Full wwPDB EM Validation Report (i)

Aug 5, 2026 – 10:47 AM EDT

PDB ID	:	8VSI / pdb_00008vsi
EMDB ID	:	EMD-43498
Title	:	Mechanistic Insights Revealed by YbtPQ in the Occluded State
Authors	:	Hu, W.; Parkinson, C.; Zheng, H.
Deposited on	:	2024-01-24
Resolution	:	3.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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:

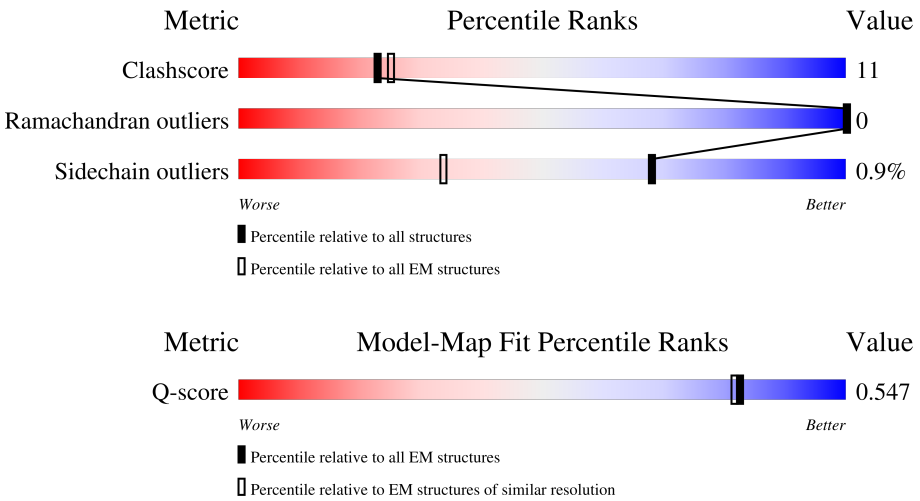
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 3.10 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	14724 (2.60 - 3.60)

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	600	18% 68% 26% 5%
2	B	600	16% 70% 25% • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8970 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 ABC transporter ATP-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	571	4428	2858	779	772	19	0	0

- Molecule 2 is a protein called Permease and ATP-binding protein of yersiniabactin-iron ABC transporter YbtQ.

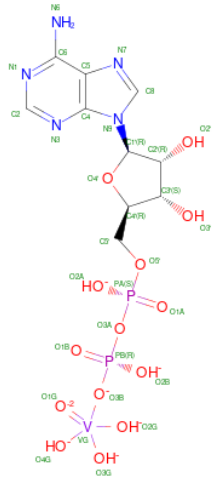
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	579	4476	2862	801	787	26	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
3	A	1	1	1	0
3	B	1	1	1	0

- Molecule 4 is ADP ORTHOVANADATE (CCD ID: AOV) (formula: $C_{10}H_{17}N_5O_{14}P_2V$) (labeled as "Ligand of Interest" by depositor).

AOV



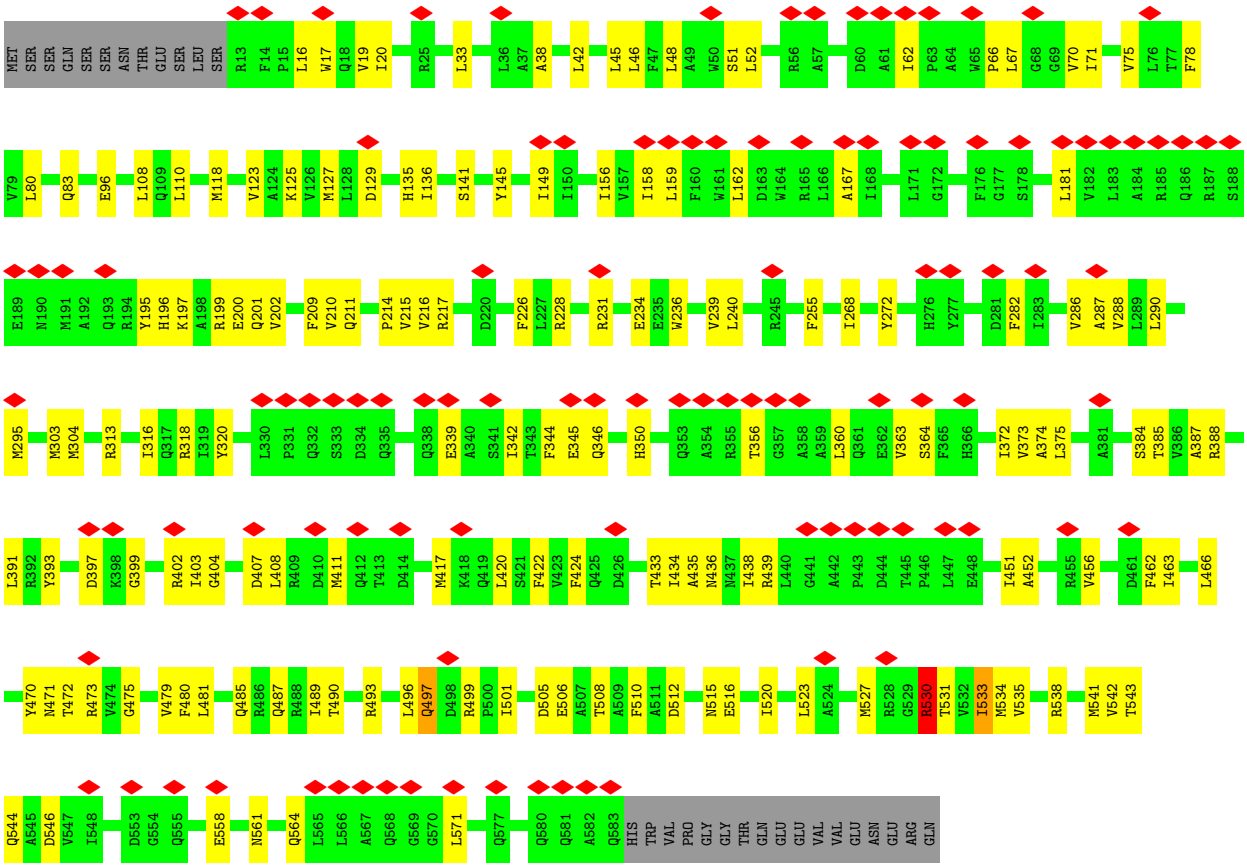
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	V	
4	A	1	32	10	5	14	2	1	0
			Total	C	N	O	P	V	
4	B	1	32	10	5	14	2	1	0

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.

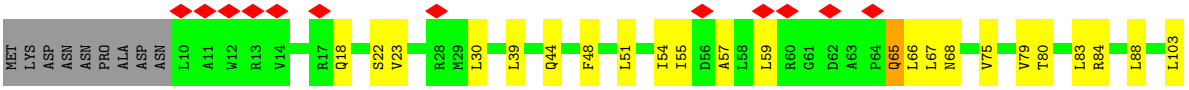
• Molecule 1: ABC transporter ATP-binding protein

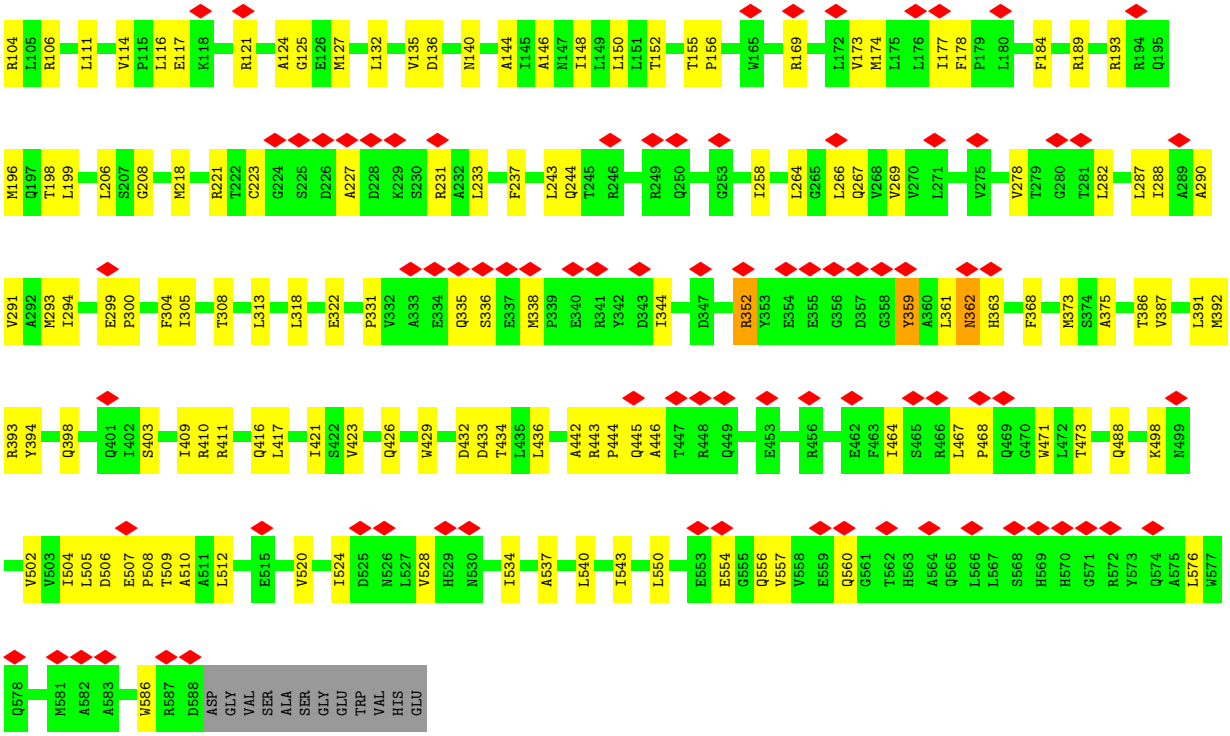
Chain A:



