Full wwPDB EM Validation Report (i)

Apr 29, 2024 – 02:52 am BST

PDB ID	:	4BTQ
EMDB ID	:	EMD-1206
Title	:	Coordinates of the bacteriophage phi6 capsid subunits fitted into the cryoEM map EMD-1206
Authors	:	Nemecek, D.; Boura, E.; Wu, W.; Cheng, N.; Plevka, P.; Qiao, J.; Mindich, L.; Heymann, J.B.; Hurley, J.H.; Steven, A.C.
Deposited on	:	2013-06-18
Resolution	:	7.50 Å(reported)
Based on initial model	:	4K7H

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 (i) 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 (i)) were used in the production of this report:

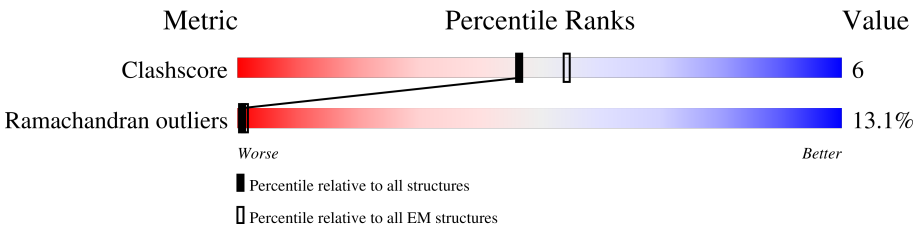
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 7.50 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

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 <=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	761	34% 73% 23% •
1	B	761	27% 66% 28% 5% •

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6086 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 INNER PROTEIN P1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	761	3043	1522	761	760	0	0
1	B	761	3043	1522	761	760	0	0

There are 2 discrepancies between the modelled and reference sequences:

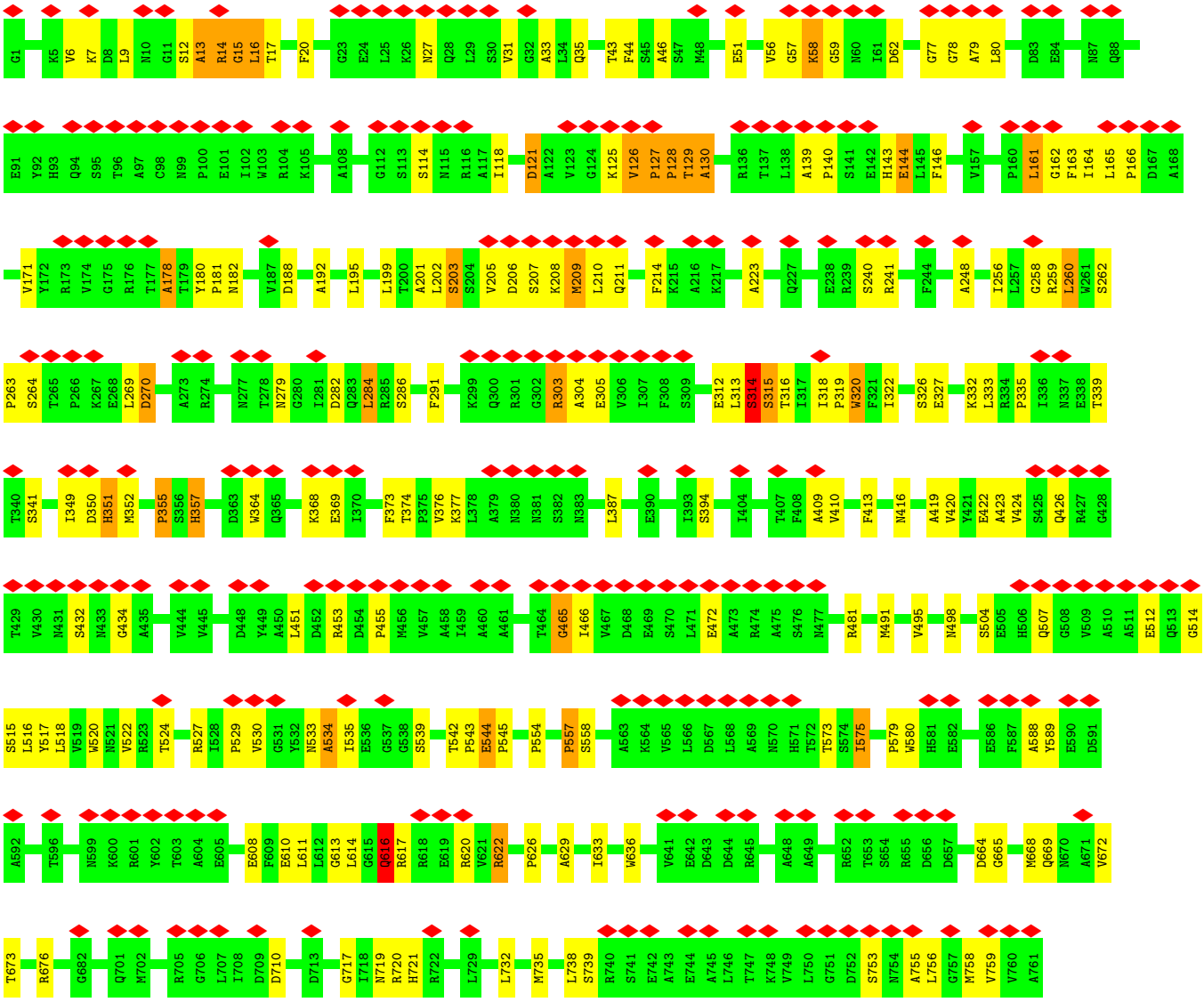
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P11126
B	1	GLY	-	expression tag	UNP P11126

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: MAJOR INNER PROTEIN P1

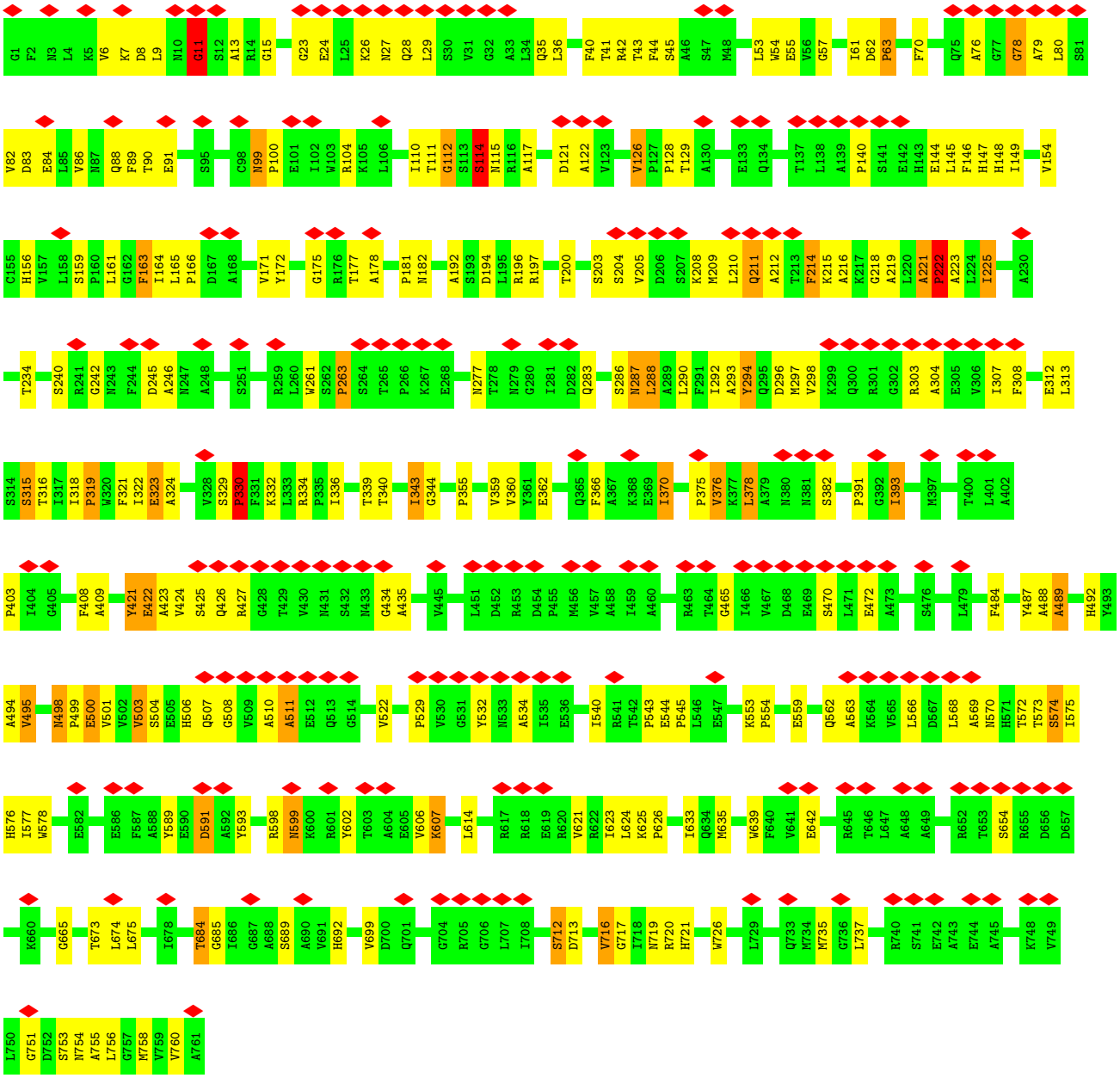
Chain A:



- Molecule 1: MAJOR INNER PROTEIN P1

Chain B:

27%
66%
28%
5%


G1 F2 N3 L4 K5 V6 K7 D8 L9 N10 G11 S12 A13 R14 G15 G23 E24 L25 K26 N27 Q28 L29 S30 V31 G32 A33 L34 Q35 L36 F40 T41 R42 T43 F44 S45 A46 S47 M48 L53 W54 E55 V56 G57 I61 D62 P63 F70 Q75 A76 G77 G78 A79 L80 S81
V82 D83 E84 L85 V86 N87 Q88 F89 T90 E91 S95 C98 N99 P100 E101 I102 W103 R104 K105 L106 I110 T111 G112 S113 S114 N115 R116 A117 D121 A122 V123 V126 P127 P128 T129 A130 E133 Q134 T137 L138 A139 P140 S141 E142 H143 E144 L145 F146 H147 H148 I149 V154
C155 H156 V157 L158 S159 P160 L161 G162 F163 I164 L165 P166 D167 A168 V171 Y172 G175 R176 T177 A178 P181 N182 A192 S193 D194 L195 R196 R197 T200 S203 S204 V205 D206 S207 K208 M209 L210 Q211 A212 T213 F214 K215 A216 K217 G218 A219 L220 A221 P222 A223 L224 I225 A230
T234 S240 R241 G242 N243 F244 D245 A246 N247 A248 S251 R259 L260 W261 S262 P263 S264 T265 P266 K267 E268 N277 T278 N279 G280 I281 D282 Q283 S286 N287 L288 A289 L290 F291 I292 A293 Y294 Q295 D296 M297 V298 K299 Q300 R301 G302 R303 A304 E305 V306 I307 F308 E312 L313
S314 S315 T316 I317 I318 P319 W320 F321 I322 E323 A324 V328 S329 P330 F331 K332 L333 R334 P335 I336 T339 T340 I343 G344 P355 V359 V360 Y361 E362 Q365 F366 A367 K368 E369 I370 P375 V376 K377 L378 A379 N380 N381 S382 P391 G392 I393 M397 T400 L401 A402
P403 I404 G405 F408 A409 Y421 E422 A423 V424 S425 Q426 R427 G428 T429 V430 M431 S432 M433 G434 A435 V445 L451 D452 R453 D454 P455 M456 V457 A458 I459 A460 R463 T464 G465 I466 V467 D468 E469 S470 L471 E472 A473 S476 L479 F484 Y487 A488 A489 H492 Y493
A494 V495 N498 P499 E500 V501 V502 V503 S504 E505 H506 Q507 G508 V509 A510 A511 E512 Q513 G514 V522 P529 V530 G531 Y532 N533 A534 I535 E536 I540 R541 T542 P543 E544 P545 L546 E547 K553 P554 E559 Q562 A563 K564 V565 L566 D567 L568 A569 N570 H571 T572 T573 S574 I575
H576 I577 W578 E582 E586 F587 A588 Y589 E590 D591 A592 Y593 R598 N599 K600 R601 Y602 T603 A604 E605 V606 K607 L614 R617 R618 E619 R620 V621 R622 I623 L624 K625 P626 I633 Q634 M635 W639 F640 V641 E642 R645 T646 L647 A648 A649 R652 T653 S654 R655 D656 D657
K660 G665 T673 L674 L675 I678 T684 G685 I686 G687 A688 S689 A690 V691 H692 V699 D700 Q701 G704 R705 G706 L707 I708 S712 D713 V716 G717 I718 N719 R720 H721 W726 L729 Q733 M734 M735 G736 L737 R740 S741 E742 A743 E744 A745 K748 V749
L750 G751 D752 S753 N754 A755 L756 G757 M758 V759 V760 A761

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	10463	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	4406.000	Depositor
Minimum map value	-2373.000	Depositor
Average map value	108.317	Depositor
Map value standard deviation	931.766	Depositor
Recommended contour level	1800.0	Depositor
Map size (Å)	589.4, 589.4, 589.4	wwPDB
Map dimensions	421, 421, 421	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	2.08	33/3042 (1.1%)	1.70	53/3801 (1.4%)
1	B	2.43	81/3041 (2.7%)	1.82	66/3798 (1.7%)
All	All	2.26	114/6083 (1.9%)	1.76	119/7599 (1.6%)

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	A	0	31
1	B	0	42
All	All	0	73

All (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	465	GLY	CA-C	-7.93	1.39	1.51
1	B	719	ASN	N-CA	-7.11	1.32	1.46
1	B	635	MET	CA-C	-7.09	1.34	1.52
1	B	100	PRO	CA-C	-6.92	1.39	1.52
1	B	288	LEU	CA-C	-6.74	1.35	1.52
1	B	685	GLY	CA-C	-6.73	1.41	1.51
1	A	721	HIS	CA-C	-6.66	1.35	1.52
1	A	319	PRO	CA-C	-6.57	1.39	1.52
1	B	104	ARG	CA-C	-6.53	1.35	1.52
1	A	721	HIS	N-CA	-6.44	1.33	1.46
1	B	484	PHE	CA-C	-6.36	1.36	1.52
1	B	112	GLY	CA-C	-6.33	1.41	1.51
1	A	315	SER	CA-C	-6.22	1.36	1.52
1	A	495	VAL	N-CA	-6.21	1.33	1.46
1	B	89	PHE	N-CA	-6.21	1.33	1.46
1	B	721	HIS	CA-C	-6.20	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	403	PRO	CA-C	-6.16	1.40	1.52
1	A	335	PRO	CA-C	-6.11	1.40	1.52
1	A	610	GLU	N-CA	-6.03	1.34	1.46
1	B	359	VAL	CA-C	-5.97	1.37	1.52
1	B	54	TRP	N-CA	-5.87	1.34	1.46
1	B	84	GLU	CA-C	-5.85	1.37	1.52
1	A	665	GLY	CA-C	-5.83	1.42	1.51
1	B	318	ILE	N-CA	-5.82	1.34	1.46
1	B	70	PHE	CA-C	-5.80	1.37	1.52
1	B	234	THR	CA-C	-5.74	1.38	1.52
1	B	492	HIS	CA-C	-5.73	1.38	1.52
1	B	623	ILE	N-CA	-5.73	1.34	1.46
1	B	720	ARG	CA-C	-5.69	1.38	1.52
1	A	514	GLY	CA-C	-5.68	1.42	1.51
1	A	633	ILE	N-CA	-5.67	1.34	1.46
1	A	720	ARG	CA-C	-5.67	1.38	1.52
1	B	192	ALA	CA-C	-5.64	1.38	1.52
1	A	332	LYS	CA-C	-5.63	1.38	1.52
1	B	726	TRP	N-CA	-5.61	1.35	1.46
1	A	554	PRO	CA-C	-5.57	1.41	1.52
1	A	355	PRO	CA-C	-5.56	1.41	1.52
1	A	260	LEU	CA-C	-5.55	1.38	1.52
1	B	261	TRP	CA-C	-5.55	1.38	1.52
1	B	297	MET	CA-C	-5.53	1.38	1.52
1	A	636	TRP	CA-C	-5.53	1.38	1.52
1	B	145	LEU	CA-C	-5.51	1.38	1.52
1	B	225	ILE	CA-C	-5.51	1.38	1.52
1	B	99	ASN	C-N	-5.50	1.23	1.34
1	B	675	LEU	N-CA	-5.47	1.35	1.46
1	B	642	GLU	CA-C	-5.47	1.38	1.52
1	A	376	VAL	CA-C	-5.45	1.38	1.52
1	B	495	VAL	N-CA	-5.41	1.35	1.46
1	B	498	ASN	C-N	-5.41	1.24	1.34
1	B	147	HIS	N-CA	-5.39	1.35	1.46
1	B	54	TRP	CA-C	-5.39	1.39	1.52
1	B	197	ARG	CA-C	-5.39	1.39	1.52
1	B	543	PRO	N-CA	-5.38	1.38	1.47
1	A	422	GLU	N-CA	-5.37	1.35	1.46
1	B	692	HIS	CA-C	-5.37	1.39	1.52
1	B	393	ILE	CA-C	-5.35	1.39	1.52
1	B	91	GLU	N-CA	-5.35	1.35	1.46
1	A	629	ALA	CA-C	-5.35	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	507	GLN	CA-C	-5.34	1.39	1.52
1	B	665	GLY	CA-C	-5.34	1.43	1.51
1	A	498	ASN	CA-C	-5.33	1.39	1.52
1	B	11	GLY	N-CA	-5.33	1.38	1.46
1	B	55	GLU	N-CA	-5.32	1.35	1.46
1	B	334	ARG	N-CA	-5.32	1.35	1.46
1	A	416	ASN	CA-C	-5.31	1.39	1.52
1	B	156	HIS	N-CA	-5.31	1.35	1.46
1	B	343	ILE	N-CA	-5.29	1.35	1.46
1	B	507	GLN	N-CA	-5.27	1.35	1.46
1	B	286	SER	N-CA	-5.27	1.35	1.46
1	A	719	ASN	N-CA	-5.26	1.35	1.46
1	B	313	LEU	N-CA	-5.26	1.35	1.46
1	B	495	VAL	CA-C	-5.26	1.39	1.52
1	A	312	GLU	N-CA	-5.25	1.35	1.46
1	B	126	VAL	CA-C	-5.23	1.39	1.52
1	B	319	PRO	N-CA	-5.23	1.38	1.47
1	B	88	GLN	CA-C	-5.23	1.39	1.52
1	B	194	ASP	CA-C	-5.23	1.39	1.52
1	B	633	ILE	CA-C	-5.22	1.39	1.52
1	B	298	VAL	N-CA	-5.22	1.35	1.46
1	B	674	LEU	CA-C	-5.21	1.39	1.52
1	A	333	LEU	CA-C	-5.21	1.39	1.52
1	B	23	GLY	CA-C	-5.20	1.43	1.51
1	B	689	SER	CA-C	-5.20	1.39	1.52
1	A	495	VAL	CA-C	-5.19	1.39	1.52
1	B	673	THR	N-CA	-5.19	1.35	1.46
1	A	248	ALA	N-CA	-5.19	1.35	1.46
1	B	545	PRO	CA-C	-5.18	1.42	1.52
1	B	318	ILE	C-N	-5.17	1.24	1.34
1	B	292	ILE	N-CA	-5.17	1.36	1.46
1	B	43	THR	N-CA	-5.16	1.36	1.46
1	A	44	PHE	N-CA	-5.16	1.36	1.46
1	A	491	MET	CA-C	-5.16	1.39	1.52
1	B	318	ILE	CA-C	-5.15	1.39	1.52
1	B	263	PRO	CA-C	-5.13	1.42	1.52
1	B	53	LEU	CA-C	-5.13	1.39	1.52
1	B	699	VAL	N-CA	-5.12	1.36	1.46
1	A	332	LYS	N-CA	-5.11	1.36	1.46
1	B	283	GLN	CA-C	-5.11	1.39	1.52
1	B	83	ASP	N-CA	-5.11	1.36	1.46
1	B	42	ARG	CA-C	-5.10	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	481	ARG	CA-C	-5.10	1.39	1.52
1	B	154	VAL	CA-C	-5.10	1.39	1.52
1	A	320	TRP	CA-C	-5.09	1.39	1.52
1	B	488	ALA	N-CA	-5.09	1.36	1.46
1	B	221	ALA	C-N	-5.09	1.24	1.34
1	A	20	PHE	CA-C	-5.08	1.39	1.52
1	B	360	VAL	N-CA	-5.08	1.36	1.46
1	B	735	MET	N-CA	-5.08	1.36	1.46
1	B	148	HIS	N-CA	-5.06	1.36	1.46
1	B	315	SER	N-CA	-5.05	1.36	1.46
1	B	330	PRO	CA-C	-5.05	1.42	1.52
1	B	639	TRP	CA-C	-5.04	1.39	1.52
1	B	208	LYS	N-CA	-5.03	1.36	1.46
1	B	296	ASP	N-CA	-5.02	1.36	1.46

