Full wwPDB EM Validation Report (i)

Aug 4, 2026 – 08:54 PM EDT

PDB ID	:	8VIX / pdb_00008vix
EMDB ID	:	EMD-43270
Title	:	Hydrogen Peroxide-bound Vanadium-dependent Bromoperoxidase from Corallina pilulifera
Authors	:	Hessefort, L.Z.; Williams, D.R.; Biegasiewicz, K.F.
Deposited on	:	2024-01-05
Resolution	:	2.31 Å(reported)
Based on initial model	:	.

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

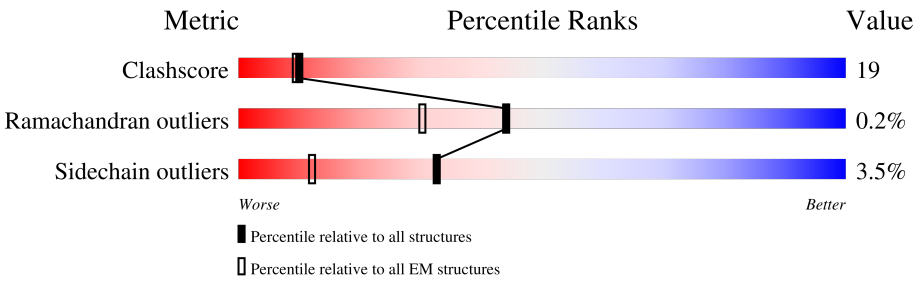
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.50

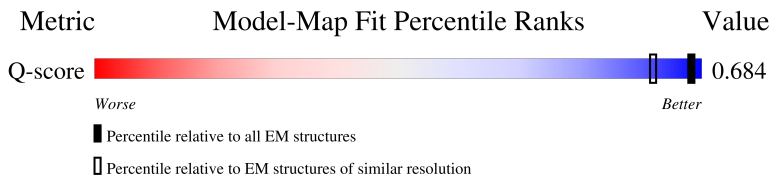
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.31 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	4306 (1.81 - 2.81)

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	634	57% 34% • 7%
1	B	634	53% 38% • 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	VO4	A	601	-	-	X	-
2	VO4	B	602	-	-	X	-
3	PER	A	602	-	X	X	-
3	PER	B	601	-	X	-	-
3	PER	B	603	-	X	X	-
3	PER	B	604	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9146 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 Vanadium-dependent bromoperoxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	590	4559	2898	761	893	7	0	0
1	B	590	4559	2898	761	893	7	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	initiating methionine	UNP O81959
A	-34	GLY	-	expression tag	UNP O81959
A	-33	SER	-	expression tag	UNP O81959
A	-32	SER	-	expression tag	UNP O81959
A	-31	HIS	-	expression tag	UNP O81959
A	-30	HIS	-	expression tag	UNP O81959
A	-29	HIS	-	expression tag	UNP O81959
A	-28	HIS	-	expression tag	UNP O81959
A	-27	HIS	-	expression tag	UNP O81959
A	-26	HIS	-	expression tag	UNP O81959
A	-25	SER	-	expression tag	UNP O81959
A	-24	SER	-	expression tag	UNP O81959
A	-23	GLY	-	expression tag	UNP O81959
A	-22	LEU	-	expression tag	UNP O81959
A	-21	VAL	-	expression tag	UNP O81959
A	-20	PRO	-	expression tag	UNP O81959
A	-19	ARG	-	expression tag	UNP O81959
A	-18	GLY	-	expression tag	UNP O81959
A	-17	SER	-	expression tag	UNP O81959
A	-16	HIS	-	expression tag	UNP O81959
A	-15	MET	-	expression tag	UNP O81959
A	-14	ALA	-	expression tag	UNP O81959
A	-13	SER	-	expression tag	UNP O81959
A	-12	MET	-	expression tag	UNP O81959
A	-11	THR	-	expression tag	UNP O81959
A	-10	GLY	-	expression tag	UNP O81959

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLY	-	expression tag	UNP O81959
A	-8	GLN	-	expression tag	UNP O81959
A	-7	GLN	-	expression tag	UNP O81959
A	-6	MET	-	expression tag	UNP O81959
A	-5	GLY	-	expression tag	UNP O81959
A	-4	ARG	-	expression tag	UNP O81959
A	-3	GLY	-	expression tag	UNP O81959
A	-2	SER	-	expression tag	UNP O81959
A	-1	GLU	-	expression tag	UNP O81959
A	0	PHE	-	expression tag	UNP O81959
B	-35	MET	-	initiating methionine	UNP O81959
B	-34	GLY	-	expression tag	UNP O81959
B	-33	SER	-	expression tag	UNP O81959
B	-32	SER	-	expression tag	UNP O81959
B	-31	HIS	-	expression tag	UNP O81959
B	-30	HIS	-	expression tag	UNP O81959
B	-29	HIS	-	expression tag	UNP O81959
B	-28	HIS	-	expression tag	UNP O81959
B	-27	HIS	-	expression tag	UNP O81959
B	-26	HIS	-	expression tag	UNP O81959
B	-25	SER	-	expression tag	UNP O81959
B	-24	SER	-	expression tag	UNP O81959
B	-23	GLY	-	expression tag	UNP O81959
B	-22	LEU	-	expression tag	UNP O81959
B	-21	VAL	-	expression tag	UNP O81959
B	-20	PRO	-	expression tag	UNP O81959
B	-19	ARG	-	expression tag	UNP O81959
B	-18	GLY	-	expression tag	UNP O81959
B	-17	SER	-	expression tag	UNP O81959
B	-16	HIS	-	expression tag	UNP O81959
B	-15	MET	-	expression tag	UNP O81959
B	-14	ALA	-	expression tag	UNP O81959
B	-13	SER	-	expression tag	UNP O81959
B	-12	MET	-	expression tag	UNP O81959
B	-11	THR	-	expression tag	UNP O81959
B	-10	GLY	-	expression tag	UNP O81959
B	-9	GLY	-	expression tag	UNP O81959
B	-8	GLN	-	expression tag	UNP O81959
B	-7	GLN	-	expression tag	UNP O81959
B	-6	MET	-	expression tag	UNP O81959
B	-5	GLY	-	expression tag	UNP O81959
B	-4	ARG	-	expression tag	UNP O81959

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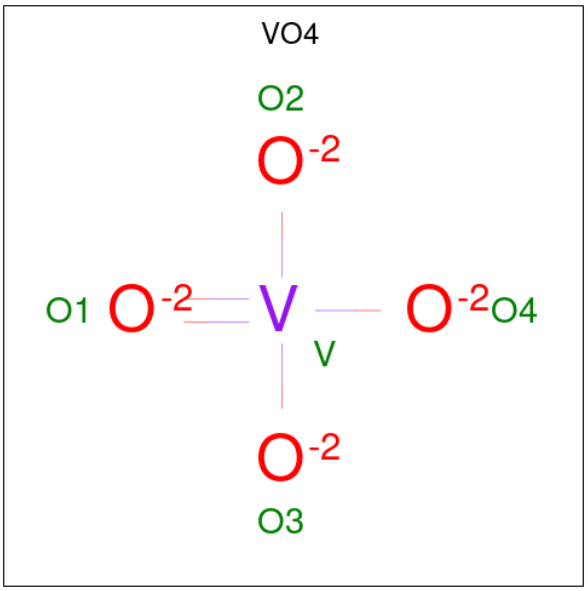
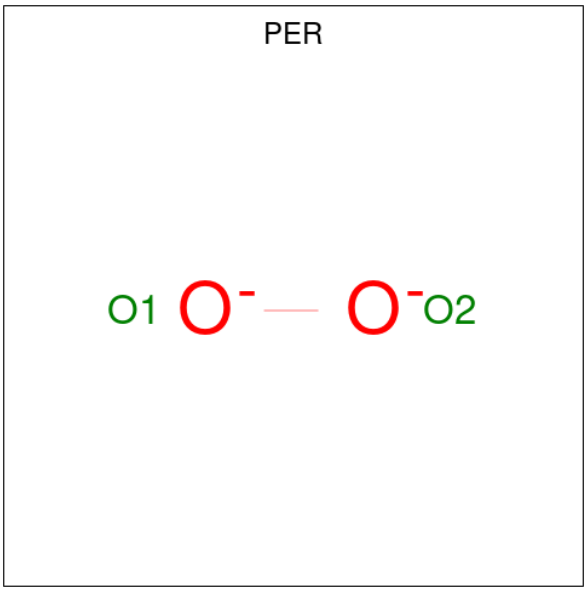
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP O81959
B	-2	SER	-	expression tag	UNP O81959
B	-1	GLU	-	expression tag	UNP O81959
B	0	PHE	-	expression tag	UNP O81959

- Molecule 2 is VANADATE ION (CCD ID: VO4) (formula: O_4V) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	O	V	
2	A	1	5	4	1	0
			Total	O	V	
2	B	1	5	4	1	0

- Molecule 3 is PEROXIDE ION (CCD ID: PER) (formula: O_2).



Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total O 2 2	0
3	B	1	Total O 2 2	0
3	B	1	Total O 2 2	0
3	B	1	Total O 2 2	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Ca 1 1	0
4	B	1	Total Ca 1 1	0

- Molecule 5 is water.

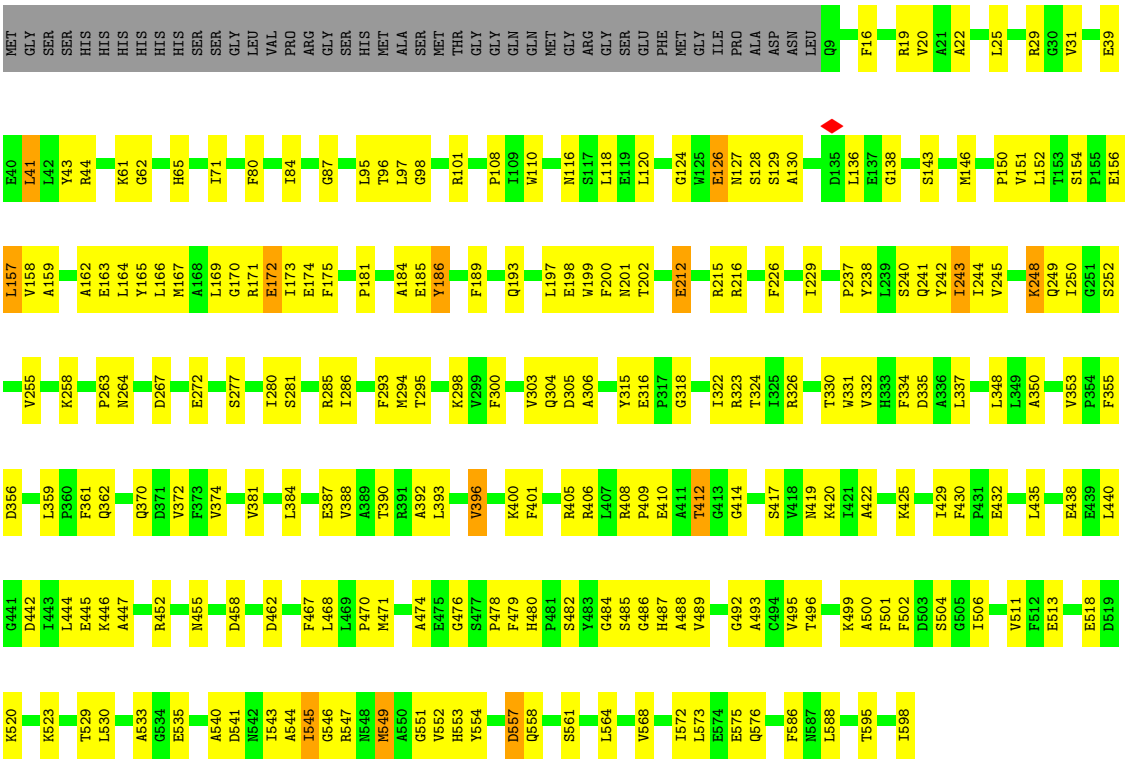
Mol	Chain	Residues	Atoms	AltConf
5	A	4	Total O 4 4	0
5	B	4	Total O 4 4	0

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.