• Molecule 2: Permease and ATP-binding protein of yersiniabactin-iron ABC transporter YbtQ

Chain B:




R104 L105 R106 L111 V114 P115 L116 E117 K118 R121 A124 G125 E126 M127 L132 V135 D136 N140 A144 I145 A146 N147 I148 L149 L150 L151 T152 T155 P156 W165 R169 L172 V173 M174 L175 L176 I177 F178 P179 L180 F184 R189 R193 R194 Q195
M196 Q197 T198 L199 L206 S207 G208 M218 R221 T222 C223 G224 S225 D226 A227 D228 K229 S230 R231 A232 L233 F237 L243 Q244 T245 R246 R249 Q250 G253 I258 L264 G265 L266 Q267 V268 V269 V270 L271 V275 V278 T279 G280 T281 L282 L287 I288 A289 A290
V291 A292 M293 I294 E299 P300 F304 I305 T308 L313 L318 E322 P331 V332 A333 E334 Q335 S336 E337 M338 P339 E340 R341 Y342 D343 I344 D347 R352 Y353 E354 E355 G356 D357 G358 Y359 A360 L361 N362 H363 F368 M373 S374 A375 T386 V387 L391 M392
R393 Y394 Q398 Q401 I402 S403 I409 R410 R411 Q416 L417 I421 S422 V423 Q426 W429 D432 D433 T434 L435 L436 A442 R443 P444 Q445 A446 T447 R448 Q449 E453 R456 E462 F463 I464 S465 R466 L467 P468 Q469 G470 W471 L472 T473 Q488 K498 N499
V502 V503 I504 L505 D506 E507 P508 T509 A510 A511 L512 E515 V520 I524 D525 N526 L527 V528 H529 N530 I534 A537 L540 I543 L550 E553 E554 G555 Q556 V557 V558 E559 Q560 G561 T562 H563 A564 Q565 L566 L567 S568 H569 H570 G571 R572 Y573 Q574 A575 L576 W577
Q578 M581 A582 A583 W586 R587 D588 ASP GLY VAL SER ALA SER GLY GLU TRP VAL HIS GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	340080	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	5.072	Depositor
Minimum map value	-2.380	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.377	Depositor
Recommended contour level	0.86	Depositor
Map size (Å)	72.21, 84.659996, 133.63	wwPDB
Map dimensions	161, 102, 87	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83000004	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: MG, AOV

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	0.22	0/4524	0.44	1/6154 (0.0%)
2	B	0.17	0/4557	0.35	1/6190 (0.0%)
All	All	0.20	0/9081	0.40	2/12344 (0.0%)

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
2	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	359	TYR	CB-CA-C	7.81	122.82	111.73
1	A	530	ARG	N-CA-CB	-5.00	102.51	110.06

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	352	ARG	Sidechain

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	4428	0	4517	115	0
2	B	4476	0	4580	114	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	32	0	12	1	0
4	B	32	0	12	1	0
All	All	8970	0	9121	203	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 11.

