Full wwPDB EM Validation Report (i)

Oct 20, 2026 – 06:22 PM JST

PDB ID	:	24DN / pdb_000024dn
EMDB ID	:	EMD-69450
Title	:	Structural snapshots of F1-ATPase catalysis in drug resistant Acinetobacter baumannii reveal novel therapeutic targets - Conformation 3b
Authors	:	Le, K.C.M.; Gruber, G.
Deposited on	:	2026-02-28
Resolution	:	2.88 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:

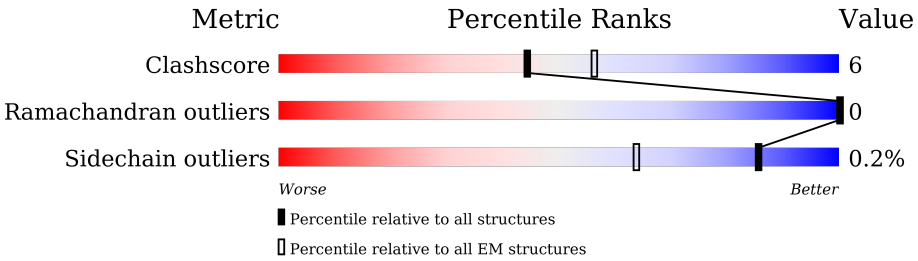
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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)	:	2.51

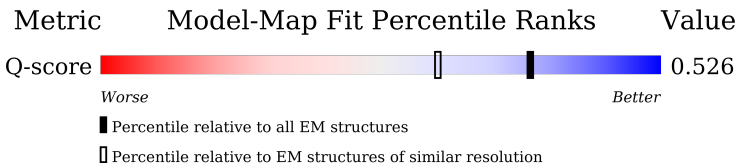
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.88 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	12111 (2.38 - 3.38)

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	e	139	8% 55% • 41%
2	A	514	87% 9% 5%
2	B	514	84% 11% 5%
2	C	514	81% 14% 5%

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Mol	Chain	Length	Quality of chain
3	D	464	87% 12%
3	E	464	84% 15%
3	F	464	82% 17%
4	g	289	74% 25%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 24510 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 ATP synthase epsilon chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	e	82	400	236	82	82	0	0

- Molecule 2 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	489	3703	2333	635	720	15	0	0
2	B	489	3703	2333	635	720	15	0	0
2	C	489	3703	2333	635	720	15	0	0

- Molecule 3 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	463	3525	2223	602	687	13	0	0
3	E	463	3525	2223	602	687	13	0	0
3	F	463	3525	2223	602	687	13	0	0

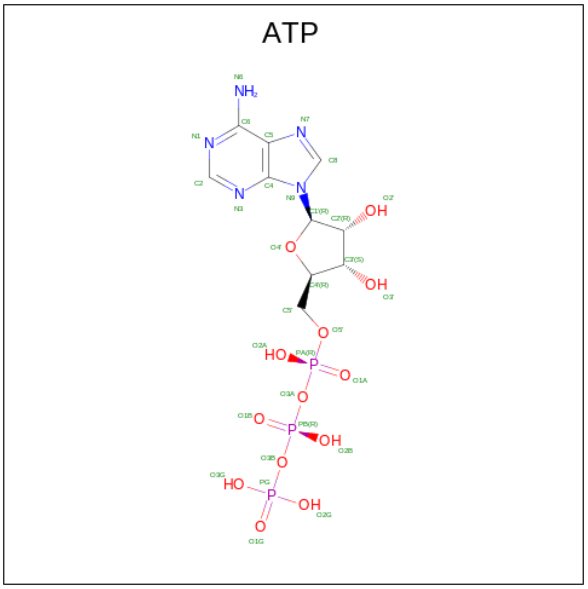
- Molecule 4 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	g	288	2243	1411	400	420	12	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