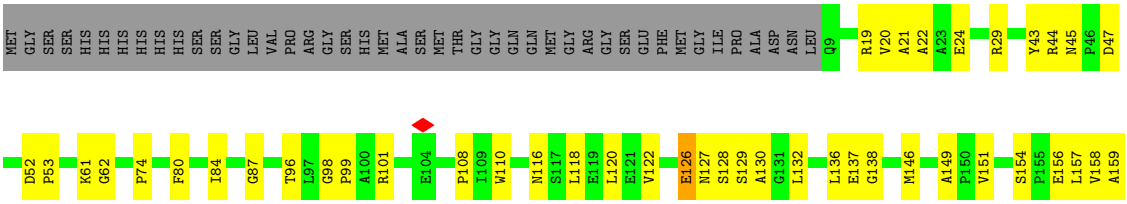
- Molecule 1: Vanadium-dependent bromoperoxidase

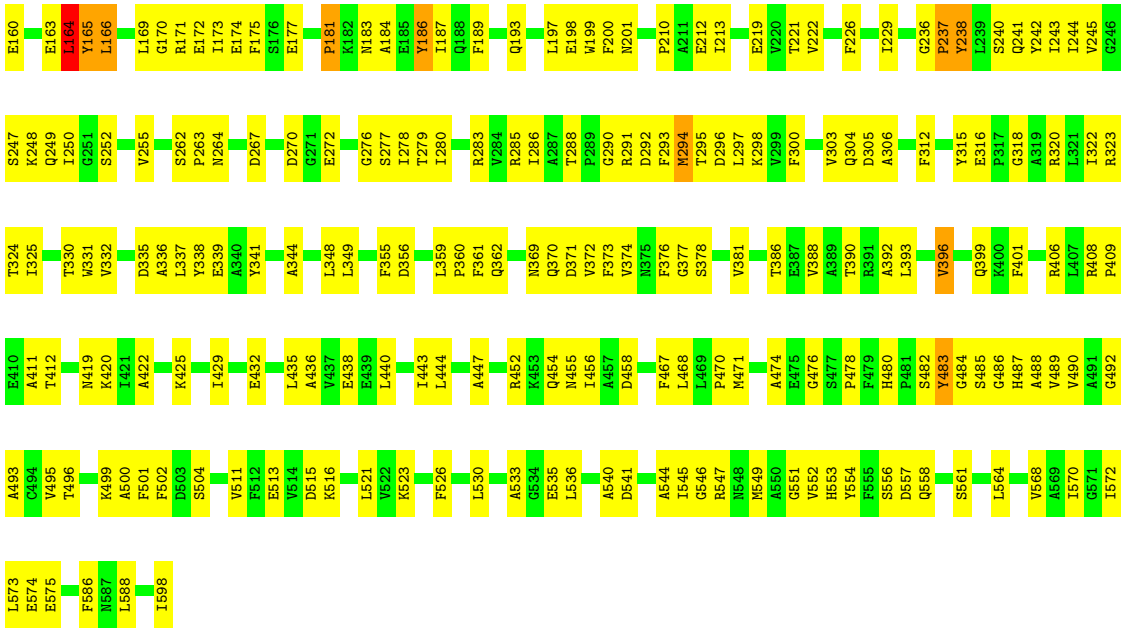
Chain A:



- Molecule 1: Vanadium-dependent bromoperoxidase

Chain B:




E160 E163 L164 Y165 L166 L169 G170 R171 E172 I173 E174 F175 S176 E177 P181 K182 N183 A184 E185 Y186 I187 Q188 F189 Q193 L197 E198 W199 F200 N201 P210 A211 E212 I213 E219 V220 T221 V222 F226 I229 G236 P237 Y238 L239 S240 Q241 Y242 I243 I244 V245 G246
S247 K248 Q249 I250 G251 S252 V255 S262 P263 N264 D267 D270 G271 E272 G276 S277 I278 T279 I280 R283 V284 R285 I286 A287 T288 P289 G290 R291 D292 F293 M294 T295 D296 L297 K298 V299 F300 V303 Q304 D305 A306 F312 Y315 E316 P317 G318 A319 R320 L321 I322 R323
T324 I325 T330 W331 V332 D335 A336 L337 Y338 E339 A340 Y341 A344 L348 L349 F355 D356 L359 P360 F361 Q362 N369 Q370 D371 V372 F373 V374 N375 F376 G377 S378 V381 T386 E387 V388 A389 T390 R391 A392 L393 V396 Q399 K400 F401 R406 L407 R408 P409
E410 A411 T412 N419 K420 I421 A422 K425 I429 E432 L435 A436 V437 E438 E439 L440 I443 L444 A447 R452 K453 Q454 N455 I456 A457 D458 F467 L468 L469 P470 M471 A474 E475 G476 S477 P478 F479 H480 P481 S482 Y483 G484 S485 G486 H487 A488 V489 V490 A491 G492
A493 C494 V495 T496 K499 A500 F501 F502 D503 S504 V511 F512 E513 V514 D515 K516 L521 V522 K523 F526 L530 A533 G534 E535 L536 A540 D541 A544 I545 G546 R547 N548 M549 A550 G551 V552 H553 Y554 F555 S556 D557 Q558 S561 L564 V568 A569 I570 G571 I572
L573 E574 E575 F586 N587 L588 I598

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, T	Depositor
Number of particles used	349552	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	-800	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	16.650	Depositor
Minimum map value	-9.108	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.236	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	527.36, 527.36, 527.36	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PER, VO4, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.26	2/4659 (0.0%)	0.38	3/6332 (0.0%)
1	B	0.60	13/4659 (0.3%)	0.58	20/6332 (0.3%)
All	All	0.46	15/9318 (0.2%)	0.49	23/12664 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	412	THR	C-O	-15.98	1.05	1.24
1	B	165	TYR	C-O	-15.64	1.05	1.24
1	B	181	PRO	N-CD	-13.77	1.28	1.47
1	B	166	LEU	C-O	-10.79	1.11	1.24
1	B	238	TYR	C-O	-10.04	1.12	1.24
1	A	412	THR	C-O	-9.65	1.12	1.24
1	B	295	THR	C-O	-9.32	1.10	1.23
1	B	483	TYR	C-O	-9.20	1.13	1.24
1	B	237	PRO	N-CD	8.11	1.59	1.47
1	B	186	TYR	C-O	-7.43	1.14	1.24
1	B	483	TYR	C-N	-7.14	1.23	1.33
1	A	186	TYR	C-O	-6.90	1.15	1.24
1	B	181	PRO	C-O	-6.36	1.16	1.24
1	B	294	MET	C-N	-5.60	1.25	1.33
1	B	237	PRO	C-N	-5.09	1.27	1.33

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	295	THR	CB-CA-C	8.98	123.58	109.03
1	B	164	LEU	CA-C-N	8.74	132.33	120.44
1	B	164	LEU	C-N-CA	8.74	132.33	120.44
1	B	295	THR	N-CA-C	-8.51	103.42	113.88
1	B	237	PRO	O-C-N	-7.82	113.45	122.91
1	B	238	TYR	CA-C-N	-7.64	110.49	121.42
1	B	238	TYR	C-N-CA	-7.64	110.49	121.42
1	B	237	PRO	CA-C-N	7.23	130.19	120.65
1	B	237	PRO	C-N-CA	7.23	130.19	120.65
1	B	166	LEU	CA-C-O	-7.17	112.95	120.55
1	B	411	ALA	CA-C-N	6.99	129.94	120.44
1	B	411	ALA	C-N-CA	6.99	129.94	120.44
1	B	412	THR	CA-CB-OG1	-6.62	99.67	109.60
1	A	185	GLU	CA-C-N	6.54	130.24	120.31
1	A	185	GLU	C-N-CA	6.54	130.24	120.31
1	B	412	THR	O-C-N	6.46	129.07	122.09
1	B	483	TYR	CA-C-O	6.05	128.20	120.57
1	A	185	GLU	O-C-N	-6.02	115.87	122.07
1	B	186	TYR	N-CA-CB	5.84	119.33	110.28
1	B	483	TYR	O-C-N	-5.30	114.90	122.96
1	B	294	MET	O-C-N	-5.13	116.55	122.86
1	B	165	TYR	CA-C-N	5.11	127.13	120.28
1	B	165	TYR	C-N-CA	5.11	127.13	120.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	238	TYR	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	4559	0	4444	188	0
1	B	4559	0	4444	190	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	5	0	0	3	0
2	B	5	0	0	3	0
3	A	2	0	0	3	0
3	B	6	0	0	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
All	All	9146	0	8888	350	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 19.

