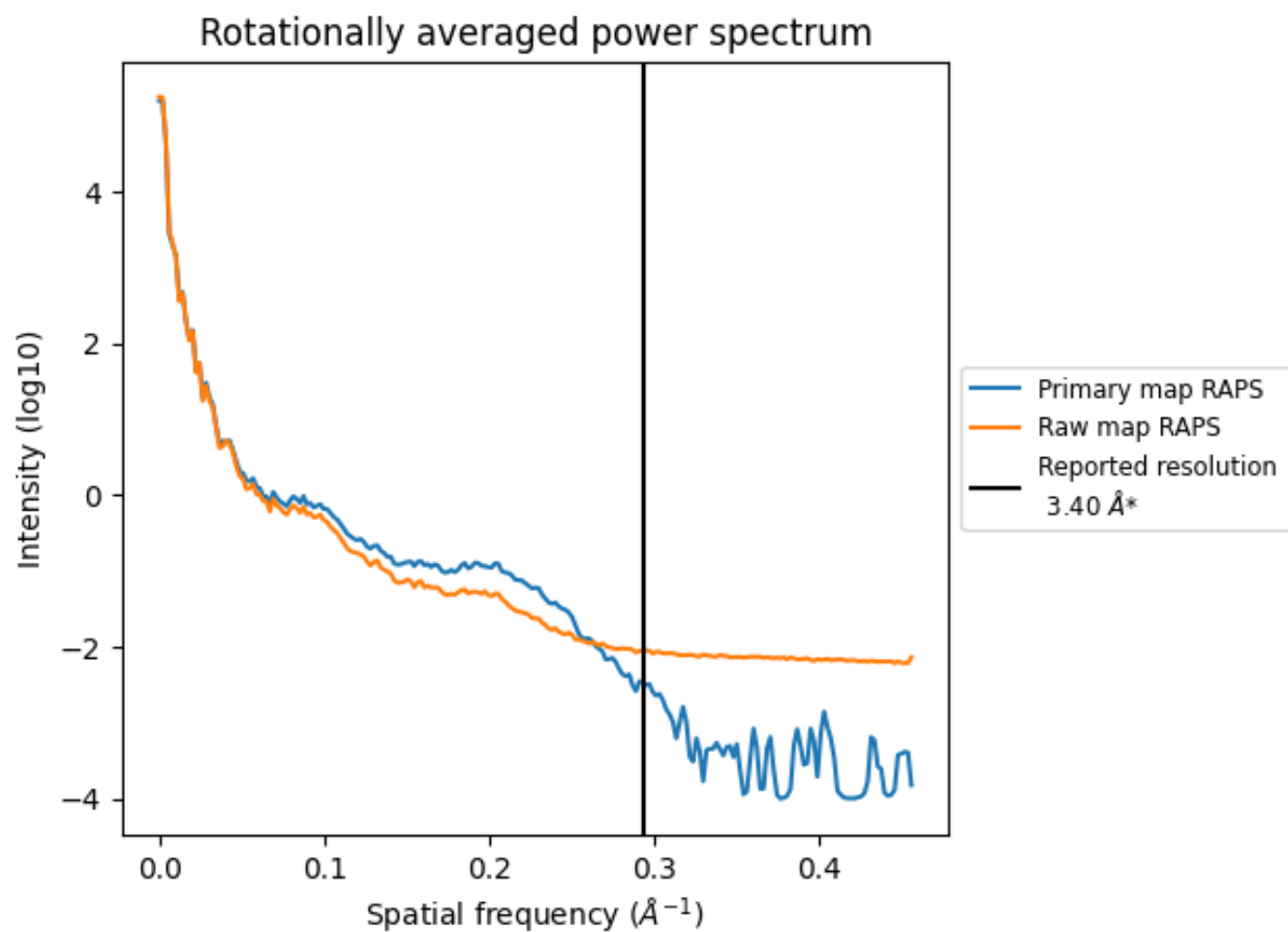
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 14728 nm^3 ; this corresponds to an approximate mass of 13304 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 ⓘ