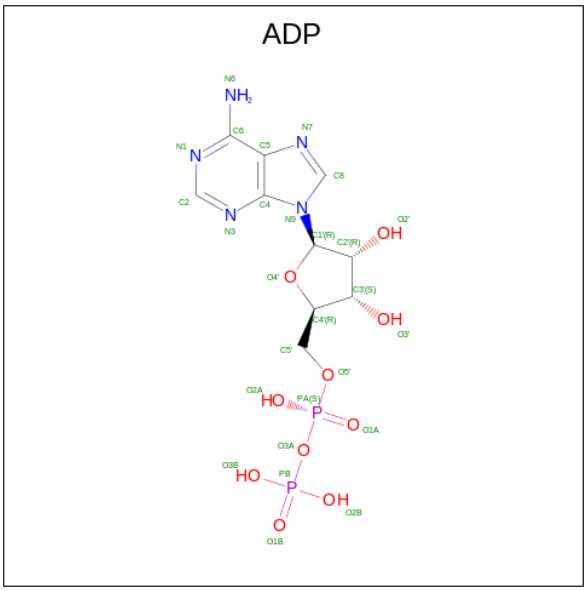
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
5	A	1	1	1	0
5	B	1	1	1	0
5	C	1	1	1	0
5	D	1	1	1	0
5	E	1	1	1	0

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	A	1	31	10	5	13	3	0
6	B	1	31	10	5	13	3	0
6	C	1	31	10	5	13	3	0
6	E	1	31	10	5	13	3	0

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



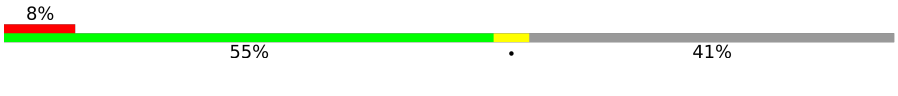
Mol	Chain	Residues	Atoms					AltConf
7	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

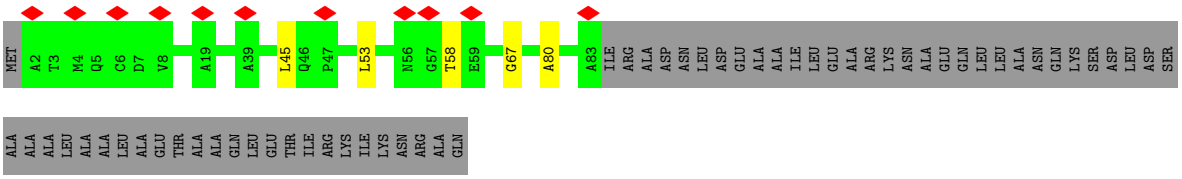
3 Residue-property plots (i)

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: ATP synthase epsilon chain

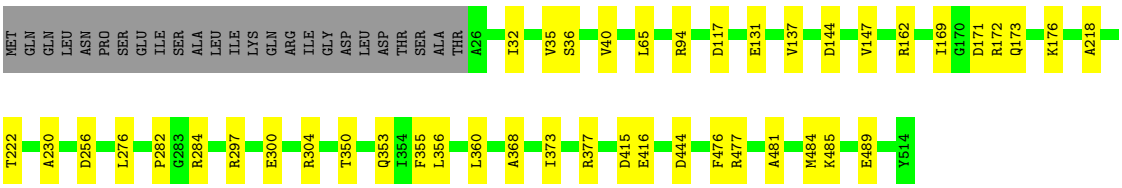
Chain e:





• Molecule 2: ATP synthase subunit alpha

Chain A:



• Molecule 2: ATP synthase subunit alpha

Chain B:

• Molecule 2: ATP synthase subunit alpha

Chain C:

MET GLN GLN LEU ASN PRO SER GLU ILE SER ALA LEU ILE LYS GLN ARG ILE GLY ASP LEU ASP THR SER ALA THR A26 T31 I32 V35 S36 D37 G38 I39 E52 N66 L67 V75 E85 C91 V100 D110 A111 D117 D128 A129 V130 E131 D144