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	287	ASN	CA-C-O	-10.94	97.14	120.10
1	B	313	LEU	N-CA-C	-10.60	82.37	111.00
1	A	15	GLY	N-CA-C	-9.85	88.48	113.10
1	A	78	GLY	N-CA-C	-9.42	89.54	113.10
1	A	426	GLN	N-CA-C	-9.32	85.83	111.00
1	A	544	GLU	CA-C-N	-8.92	92.12	117.10
1	B	735	MET	N-CA-C	-8.82	87.20	111.00
1	A	616	GLN	N-CA-C	-8.67	87.60	111.00
1	B	408	PHE	N-CA-C	8.63	134.30	111.00
1	A	264	SER	N-CA-C	-8.50	88.06	111.00
1	B	500	GLU	N-CA-C	-7.90	89.66	111.00
1	B	489	ALA	CA-C-N	-7.57	100.55	117.20
1	A	613	GLY	N-CA-C	-7.47	94.42	113.10
1	B	294	TYR	CA-C-N	-7.44	100.83	117.20
1	B	163	PHE	C-N-CA	7.41	140.22	121.70
1	B	78	GLY	N-CA-C	-7.40	94.61	113.10
1	B	211	GLN	N-CA-C	-7.17	91.66	111.00
1	B	172	TYR	N-CA-C	-7.06	91.93	111.00
1	A	351	HIS	C-N-CA	6.94	139.06	121.70
1	A	171	VAL	N-CA-C	-6.85	92.49	111.00
1	A	129	THR	N-CA-C	-6.72	92.85	111.00
1	B	23	GLY	N-CA-C	-6.69	96.38	113.10
1	B	13	ALA	N-CA-C	-6.48	93.50	111.00
1	A	143	HIS	N-CA-C	-6.47	93.53	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	329	SER	N-CA-C	-6.47	93.53	111.00
1	A	58	LYS	C-N-CA	6.43	135.81	122.30
1	B	82	VAL	C-N-CA	6.42	137.74	121.70
1	A	62	ASP	N-CA-C	-6.35	93.86	111.00
1	B	111	THR	N-CA-C	-6.34	93.88	111.00
1	A	545	PRO	N-CA-C	6.32	128.54	112.10
1	B	507	GLN	C-N-CA	6.31	135.55	122.30
1	B	112	GLY	N-CA-C	-6.27	97.43	113.10
1	A	739	SER	N-CA-C	-6.24	94.16	111.00
1	A	43	THR	N-CA-C	-6.22	94.21	111.00
1	A	180	TYR	N-CA-C	-6.21	94.23	111.00
1	B	522	VAL	N-CA-C	-6.21	94.23	111.00
1	B	336	ILE	C-N-CA	6.21	137.22	121.70
1	B	221	ALA	CA-C-N	6.19	134.42	117.10
1	A	31	VAL	N-CA-C	-6.16	94.36	111.00
1	B	315	SER	N-CA-C	-6.16	94.38	111.00
1	A	377	LYS	N-CA-C	-6.15	94.39	111.00
1	A	350	ASP	C-N-CA	6.12	136.99	121.70
1	A	394	SER	C-N-CA	6.10	136.95	121.70
1	B	146	PHE	CA-C-N	-6.04	103.92	117.20
1	B	510	ALA	C-N-CA	6.02	136.75	121.70
1	B	344	GLY	N-CA-C	-5.97	98.18	113.10
1	B	755	ALA	C-N-CA	5.96	136.60	121.70
1	B	222	PRO	N-CA-C	5.94	127.55	112.10
1	A	423	ALA	N-CA-C	-5.92	95.02	111.00
1	A	518	LEU	CA-C-N	-5.91	104.19	117.20
1	B	574	SER	C-N-CA	5.91	136.47	121.70
1	A	753	SER	C-N-CA	5.88	136.41	121.70
1	A	16	LEU	C-N-CA	5.86	136.36	121.70
1	A	77	GLY	C-N-CA	5.85	134.59	122.30
1	B	121	ASP	N-CA-C	-5.83	95.26	111.00
1	A	80	LEU	N-CA-C	-5.82	95.29	111.00
1	B	63	PRO	CA-C-N	-5.81	104.42	117.20
1	B	422	GLU	N-CA-C	-5.80	95.34	111.00
1	A	201	ALA	N-CA-C	5.76	126.56	111.00
1	B	607	LYS	N-CA-C	-5.75	95.46	111.00
1	A	303	ARG	N-CA-C	-5.72	95.56	111.00
1	B	716	VAL	N-CA-C	-5.63	95.79	111.00
1	B	506	HIS	N-CA-C	-5.57	95.96	111.00
1	A	534	ALA	N-CA-C	-5.57	95.97	111.00
1	B	11	GLY	N-CA-C	-5.56	99.20	113.10
1	B	712	SER	C-N-CA	5.56	135.59	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	314	SER	CA-C-N	-5.55	104.99	117.20
1	B	114	SER	N-CA-C	5.55	125.97	111.00
1	B	624	LEU	C-N-CA	5.54	135.55	121.70
1	A	56	VAL	C-N-CA	5.53	133.92	122.30
1	B	78	GLY	C-N-CA	5.53	135.52	121.70
1	B	322	ILE	C-N-CA	5.52	135.49	121.70
1	B	319	PRO	N-CA-C	-5.51	97.78	112.10
1	B	753	SER	C-N-CA	5.49	135.42	121.70
1	A	209	MET	C-N-CA	5.48	135.39	121.70
1	A	270	ASP	CA-C-N	5.48	132.43	117.10
1	B	332	LYS	N-CA-C	-5.46	96.26	111.00
1	A	305	GLU	C-N-CA	5.46	135.34	121.70
1	B	534	ALA	C-N-CA	5.43	135.27	121.70
1	B	115	ASN	N-CA-C	5.42	125.63	111.00
1	B	322	ILE	N-CA-C	-5.42	96.37	111.00
1	B	287	ASN	N-CA-C	-5.38	96.47	111.00
1	B	421	TYR	CA-C-N	-5.36	105.41	117.20
1	A	357	HIS	N-CA-C	-5.34	96.57	111.00
1	B	370	ILE	CA-C-N	-5.34	105.46	117.20
1	B	569	ALA	N-CA-C	-5.33	96.61	111.00
1	A	202	LEU	CA-C-N	-5.33	105.48	117.20
1	A	376	VAL	N-CA-C	-5.28	96.75	111.00
1	B	44	PHE	N-CA-C	-5.24	96.85	111.00
1	B	684	THR	N-CA-C	-5.23	96.87	111.00
1	B	504	SER	N-CA-C	-5.22	96.89	111.00
1	A	498	ASN	N-CA-C	-5.22	96.91	111.00
1	A	203	SER	N-CA-C	-5.22	96.92	111.00
1	A	575	ILE	N-CA-C	-5.21	96.92	111.00
1	A	211	GLN	N-CA-C	-5.19	96.98	111.00
1	A	376	VAL	CA-C-N	-5.19	105.79	117.20
1	A	534	ALA	C-N-CA	5.18	134.64	121.70
1	B	376	VAL	N-CA-C	-5.17	97.04	111.00
1	A	127	PRO	CA-C-N	5.17	131.57	117.10
1	A	258	GLY	C-N-CA	5.16	134.61	121.70
1	A	14	ARG	C-N-CA	5.16	133.14	122.30
1	B	606	VAL	N-CA-C	-5.16	97.06	111.00
1	B	511	ALA	N-CA-C	-5.16	97.08	111.00
1	B	122	ALA	N-CA-C	-5.15	97.09	111.00
1	B	378	LEU	N-CA-C	-5.15	97.11	111.00
1	B	553	LYS	N-CA-C	-5.14	97.13	111.00
1	A	128	PRO	N-CA-C	-5.13	98.76	112.10
1	B	177	THR	C-N-CA	5.12	134.49	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	737	LEU	N-CA-C	-5.12	97.19	111.00
1	A	374	THR	N-CA-C	-5.08	97.27	111.00
1	B	434	GLY	N-CA-C	-5.08	100.40	113.10
1	A	422	GLU	CA-C-N	-5.07	106.04	117.20
1	A	208	LYS	C-N-CA	5.05	134.33	121.70
1	A	78	GLY	C-N-CA	5.03	134.27	121.70
1	B	487	TYR	CA-C-N	-5.02	106.15	117.20
1	B	149	ILE	CA-C-N	-5.02	106.15	117.20
1	B	175	GLY	N-CA-C	-5.02	100.55	113.10
1	A	260	LEU	N-CA-C	-5.01	97.48	111.00
1	B	42	ARG	N-CA-C	-5.00	97.50	111.00

There are no chirality outliers.

All (73) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	THR	Peptide
1	A	130	ALA	Mainchain
1	A	161	LEU	Peptide
1	A	162	GLY	Peptide
1	A	178	ALA	Peptide
1	A	182	ASN	Peptide,Mainchain
1	A	203	SER	Mainchain
1	A	284	LEU	Mainchain
1	A	291	PHE	Mainchain
1	A	314	SER	Peptide,Mainchain
1	A	339	THR	Mainchain
1	A	35	GLN	Peptide,Mainchain
1	A	357	HIS	Peptide,Mainchain
1	A	387	LEU	Mainchain
1	A	419	ALA	Mainchain
1	A	455	PRO	Peptide,Mainchain
1	A	516	LEU	Mainchain
1	A	520	TRP	Mainchain
1	A	544	GLU	Peptide,Mainchain
1	A	557	PRO	Mainchain
1	A	616	GLN	Mainchain
1	A	622	ARG	Mainchain
1	A	717	GLY	Peptide,Mainchain
1	A	758	MET	Peptide
1	B	110	ILE	Peptide,Mainchain
1	B	114	SER	Peptide,Mainchain

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Mol	Chain	Res	Type	Group
1	B	159	SER	Peptide
1	B	182	ASN	Mainchain
1	B	203	SER	Peptide
1	B	222	PRO	Peptide
1	B	240	SER	Mainchain
1	B	242	GLY	Peptide
1	B	277	ASN	Peptide,Mainchain
1	B	294	TYR	Peptide,Mainchain
1	B	330	PRO	Mainchain
1	B	340	THR	Peptide,Mainchain
1	B	343	ILE	Peptide
1	B	362	GLU	Mainchain
1	B	370	ILE	Peptide,Mainchain
1	B	393	ILE	Mainchain
1	B	40	PHE	Mainchain
1	B	421	TYR	Peptide
1	B	425	SER	Mainchain
1	B	489	ALA	Peptide,Mainchain
1	B	500	GLU	Mainchain
1	B	503	VAL	Mainchain
1	B	532	TYR	Peptide,Mainchain
1	B	544	GLU	Peptide,Mainchain
1	B	591	ASP	Mainchain
1	B	599	ASN	Mainchain
1	B	602	TYR	Peptide,Mainchain
1	B	63	PRO	Peptide,Mainchain
1	B	716	VAL	Peptide
1	B	717	GLY	Peptide,Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3043	0	820	25	0
1	B	3043	0	817	25	0
All	All	6086	0	1637	50	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 6.