All (350) 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:408:ARG:HD3	1:A:482:SER:HB3	1.57	0.85
1:B:408:ARG:HD3	1:B:482:SER:HB3	1.60	0.82
1:A:126:GLU:HG3	1:A:480:HIS:HD2	1.42	0.82
1:B:504:SER:HB2	1:B:533:ALA:HB2	1.62	0.81
1:B:294:MET:HE1	1:B:476:GLY:HA3	1.63	0.80
1:A:478:PRO:HG2	3:A:602:PER:O1	1.82	0.78
1:A:504:SER:HB2	1:A:533:ALA:HB2	1.64	0.77
1:A:544:ALA:HB1	1:A:558:GLN:HB3	1.69	0.75
1:A:406:ARG:NH1	1:A:557:ASP:OD1	2.23	0.71
1:A:101:ARG:HA	1:A:108:PRO:HA	1.71	0.71
1:A:189:PHE:O	1:A:193:GLN:HG2	1.91	0.71
1:B:101:ARG:HA	1:B:108:PRO:HA	1.72	0.70
1:A:422:ALA:HA	1:A:425:LYS:HE3	1.73	0.70
1:B:544:ALA:HB1	1:B:558:GLN:HB3	1.75	0.69
1:A:146:MET:HG3	1:A:564:LEU:HD13	1.74	0.69
1:B:110:TRP:O	1:B:116:ASN:ND2	2.26	0.68
1:A:393:LEU:HD13	1:B:374:VAL:HG22	1.76	0.68
1:B:406:ARG:NH1	1:B:557:ASP:OD1	2.27	0.68
1:A:127:ASN:HB3	1:A:130:ALA:HB2	1.76	0.67
1:A:280:ILE:HG12	1:B:280:ILE:HG12	1.76	0.67
1:A:478:PRO:CG	3:A:602:PER:O1	2.42	0.67
1:B:189:PHE:O	1:B:193:GLN:HG2	1.94	0.67
1:B:267:ASP:HB3	1:B:272:GLU:HB3	1.77	0.66
1:A:374:VAL:HG22	1:B:393:LEU:HD13	1.78	0.66
1:A:545:ILE:O	1:A:549:MET:HG3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LEU:O	1:B:369:ASN:ND2	2.30	0.65
1:B:478:PRO:HG2	3:B:603:PER:O1	1.96	0.65
1:A:29:ARG:NH2	1:A:575:GLU:OE2	2.27	0.64
1:B:127:ASN:HB3	1:B:130:ALA:HB2	1.80	0.64
1:B:573:LEU:HB3	1:B:598:ILE:HG21	1.79	0.64
1:A:264:ASN:OD1	1:B:318:GLY:N	2.28	0.64
1:A:396:VAL:HG11	1:A:486:GLY:HA2	1.80	0.64
1:B:159:ALA:HA	1:B:197:LEU:HD13	1.81	0.63
1:A:388:VAL:HG23	1:A:572:ILE:HD12	1.80	0.63
1:B:388:VAL:HG23	1:B:572:ILE:HD12	1.80	0.63
2:A:601:VO4:O3	2:A:601:VO4:V	1.55	0.63
1:A:485:SER:HB2	1:A:558:GLN:HE22	1.63	0.63
1:B:396:VAL:HG11	1:B:486:GLY:HA2	1.80	0.62
2:B:602:VO4:O3	2:B:602:VO4:V	1.55	0.62
1:A:159:ALA:HA	1:A:197:LEU:HD13	1.82	0.62
1:B:171:ARG:NH1	1:B:292:ASP:OD1	2.33	0.62
1:A:151:VAL:HG22	1:A:154:SER:HB3	1.83	0.61
1:B:146:MET:HG2	1:B:564:LEU:HD13	1.82	0.61
1:B:29:ARG:NH2	1:B:575:GLU:OE2	2.27	0.61
1:A:158:VAL:HG21	1:A:435:LEU:HG	1.81	0.60
1:B:408:ARG:NH1	1:B:552:VAL:O	2.31	0.60
1:B:164:LEU:HD23	1:B:409:PRO:HB3	1.84	0.59
1:B:361:PHE:CG	1:B:370:GLN:HG2	2.37	0.59
1:A:110:TRP:O	1:A:116:ASN:ND2	2.31	0.59
1:A:335:ASP:N	1:A:335:ASP:OD1	2.34	0.59
1:A:19:ARG:HG2	1:B:136:LEU:HA	1.84	0.58
1:B:388:VAL:HG22	1:B:493:ALA:HB1	1.84	0.58
1:A:189:PHE:CE2	1:A:446:LYS:HE2	2.37	0.58
1:A:361:PHE:CG	1:A:370:GLN:HG2	2.37	0.58
1:A:19:ARG:NH1	1:B:575:GLU:OE1	2.33	0.58
1:A:500:ALA:HB1	1:A:586:PHE:HB3	1.84	0.58
1:A:226:PHE:O	1:A:238:TYR:OH	2.20	0.57
1:B:356:ASP:HB3	1:B:359:LEU:HG	1.86	0.57
1:A:174:GLU:HG2	1:A:323:ARG:HB2	1.85	0.57
1:A:249:GLN:NE2	1:A:272:GLU:O	2.37	0.57
1:B:126:GLU:HG3	1:B:480:HIS:HD2	1.69	0.57
1:A:146:MET:HE1	1:A:484:GLY:HA3	1.87	0.57
1:B:487:HIS:ND1	2:B:602:VO4:O4	2.32	0.57
1:B:432:GLU:CD	1:B:432:GLU:H	2.12	0.57
1:A:495:VAL:HG21	1:A:540:ALA:HB2	1.86	0.56
1:B:160:GLU:OE2	1:B:556:SER:OG	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:500:ALA:HB1	1:B:586:PHE:HB3	1.87	0.56
1:A:322:ILE:HD11	1:A:331:TRP:CD1	2.40	0.56
1:B:293:PHE:CG	1:B:474:ALA:HA	2.41	0.56
1:A:355:PHE:HA	1:A:502:PHE:HA	1.87	0.56
1:B:62:GLY:HA2	1:B:306:ALA:HB2	1.86	0.56
1:A:174:GLU:HG3	1:A:324:THR:HG22	1.87	0.56
1:A:419:ASN:ND2	1:A:430:PHE:O	2.38	0.56
1:B:322:ILE:HD11	1:B:331:TRP:CD1	2.41	0.56
1:B:545:ILE:O	1:B:549:MET:HG3	2.06	0.56
1:A:420:LYS:HD2	1:A:444:LEU:HD13	1.87	0.55
1:B:323:ARG:NH2	1:B:515:ASP:O	2.39	0.55
1:B:492:GLY:O	1:B:496:THR:OG1	2.22	0.55
1:A:138:GLY:N	1:A:575:GLU:OE1	2.38	0.55
1:A:156:GLU:HG3	1:A:199:TRP:CZ2	2.42	0.55
1:B:187:ILE:HG21	1:B:222:VAL:HG23	1.87	0.55
1:A:573:LEU:HB3	1:A:598:ILE:HG21	1.89	0.55
1:A:432:GLU:H	1:A:432:GLU:CD	2.15	0.54
1:B:249:GLN:NE2	1:B:272:GLU:O	2.40	0.54
1:A:295:THR:OG1	1:A:455:ASN:OD1	2.20	0.54
1:A:157:LEU:HD23	1:A:406:ARG:HH21	1.73	0.54
1:A:485:SER:HB3	1:A:488:ALA:HB3	1.89	0.54
1:B:174:GLU:HA	1:B:324:THR:HA	1.89	0.54
1:B:335:ASP:OD1	1:B:335:ASP:N	2.39	0.54
1:B:545:ILE:HG22	1:B:549:MET:HE3	1.89	0.54
1:A:164:LEU:HD13	1:A:409:PRO:HB3	1.90	0.54
1:A:258:LYS:HE2	1:B:118:LEU:HD21	1.90	0.54
1:B:20:VAL:HG12	1:B:24:GLU:OE1	2.06	0.54
1:B:422:ALA:HA	1:B:425:LYS:HE3	1.90	0.54
1:B:570:ILE:HG22	1:B:574:GLU:OE1	2.08	0.54
1:A:388:VAL:HG22	1:A:493:ALA:HB1	1.90	0.54
1:A:553:HIS:NE2	2:A:601:VO4:O3	2.40	0.54
1:A:169:LEU:HD21	1:A:447:ALA:HA	1.89	0.53
1:A:173:ILE:HD13	1:A:186:TYR:CD2	2.43	0.53
1:B:169:LEU:HD21	1:B:447:ALA:HA	1.89	0.53
1:B:495:VAL:HG12	1:B:499:LYS:HE2	1.89	0.53
1:A:120:LEU:HD21	1:B:255:VAL:HG12	1.89	0.53
1:A:124:GLY:C	1:A:479:PHE:HD2	2.16	0.53
1:B:21:ALA:HA	1:B:24:GLU:OE2	2.08	0.53
1:B:43:TYR:CD1	1:B:432:GLU:HG2	2.43	0.53
1:A:381:VAL:HB	1:A:501:PHE:CD1	2.44	0.53
1:A:127:ASN:OD1	1:B:374:VAL:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:VAL:HB	1:B:501:PHE:CD1	2.44	0.53
1:A:16:PHE:HE1	1:B:24:GLU:HG3	1.74	0.53
1:A:255:VAL:HG12	1:B:120:LEU:HD21	1.91	0.53
1:A:408:ARG:NH1	1:A:552:VAL:O	2.38	0.53
1:A:487:HIS:ND1	2:A:601:VO4:O4	2.36	0.53
1:A:62:GLY:HA3	1:A:479:PHE:HZ	1.73	0.52
1:A:285:ARG:HG3	1:B:250:ILE:HB	1.91	0.52
1:B:166:LEU:O	1:B:186:TYR:OH	2.22	0.52
1:B:181:PRO:HA	1:B:184:ALA:HB2	1.90	0.52
1:B:61:LYS:HE3	1:B:303:VAL:HG12	1.92	0.52
1:A:500:ALA:HB2	1:A:588:LEU:HD13	1.91	0.52
1:A:240:SER:O	1:A:243:ILE:HG22	2.10	0.52
1:A:576:GLN:HE22	1:A:586:PHE:HE2	1.58	0.52
1:B:440:LEU:HD22	1:B:443:ILE:HD12	1.91	0.52
1:A:412:THR:HG1	1:A:554:TYR:HH	1.54	0.52
1:B:126:GLU:HG3	1:B:480:HIS:CD2	2.44	0.52
1:A:293:PHE:CG	1:A:474:ALA:HA	2.45	0.51
1:B:226:PHE:O	1:B:545:ILE:HG21	2.10	0.51
1:A:243:ILE:HG23	1:A:244:ILE:HG23	1.92	0.51
1:B:249:GLN:HG3	1:B:267:ASP:HB2	1.91	0.51
1:B:252:SER:HB2	1:B:262:SER:HB2	1.92	0.51
1:A:553:HIS:HB3	1:A:558:GLN:NE2	2.25	0.51
1:B:488:ALA:HB3	1:B:561:SER:HB2	1.93	0.51
1:A:330:THR:O	1:B:277:SER:OG	2.20	0.51
1:B:243:ILE:HG23	1:B:244:ILE:HG23	1.93	0.51
1:A:356:ASP:HB3	1:A:359:LEU:HG	1.94	0.50
1:B:157:LEU:HD23	1:B:406:ARG:HH21	1.76	0.50
1:A:170:GLY:HA2	1:A:173:ILE:HD12	1.92	0.50
1:B:210:PRO:HA	1:B:213:ILE:HD12	1.92	0.50
1:B:420:LYS:HD2	1:B:444:LEU:HD13	1.93	0.50
1:A:294:MET:HE1	1:A:476:GLY:HA3	1.93	0.50
1:A:495:VAL:HG12	1:A:499:LYS:HE2	1.92	0.50
1:B:151:VAL:HG22	1:B:154:SER:HB3	1.93	0.50
1:A:80:PHE:CZ	1:A:84:ILE:HD11	2.46	0.50
1:B:146:MET:HG3	1:B:399:GLN:HG3	1.94	0.50
1:B:471:MET:HE1	1:B:551:GLY:C	2.36	0.50
1:B:485:SER:HB3	1:B:488:ALA:HB3	1.94	0.50
1:A:478:PRO:HB2	1:A:480:HIS:NE2	2.26	0.49
1:B:361:PHE:HB2	1:B:372:VAL:HG13	1.94	0.49
1:A:156:GLU:HG3	1:A:199:TRP:CH2	2.47	0.49
1:A:166:LEU:O	1:A:186:TYR:OH	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:GLY:N	1:B:264:ASN:OD1	2.36	0.49
1:A:452:ARG:NH2	1:A:462:ASP:OD1	2.45	0.49
1:B:29:ARG:NH1	1:B:574:GLU:OE2	2.45	0.49
1:B:323:ARG:HG3	1:B:324:THR:HG23	1.94	0.49
1:B:158:VAL:HG21	1:B:435:LEU:HG	1.95	0.49
1:B:291:ARG:HA	1:B:454:GLN:HE22	1.78	0.49
1:B:419:ASN:ND2	1:B:429:ILE:O	2.29	0.49
1:A:410:GLU:HB3	1:A:471:MET:HE2	1.95	0.49
1:A:277:SER:OG	1:B:330:THR:O	2.22	0.49
1:A:193:GLN:O	1:A:197:LEU:HG	2.13	0.49
1:B:245:VAL:HA	1:B:521:LEU:HD11	1.95	0.49
1:A:146:MET:HE1	1:A:484:GLY:CA	2.43	0.48
1:A:62:GLY:HA2	1:A:306:ALA:HB2	1.94	0.48
1:A:414:GLY:HA2	1:A:468:LEU:HD23	1.94	0.48
1:B:288:THR:HA	1:B:316:GLU:OE1	2.12	0.48
1:A:400:LYS:NZ	1:A:484:GLY:O	2.32	0.48
1:B:270:ASP:O	1:B:283:ARG:NH1	2.46	0.48
1:B:272:GLU:HG3	1:B:279:THR:HB	1.95	0.48
1:A:267:ASP:HB3	1:A:272:GLU:HB2	1.94	0.48
1:B:242:TYR:CE2	1:B:535:GLU:HB3	2.48	0.48
1:B:495:VAL:HG13	1:B:536:LEU:HB3	1.94	0.48
1:A:16:PHE:CE1	1:B:24:GLU:HG3	2.48	0.48
1:A:174:GLU:HA	1:A:324:THR:HA	1.94	0.48
1:A:118:LEU:HB2	1:A:120:LEU:HG	1.95	0.48
1:A:136:LEU:HA	1:B:19:ARG:HG2	1.95	0.48
1:B:101:ARG:NH1	1:B:108:PRO:HD3	2.29	0.48
1:A:417:SER:HA	1:A:467:PHE:HB2	1.95	0.48
1:A:485:SER:HB2	1:A:558:GLN:NE2	2.28	0.48
1:A:156:GLU:HG3	1:A:199:TRP:CE2	2.49	0.47
1:A:165:TYR:OH	1:A:467:PHE:O	2.23	0.47
1:A:181:PRO:HA	1:A:184:ALA:HB2	1.96	0.47
1:B:248:LYS:HG2	1:B:252:SER:HB3	1.95	0.47
1:B:297:LEU:HA	1:B:468:LEU:HD11	1.97	0.47
1:B:553:HIS:NE2	2:B:602:VO4:O3	2.48	0.47
1:A:242:TYR:CE2	1:A:535:GLU:HB3	2.48	0.47
1:B:198:GLU:HA	1:B:201:ASN:OD1	2.15	0.47
1:B:219:GLU:OE1	1:B:221:THR:HG23	2.14	0.47
1:B:478:PRO:HB2	1:B:480:HIS:NE2	2.29	0.47
1:B:547:ARG:HB2	1:B:558:GLN:NE2	2.30	0.47
1:A:128:SER:HA	1:A:401:PHE:CE2	2.50	0.47
1:A:300:PHE:O	1:A:304:GLN:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:ALA:HB1	1:A:489:VAL:HG22	1.96	0.47
1:A:396:VAL:HB	1:A:489:VAL:HG11	1.97	0.47
1:B:241:GLN:O	1:B:245:VAL:HG22	2.14	0.47
1:A:355:PHE:HB3	1:A:359:LEU:HD12	1.97	0.47
1:A:392:ALA:HA	1:A:568:VAL:HG21	1.97	0.47
1:A:530:LEU:HD13	1:A:535:GLU:OE1	2.15	0.47
1:A:164:LEU:HD21	1:A:553:HIS:O	2.15	0.47
1:B:331:TRP:CH2	1:B:339:GLU:HG2	2.50	0.46
1:B:325:ILE:HG23	1:B:549:MET:SD	2.55	0.46
1:A:401:PHE:O	1:A:405:ARG:NH1	2.45	0.46
1:A:412:THR:OG1	1:A:554:TYR:OH	2.29	0.46
1:A:471:MET:HE1	1:A:551:GLY:C	2.41	0.46
1:B:172:GLU:CD	1:B:290:GLY:H	2.23	0.46
1:A:62:GLY:CA	1:A:479:PHE:HZ	2.29	0.46
1:A:543:ILE:O	1:A:547:ARG:HG2	2.16	0.46
1:B:478:PRO:CG	3:B:603:PER:O1	2.62	0.46
1:B:247:SER:O	1:B:249:GLN:NE2	2.39	0.46
1:A:552:VAL:HG23	1:A:553:HIS:CD2	2.52	0.45
1:A:20:VAL:HG22	1:B:20:VAL:HG22	1.97	0.45
1:A:39:GLU:OE2	1:A:152:LEU:N	2.40	0.45
1:B:396:VAL:HB	1:B:489:VAL:HG11	1.97	0.45
1:B:199:TRP:HH2	1:B:212:GLU:HG2	1.81	0.45
1:B:511:VAL:H	1:B:523:LYS:NZ	2.15	0.45
1:A:198:GLU:HA	1:A:201:ASN:OD1	2.17	0.45
1:A:250:ILE:HB	1:B:285:ARG:HG3	1.98	0.45
1:B:174:GLU:HG2	1:B:324:THR:HG22	1.99	0.45
1:B:495:VAL:HG21	1:B:540:ALA:HB2	1.98	0.45
1:B:128:SER:HA	1:B:401:PHE:CE2	2.51	0.45
1:A:241:GLN:O	1:A:245:VAL:HG22	2.16	0.45
1:A:171:ARG:HH12	1:A:470:PRO:C	2.24	0.45
1:A:172:GLU:CD	1:A:326:ARG:HE	2.23	0.45
1:B:87:GLY:HA2	1:B:129:SER:OG	2.17	0.45
1:B:243:ILE:HD12	1:B:243:ILE:HA	1.84	0.45
1:B:341:TYR:CE2	1:B:490:VAL:HG12	2.52	0.45
1:B:349:LEU:HD13	1:B:378:SER:HB2	1.98	0.45
1:A:101:ARG:NH1	1:A:108:PRO:HD3	2.32	0.44
1:A:175:PHE:HE1	1:A:549:MET:HE1	1.82	0.44
1:B:489:VAL:HA	1:B:561:SER:O	2.17	0.44
1:A:41:LEU:O	1:A:44:ARG:NH1	2.44	0.44
1:A:387:GLU:OE1	1:A:572:ILE:HG21	2.17	0.44
1:B:137:GLU:HG3	1:B:572:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:TRP:CZ2	1:A:216:ARG:HA	2.53	0.44
1:B:409:PRO:HB2	1:B:551:GLY:O	2.18	0.44
1:A:315:TYR:O	1:B:263:PRO:HG3	2.17	0.44
1:B:61:LYS:HG3	1:B:304:GLN:HA	1.99	0.44
1:B:554:TYR:HD1	1:B:557:ASP:OD2	2.00	0.44
1:B:22:ALA:HB1	1:B:575:GLU:HG2	1.98	0.44
1:A:361:PHE:HB2	1:A:372:VAL:HG13	2.00	0.44
1:B:170:GLY:HA2	1:B:173:ILE:HD12	2.00	0.44
1:B:355:PHE:CE2	1:B:377:GLY:HA2	2.52	0.44
1:A:471:MET:HE1	1:A:551:GLY:O	2.18	0.44
1:A:286:ILE:HB	1:A:316:GLU:HB2	2.00	0.44
1:B:360:PRO:HG2	1:B:376:PHE:CE2	2.53	0.44
1:B:455:ASN:HA	1:B:458:ASP:HB2	2.00	0.44
1:B:159:ALA:HB1	1:B:200:PHE:CE2	2.53	0.43
1:B:332:VAL:HG21	1:B:546:GLY:C	2.43	0.43
1:A:43:TYR:CD1	1:A:432:GLU:HG2	2.54	0.43
1:A:226:PHE:O	1:A:545:ILE:HG21	2.17	0.43
1:B:336:ALA:O	1:B:338:TYR:N	2.51	0.43
1:B:362:GLN:HE22	1:B:372:VAL:HG21	1.83	0.43
1:B:483:TYR:HA	1:B:484:GLY:HA2	1.55	0.43
1:A:19:ARG:NH2	1:B:575:GLU:OE1	2.51	0.43
1:A:80:PHE:CE2	1:A:84:ILE:HD11	2.53	0.43
1:A:442:ASP:HA	1:A:445:GLU:OE1	2.19	0.43
1:B:129:SER:HB3	1:B:132:LEU:HD12	1.99	0.43
1:B:286:ILE:HG13	1:B:320:ARG:HG2	2.00	0.43
1:B:500:ALA:HB2	1:B:588:LEU:HD13	1.99	0.43
1:A:150:PRO:HB3	1:A:156:GLU:HB3	2.00	0.43
1:A:186:TYR:CD2	1:A:186:TYR:C	2.95	0.43
1:A:489:VAL:HA	1:A:561:SER:O	2.19	0.43
1:B:156:GLU:HB2	1:B:199:TRP:CZ3	2.53	0.43
1:A:575:GLU:OE1	1:B:19:ARG:NH1	2.44	0.43
1:B:146:MET:HE1	1:B:484:GLY:HA3	1.99	0.43
1:B:193:GLN:O	1:B:197:LEU:HG	2.18	0.43
1:A:163:GLU:HG2	1:A:167:MET:SD	2.58	0.43
1:A:281:SER:O	1:B:278:ILE:HB	2.18	0.43
1:A:362:GLN:HE22	1:A:372:VAL:HG21	1.83	0.43
1:A:492:GLY:O	1:A:496:THR:OG1	2.25	0.43
1:B:165:TYR:OH	1:B:467:PHE:O	2.30	0.43
1:B:300:PHE:O	1:B:304:GLN:HG2	2.19	0.43
1:A:97:LEU:HD22	1:B:369:ASN:HA	2.00	0.43
1:A:485:SER:HA	1:A:553:HIS:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ASN:HD22	1:B:47:ASP:H	1.67	0.43
1:B:291:ARG:HA	1:B:454:GLN:NE2	2.33	0.43
1:B:360:PRO:HG2	1:B:376:PHE:CD2	2.54	0.43
1:A:156:GLU:CD	1:A:215:ARG:HE	2.27	0.42
1:A:263:PRO:HG3	1:B:315:TYR:O	2.19	0.42
1:A:557:ASP:HB2	1:A:558:GLN:HE21	1.83	0.42
1:B:173:ILE:HG12	1:B:183:ASN:ND2	2.35	0.42
1:A:488:ALA:HB3	1:A:561:SER:OG	2.20	0.42
1:A:511:VAL:H	1:A:523:LYS:NZ	2.17	0.42
1:B:146:MET:HE1	1:B:484:GLY:CA	2.49	0.42
1:B:237:PRO:HD2	1:B:530:LEU:HD11	2.00	0.42
1:A:167:MET:HE2	1:A:545:ILE:HG23	2.01	0.42
1:A:248:LYS:HD2	1:A:350:ALA:O	2.19	0.42
1:A:575:GLU:OE1	1:B:19:ARG:NH2	2.50	0.42
1:B:158:VAL:HG13	1:B:436:ALA:HA	2.01	0.42
1:A:523:LYS:HE3	1:A:523:LYS:HB3	1.83	0.42
1:B:355:PHE:HA	1:B:502:PHE:HA	2.02	0.42
1:B:392:ALA:HA	1:B:568:VAL:HG21	2.02	0.42
1:B:523:LYS:HD2	1:B:523:LYS:HA	1.91	0.42
1:A:98:GLY:HA2	1:A:305:ASP:O	2.19	0.42
1:B:240:SER:O	1:B:243:ILE:HG22	2.18	0.42
1:A:277:SER:HB2	1:B:331:TRP:HA	2.02	0.42
1:B:122:VAL:HA	1:B:306:ALA:O	2.20	0.42
1:B:175:PHE:HE1	1:B:549:MET:HE1	1.84	0.42
1:A:486:GLY:O	1:A:489:VAL:HG12	2.19	0.42
1:B:173:ILE:HD13	1:B:186:TYR:CD2	2.54	0.42
1:B:80:PHE:CZ	1:B:84:ILE:HD11	2.54	0.42
1:B:171:ARG:HH12	1:B:470:PRO:C	2.27	0.42
1:B:242:TYR:CZ	1:B:348:LEU:HD21	2.55	0.42
1:B:312:PHE:HB3	1:B:474:ALA:CB	2.49	0.42
1:A:518:GLU:HB2	1:A:520:LYS:HE3	2.01	0.42
1:A:65:HIS:HA	1:A:71:ILE:HA	2.02	0.41
1:A:159:ALA:HB1	1:A:200:PHE:CE2	2.55	0.41
1:A:189:PHE:CD2	1:A:446:LYS:HE2	2.55	0.41
1:B:236:GLY:HA2	1:B:526:PHE:CG	2.55	0.41
1:B:489:VAL:HG21	1:B:564:LEU:HD23	2.02	0.41
1:A:198:GLU:O	1:A:202:THR:HB	2.19	0.41
1:A:237:PRO:HB3	1:A:513:GLU:OE2	2.21	0.41
1:A:348:LEU:HD22	1:A:353:VAL:HG11	2.01	0.41
1:A:409:PRO:HB2	1:A:551:GLY:O	2.19	0.41
1:B:52:ASP:HB3	1:B:74:PRO:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:GLY:HA2	1:B:305:ASP:O	2.20	0.41
1:A:31:VAL:HG22	1:A:143:SER:HA	2.03	0.41
1:A:61:LYS:NZ	1:A:410:GLU:OE2	2.38	0.41
1:A:159:ALA:HB2	1:A:199:TRP:HB3	2.02	0.41
1:A:554:TYR:HD1	1:A:557:ASP:OD2	2.02	0.41
1:B:511:VAL:H	1:B:523:LYS:HZ1	1.67	0.41
1:A:22:ALA:HB1	1:A:575:GLU:HG2	2.01	0.41
1:B:177:GLU:CG	1:B:516:LYS:HG2	2.50	0.41
1:A:243:ILE:HD11	1:A:331:TRP:CE2	2.56	0.41
1:A:419:ASN:HB2	1:A:430:PHE:HB2	2.02	0.41
1:A:193:GLN:HG2	1:A:193:GLN:H	1.71	0.41
1:B:344:ALA:O	1:B:348:LEU:HG	2.21	0.41
1:A:25:LEU:O	1:A:29:ARG:HG3	2.21	0.41
1:A:429:ILE:HG12	1:A:430:PHE:N	2.35	0.41
1:A:87:GLY:HA2	1:A:129:SER:OG	2.20	0.41
1:A:212:GLU:OE2	1:A:216:ARG:HD2	2.21	0.41
1:A:332:VAL:HG21	1:A:546:GLY:C	2.46	0.41
1:A:334:PHE:O	1:B:276:GLY:HA2	2.21	0.41
1:A:384:LEU:HD23	1:A:384:LEU:HA	1.85	0.41
1:A:478:PRO:HG2	3:A:602:PER:O2	2.20	0.41
1:B:138:GLY:N	1:B:575:GLU:OE1	2.51	0.41
1:B:159:ALA:HB2	1:B:199:TRP:HB3	2.02	0.41
1:B:483:TYR:HD2	1:B:557:ASP:OD1	2.04	0.41
1:A:162:ALA:HB2	1:A:440:LEU:CD2	2.51	0.41
1:B:286:ILE:CG1	1:B:320:ARG:HG2	2.51	0.41
1:B:564:LEU:O	1:B:568:VAL:HG23	2.21	0.41
1:A:127:ASN:OD1	1:B:373:PHE:N	2.50	0.40
1:B:452:ARG:NH1	1:B:456:ILE:HD11	2.36	0.40
1:A:61:LYS:HE3	1:A:303:VAL:HG12	2.03	0.40
1:B:149:ALA:HB1	1:B:406:ARG:HD2	2.04	0.40
1:B:486:GLY:O	1:B:489:VAL:HG12	2.22	0.40
1:B:44:ARG:HA	1:B:53:PRO:HA	2.04	0.40
1:A:489:VAL:HG21	1:A:564:LEU:HD23	2.03	0.40
1:B:359:LEU:HD21	1:B:586:PHE:CD1	2.57	0.40
1:A:455:ASN:HA	1:A:458:ASP:HB2	2.03	0.40
1:A:499:LYS:HA	1:A:504:SER:HB3	2.04	0.40
1:B:99:PRO:HD3	1:B:305:ASP:HB3	2.03	0.40
1:B:338:TYR:CD1	1:B:386:THR:HG22	2.56	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	588/634 (93%)	576 (98%)	11 (2%)	1 (0%)	43	53
1	B	588/634 (93%)	572 (97%)	15 (3%)	1 (0%)	43	53
All	All	1176/1268 (93%)	1148 (98%)	26 (2%)	2 (0%)	44	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	337	LEU
1	A	337	LEU