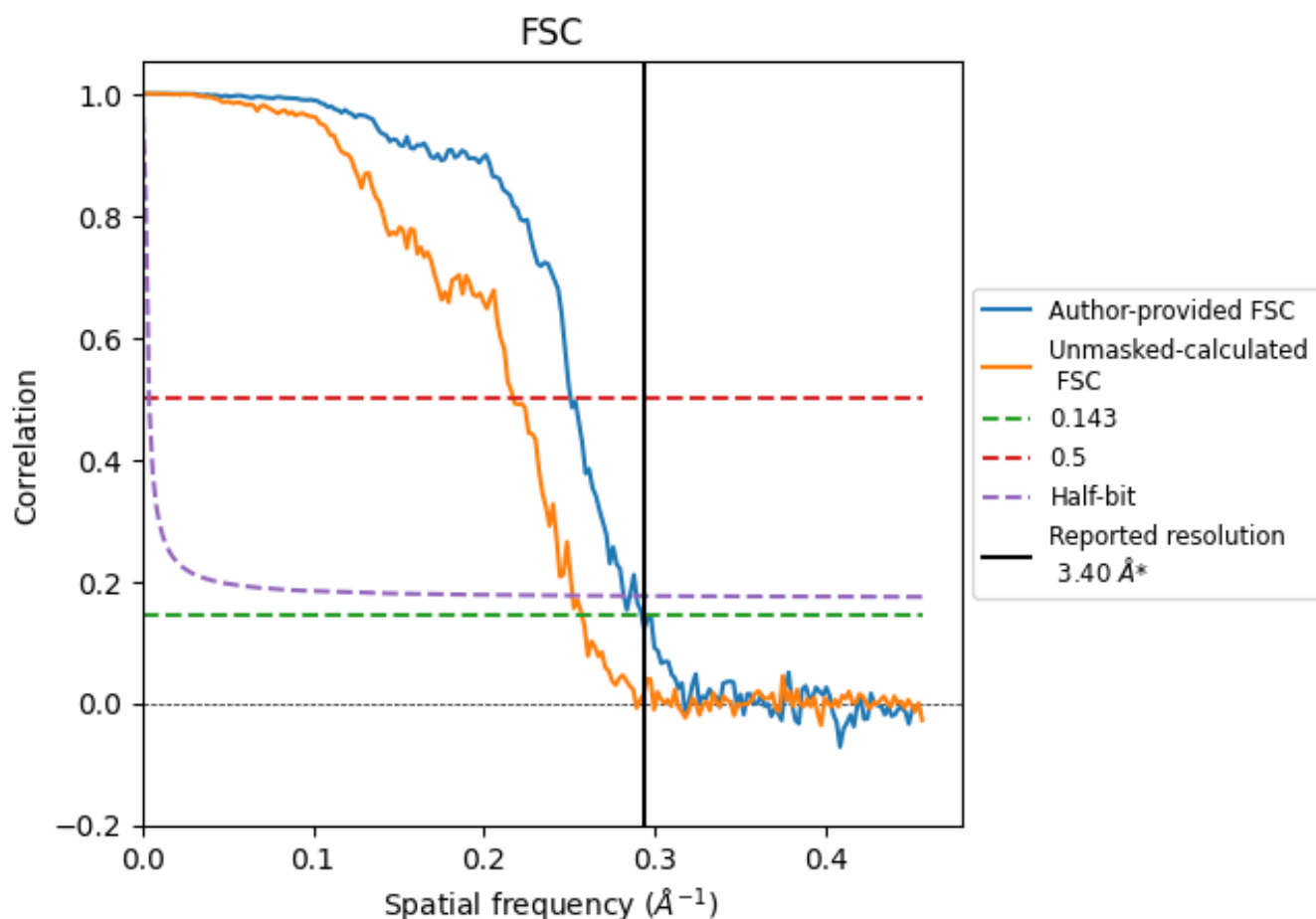


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 $0.294 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.42	3.99	3.55
Unmasked-calculated*	3.89	4.61	3.97