All (50) 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:A:14:ARG:H	1:A:465:GLY:HA3	1.67	0.59
1:B:222:PRO:CA	1:B:225:ILE:H	2.17	0.58
1:A:504:SER:H	1:A:517:TYR:H	1.52	0.57
1:B:171:VAL:N	1:B:576:HIS:H	2.03	0.56
1:A:118:ILE:N	1:A:121:ASP:H	2.05	0.55
1:B:209:MET:H	1:B:214:PHE:N	2.06	0.53
1:B:495:VAL:C	1:B:498:ASN:H	2.15	0.50
1:A:451:LEU:C	1:A:453:ARG:H	2.14	0.50
1:A:144:GLU:C	1:A:146:PHE:H	2.14	0.49
1:B:36:LEU:N	1:B:503:VAL:H	2.10	0.49
1:B:76:ALA:C	1:B:78:GLY:H	2.15	0.49
1:A:318:ILE:C	1:A:320:TRP:H	2.15	0.49
1:B:9:LEU:C	1:B:11:GLY:H	2.14	0.48
1:A:9:LEU:C	1:A:12:SER:H	2.17	0.48
1:A:672:VAL:O	1:A:676:ARG:N	2.46	0.48
1:B:161:LEU:C	1:B:163:PHE:H	2.17	0.47
1:B:290:LEU:C	1:B:293:ALA:H	2.19	0.46
1:B:6:VAL:H	1:B:435:ALA:H	1.64	0.46
1:A:313:LEU:O	1:A:315:SER:N	2.49	0.45
1:A:410:VAL:C	1:A:413:PHE:H	2.20	0.45
1:B:15:GLY:H	1:B:465:GLY:HA3	1.82	0.45
1:B:45:SER:O	1:B:330:PRO:O	2.35	0.45
1:B:321:PHE:C	1:B:323:GLU:N	2.69	0.44
1:B:221:ALA:O	1:B:223:ALA:N	2.51	0.44
1:A:573:THR:C	1:A:575:ILE:H	2.17	0.44
1:B:86:VAL:O	1:B:90:THR:N	2.51	0.44
1:B:219:ALA:O	1:B:221:ALA:O	2.36	0.43
1:B:36:LEU:H	1:B:503:VAL:H	1.66	0.43
1:B:312:GLU:O	1:B:316:THR:N	2.51	0.43
1:A:14:ARG:H	1:A:465:GLY:CA	2.31	0.43
1:B:126:VAL:C	1:B:165:LEU:H	2.22	0.43
1:A:188:ASP:O	1:A:192:ALA:N	2.52	0.42
1:A:732:LEU:C	1:A:735:MET:H	2.23	0.42
1:B:494:ALA:O	1:B:498:ASN:N	2.53	0.42
1:A:6:VAL:O	1:A:434:GLY:HA2	2.20	0.42
1:A:673:THR:C	1:A:676:ARG:H	2.23	0.41
1:A:13:ALA:C	1:A:15:GLY:H	2.24	0.41
1:A:504:SER:O	1:A:517:TYR:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:GLU:C	1:A:611:LEU:H	2.24	0.41
1:A:373:PHE:O	1:A:622:ARG:O	2.39	0.41
1:A:195:LEU:O	1:A:199:LEU:N	2.53	0.41
1:A:256:ILE:O	1:A:259:ARG:O	2.39	0.41
1:B:287:ASN:C	1:B:288:LEU:N	2.74	0.41
1:B:570:ASN:C	1:B:572:THR:H	2.23	0.41
1:A:126:VAL:CA	1:A:163:PHE:H	2.35	0.40
1:A:504:SER:N	1:A:517:TYR:H	2.17	0.40
1:B:196:ARG:O	1:B:200:THR:N	2.55	0.40
1:B:211:GLN:C	1:B:215:LYS:O	2.60	0.40
1:A:14:ARG:N	1:A:465:GLY:CA	2.84	0.40
1:B:495:VAL:O	1:B:498:ASN:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	759/761 (100%)	561 (74%)	98 (13%)	100 (13%)	0 4
1	B	757/761 (100%)	559 (74%)	100 (13%)	98 (13%)	0 5
All	All	1516/1522 (100%)	1120 (74%)	198 (13%)	198 (13%)	1 4

All (198) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	ALA
1	A	16	LEU
1	A	17	THR
1	A	46	ALA
1	A	51	GLU
1	A	57	GLY

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Mol	Chain	Res	Type
1	A	58	LYS
1	A	126	VAL
1	A	127	PRO
1	A	140	PRO
1	A	144	GLU
1	A	164	ILE
1	A	165	LEU
1	A	166	PRO
1	A	178	ALA
1	A	205	VAL
1	A	209	MET
1	A	210	LEU
1	A	240	SER
1	A	270	ASP
1	A	279	ASN
1	A	314	SER
1	A	326	SER
1	A	327	GLU
1	A	341	SER
1	A	349	ILE
1	A	351	HIS
1	A	368	LYS
1	A	369	GLU
1	A	424	VAL
1	A	432	SER
1	A	472	GLU
1	A	512	GLU
1	A	527	ARG
1	A	530	VAL
1	A	579	PRO
1	A	580	TRP
1	A	588	ALA
1	A	589	TYR
1	A	614	LEU
1	A	617	ARG
1	A	620	ARG
1	A	668	MET
1	A	738	LEU
1	A	755	ALA
1	A	759	VAL
1	B	8	ASP
1	B	24	GLU

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Mol	Chain	Res	Type
1	B	26	LYS
1	B	28	GLN
1	B	79	ALA
1	B	99	ASN
1	B	117	ALA
1	B	164	ILE
1	B	166	PRO
1	B	178	ALA
1	B	181	PRO
1	B	204	SER
1	B	205	VAL
1	B	222	PRO
1	B	246	ALA
1	B	263	PRO
1	B	303	ARG
1	B	304	ALA
1	B	378	LEU
1	B	382	SER
1	B	391	PRO
1	B	409	ALA
1	B	422	GLU
1	B	424	VAL
1	B	470	SER
1	B	508	GLY
1	B	554	PRO
1	B	563	ALA
1	B	566	LEU
1	B	575	ILE
1	B	577	ILE
1	B	578	TRP
1	B	589	TYR
1	B	591	ASP
1	B	599	ASN
1	B	625	LYS
1	B	626	PRO
1	B	713	ASP
1	B	754	ASN
1	B	756	LEU
1	B	758	MET
1	B	760	VAL
1	A	27	ASN
1	A	59	GLY

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Mol	Chain	Res	Type
1	A	79	ALA
1	A	130	ALA
1	A	206	ASP
1	A	207	SER
1	A	214	PHE
1	A	241	ARG
1	A	260	LEU
1	A	262	SER
1	A	304	ALA
1	A	322	ILE
1	A	409	ALA
1	A	420	VAL
1	A	466	ILE
1	A	515	SER
1	A	524	THR
1	A	535	ILE
1	A	539	SER
1	A	664	ASP
1	A	669	GLN
1	B	7	LYS
1	B	11	GLY
1	B	35	GLN
1	B	61	ILE
1	B	80	LEU
1	B	129	THR
1	B	210	LEU
1	B	323	GLU
1	B	366	PHE
1	B	423	ALA
1	B	426	GLN
1	B	511	ALA
1	B	540	ILE
1	B	568	LEU
1	B	593	TYR
1	B	654	SER
1	B	684	THR
1	B	712	SER
1	A	33	ALA
1	A	114	SER
1	A	161	LEU
1	A	223	ALA
1	A	269	LEU

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Mol	Chain	Res	Type
1	A	282	ASP
1	A	284	LEU
1	A	286	SER
1	A	303	ARG
1	A	352	MET
1	A	355	PRO
1	A	507	GLN
1	A	533	ASN
1	A	534	ALA
1	A	542	THR
1	A	557	PRO
1	A	626	PRO
1	A	710	ASP
1	A	756	LEU
1	B	27	ASN
1	B	41	THR
1	B	144	GLU
1	B	216	ALA
1	B	218	GLY
1	B	308	PHE
1	B	315	SER
1	B	324	ALA
1	B	559	GLU
1	B	562	GLN
1	B	573	THR
1	B	751	GLY
1	A	121	ASP
1	A	125	LYS
1	A	181	PRO
1	A	316	THR
1	A	558	SER
1	A	616	GLN
1	B	214	PHE
1	B	245	ASP
1	B	375	PRO
1	B	499	PRO
1	B	574	SER
1	A	7	LYS
1	A	364	TRP
1	A	522	VAL
1	B	29	LEU
1	B	128	PRO

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Mol	Chain	Res	Type
1	B	140	PRO
1	B	212	ALA
1	B	307	ILE
1	B	339	THR
1	B	376	VAL
1	B	427	ARG
1	B	472	GLU
1	B	529	PRO
1	B	598	ARG
1	B	607	LYS
1	B	614	LEU
1	A	543	PRO
1	B	114	SER
1	B	319	PRO
1	B	621	VAL
1	A	139	ALA
1	B	62	ASP
1	B	57	GLY
1	A	529	PRO
1	B	355	PRO
1	B	501	VAL
1	B	112	GLY
1	A	128	PRO
1	A	263	PRO

5.3.2 Protein sidechains (i)

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	287:ASN	C	288:LEU	N	2.74

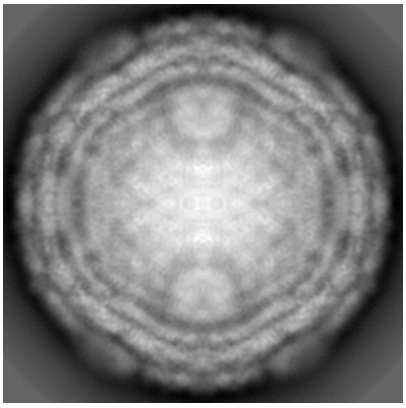
6 Map visualisation (i)

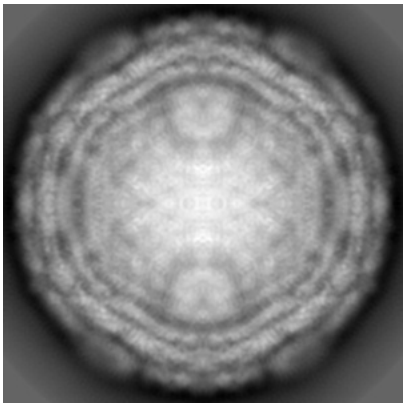
This section contains visualisations of the EMDB entry EMD-1206. These allow visual inspection of the internal detail of the map and identification of artifacts.