5.3.2 Protein sidechains (i)

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	486/520 (94%)	465 (96%)	21 (4%)	26	38
1	B	486/520 (94%)	473 (97%)	13 (3%)	39	56
All	All	972/1040 (94%)	938 (96%)	34 (4%)	32	46

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LEU
1	A	96	THR
1	A	126	GLU
1	A	157	LEU

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Mol	Chain	Res	Type
1	A	172	GLU
1	A	212	GLU
1	A	229	ILE
1	A	243	ILE
1	A	248	LYS
1	A	252	SER
1	A	298	LYS
1	A	390	THR
1	A	396	VAL
1	A	438	GLU
1	A	506	ILE
1	A	529	THR
1	A	541	ASP
1	A	545	ILE
1	A	549	MET
1	A	557	ASP
1	A	595	THR
1	B	96	THR
1	B	126	GLU
1	B	163	GLU
1	B	164	LEU
1	B	229	ILE
1	B	296	ASP
1	B	298	LYS
1	B	371	ASP
1	B	390	THR
1	B	396	VAL
1	B	438	GLU
1	B	513	GLU
1	B	541	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	304	GLN
1	A	370	GLN
1	A	424	GLN
1	A	454	GLN
1	A	510	GLN
1	A	558	GLN
1	A	567	GLN
1	A	597	GLN

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Mol	Chain	Res	Type
1	B	45	ASN
1	B	68	ASN
1	B	183	ASN
1	B	454	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PER	A	602	-	1,1,1	2.03	1 (100%)	-		
2	VO4	B	602	1	0,4,4	-	-	-		
2	VO4	A	601	1	0,4,4	-	-	-		
3	PER	B	601	-	1,1,1	2.17	1 (100%)	-		
3	PER	B	604	-	1,1,1	2.14	1 (100%)	-		
3	PER	B	603	-	1,1,1	2.02	1 (100%)	-		

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	PER	O2-O1	-2.17	1.12	1.42
3	B	604	PER	O2-O1	-2.14	1.12	1.42
3	A	602	PER	O2-O1	-2.03	1.14	1.42
3	B	603	PER	O2-O1	-2.02	1.14	1.42

There are no bond angle outliers.