*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 3.89 differs from the reported value 3.4 by more than 10 %

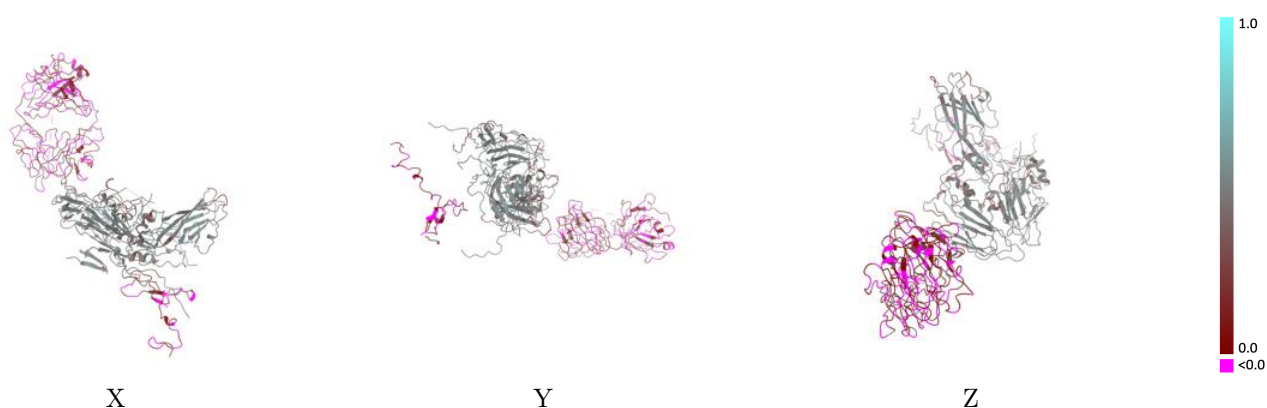
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-20546 and PDB model 6Q0B. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

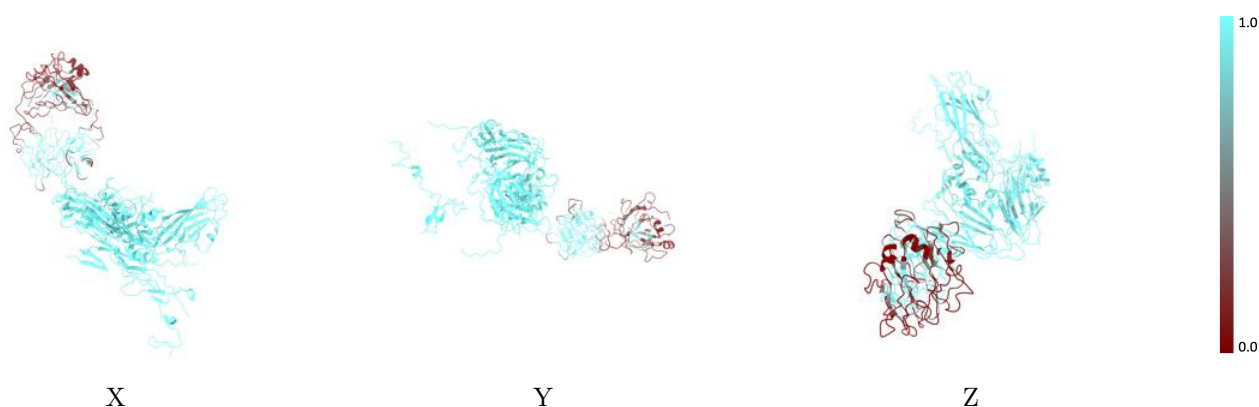
This section was not generated.