V147 Q148 R162 G163 Q164 R165 E166 I169 A180 Q187 I199 A230 Y241 T245 M246 D256 I260 D263 Y271 I274 L277 R280 R297 L298 L299 R304 P329 I330 I331 E357 R366 P367 N370 R377 K389 L390

L398 A399 Q400 Y401 R402 E403 Q409 L414 D415 E416 R419 K420 Q421 L422 E423 R427 D444 Y450 D459 D469 A470 I473 Y493 N494 I497 Y514

- Molecule 3: ATP synthase subunit beta

Chain D: 87% 12%

MET S2 I9 I14 D15 V16 D28 A29 T38 V41 T52 I53 A54 M55 V67 T70 I74 A81 M87 T102 E103 I108 V131 L134 G153 E160 N164 H169 S170 G171 L172 E180 R181 D199 Q207 E210

N214 R215 L216 R217 V218 L223 R230 D231 N248 A255 V259 M280 I287 T288 S289 S294 I295 D310 P313 R363 L375 I378 R403 F404 F405 K426 E427 F432 F448 L464

- Molecule 3: ATP synthase subunit beta

Chain E: 84% 15%

MET S2 R5 V13 I14 R20 A29 V32 T38 V41 Q42 Q43 Q44 L45 G46 D47 R51 T52 M55 T58 L61 V67 T70 V76 R85 I86 D95 G98 T122 D123 K140 L161 I165 R181 N186 Y189

D199 M203 N209 T221 G222 L223 T224 M225 F229 D234 R240 D241 A255 V259 L262 R265 S268 A269 E278 V282 E285 R286 I287 T288 S289 S294 D310 P313 L349 R363 A364 V365 Q366 M384 V395 Y396 R397

K400 P424 E427 L436 A437 G438 I443 V451 E456 V457 L464

- Molecule 3: ATP synthase subunit beta

Chain F: 82% 17%

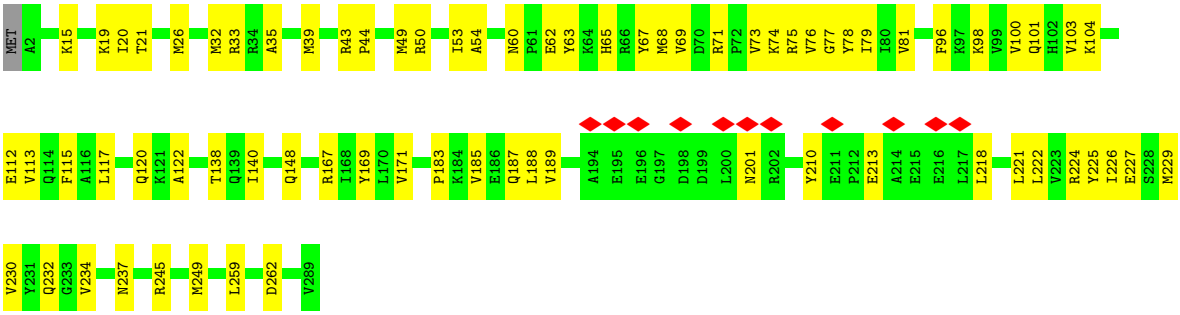
MET S2 T21 S22 A29 V32 T35 E36 T37 V41 Q42 Q43 V50 R51 T52 S57 T58 E59 G60 L61 K62 R63 V67 T70 V76 I86 E103 G151 V152 G153 N157 K167 N186 Y189 M192 L198 M203 Q207

E210 R215 T221 E232 R240 D247 N248 L254 M266 P267 S268 A269 V270 G271 Y272 Q273 P274 T275 L276 A277 E278 V282 E285 R286 I287 T290 K291 S292 I295 D310 P313 L326 Y336 R347 R371 E374 L375 I378 I379 A380 I381