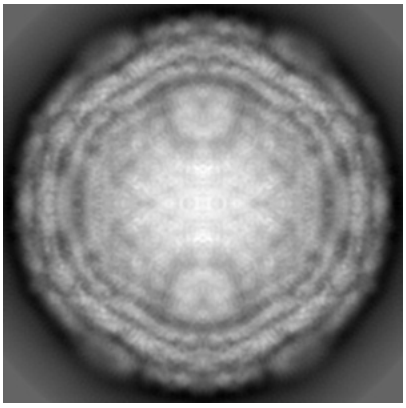
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

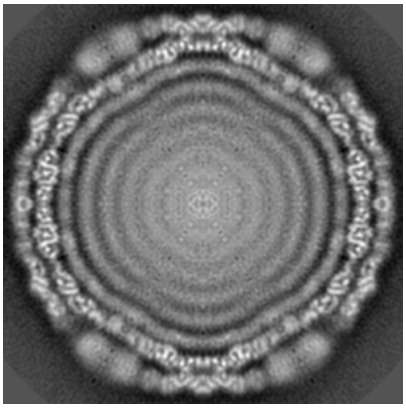

Y

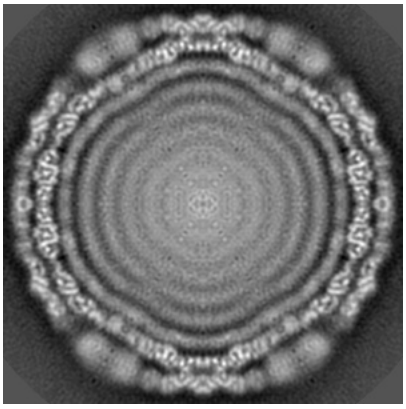

Z

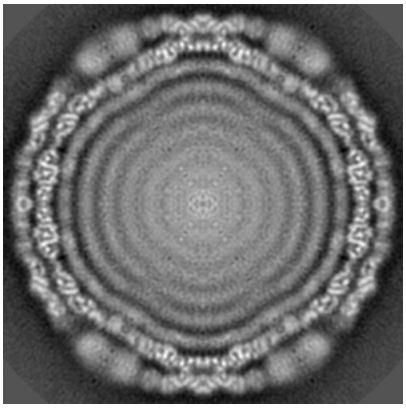
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 210

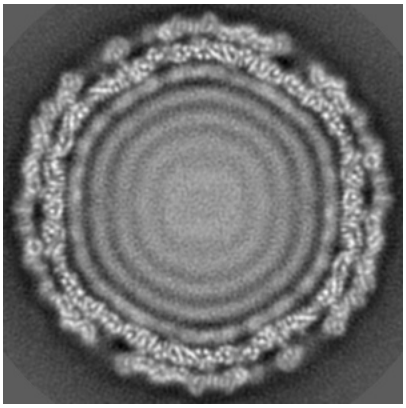

Y Index: 210

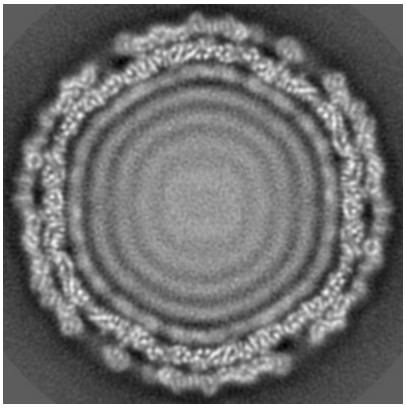

Z Index: 210

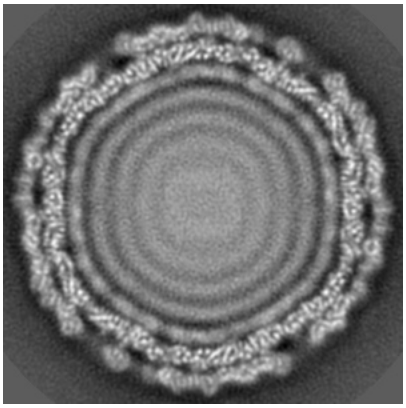
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 165

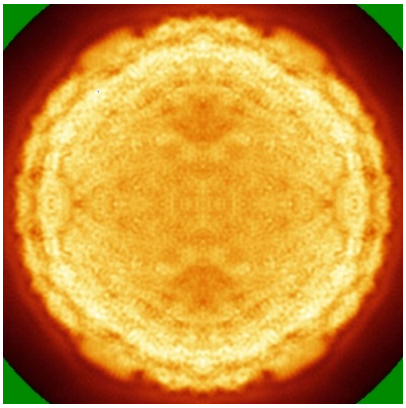

Y Index: 255

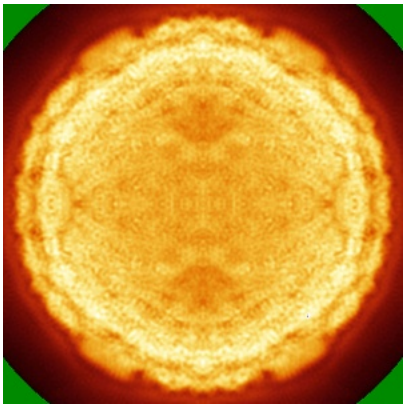

Z Index: 255

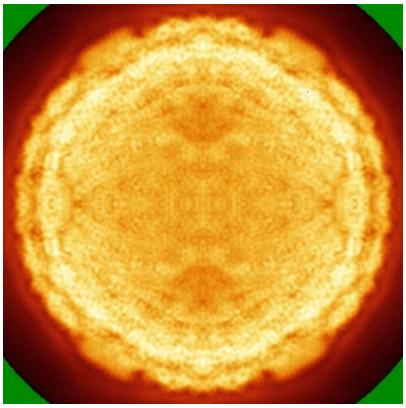
The images above show the largest variance slices of the map in three orthogonal directions.

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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1800.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

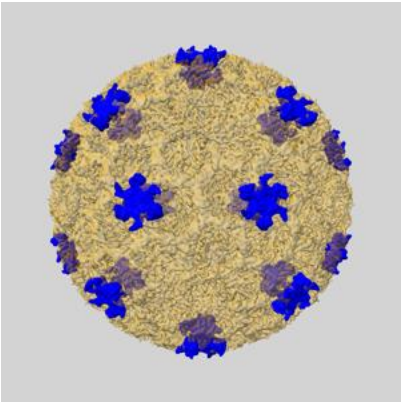
6.6 Mask visualisation (i)

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

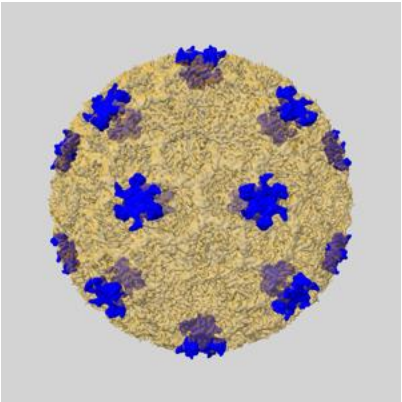
A mask typically either:

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

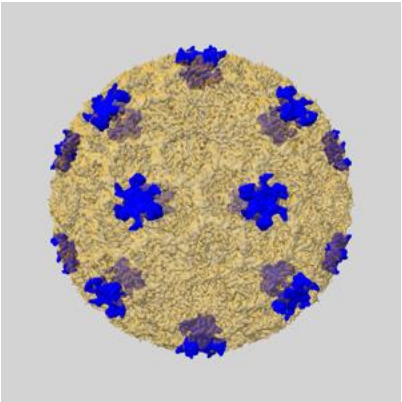
6.6.1 emd_1206_msk_6.map (i)



X

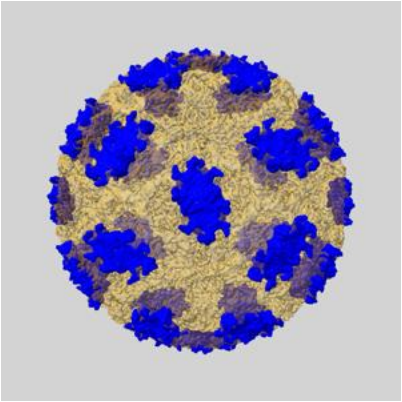


Y

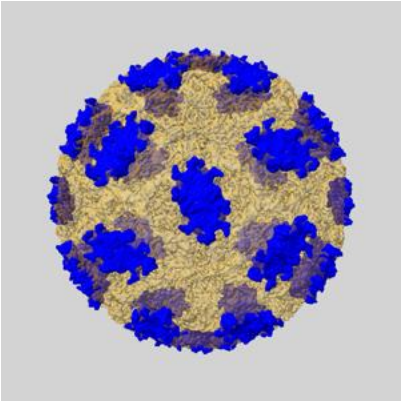


Z

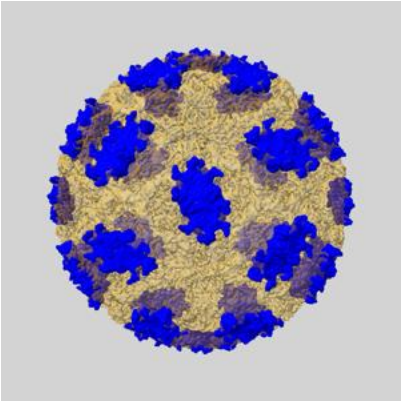
6.6.2 emd_1206_msk_5.map (i)