There are no chirality outliers.

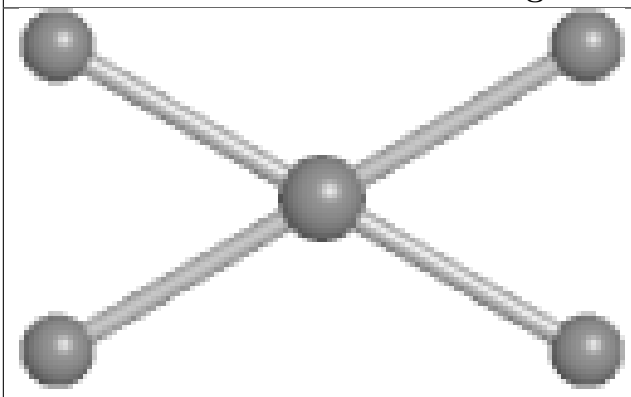
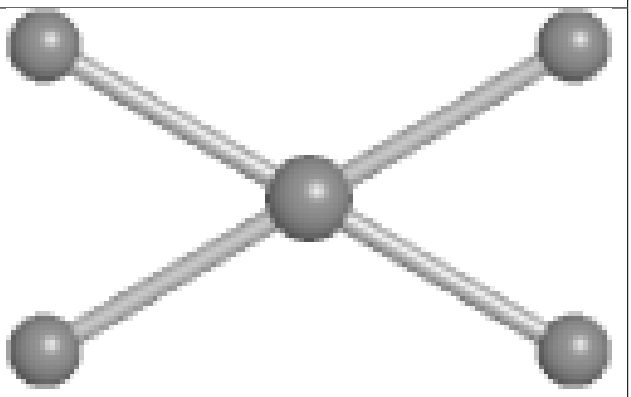
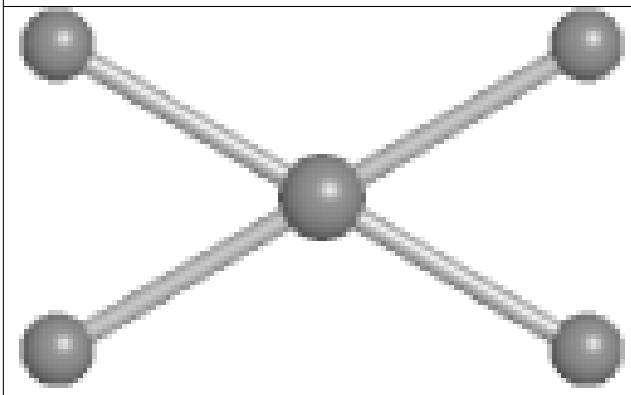
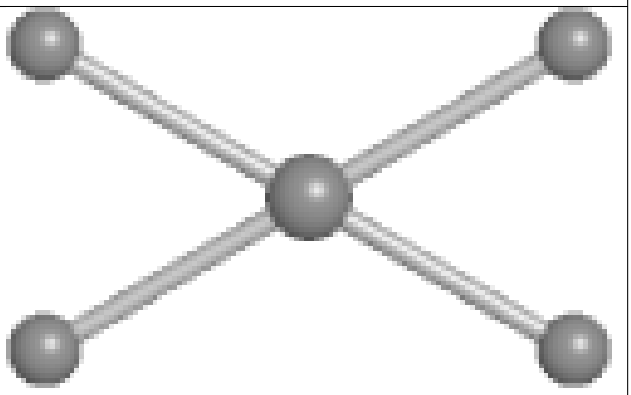
There are no torsion outliers.

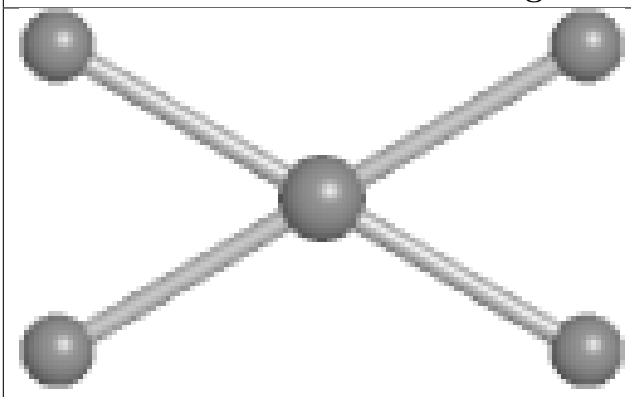
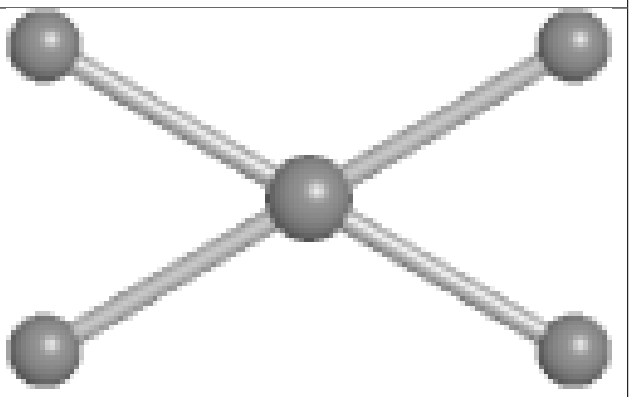
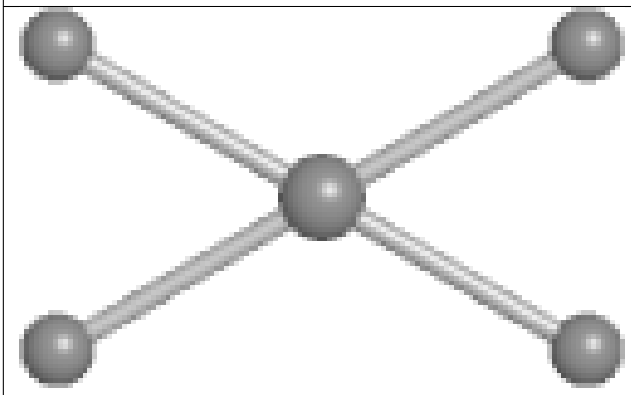
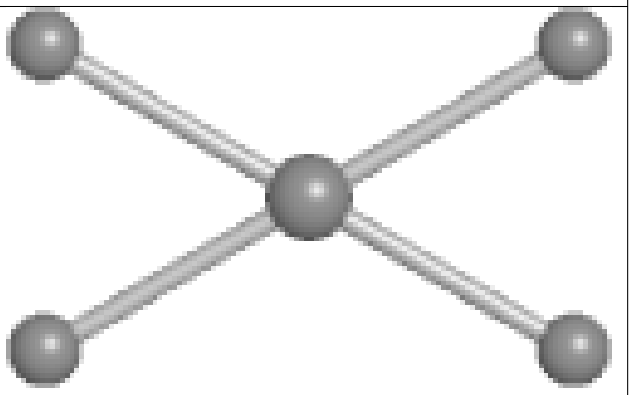
There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	PER	3	0
2	B	602	VO4	3	0
2	A	601	VO4	3	0
3	B	603	PER	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand VO4 B 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand VO4 A 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

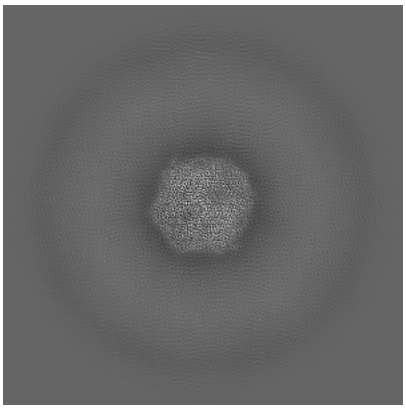
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-43270. These allow visual inspection of the internal detail of the map and identification of artifacts.

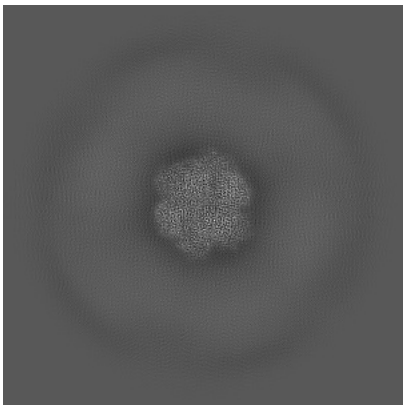
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

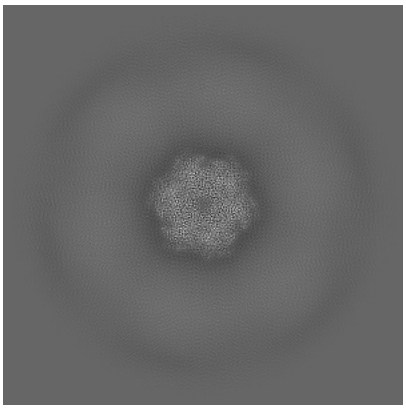
6.1.1 Primary map



X

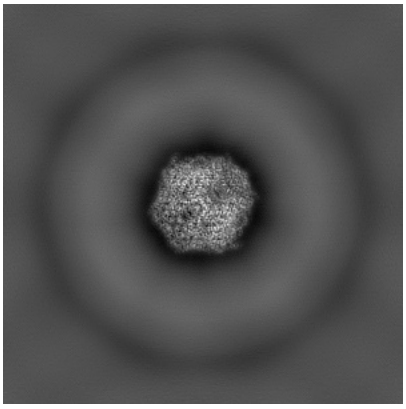


Y

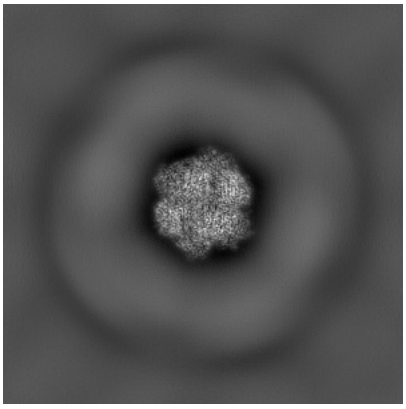


Z

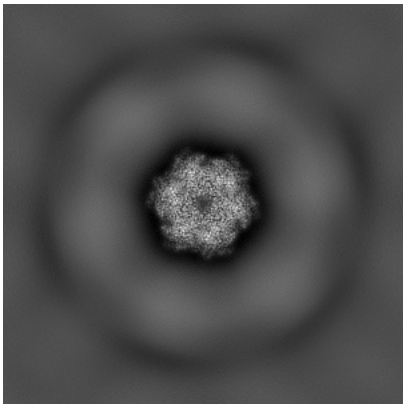
6.1.2 Raw map



X



Y

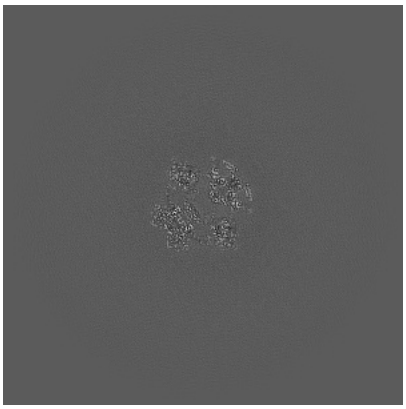


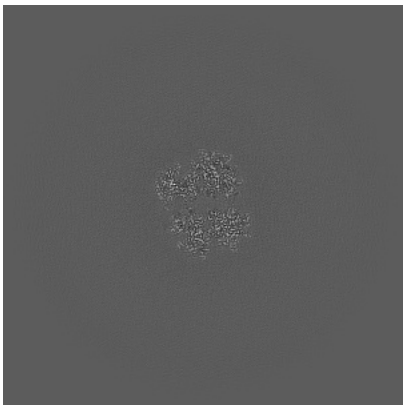
Z

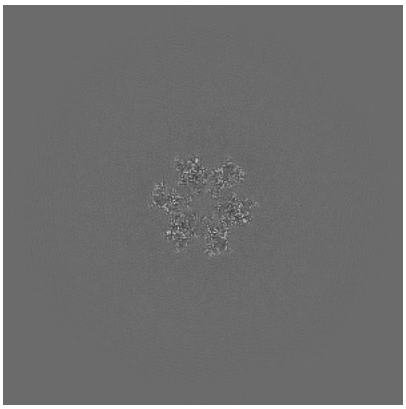
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