L382 G383 M384 D385 E386 L387 D391 K392 R399 R403 K421 L422 V423 P424 E427 M450 G453 I454 D455 E456 V457 I458 L464

- Molecule 4: ATP synthase gamma chain

Chain g: 74% 25%


MET
A2
K15
K19
I20
T21
M26
M32
R33
R34
A35
M39
R43
P44
M49
R50
I53
A54
N60
P61
E62
Y63
K64
H65
R66
Y67
M68
V69
D70
R71
P72
V73
K74
R75
V76
G77
Y78
I79
I80
V81
F96
K97
K98
V99
V100
Q101
H102
V103
K104
E112
V113
Q114
F115
A116
L117
Q120
K121
A122
T138
Q139
I140
Q148
R167
I168
Y169
L170
V171
P183
K184
V185
E186
Q187
L188
V189
A194
E195
E196
G197
D198
D199
L200
N201
R202
Y210
E211
P212
E213
A214
E215
E216
L217
L218
L221
L222
V223
R224
Y225
I226
E227
S228
M229
V230
Y231
Q232
G233
V234
N237
R245
M249
L259
D262
V289

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	117344	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	68.6	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	160000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.703	Depositor
Minimum map value	-0.288	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.0712	Depositor
Map size (Å)	300.3, 300.3, 300.3	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.858, 0.858, 0.858	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: ATP, ADP, MG

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	e	0.14	0/399	0.38	0/551
2	A	0.16	0/3759	0.28	0/5086
2	B	0.15	0/3759	0.27	0/5086
2	C	0.15	0/3759	0.30	0/5086
3	D	0.15	0/3582	0.28	0/4854
3	E	0.15	0/3582	0.30	0/4854
3	F	0.17	0/3582	0.31	0/4854
4	g	0.15	0/2273	0.36	0/3062
All	All	0.16	0/24695	0.30	0/33433