All (203) 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:304:MET:HE2	2:B:148:ILE:HD11	1.57	0.86
2:B:196:MET:HE3	2:B:313:LEU:HB2	1.60	0.82
1:A:435:ALA:HB2	1:A:470:TYR:HB3	1.70	0.74
2:B:18:GLN:NE2	2:B:322:GLU:OE1	2.22	0.71
2:B:23:VAL:HG21	2:B:30:LEU:HD22	1.72	0.71
2:B:423:VAL:HG22	2:B:504:ILE:HB	1.77	0.66
1:A:129:ASP:OD2	1:A:199:ARG:NH2	2.28	0.66
2:B:335:GLN:NE2	2:B:336:SER:O	2.30	0.65
1:A:384:SER:OG	1:A:388:ARG:NH1	2.30	0.65
1:A:487:GLN:NE2	1:A:506:GLU:O	2.31	0.63
2:B:505:LEU:HB3	2:B:508:PRO:HG3	1.80	0.63
2:B:198:THR:HG22	2:B:243:LEU:HD21	1.81	0.63
1:A:75:VAL:HA	1:A:78:PHE:CE1	2.34	0.62
1:A:339:GLU:HB2	1:A:404:GLY:HA2	1.81	0.62
1:A:480:PHE:HZ	2:B:121:ARG:HA	1.64	0.61
1:A:156:ILE:HA	1:A:295:MET:HE2	1.82	0.61
2:B:103:LEU:HD23	2:B:135:VAL:HG13	1.82	0.61
2:B:266:LEU:HD12	2:B:294:ILE:HD12	1.83	0.60
2:B:442:ALA:HB1	2:B:498:LYS:HB2	1.84	0.59
1:A:48:LEU:HB2	1:A:70:VAL:HG21	1.84	0.59
1:A:374:ALA:HA	1:A:534:MET:HB3	1.84	0.59
1:A:195:TYR:HA	1:A:239:VAL:HG11	1.85	0.59
2:B:173:VAL:HG22	2:B:269:VAL:HG22	1.85	0.59
2:B:189:ARG:HH21	2:B:193:ARG:HH22	1.49	0.58
1:A:344:PHE:O	1:A:364:SER:HA	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:554:GLU:O	2:B:556:GLN:NE2	2.37	0.58
1:A:214:PRO:HG3	2:B:116:LEU:HD21	1.86	0.58
1:A:561:ASN:OD1	1:A:564:GLN:NE2	2.36	0.58
2:B:266:LEU:HD12	2:B:294:ILE:HG23	1.85	0.58
1:A:226:PHE:CE2	1:A:228:ARG:HB2	2.38	0.57
1:A:543:THR:HG23	1:A:544:GLN:HG3	1.86	0.57
2:B:488:GLN:HE22	2:B:510:ALA:H	1.52	0.57
1:A:546:ASP:O	1:A:561:ASN:ND2	2.38	0.57
1:A:228:ARG:NH2	2:B:432:ASP:O	2.38	0.57
1:A:433:THR:HG23	1:A:471:ASN:HA	1.86	0.57
1:A:268:ILE:HD13	2:B:54:ILE:HD13	1.88	0.56
2:B:375:ALA:HB1	2:B:543:ILE:HD12	1.87	0.56
1:A:516:GLU:O	1:A:520:ILE:HG12	2.06	0.56
1:A:108:LEU:O	2:B:221:ARG:NH2	2.39	0.56
1:A:475:GLY:HA3	1:A:479:VAL:HG12	1.88	0.56
1:A:360:LEU:HD22	1:A:363:VAL:HG21	1.88	0.55
2:B:426:GLN:HB2	2:B:506:ASP:OD2	2.07	0.54
2:B:75:VAL:O	2:B:79:VAL:HG23	2.07	0.54
2:B:80:THR:HG22	2:B:84:ARG:HH12	1.72	0.54
2:B:177:ILE:HG12	2:B:266:LEU:HD22	1.90	0.54
2:B:57:ALA:HB1	2:B:66:LEU:HB2	1.90	0.54
1:A:272:TYR:CE1	2:B:67:LEU:HB2	2.43	0.54
1:A:19:VAL:HG11	1:A:316:ILE:HG12	1.89	0.54
1:A:52:LEU:HD13	2:B:288:ILE:HG12	1.90	0.53
2:B:393:ARG:HH12	2:B:410:ARG:HG2	1.73	0.53
1:A:523:LEU:HD23	2:B:586:TRP:HH2	1.73	0.53
2:B:305:ILE:O	2:B:308:THR:OG1	2.26	0.52
1:A:420:LEU:HD23	1:A:501:ILE:HB	1.91	0.52
1:A:433:THR:HB	1:A:436:ASN:HB2	1.91	0.52
2:B:331:PRO:O	2:B:393:ARG:NH2	2.42	0.52
2:B:509:THR:HG22	2:B:512:LEU:HD12	1.91	0.52
1:A:433:THR:CG2	1:A:471:ASN:HA	2.40	0.52
1:A:497:GLN:HB3	1:A:499:ARG:HG3	1.91	0.52
1:A:527:MET:HA	1:A:530:ARG:HG3	1.91	0.52
1:A:387:ALA:HB1	1:A:422:PHE:HE1	1.75	0.52
1:A:403:ILE:HB	1:A:411:MET:HE1	1.91	0.51
1:A:342:ILE:HD11	1:A:501:ILE:HG21	1.93	0.51
1:A:434:ILE:HD12	1:A:472:THR:HB	1.93	0.51
2:B:290:ALA:O	2:B:294:ILE:HG12	2.11	0.51
1:A:159:LEU:HD22	1:A:295:MET:HE3	1.93	0.50
2:B:174:MET:HE3	2:B:294:ILE:HD11	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:GLN:HB2	2:B:80:THR:HG21	1.93	0.50
2:B:116:LEU:HD23	2:B:394:TYR:HD2	1.77	0.50
1:A:286:VAL:HG21	2:B:288:ILE:HD13	1.93	0.50
1:A:407:ASP:OD1	1:A:408:LEU:N	2.44	0.49
2:B:391:LEU:HD23	2:B:504:ILE:HD11	1.94	0.49
2:B:464:ILE:HA	2:B:467:LEU:HD12	1.95	0.49
1:A:217:ARG:NH2	2:B:114:VAL:O	2.44	0.49
1:A:127:MET:HE1	2:B:233:LEU:HD21	1.96	0.48
2:B:361:LEU:HD22	2:B:386:THR:HG22	1.95	0.48
2:B:433:ASP:CG	2:B:434:THR:H	2.21	0.48
1:A:196:HIS:CE1	1:A:318:ARG:HB2	2.48	0.48
1:A:231:ARG:HH21	1:A:234:GLU:CD	2.21	0.48
1:A:480:PHE:CZ	2:B:121:ARG:HA	2.48	0.48
1:A:46:LEU:HD21	1:A:158:ILE:HG21	1.96	0.48
2:B:206:LEU:HD11	2:B:237:PHE:CE1	2.49	0.48
1:A:16:LEU:HD11	1:A:313:ARG:HE	1.79	0.48
1:A:67:LEU:HA	1:A:70:VAL:HG12	1.96	0.48
2:B:373:MET:HB2	2:B:528:VAL:HG22	1.95	0.48
1:A:231:ARG:NH2	1:A:234:GLU:OE1	2.46	0.47
2:B:443:ARG:HE	2:B:446:ALA:HB2	1.79	0.47
1:A:346:GLN:H	1:A:364:SER:HB2	1.80	0.47
2:B:51:LEU:O	2:B:55:ILE:HG12	2.13	0.47
2:B:423:VAL:HA	2:B:504:ILE:O	2.15	0.47
2:B:338:MET:HE1	2:B:416:GLN:HB3	1.96	0.47
1:A:62:ILE:HD11	2:B:278:VAL:HG21	1.95	0.47
1:A:159:LEU:HB3	1:A:167:ALA:HB2	1.96	0.47
1:A:520:ILE:HD11	1:A:541:MET:HE3	1.96	0.47
1:A:558:GLU:OE2	1:A:571:LEU:N	2.46	0.47
2:B:409:ILE:HG23	2:B:417:LEU:HD13	1.96	0.46
2:B:421:ILE:HD13	2:B:502:VAL:HB	1.96	0.46
2:B:264:LEU:HA	2:B:267:GLN:HB2	1.97	0.46
2:B:436:LEU:HB2	2:B:471:TRP:HB3	1.97	0.46
2:B:39:LEU:HB3	2:B:83:LEU:HD13	1.96	0.46
2:B:504:ILE:HG12	2:B:534:ILE:HD12	1.97	0.46
1:A:215:VAL:HG21	2:B:429:TRP:HB2	1.98	0.46
2:B:111:LEU:HD21	2:B:127:MET:HE3	1.97	0.46
1:A:350:HIS:ND1	1:A:397:ASP:OD2	2.34	0.46
2:B:344:ILE:HB	2:B:368:PHE:HB2	1.97	0.46
1:A:159:LEU:HG	1:A:288:VAL:HG22	1.98	0.46
1:A:391:LEU:HG	1:A:417:MET:HE1	1.97	0.46
1:A:403:ILE:HG13	1:A:408:LEU:HD21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:LEU:O	2:B:291:VAL:HG23	2.16	0.45
2:B:444:PRO:HG2	2:B:445:GLN:HE22	1.81	0.45
1:A:110:LEU:O	2:B:221:ARG:NH2	2.50	0.45
1:A:373:VAL:HG13	1:A:533:ILE:HA	1.99	0.45
1:A:463:ILE:HA	1:A:466:LEU:HD12	1.98	0.45
2:B:117:GLU:O	2:B:121:ARG:HG2	2.16	0.45
1:A:387:ALA:HB1	1:A:422:PHE:CE1	2.52	0.45
1:A:452:ALA:O	1:A:456:VAL:HG23	2.16	0.45
2:B:146:ALA:O	2:B:150:LEU:HG	2.17	0.45
1:A:402:ARG:HG2	1:A:407:ASP:HA	1.99	0.45
1:A:512:ASP:OD1	1:A:512:ASP:N	2.49	0.45
2:B:65:GLN:HA	2:B:68:ASN:HB2	1.99	0.45
2:B:104:ARG:NH2	2:B:132:LEU:HD12	2.31	0.45
2:B:299:GLU:HB3	2:B:300:PRO:HD3	1.99	0.45
2:B:362:ASN:O	2:B:363:HIS:C	2.60	0.44
1:A:485:GLN:O	1:A:489:ILE:HG12	2.18	0.44
1:A:438:ILE:HG22	1:A:496:LEU:HD22	2.00	0.44
1:A:123:VAL:O	1:A:127:MET:HB2	2.18	0.44
1:A:228:ARG:HE	2:B:433:ASP:HB2	1.83	0.44
2:B:344:ILE:HG12	2:B:391:LEU:HD21	1.99	0.44
2:B:467:LEU:HD22	2:B:473:THR:HG21	1.99	0.44
1:A:96:GLU:OE2	1:A:135:HIS:HB2	2.18	0.44
2:B:173:VAL:HG13	2:B:269:VAL:HG13	1.99	0.44
2:B:537:ALA:HB3	2:B:543:ILE:HD13	2.00	0.44
1:A:197:LYS:O	1:A:201:GLN:HG2	2.18	0.44
2:B:18:GLN:HB3	2:B:318:LEU:HD22	2.00	0.44
1:A:424:PHE:CE2	2:B:218:MET:HB3	2.53	0.44
2:B:22:SER:O	2:B:106:ARG:NH2	2.51	0.44
2:B:540:LEU:HD11	2:B:576:LEU:HB3	1.99	0.44
1:A:211:GLN:HG3	2:B:124:ALA:HB2	2.00	0.43
1:A:499:ARG:HH22	2:B:223:CYS:HA	1.82	0.43
2:B:152:THR:HG21	2:B:304:PHE:HB2	2.00	0.43
2:B:361:LEU:HD11	2:B:387:VAL:HG23	2.00	0.43
1:A:162:LEU:HD21	1:A:287:ALA:HB1	2.01	0.43
2:B:392:MET:SD	2:B:423:VAL:HG21	2.58	0.43
1:A:210:VAL:HG11	2:B:124:ALA:HA	1.99	0.43
1:A:181:LEU:HD13	1:A:303:MET:HE2	2.00	0.43
1:A:508:THR:HB	1:A:516:GLU:HG3	1.99	0.43
1:A:17:TRP:CE3	1:A:20:ILE:HD11	2.54	0.43
1:A:141:SER:HB3	1:A:145:TYR:CE2	2.53	0.43
1:A:145:TYR:O	1:A:149:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:THR:N	4:A:702:AOV:O1A	2.50	0.43
2:B:199:LEU:HD11	2:B:244:GLN:HG2	2.00	0.43
1:A:282:PHE:CE2	2:B:59:LEU:HD12	2.54	0.43
1:A:345:GLU:O	1:A:399:GLY:CA	2.67	0.43
1:A:473:ARG:HD2	1:A:473:ARG:HA	1.86	0.43
1:A:490:THR:HG22	1:A:493:ARG:NH2	2.34	0.43
1:A:202:VAL:HG21	1:A:236:TRP:HB2	2.00	0.43
2:B:352:ARG:H	2:B:398:GLN:HE22	1.67	0.43
2:B:444:PRO:HG2	2:B:445:GLN:NE2	2.34	0.43
1:A:33:LEU:HD12	1:A:80:LEU:HD22	2.00	0.42
1:A:209:PHE:CE1	1:A:216:VAL:HG11	2.54	0.42
2:B:344:ILE:HA	2:B:403:SER:O	2.19	0.42
2:B:206:LEU:HD11	2:B:237:PHE:HE1	1.84	0.42
1:A:462:PHE:HE1	1:A:481:LEU:HD11	1.83	0.42
2:B:169:ARG:NH2	2:B:282:LEU:HB2	2.35	0.42
1:A:356:THR:H	2:B:468:PRO:HD3	1.85	0.42
1:A:67:LEU:O	1:A:71:ILE:HG22	2.19	0.42
1:A:505:ASP:HA	1:A:535:VAL:HB	2.01	0.42
1:A:516:GLU:OE1	1:A:538:ARG:NH1	2.46	0.42
2:B:336:SER:HB2	2:B:411:ARG:NH2	2.34	0.42
1:A:388:ARG:HD2	1:A:393:TYR:CD1	2.54	0.42
1:A:515:ASN:C	1:A:515:ASN:HD22	2.28	0.42
2:B:520:VAL:O	2:B:524:ILE:HG12	2.20	0.42
2:B:125:GLY:HA3	2:B:208:GLY:HA2	2.02	0.42
2:B:227:ALA:O	2:B:231:ARG:HB2	2.20	0.42
1:A:374:ALA:HB1	1:A:542:VAL:HG12	2.01	0.41
1:A:375:LEU:HB2	1:A:534:MET:O	2.20	0.41
2:B:104:ARG:HD2	2:B:135:VAL:HG11	2.01	0.41
2:B:155:THR:HB	2:B:156:PRO:HD3	2.02	0.41
2:B:361:LEU:HD11	2:B:387:VAL:CG2	2.51	0.41
2:B:136:ASP:HB2	2:B:140:ASN:ND2	2.35	0.41
2:B:421:ILE:HG22	2:B:423:VAL:HG23	2.01	0.41
1:A:33:LEU:HG	1:A:83:GLN:OE1	2.21	0.41
1:A:451:ILE:HG12	1:A:470:TYR:CE1	2.55	0.41
1:A:118:MET:HE2	1:A:123:VAL:HG22	2.02	0.41
1:A:136:ILE:HD13	1:A:136:ILE:HA	1.97	0.41
1:A:480:PHE:HA	4:B:702:AOV:C6	2.50	0.41
1:A:125:LYS:HD2	1:A:200:GLU:OE2	2.20	0.41
1:A:19:VAL:HG12	1:A:320:TYR:CE1	2.56	0.41
1:A:38:ALA:O	1:A:42:LEU:HD23	2.20	0.41
1:A:255:PHE:HD2	2:B:88:LEU:HD13	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:MET:HE3	2:B:221:ARG:HG2	2.02	0.41
2:B:144:ALA:O	2:B:148:ILE:HG12	2.21	0.41
1:A:510:PHE:HD1	2:B:507:GLU:OE1	2.04	0.41
2:B:156:PRO:HB2	2:B:178:PHE:HZ	1.86	0.41
1:A:240:LEU:HD23	1:A:240:LEU:HA	1.96	0.40
1:A:435:ALA:O	1:A:439:ARG:HG2	2.21	0.40
2:B:48:PHE:O	2:B:293:MET:HE2	2.21	0.40
2:B:392:MET:HE3	2:B:392:MET:HB2	1.89	0.40
2:B:550:LEU:HD12	2:B:557:VAL:HG11	2.03	0.40
1:A:51:SER:OG	1:A:66:PRO:HB2	2.22	0.40
2:B:550:LEU:HD13	2:B:560:GLN:HG3	2.02	0.40
1:A:45:LEU:HD12	1:A:290:LEU:HB3	2.03	0.40
2:B:184:PHE:CD2	2:B:258:ILE:HG12	2.56	0.40
2:B:344:ILE:HD12	2:B:344:ILE:H	1.87	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	569/600 (95%)	547 (96%)	22 (4%)	0	100	100
2	B	577/600 (96%)	572 (99%)	5 (1%)	0	100	100
All	All	1146/1200 (96%)	1119 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	457/490 (93%)	452 (99%)	5 (1%)	65	78
2	B	458/486 (94%)	455 (99%)	3 (1%)	76	82
All	All	915/976 (94%)	907 (99%)	8 (1%)	68	80