X

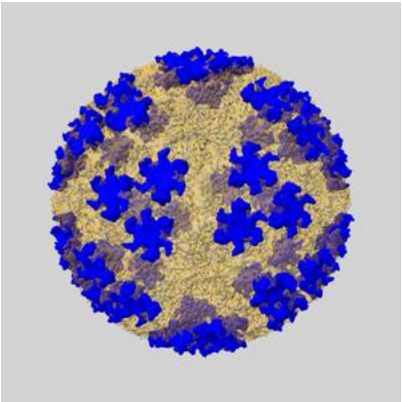


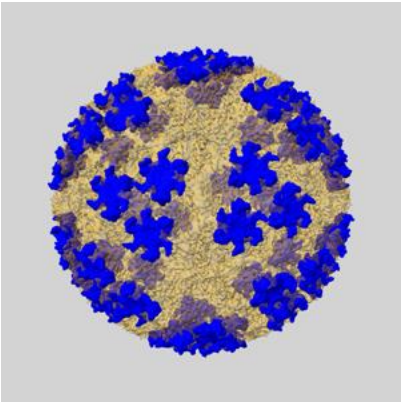
Y

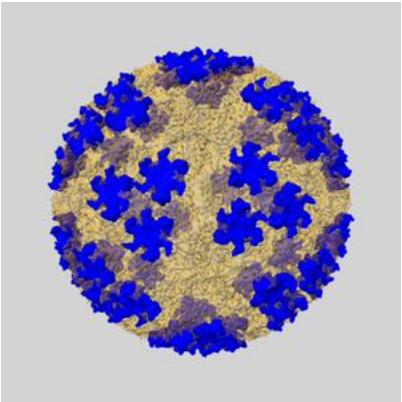


Z

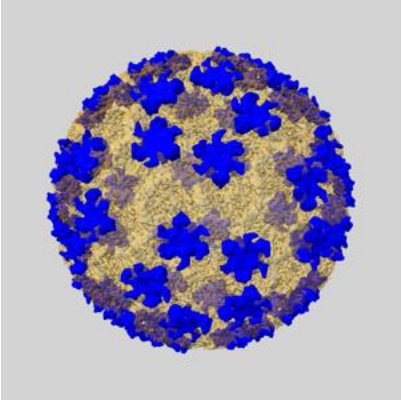
6.6.3 emd_1206_msk_4.map (i)

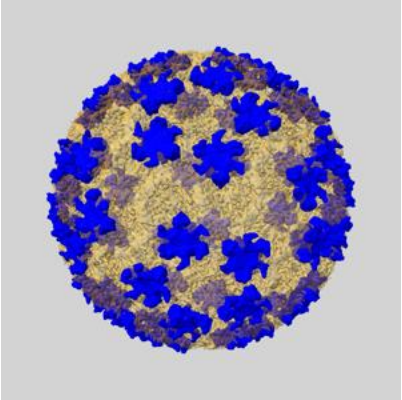

X

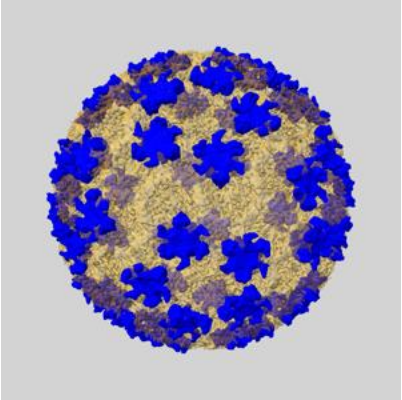

Y


Z

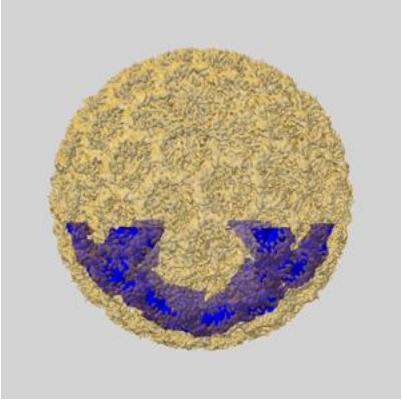
6.6.4 emd_1206_msk_3.map (i)

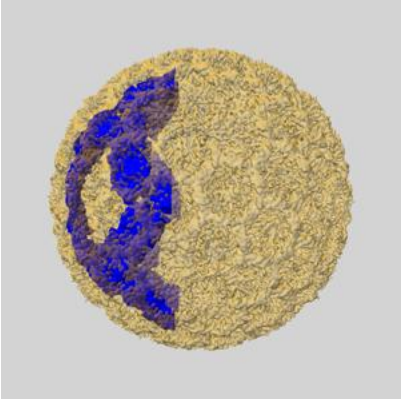

X

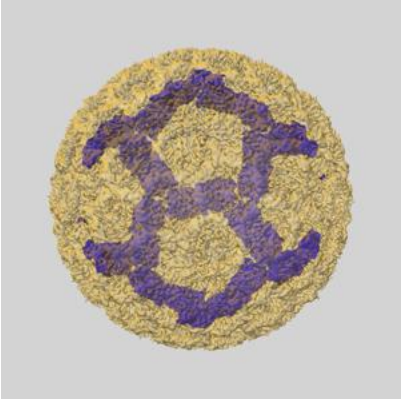

Y


Z

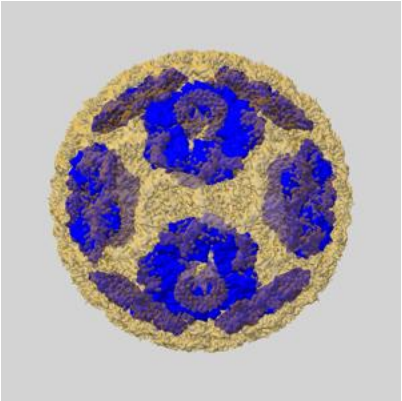
6.6.5 emd_1206_msk_2.map (i)


X

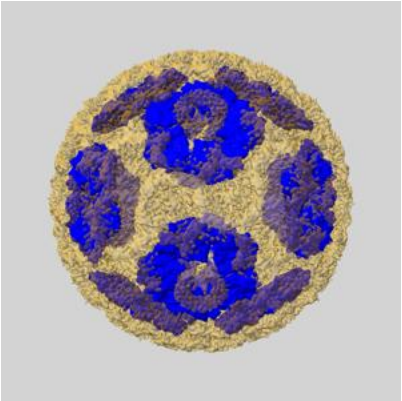

Y


Z

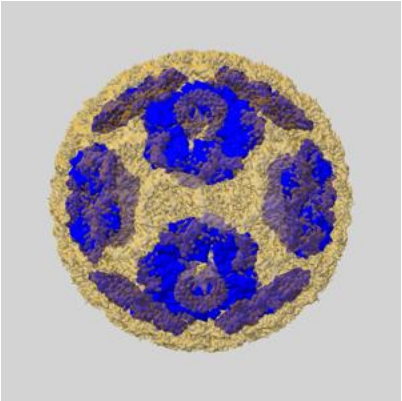
6.6.6 emd_1206_msk_1.map (i)



X

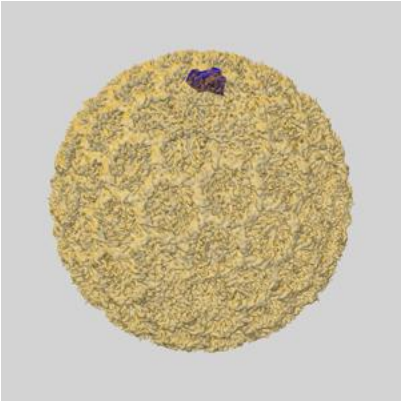


Y

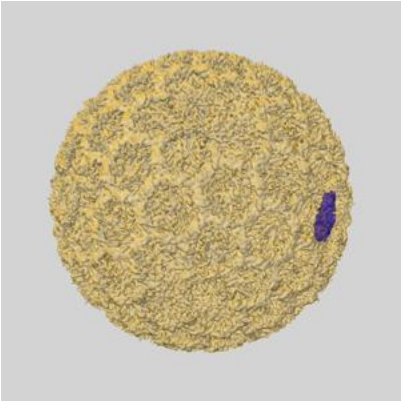


Z

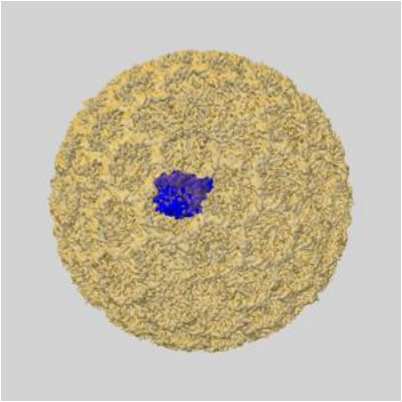
6.6.7 emd_1206_msk_7.map (i)