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	e	400	0	189	4	0
2	A	3703	0	3729	31	0
2	B	3703	0	3729	35	0
2	C	3703	0	3728	49	0
3	D	3525	0	3555	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	3525	0	3555	51	0
3	F	3525	0	3555	64	0
4	g	2243	0	2294	56	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
6	A	31	0	12	0	0
6	B	31	0	12	1	0
6	C	31	0	12	0	0
6	E	31	0	12	1	0
7	D	27	0	12	1	0
7	F	27	0	12	7	0
All	All	24510	0	24406	314	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (314) 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)
3:F:336:TYR:HD2	7:F:501:ADP:C2	1.59	1.18
3:F:336:TYR:CD2	7:F:501:ADP:C2	2.31	1.16
3:D:74:ILE:HB	3:D:108:ILE:HD12	1.19	1.08
3:D:74:ILE:HB	3:D:108:ILE:CD1	2.03	0.89
3:D:53:ILE:HD11	3:D:259:VAL:HG11	1.56	0.88
3:D:214:ASN:O	3:D:218:VAL:HG23	1.76	0.86
3:F:336:TYR:CD2	7:F:501:ADP:N3	2.44	0.85
3:F:268:SER:HB2	3:F:274:PRO:HA	1.57	0.84
3:F:336:TYR:HB3	7:F:501:ADP:N1	1.95	0.81
3:F:278:GLU:O	3:F:282:VAL:HG23	1.90	0.71
2:A:300:GLU:HG2	3:E:209:ASN:HB3	1.70	0.71
3:D:103:GLU:OE2	3:D:103:GLU:N	2.24	0.71
3:E:223:LEU:HD11	3:E:287:ILE:HG12	1.74	0.70
2:C:162:ARG:NH1	2:C:256:ASP:OD2	2.23	0.70
3:E:278:GLU:O	3:E:282:VAL:HG23	1.93	0.69
2:B:400:GLN:NE2	2:B:421:GLN:OE1	2.26	0.68
3:F:151:GLY:H	7:F:501:ADP:PB	2.16	0.68
3:D:74:ILE:CB	3:D:108:ILE:HD12	2.10	0.68
3:E:161:LEU:O	3:E:165:ILE:HG12	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:131:GLU:OE2	2:C:297:ARG:NH1	2.27	0.67
4:g:245:ARG:O	4:g:249:MET:HG2	1.95	0.66
3:F:268:SER:HB2	3:F:274:PRO:CA	2.26	0.65
4:g:68:MET:N	4:g:68:MET:SD	2.70	0.65
2:B:476:PHE:HB3	2:B:484:MET:HE2	1.78	0.65
3:E:20:ARG:HH12	3:E:47:ASP:HA	1.62	0.65
3:F:35:THR:HG22	3:F:37:THR:H	1.62	0.65
2:B:162:ARG:NH1	2:B:256:ASP:OD2	2.30	0.64
2:B:165:ARG:NH2	2:B:351:ASP:OD1	2.30	0.64
3:E:32:VAL:HG22	3:E:67:VAL:HG22	1.79	0.64
2:C:147:VAL:HG23	2:C:162:ARG:HG2	1.78	0.64
1:e:67:GLY:HA3	1:e:80:ALA:HA	1.79	0.63
2:A:162:ARG:NH1	2:A:256:ASP:OD2	2.30	0.63
4:g:35:ALA:O	4:g:39:MET:HG2	1.99	0.63
2:C:357:GLU:OE1	2:C:370:ASN:ND2	2.32	0.63
3:F:152:VAL:HG23	3:F:326:LEU:HD23	1.81	0.62
4:g:120:GLN:HG2	4:g:138:THR:HG23	1.80	0.62
3:F:210:GLU:O	3:F:215:ARG:NH1	2.32	0.62
2:A:172:ARG:HG2	2:A:173:GLN:HG2	1.80	0.62
2:B:478:SER:OG	2:B:479:GLU:OE1	2.18	0.62
3:F:455:ASP:HA	3:F:458:ILE:HD12	1.81	0.62
3:D:38:THR:HG23	3:D:55:MET:HB2	1.82	0.62
2:B:153:SER:HA	2:B:432:MET:HE1	1.82	0.61
3:E:45:LEU:HD11	3:E:51:ARG:HG3	1.80	0.61
4:g:96:PHE:O	4:g:100:VAL:HG23	2.00	0.61