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	372	ILE
1	A	497	GLN
1	A	530	ARG
1	A	531	THR
1	A	533	ILE
2	B	65	GLN
2	B	359	TYR
2	B	362	ASN

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

Mol	Chain	Res	Type
1	A	335	GLN
1	A	336	GLN
1	A	371	GLN
1	A	412	GLN
1	A	561	ASN
1	A	564	GLN
2	B	128	ASN
2	B	363	HIS
2	B	445	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
4	AOV	A	702	3	32,34,34	2.25	6 (18%)	42,56,56	2.82	14 (33%)
4	AOV	B	702	3	32,34,34	2.25	6 (18%)	42,56,56	2.81	14 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AOV	A	702	3	-	6/16/39/39	0/3/3/3
4	AOV	B	702	3	-	6/16/39/39	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	702	AOV	O1G-VG	10.07	1.78	1.61
4	A	702	AOV	O1G-VG	10.07	1.78	1.61
4	A	702	AOV	C5-C4	4.23	1.46	1.39
4	B	702	AOV	C5-C4	4.16	1.46	1.39
4	B	702	AOV	C5-C6	3.05	1.49	1.41
4	A	702	AOV	C5-C6	3.05	1.49	1.41
4	A	702	AOV	C4-N9	-2.51	1.32	1.37
4	B	702	AOV	C4-N9	-2.49	1.32	1.37
4	A	702	AOV	C5-N7	-2.33	1.34	1.39
4	B	702	AOV	C5-N7	-2.29	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	702	AOV	C8-N7	2.05	1.35	1.31
4	A	702	AOV	C8-N7	2.02	1.35	1.31

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	702	AOV	N3-C4-N9	8.71	141.99	127.17
4	B	702	AOV	N3-C4-N9	8.67	141.91	127.17
4	A	702	AOV	C4-N9-C8	7.72	113.85	105.74
4	B	702	AOV	C4-N9-C8	7.72	113.84	105.74
4	A	702	AOV	C5-C4-N3	-6.24	118.12	126.72
4	B	702	AOV	C5-C4-N3	-6.22	118.16	126.72
4	A	702	AOV	C5-C4-N9	-5.43	99.89	105.81
4	B	702	AOV	C5-C4-N9	-5.40	99.93	105.81
4	A	702	AOV	C2-N3-C4	4.41	122.61	111.83
4	B	702	AOV	C2-N3-C4	4.39	122.56	111.83
4	B	702	AOV	O3A-PA-O1A	-3.80	99.28	110.70
4	A	702	AOV	O3A-PA-O1A	-3.79	99.30	110.70
4	B	702	AOV	N3-C2-N1	-3.64	123.07	128.58
4	A	702	AOV	N3-C2-N1	-3.63	123.08	128.58
4	A	702	AOV	O2A-PA-O1A	3.06	126.69	112.44
4	B	702	AOV	O2A-PA-O1A	3.06	126.68	112.44
4	A	702	AOV	N9-C8-N7	-2.95	109.75	113.94
4	B	702	AOV	N9-C8-N7	-2.95	109.75	113.94
4	B	702	AOV	C2'-C3'-C4'	-2.85	97.10	102.61
4	A	702	AOV	C2'-C3'-C4'	-2.84	97.12	102.61
4	B	702	AOV	O4'-C1'-N9	2.64	113.15	108.09
4	A	702	AOV	O4'-C1'-N9	2.63	113.13	108.09
4	A	702	AOV	O3'-C3'-C4'	-2.54	103.78	111.08
4	B	702	AOV	O3'-C3'-C4'	-2.54	103.79	111.08
4	B	702	AOV	O4'-C4'-C3'	2.51	110.14	105.15
4	A	702	AOV	O4'-C4'-C3'	2.50	110.11	105.15
4	A	702	AOV	C3'-C2'-C1'	2.45	106.10	101.46
4	B	702	AOV	C3'-C2'-C1'	2.44	106.08	101.46

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	702	AOV	C5'-O5'-PA-O1A
4	B	702	AOV	C5'-O5'-PA-O1A
4	A	702	AOV	O4'-C4'-C5'-O5'

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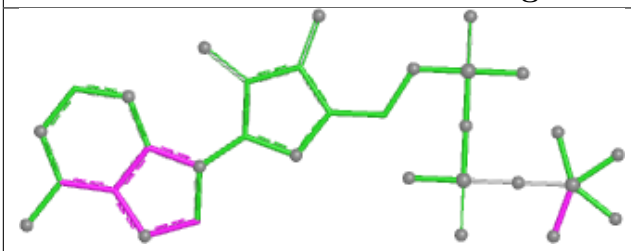
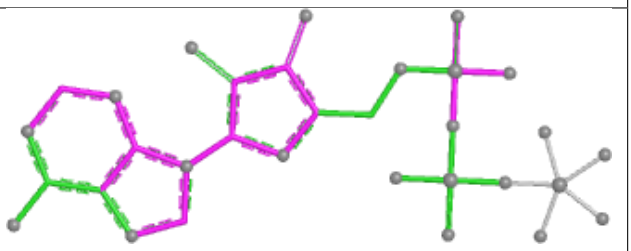
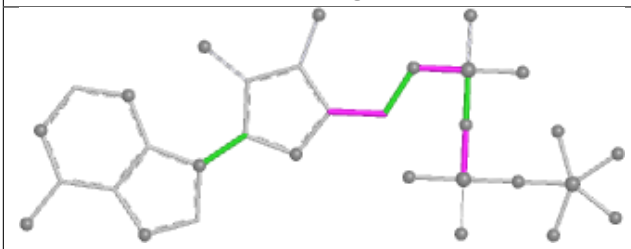
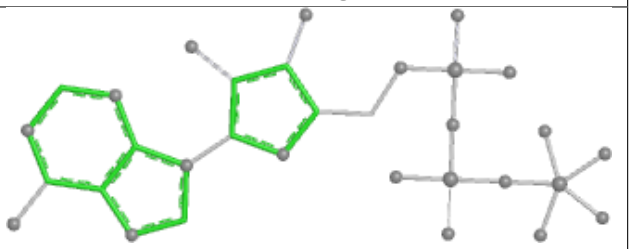
Mol	Chain	Res	Type	Atoms
4	B	702	AOV	O4'-C4'-C5'-O5'
4	A	702	AOV	C3'-C4'-C5'-O5'
4	B	702	AOV	C3'-C4'-C5'-O5'
4	A	702	AOV	C5'-O5'-PA-O2A
4	A	702	AOV	C5'-O5'-PA-O3A
4	B	702	AOV	C5'-O5'-PA-O2A
4	B	702	AOV	C5'-O5'-PA-O3A
4	A	702	AOV	PA-O3A-PB-O2B
4	B	702	AOV	PA-O3A-PB-O2B