X



Y

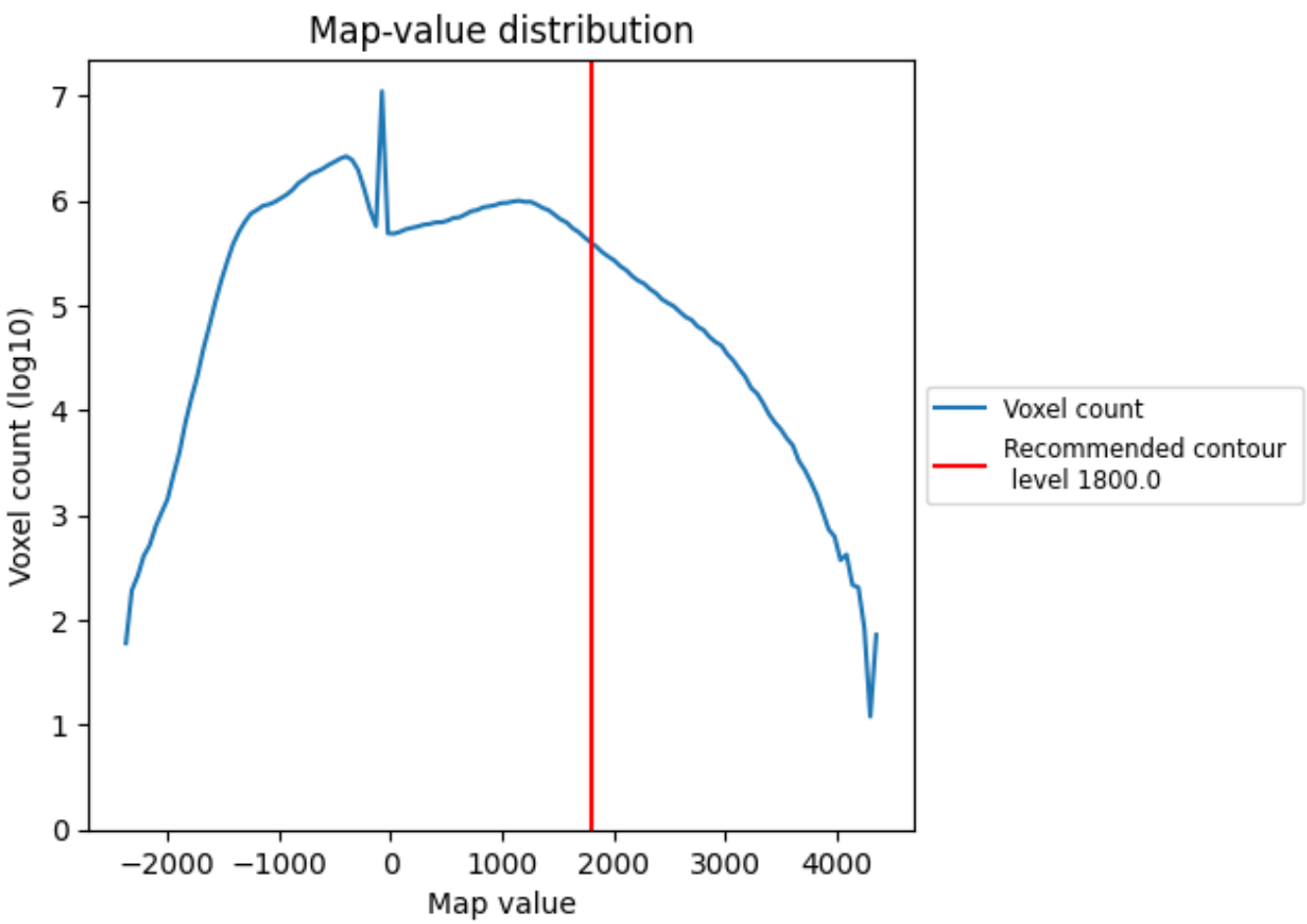


Z

7 Map analysis (i)

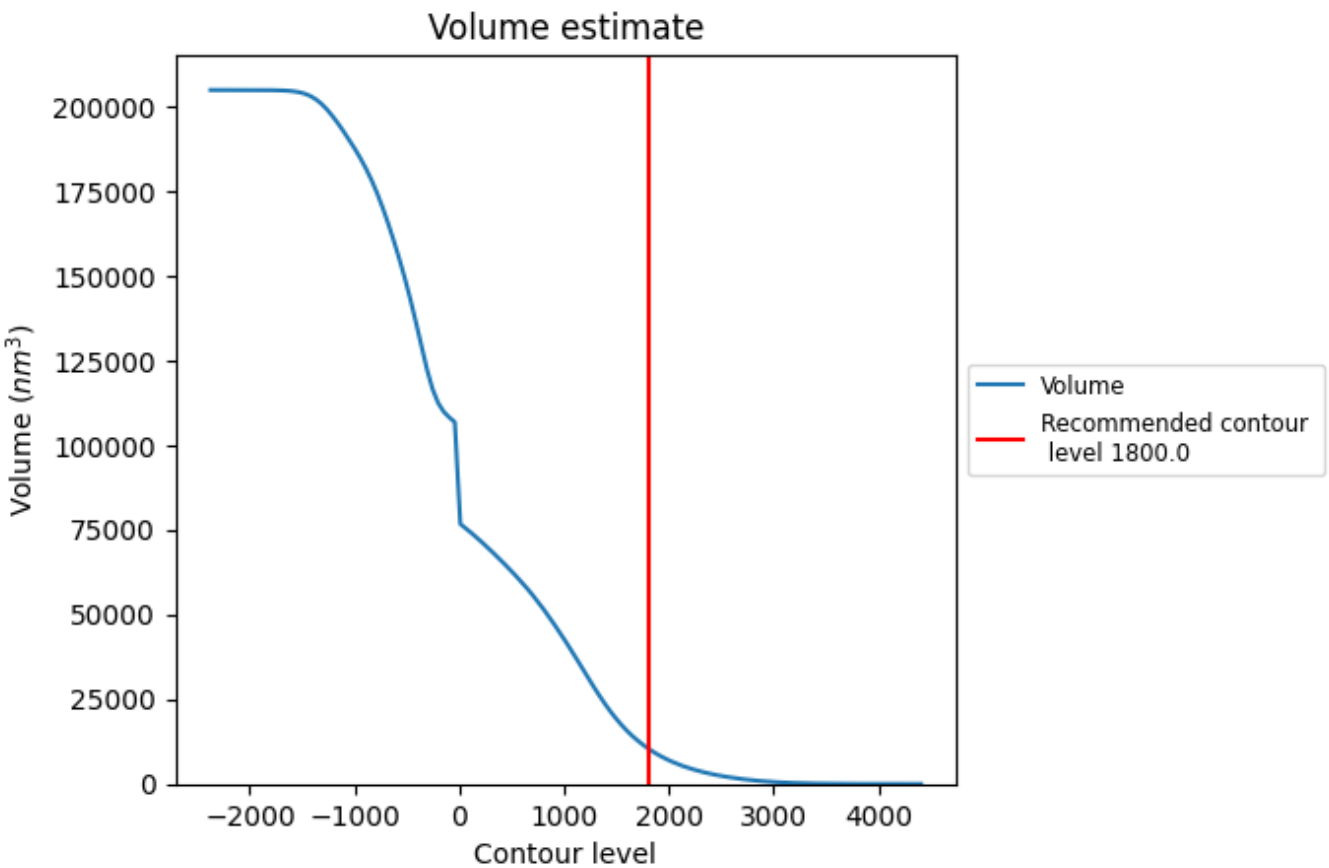
This section contains the results of statistical analysis of the map.

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.

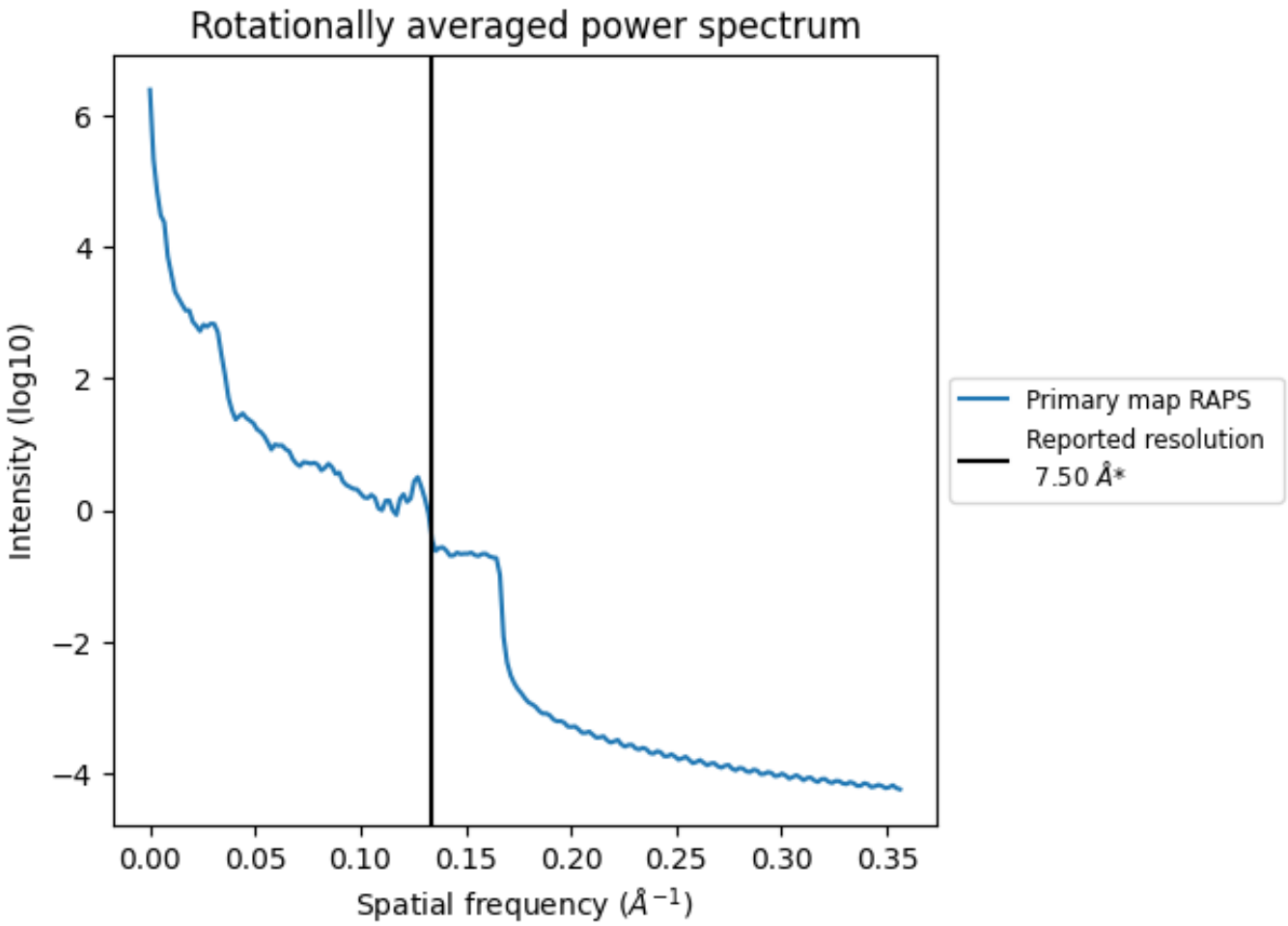
7.2 Volume estimate (i)



The volume at the recommended contour level is 10518 nm^3; this corresponds to an approximate mass of 9501 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 (i)



*Reported resolution corresponds to spatial frequency of 0.133 Å^{-1}

8 Fourier-Shell correlation (i)

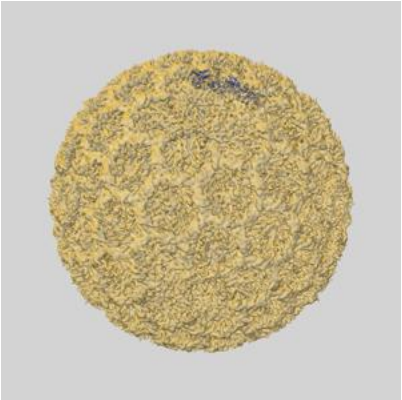
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