3:F:371:ARG:NH1	3:F:374:GLU:OE2	2.33	0.61
3:D:74:ILE:CG2	3:D:108:ILE:HD11	2.30	0.61
2:A:35:VAL:HG12	2:A:40:VAL:HG22	1.82	0.61
3:D:403:ARG:HG3	3:D:403:ARG:HH11	1.65	0.61
4:g:167:ARG:HA	4:g:189:VAL:HG11	1.83	0.61
1:e:67:GLY:HA2	4:g:224:ARG:HH12	1.66	0.60
2:C:230:ALA:HB2	3:E:285:GLU:HG3	1.83	0.60
2:C:414:LEU:HD11	2:C:419:ARG:HB3	1.83	0.60
2:A:131:GLU:OE2	2:A:297:ARG:NH1	2.34	0.60
2:B:248:GLU:OE1	2:B:251:ARG:NH2	2.33	0.60
3:D:378:ILE:HG21	4:g:20:ILE:CD1	2.31	0.60
2:C:199:ILE:HD11	2:C:263:ASP:O	2.02	0.60
2:C:169:ILE:HG13	2:C:331:ILE:HG23	1.83	0.59
2:C:31:THR:HG22	2:C:32:ILE:N	2.18	0.59
2:C:144:ASP:OD1	2:C:304:ARG:NH1	2.35	0.59
2:C:75:VAL:HG11	2:C:274:ILE:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:390:LEU:HD21	2:C:450:TYR:HB2	1.84	0.59
3:E:397:ARG:HH21	3:E:438:GLY:HA2	1.66	0.58
2:C:414:LEU:O	2:C:419:ARG:NH1	2.36	0.58
1:e:45:LEU:N	1:e:67:GLY:O	2.37	0.58
2:B:271:TYR:CD2	2:B:294:LEU:HD22	2.40	0.57
3:E:58:THR:HG22	3:E:61:LEU:HD12	1.86	0.57
2:A:476:PHE:HB3	2:A:484:MET:HE2	1.87	0.57
2:B:177:THR:OG1	6:B:601:ATP:O3G	2.23	0.57
3:D:180:GLU:OE2	3:D:248:ASN:ND2	2.37	0.57
3:D:230:ARG:HD3	3:D:295:ILE:HG13	1.86	0.57
3:E:310:ASP:HB3	3:E:313:PRO:HD2	1.86	0.57
3:F:386:GLU:N	3:F:386:GLU:OE1	2.35	0.56
4:g:81:VAL:HG21	4:g:234:VAL:HG12	1.87	0.56
3:D:29:ALA:O	3:D:70:THR:OG1	2.23	0.56
3:F:232:GLU:OE1	3:F:240:ARG:NH2	2.37	0.56
3:D:230:ARG:NH1	3:D:231:ASP:OD1	2.39	0.56
4:g:78:TYR:HB2	4:g:115:PHE:HB3	1.88	0.55
2:C:128:ASP:N	2:C:128:ASP:OD1	2.38	0.55
2:C:389:LYS:O	2:C:389:LYS:NZ	2.29	0.55
3:F:32:VAL:HG22	3:F:67:VAL:HG22	1.88	0.55
3:F:386:GLU:OE2	4:g:33:ARG:NH1	2.40	0.55
3:F:86:ILE:HG12	3:F:203:MET:HE2	1.88	0.55
3:D:199:ASP:OD1	3:D:199:ASP:N	2.39	0.55
3:D:207:GLN:N	3:D:210:GLU:OE1	2.40	0.55
3:F:76:VAL:HG11	3:F:221:THR:HG23	1.89	0.55
3:F:336:TYR:CE2	7:F:501:ADP:N3	2.74	0.55
3:E:268:SER:OG	3:E:269:ALA:N	2.38	0.54
2:B:147:VAL:HG23	2:B:162:ARG:HG2	1.90	0.54
4:g:98:LYS:O	4:g:101:GLN:HG3	2.08	0.54
3:F:375:LEU:HD12	3:F:378:ILE:HD12	1.89	0.54
4:g:187:GLN:OE1	4:g:189:VAL:N	2.33	0.54
4:g:140:ILE:O	4:g:148:GLN:NE2	2.40	0.53
2:B:414:LEU:O	2:B:419:ARG:NH2	2.42	0.53
2:B:164:GLN:NE2	2:B:166:GLU:OE1	2.42	0.53
2:B:412:SER:O	2:B:419:ARG:NH2	2.42	0.53
2:C:180:ALA:HB1	2:C:260:ILE:HD13	1.90	0.53
3:E:451:VAL:HG22	3:E:456:GLU:HB2	1.91	0.53
4:g:222:LEU:O	4:g:226:ILE:HG12	2.08	0.53
3:D:169:HIS:CD2	3:D:171:GLY:H	2.27	0.53
4:g:229:MET:SD	4:g:229:MET:N	2.81	0.53