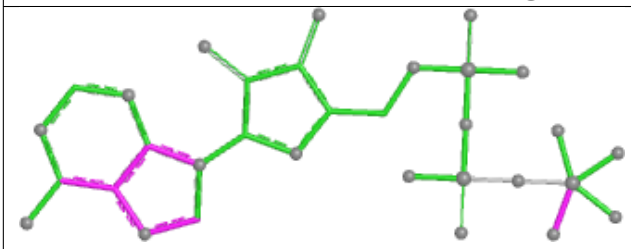
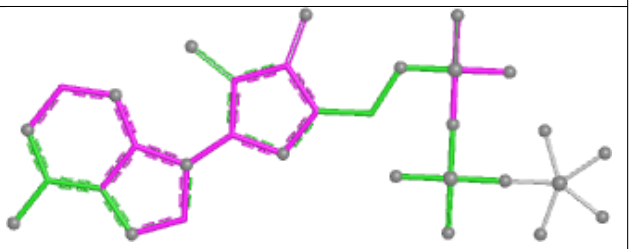
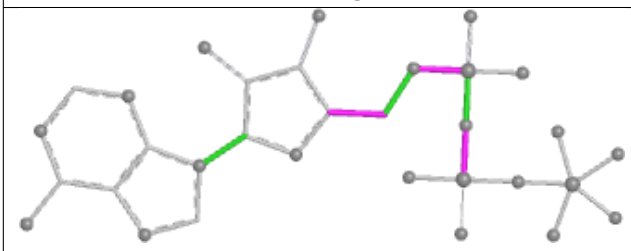
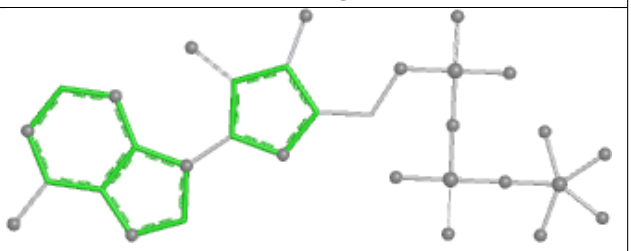
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	702	AOV	1	0
4	B	702	AOV	1	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 AOV A 702	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AOV B 702	
 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.

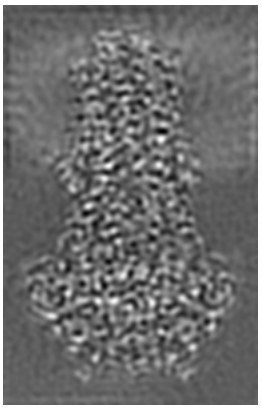
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-43498. These allow visual inspection of the internal detail of the map and identification of artifacts.

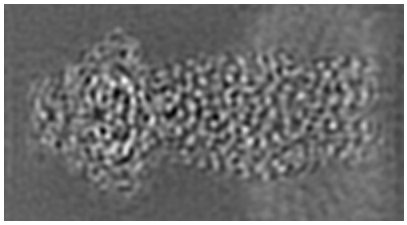
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

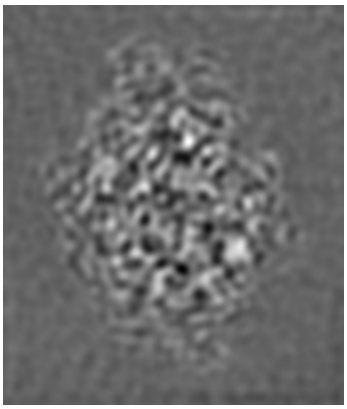
6.1.1 Primary map



X

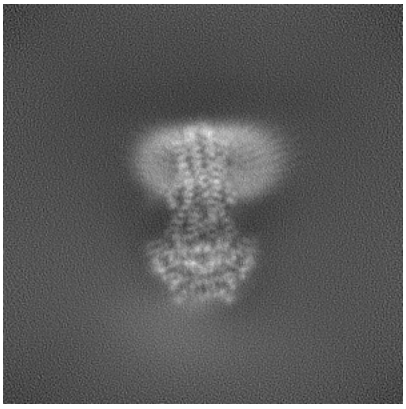


Y

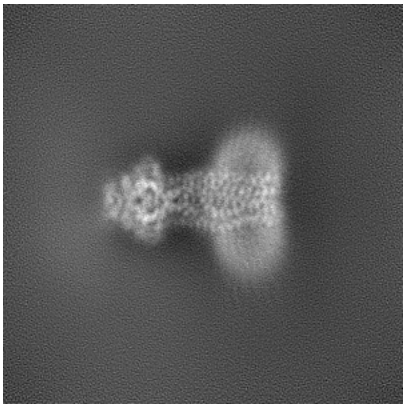


Z

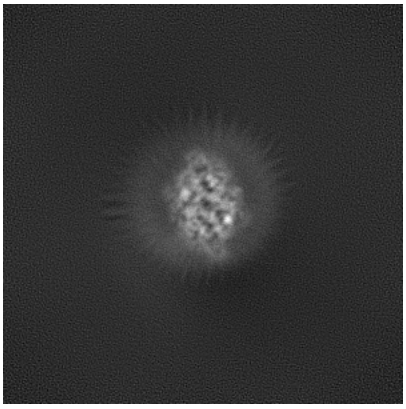
6.1.2 Raw map



X



Y

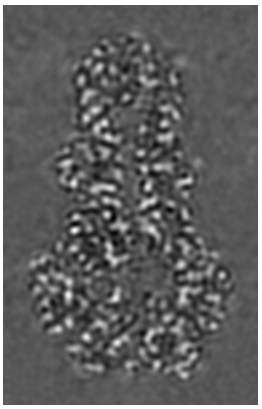


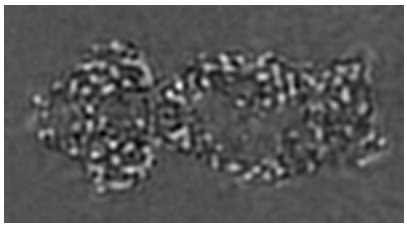
Z

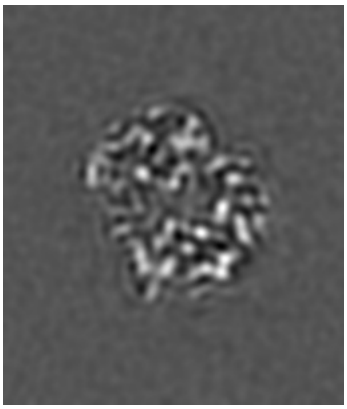
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

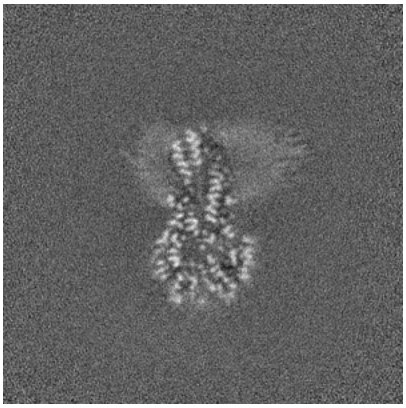
6.2.1 Primary map

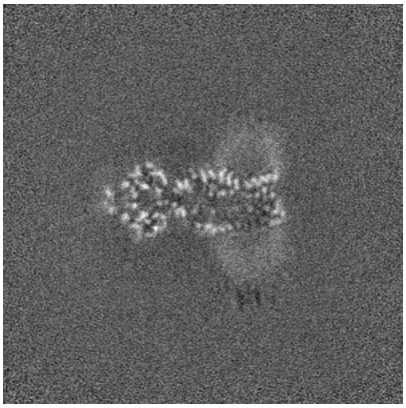

X Index: 43

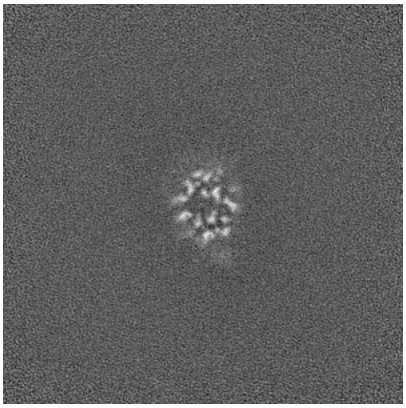

Y Index: 51


Z Index: 80

6.2.2 Raw map


X Index: 160

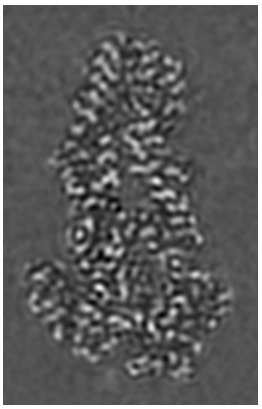

Y Index: 160


Z Index: 160

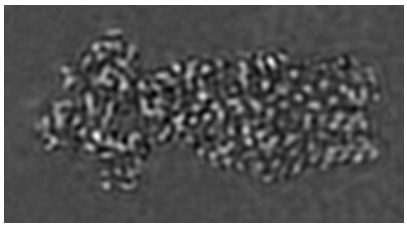
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