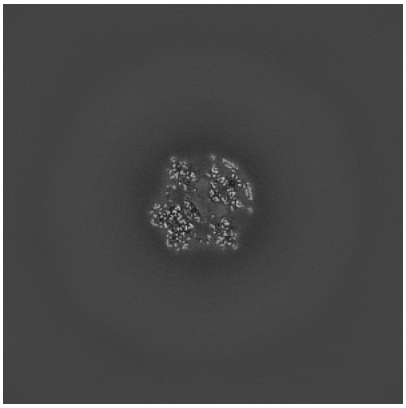
6.2.1 Primary map

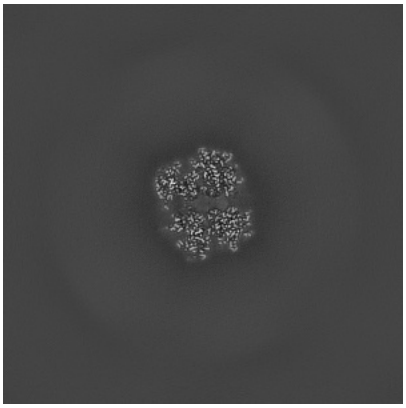

X Index: 256

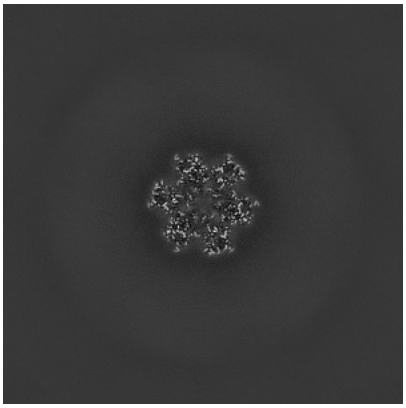

Y Index: 256


Z Index: 256

6.2.2 Raw map


X Index: 256

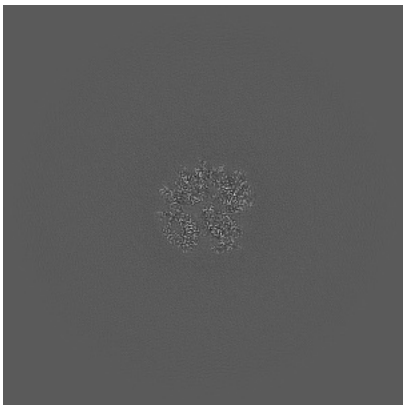

Y Index: 256


Z Index: 256

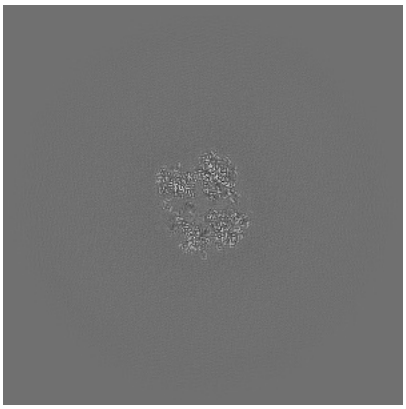
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

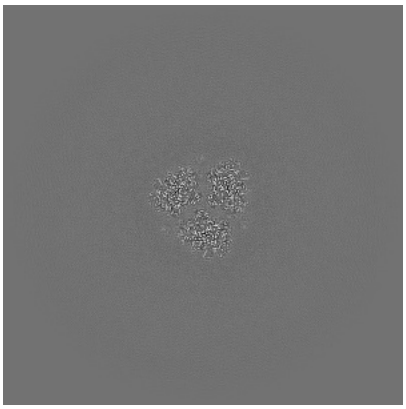
6.3.1 Primary map



X Index: 242

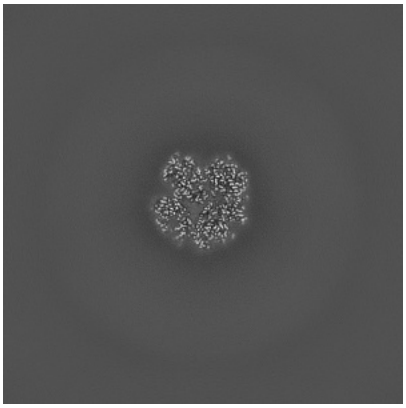


Y Index: 252

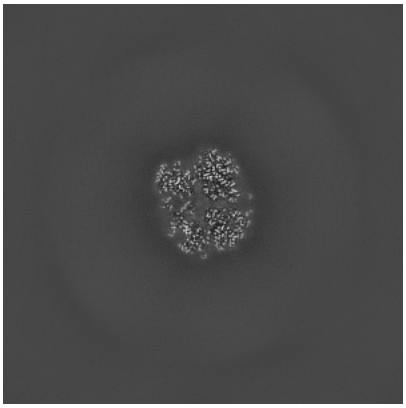


Z Index: 245

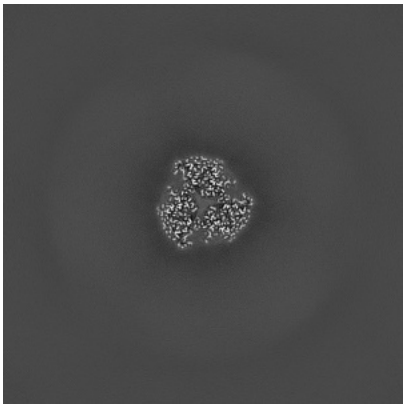
6.3.2 Raw map



X Index: 272



Y Index: 251

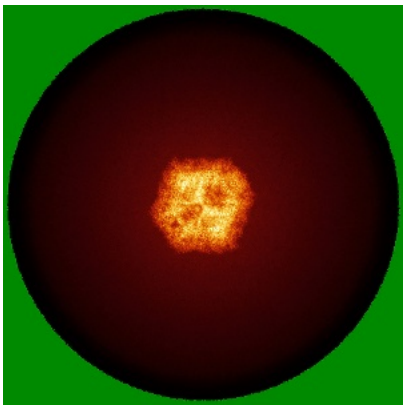


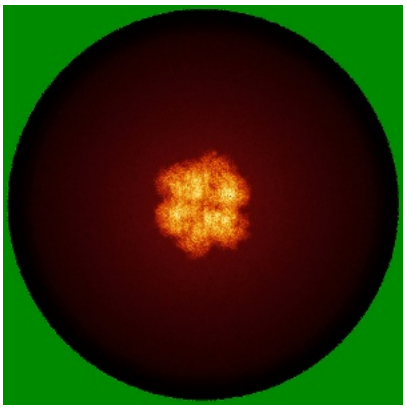
Z Index: 281

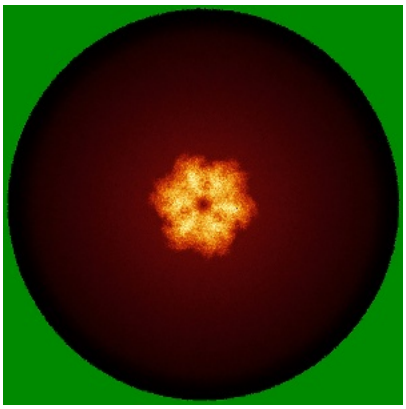
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

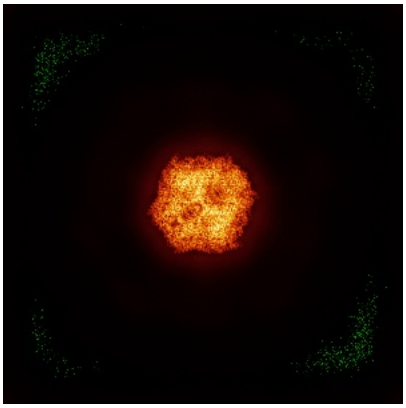
6.4.1 Primary map

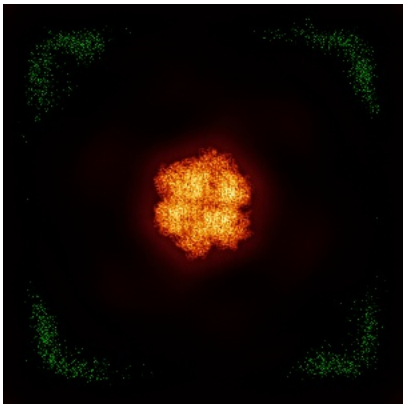

X

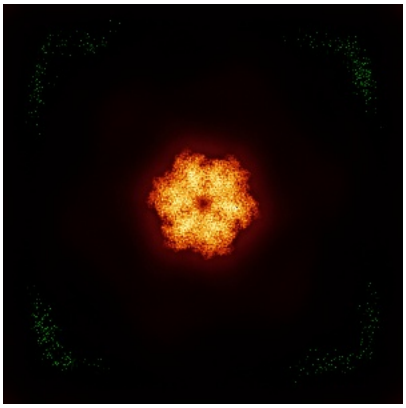

Y


Z

6.4.2 Raw map


X

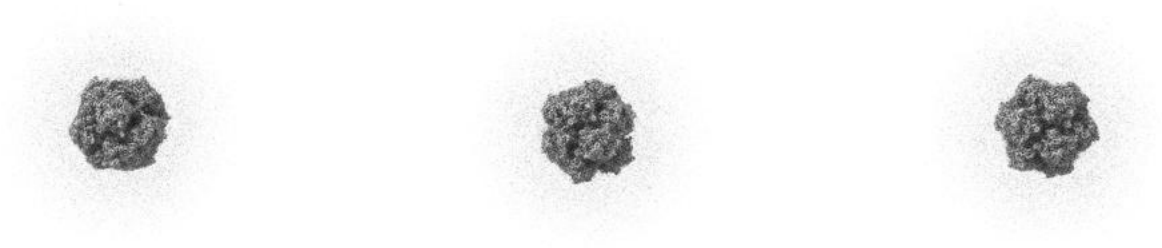

Y


Z

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

6.5 Orthogonal surface views (i)

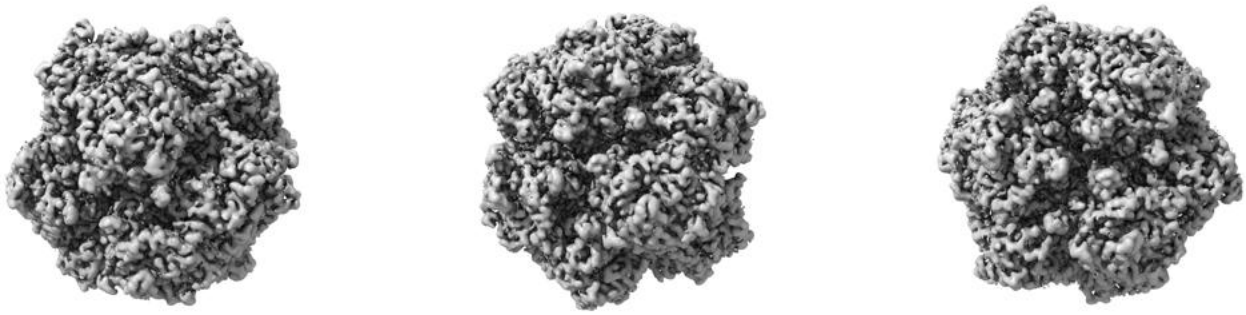
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