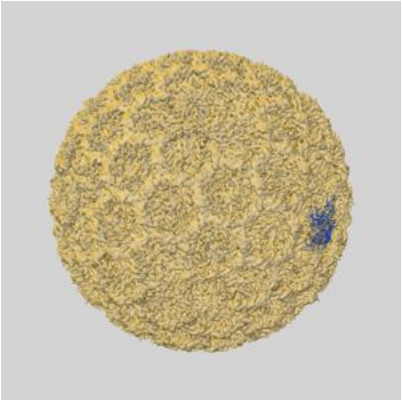
This section contains information regarding the fit between EMDB map EMD-1206 and PDB model 4BTQ. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlays

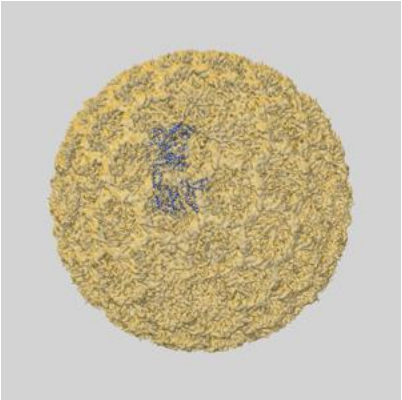
9.1.1 Map-model overlay (i)



X

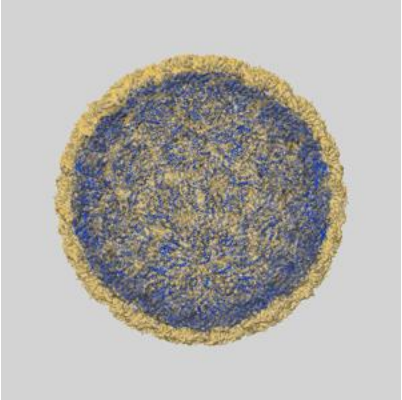


Y

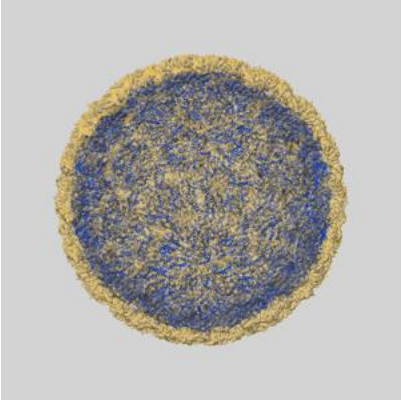


Z

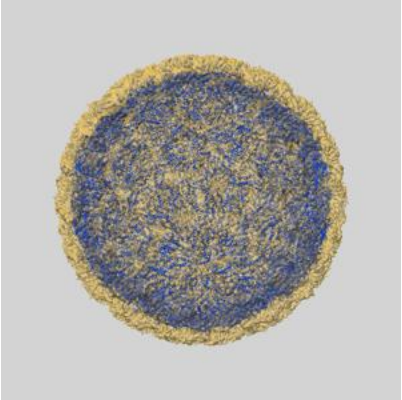
9.1.2 Map-model assembly overlay (i)



X



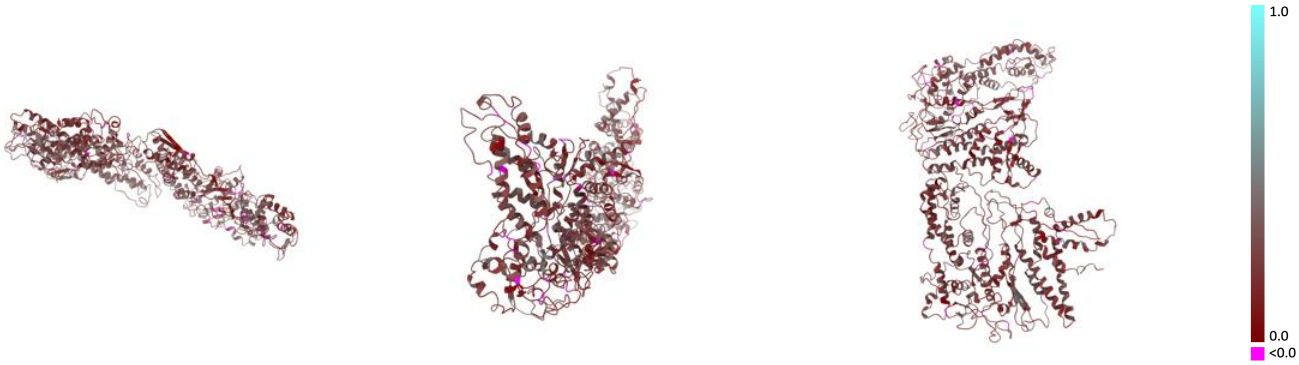
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1800.0 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.

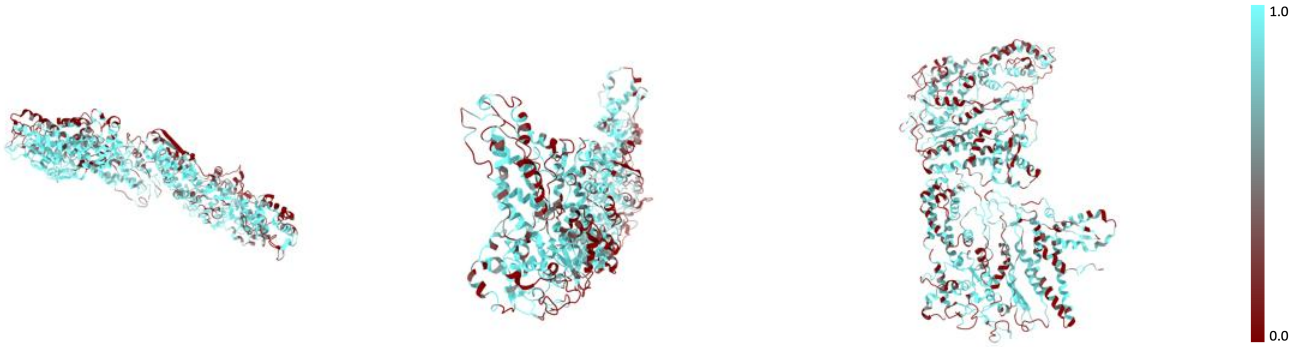
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

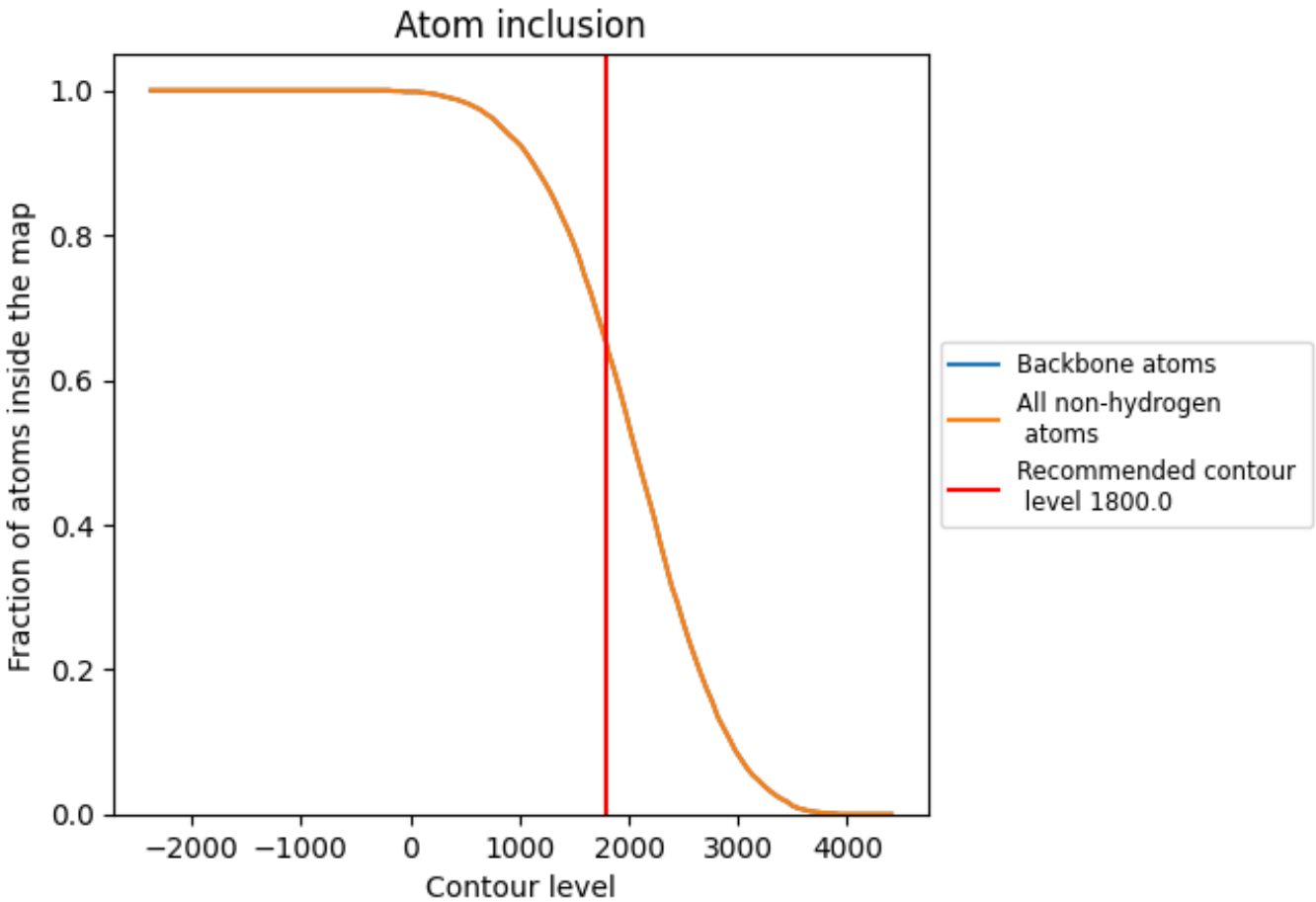
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (1800.0).

9.4 Atom inclusion (i)



At the recommended contour level, 65% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (1800.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6480	0.2460
A	0.6130	0.2400
B	0.6830	0.2520