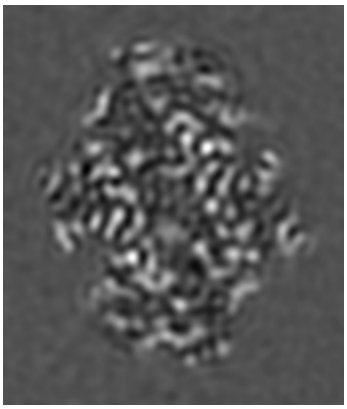
6.3.1 Primary map



X Index: 48

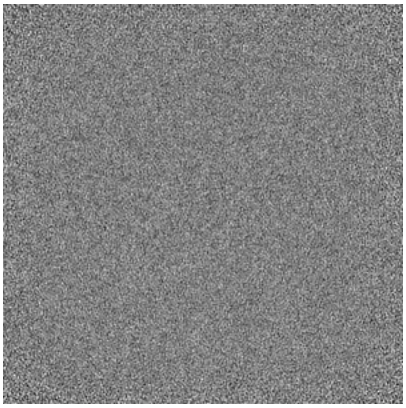


Y Index: 43

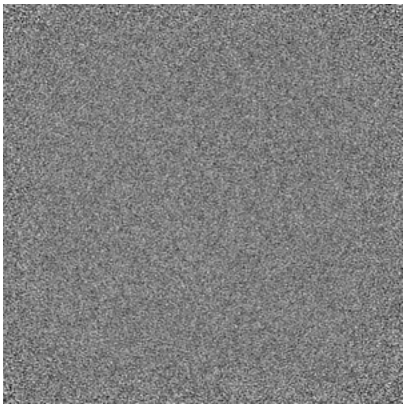


Z Index: 41

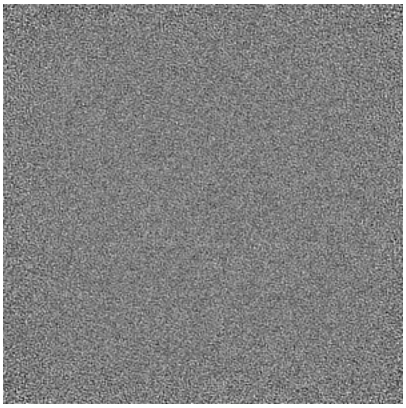
6.3.2 Raw map



X Index: 0



Y Index: 0

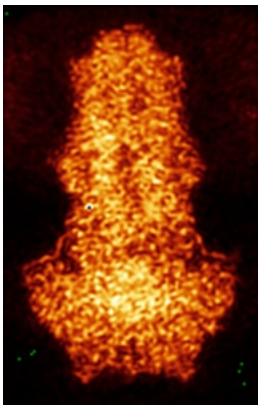


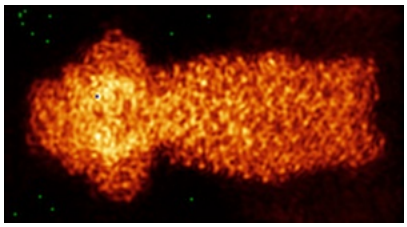
Z Index: 0

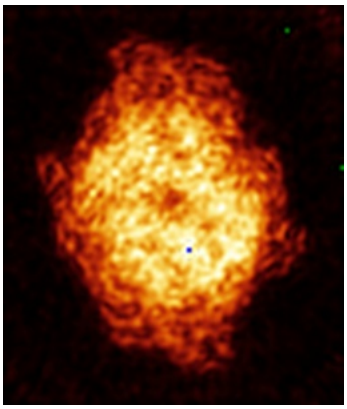
The images above show the largest variance slices of the map in three orthogonal directions.

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

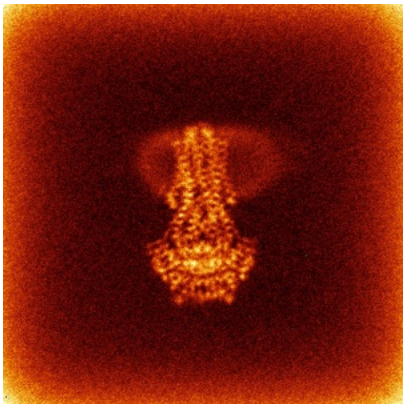
6.4.1 Primary map

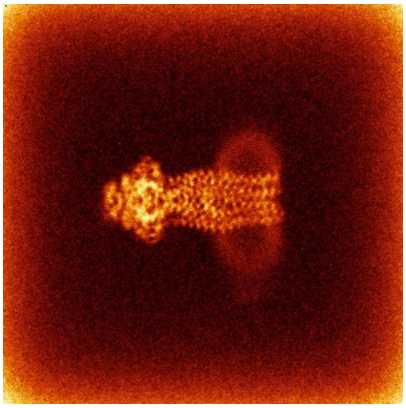

X

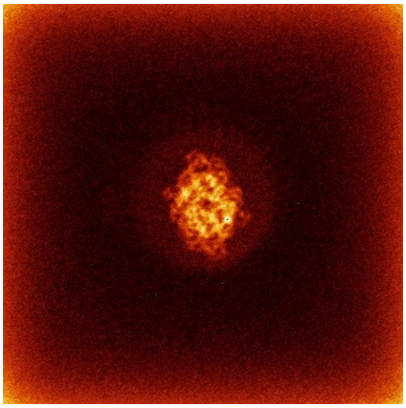

Y


Z

6.4.2 Raw map


X

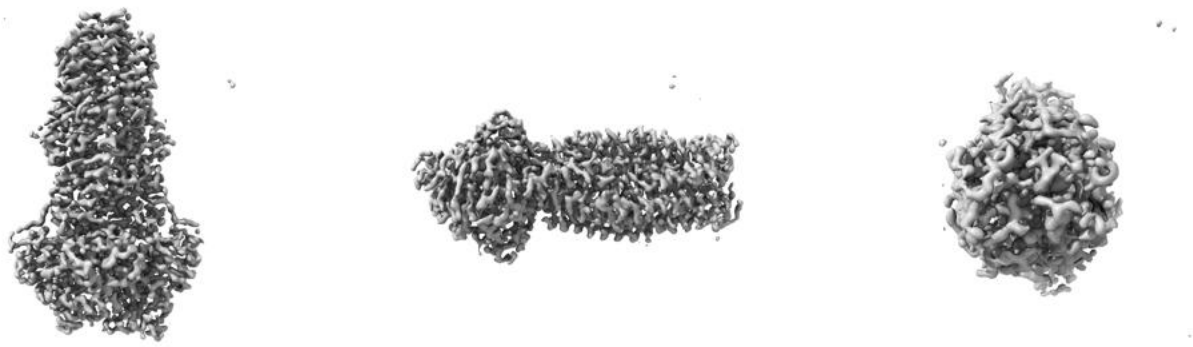

Y


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 0.86. 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.

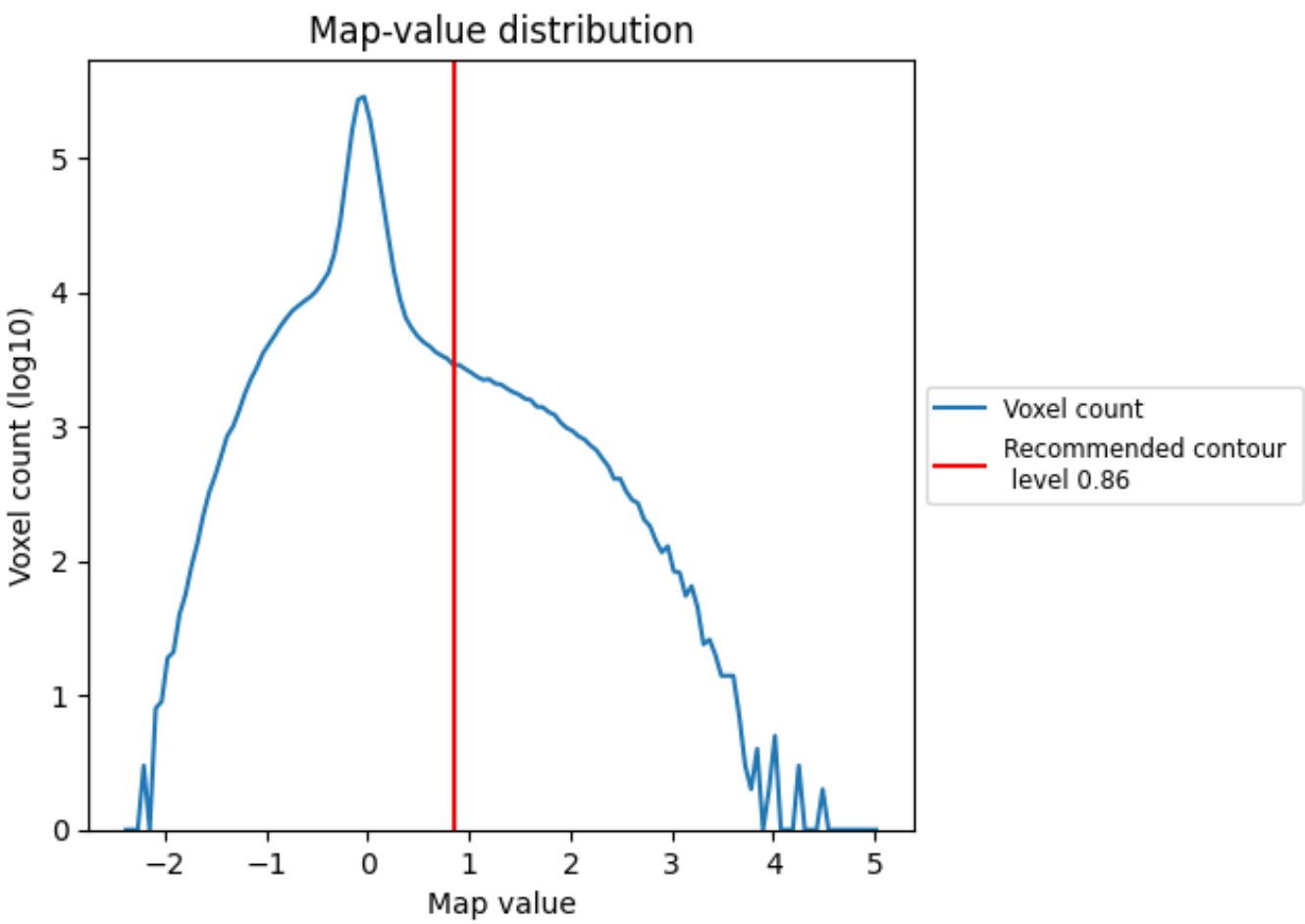
6.6 Mask visualisation (i)