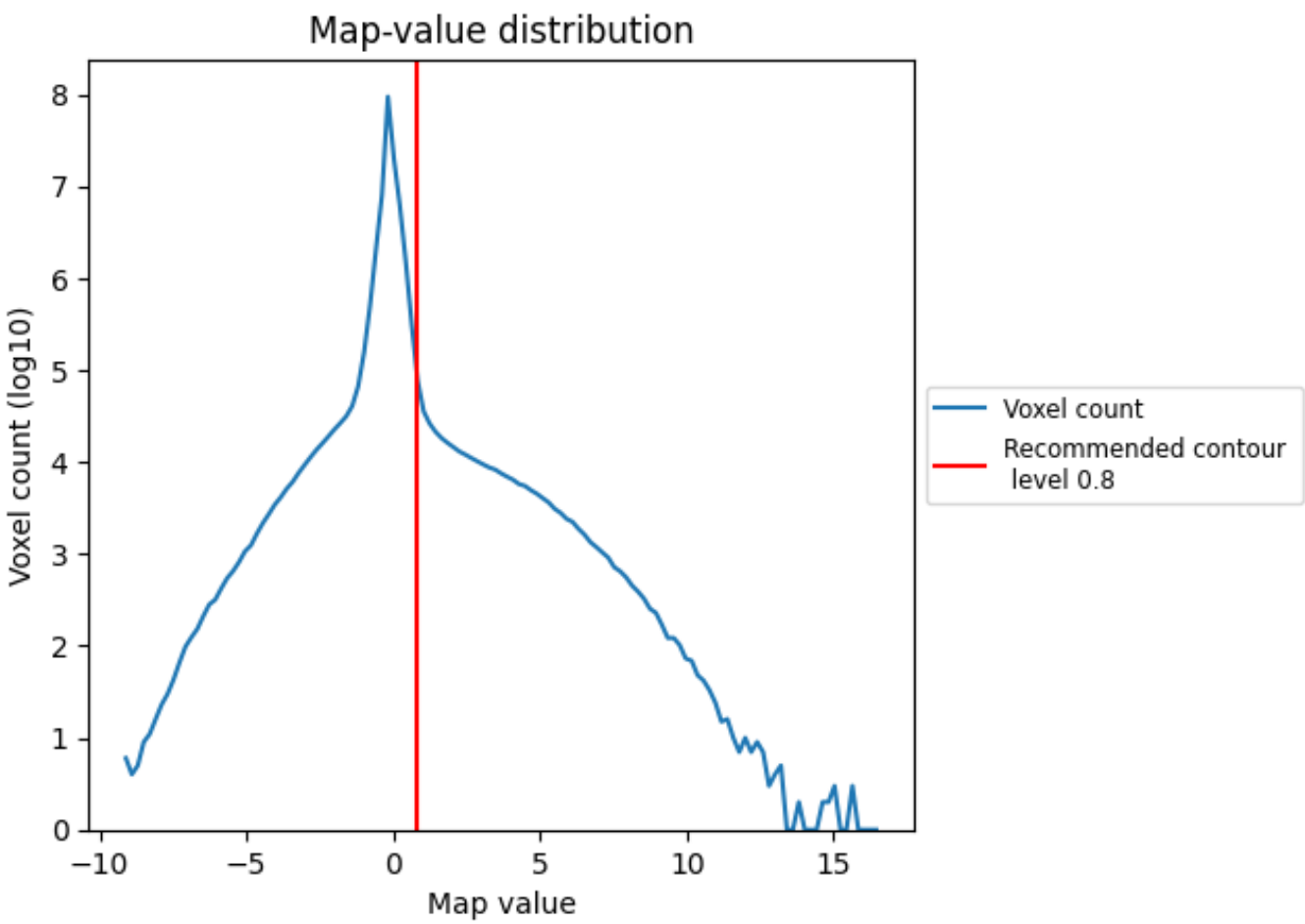
6.6 Mask visualisation (i)

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

7 Map analysis (i)

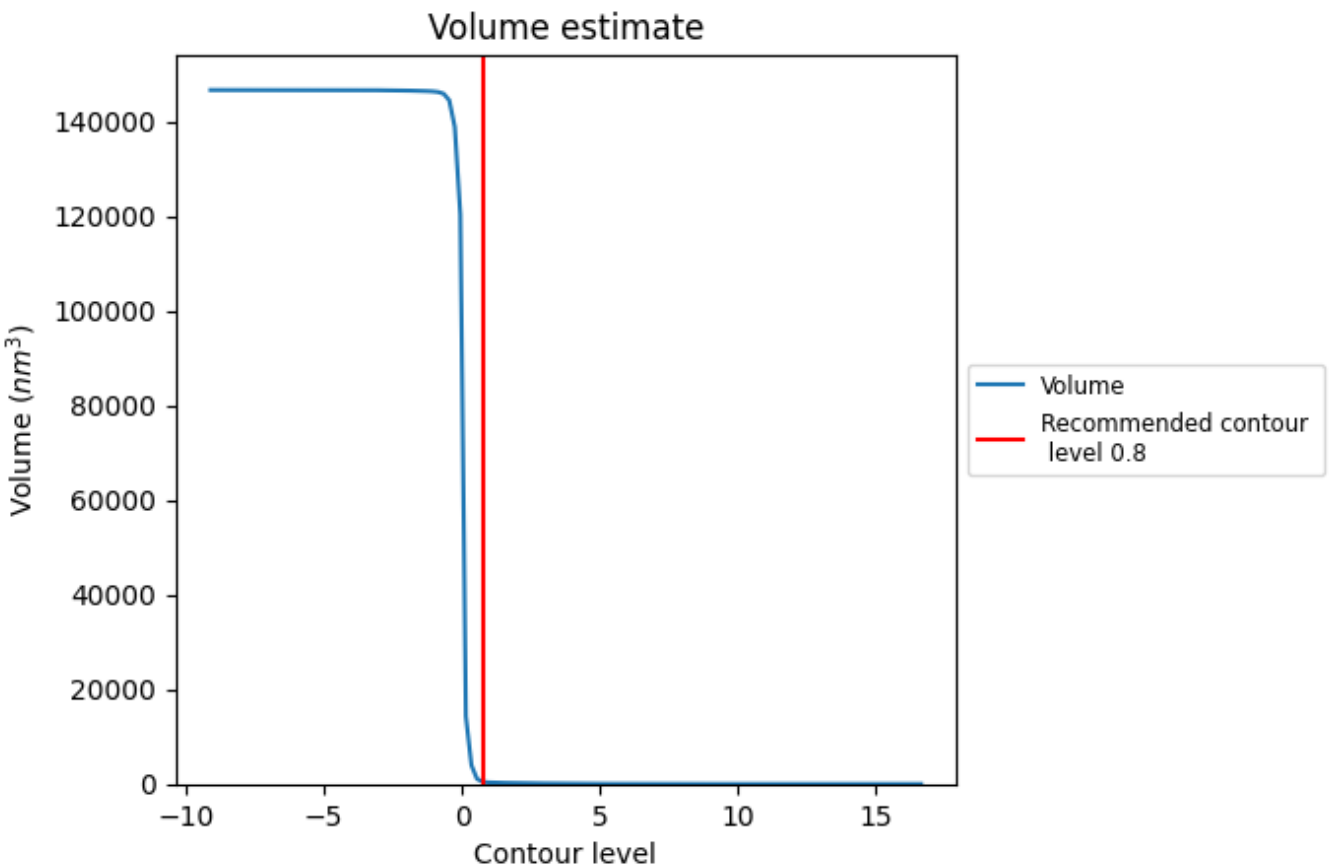
This section contains the results of statistical analysis of the map.

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.

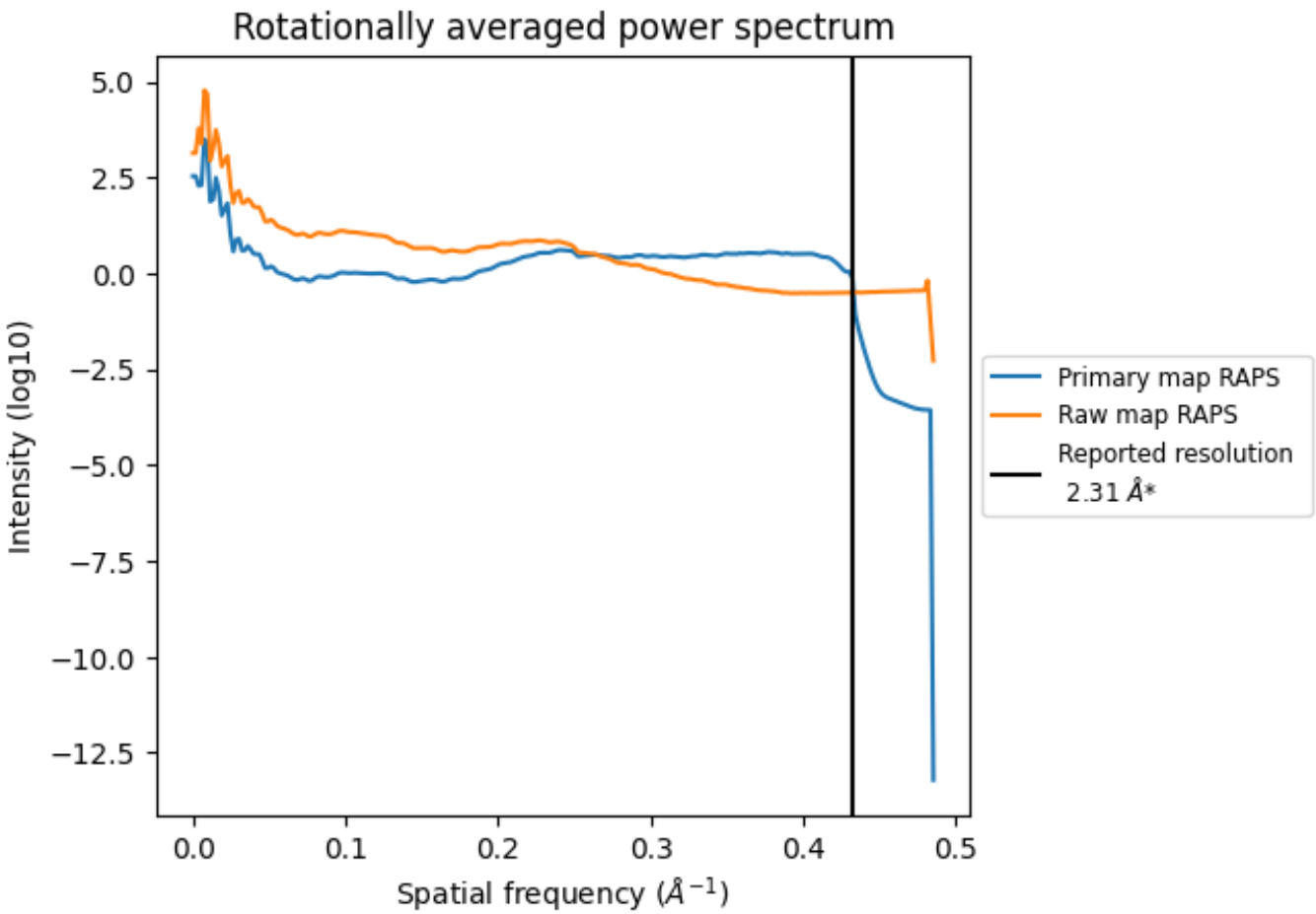
7.2 Volume estimate (i)



The volume at the recommended contour level is 429 nm^3; this corresponds to an approximate mass of 388 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)