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



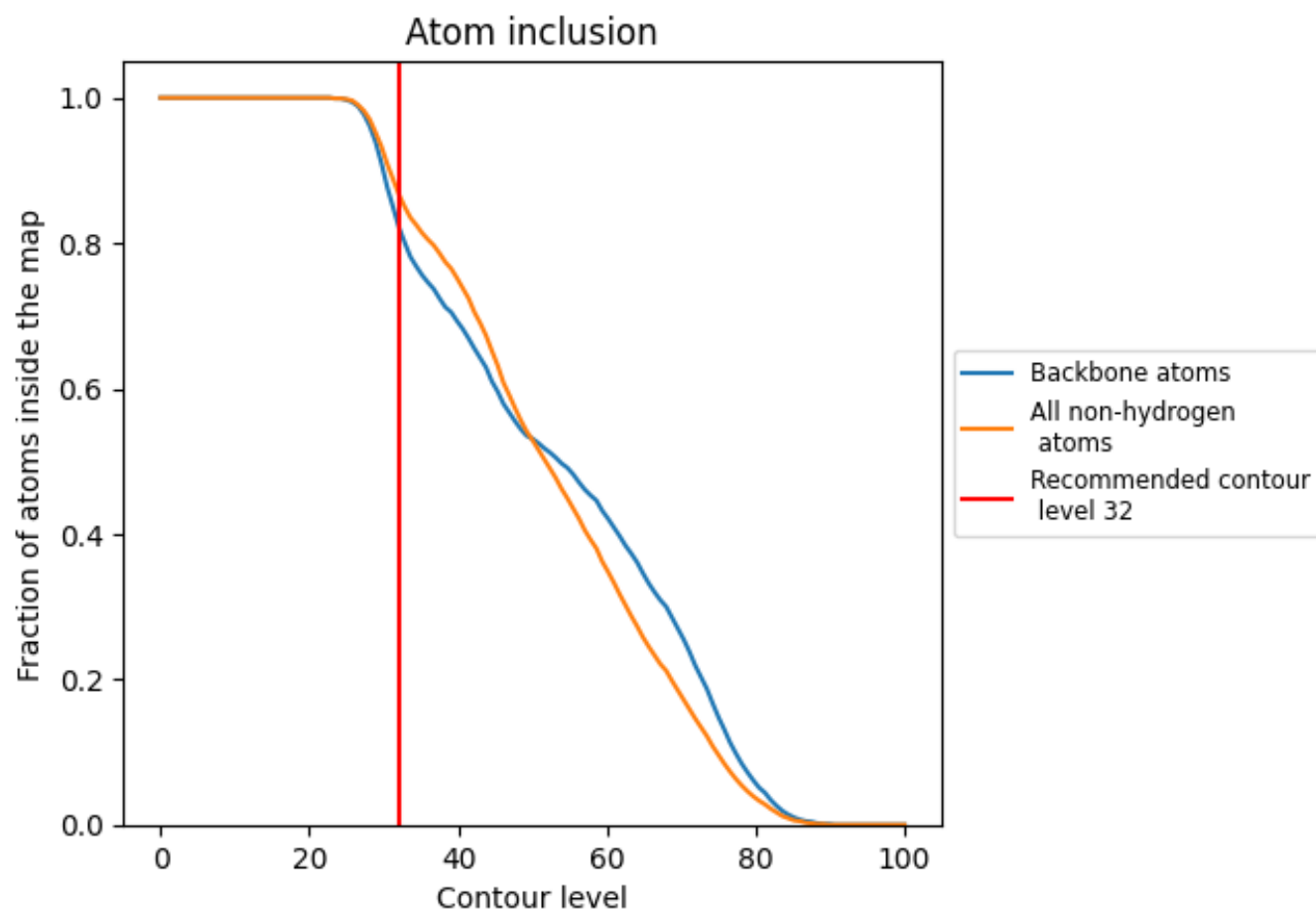
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (32).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 87% 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 (32) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8670	0.3330
1	0.9990	0.4710
2	0.9990	0.4590
3	0.9990	0.4590
4	1.0000	0.0610
7	0.5280	0.0940