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

7 Map analysis (i)

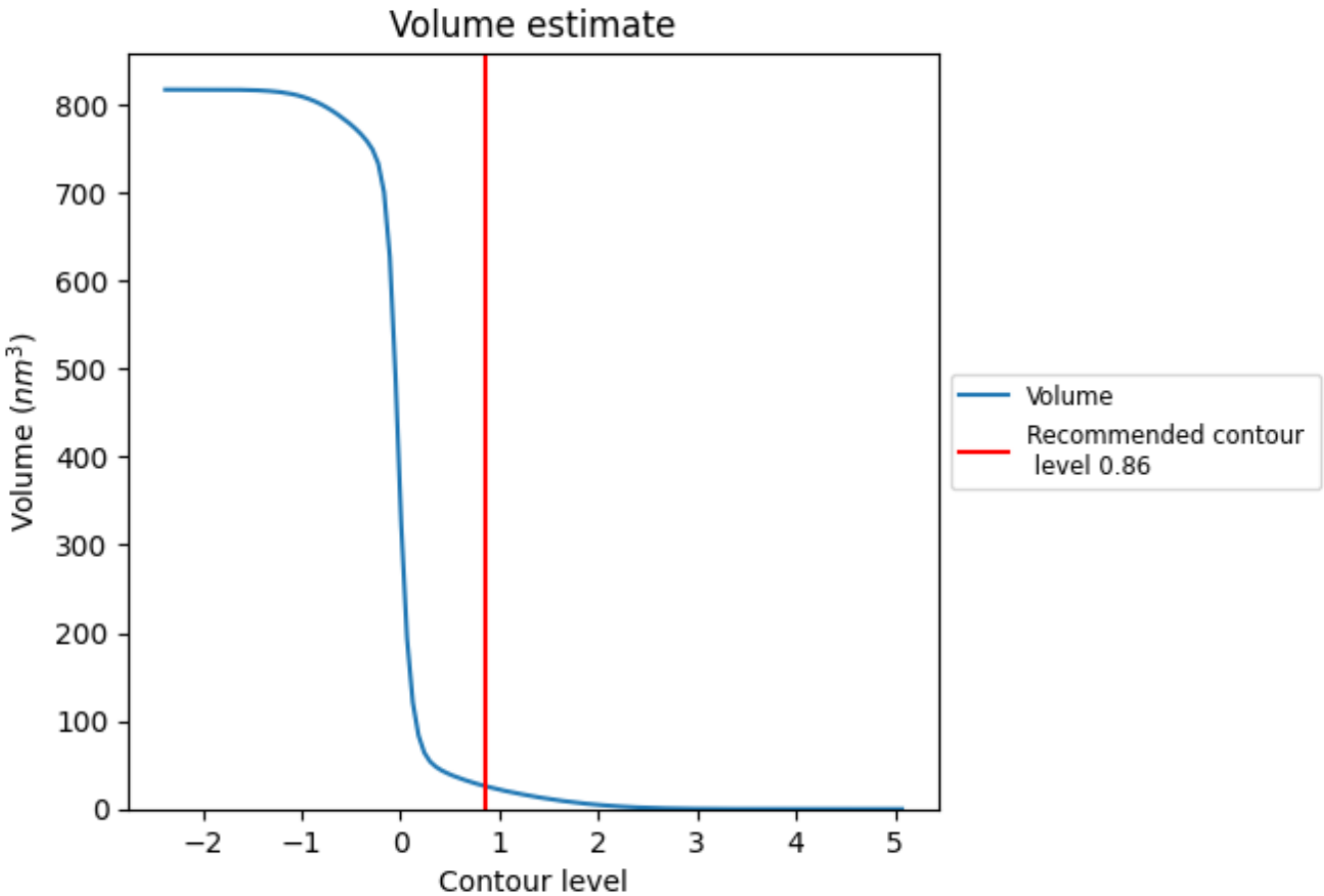
This section contains the results of statistical analysis of the map.

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 26 nm^3; this corresponds to an approximate mass of 23 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.

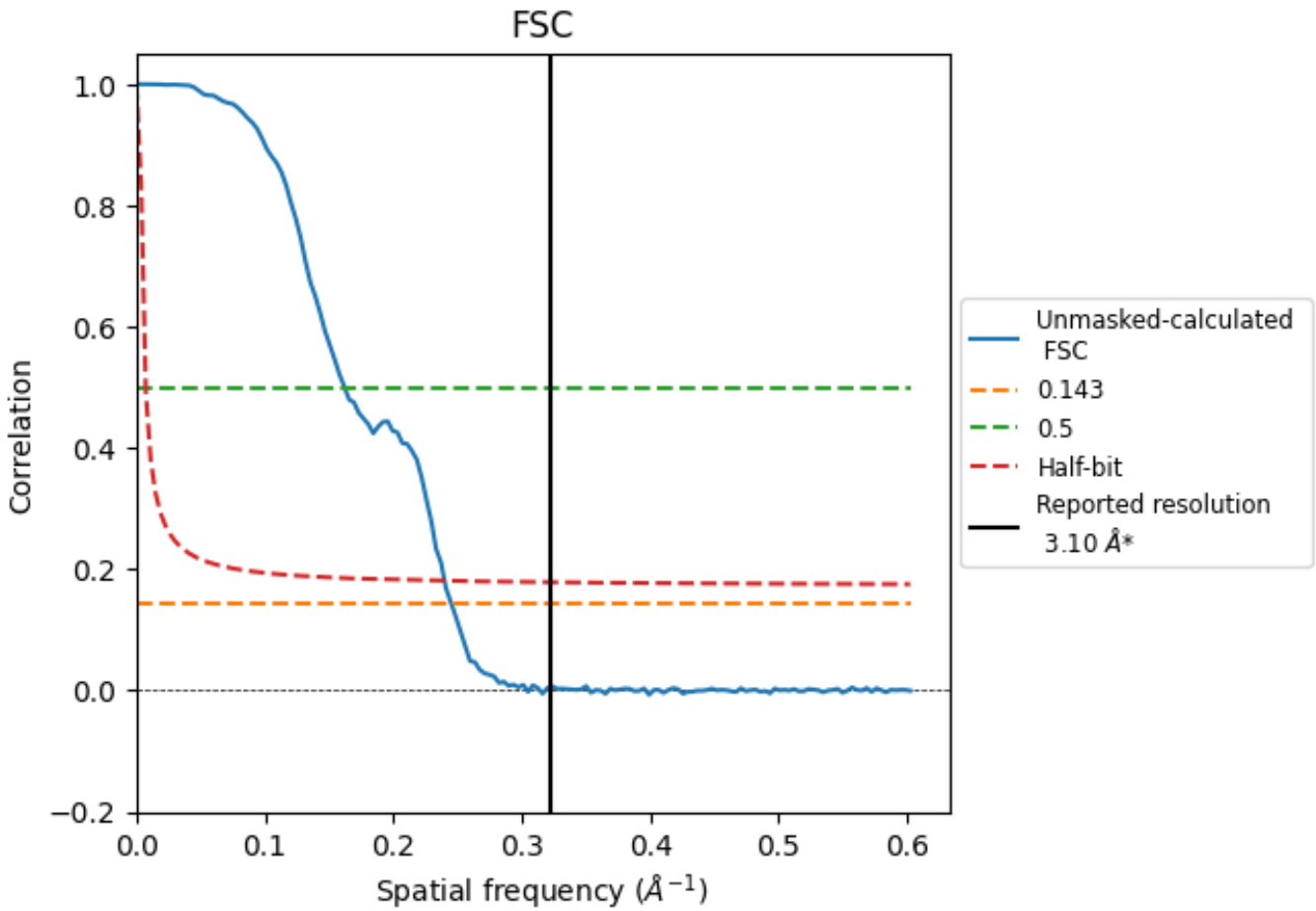
7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.323 Å^{-1}