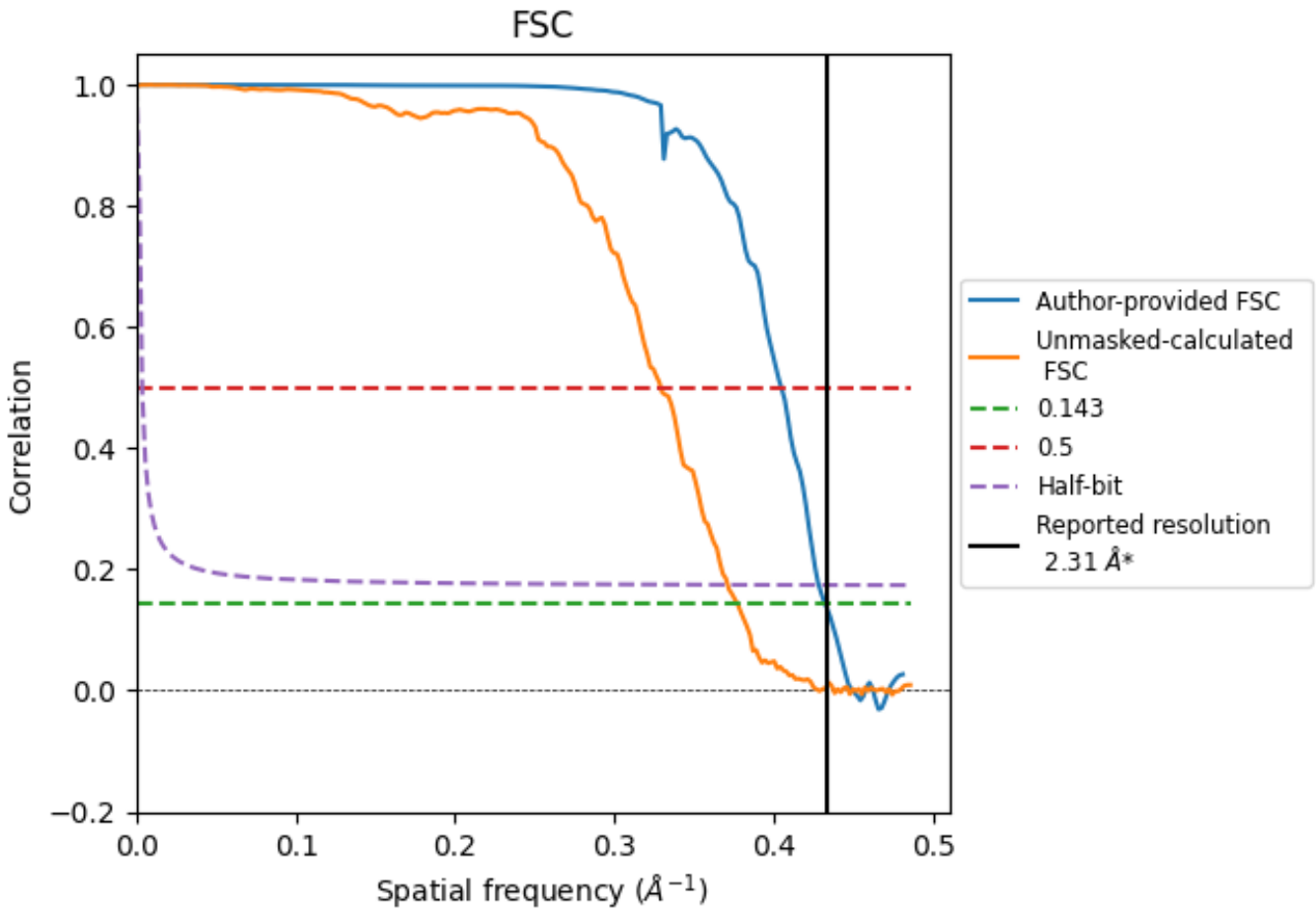


*Reported resolution corresponds to spatial frequency of 0.433 Å^{-1}

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 0.433 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.31	-	-
Author-provided FSC curve	2.31	2.47	2.34
Unmasked-calculated*	2.65	3.04	2.70

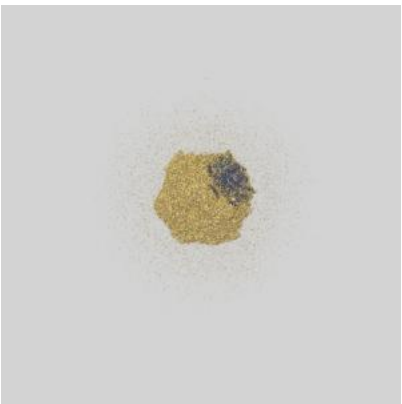
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.65 differs from the reported value 2.31 by more than 10 %

9 Map-model fit (i)

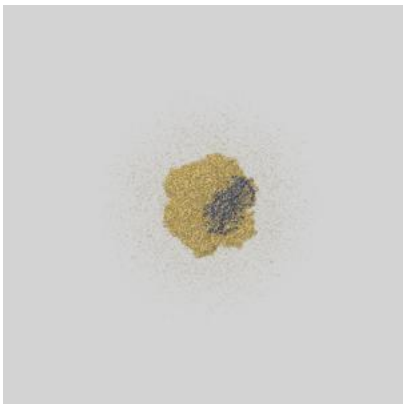
This section contains information regarding the fit between EMDB map EMD-43270 and PDB model 8VIX. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlays

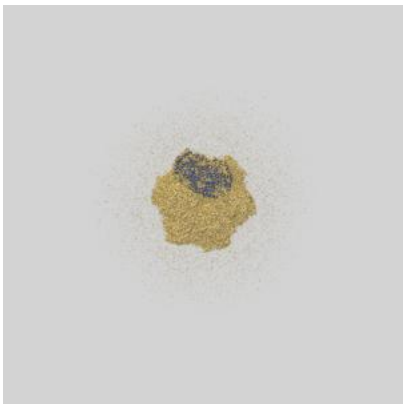
9.1.1 Map-model overlay (i)



X

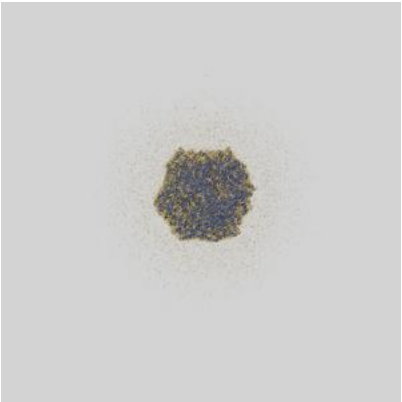


Y

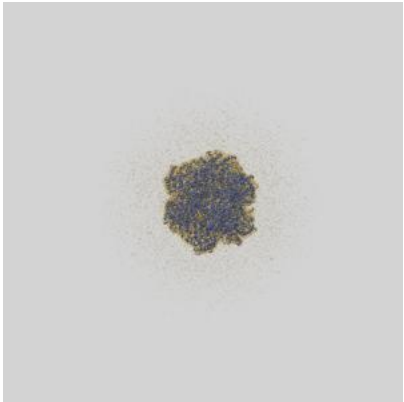


Z

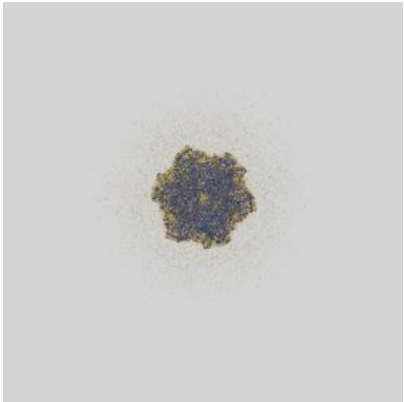
9.1.2 Map-model assembly overlay (i)



X



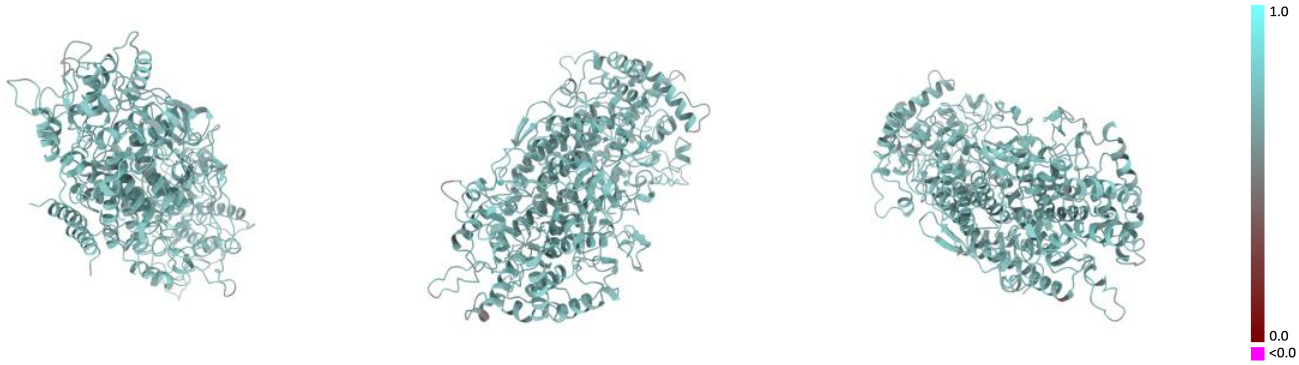
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.8 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.

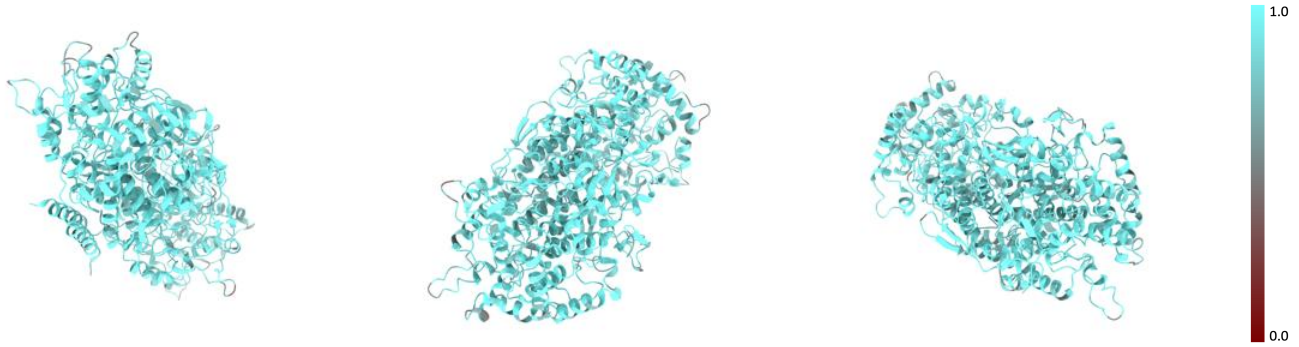
9.2 Q-score mapped to coordinate model (i)



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.

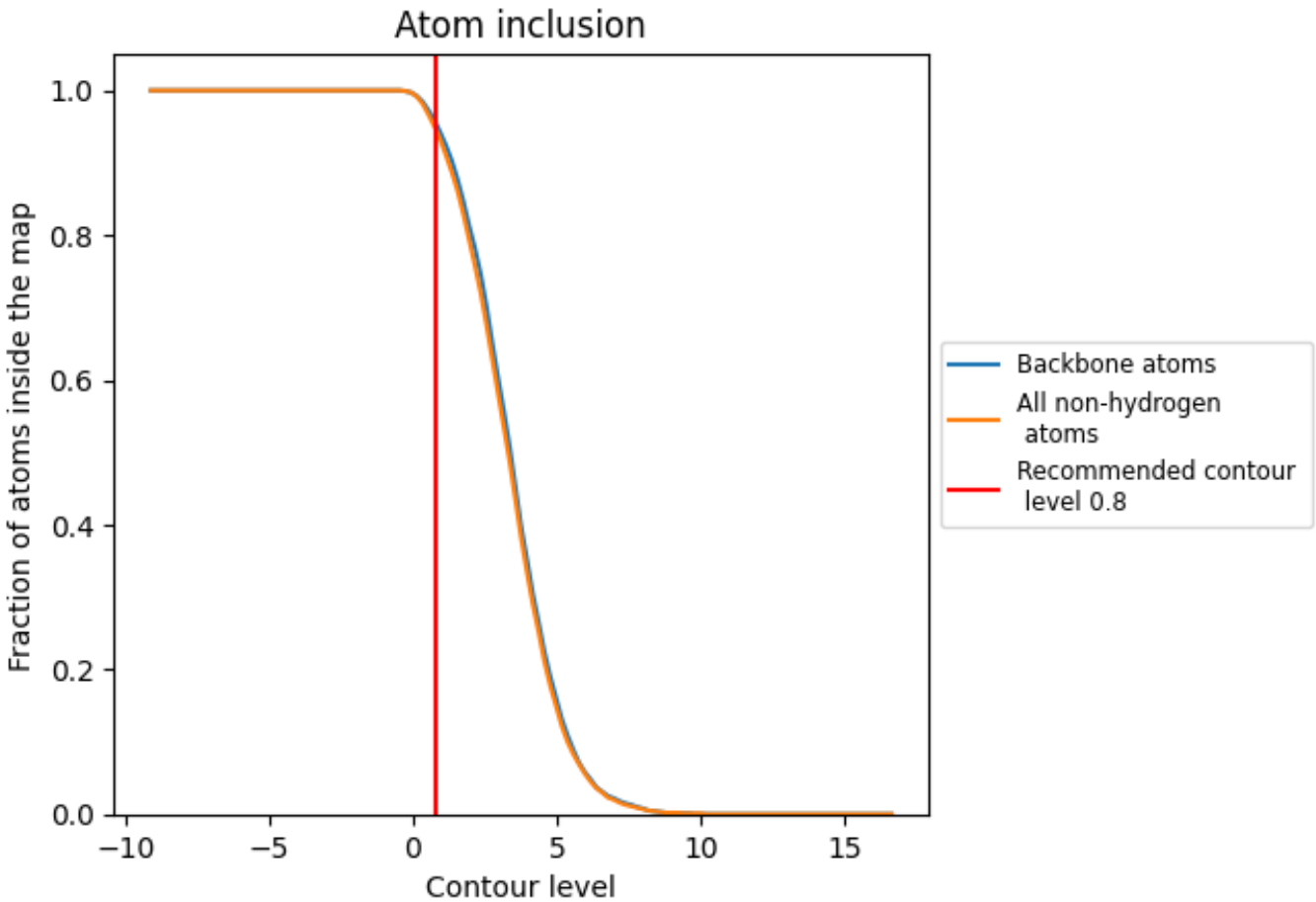
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.8).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9460	0.6840
A	0.9470	0.6830
B	0.9450	0.6840