8.2 Resolution estimates (i)

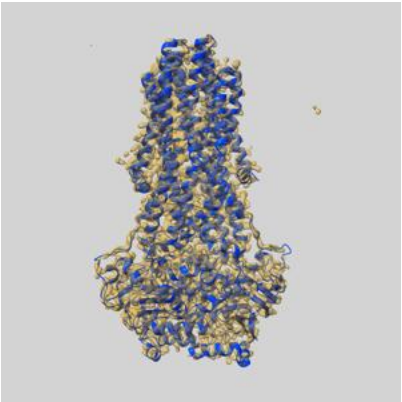
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.08	6.17	4.17

*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 4.08 differs from the reported value 3.1 by more than 10 %

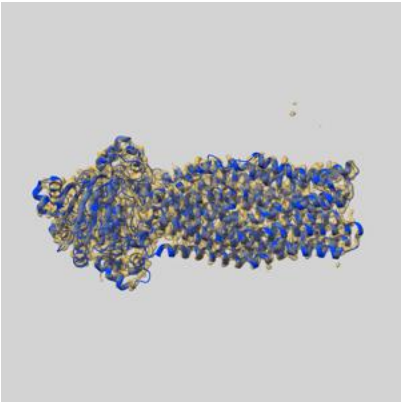
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-43498 and PDB model 8VSI. Per-residue inclusion information can be found in section 3 on page 5.

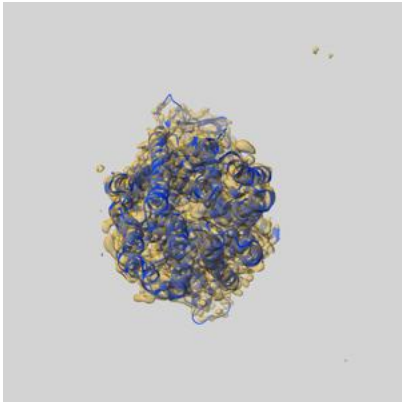
9.1 Map-model overlay (i)



X



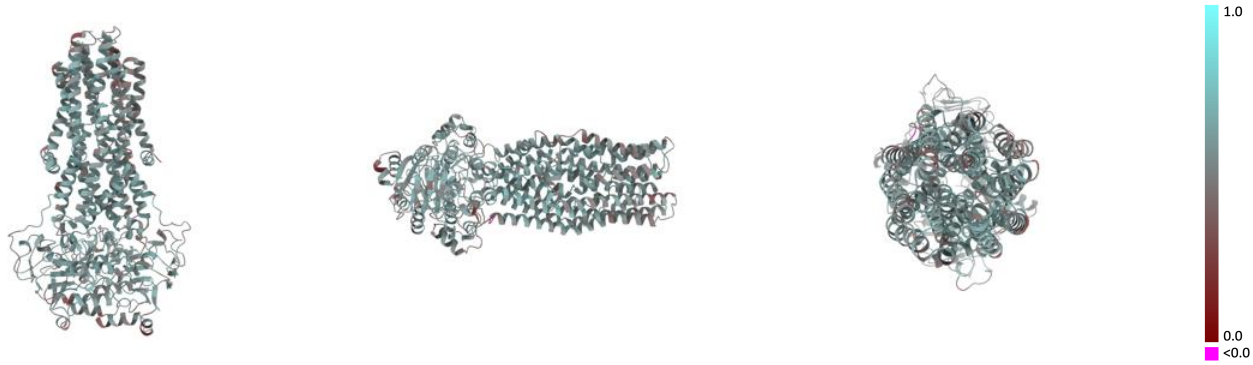
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.86 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.

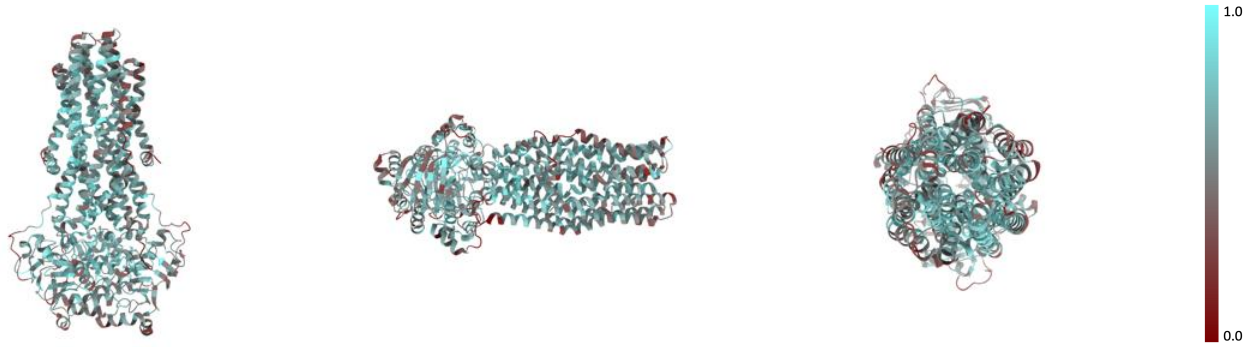
9.2 Q-score mapped to coordinate model (i)



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.

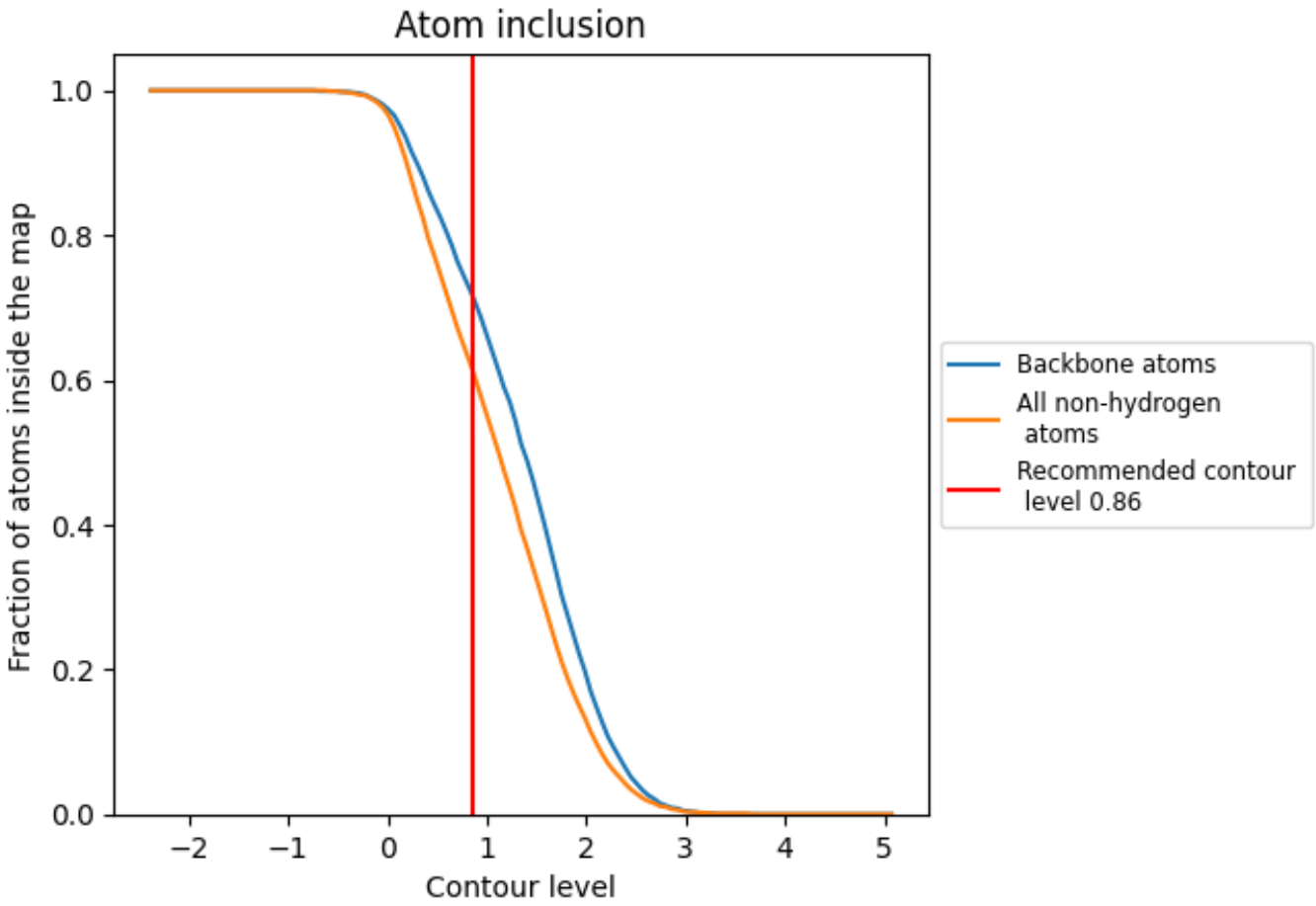
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.86).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 61% 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 (0.86) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6120	0.5470
A	0.6020	0.5430
B	0.6220	0.5510