2:C:130:VAL:HA	2:C:245:THR:HG21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:378:ILE:HG21	4:g:20:ILE:HD12	1.89	0.53
3:E:41:VAL:HA	3:E:52:THR:HG22	1.91	0.53
2:C:67:LEU:HD12	3:D:9:ILE:HD11	1.89	0.53
2:B:144:ASP:OD1	2:B:304:ARG:NH1	2.41	0.52
3:E:400:LYS:NZ	3:E:443:ILE:O	2.34	0.52
3:D:74:ILE:CB	3:D:108:ILE:CD1	2.81	0.52
3:D:310:ASP:HB3	3:D:313:PRO:HD2	1.91	0.52
3:E:14:ILE:HD11	3:E:58:THR:HG21	1.90	0.52
2:B:157:MET:HE1	2:B:398:LEU:HD12	1.92	0.52
2:B:27:LYS:HD2	2:B:27:LYS:C	2.34	0.52
2:C:85:GLU:OE2	3:E:20:ARG:NH2	2.43	0.52
3:E:38:THR:HG23	3:E:55:MET:HB3	1.91	0.52
3:E:199:ASP:OD1	3:E:199:ASP:N	2.42	0.52
3:E:85:ARG:NH2	3:E:98:GLY:O	2.38	0.52
3:F:310:ASP:HB3	3:F:313:PRO:HD2	1.91	0.51
4:g:74:LYS:HG3	4:g:75:ARG:HG2	1.91	0.51
4:g:78:TYR:HD1	4:g:169:TYR:HB2	1.75	0.51
4:g:171:VAL:HG12	4:g:185:VAL:HA	1.92	0.51
2:C:390:LEU:HD11	2:C:450:TYR:HD1	1.74	0.51
4:g:187:GLN:OE1	4:g:188:LEU:N	2.43	0.51
2:B:419:ARG:O	2:B:423:GLU:HG2	2.11	0.51
3:D:223:LEU:HD21	3:D:287:ILE:HG12	1.92	0.51
2:C:66:ASN:HB3	2:C:280:ARG:HH21	1.75	0.51
3:E:29:ALA:O	3:E:70:THR:OG1	2.26	0.51
3:F:269:ALA:O	3:F:272:TYR:N	2.44	0.50
4:g:50:ARG:HH21	4:g:54:ALA:HB2	1.76	0.50
3:D:16:VAL:HG11	3:D:67:VAL:HG11	1.92	0.50
2:B:100:VAL:HG23	2:B:246:MET:HA	1.94	0.50
2:C:110:ASP:OD1	2:C:111:ALA:N	2.43	0.50
3:D:74:ILE:HG22	3:D:108:ILE:HD11	1.94	0.50
3:F:41:VAL:HA	3:F:52:THR:HG22	1.94	0.50
3:E:451:VAL:HG11	3:E:457:VAL:HG22	1.93	0.50
4:g:74:LYS:HG3	4:g:75:ARG:HE	1.77	0.49
3:F:290:THR:HG22	3:F:292:SER:H	1.76	0.49
2:B:137:VAL:O	3:F:186:ASN:ND2	2.45	0.49
3:F:287:ILE:HG23	3:F:295:ILE:HG22	1.94	0.49
2:B:407:PHE:HZ	4:g:26:MET:HG3	1.77	0.49
2:A:481:ALA:O	2:A:485:LYS:HG2	2.12	0.49
3:F:268:SER:N	3:F:272:TYR:O	2.45	0.49
2:C:164:GLN:NE2	2:C:166:GLU:OE1	2.45	0.49
3:F:424:PRO:HG2	3:F:427:GLU:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:423:GLU:O	2:C:427:ARG:HG2	2.13	0.49
3:D:41:VAL:HA	3:D:52:THR:HG22	1.93	0.49
3:E:181:ARG:NH2	6:E:502:ATP:O2G	2.45	0.49
2:C:377:ARG:HH22	3:D:181:ARG:NH1	2.11	0.48
3:D:74:ILE:O	3:D:108:ILE:HG13	2.12	0.48
3:D:74:ILE:CG2	3:D:108:ILE:CD1	2.91	0.48
3:F:387:LEU:O	3:F:392:LYS:NZ	2.46	0.48
2:C:37:ASP:OD1	3:E:265:ARG:NH1	2.46	0.48
3:F:382:LEU:HD11	4:g:32:MET:HE1	1.95	0.48
2:A:137:VAL:O	3:E:186:ASN:ND2	2.44	0.48
4:g:201:ASN:OD1	4:g:201:ASN:N	2.44	0.48
4:g:21:THR:HG23	4:g:249:MET:CE	2.43	0.48
2:A:356:LEU:HA	2:A:368:ALA:O	2.14	0.48
2:A:169:ILE:HG23	2:A:355:PHE:HD1	1.79	0.48
3:F:269:ALA:O	3:F:270:VAL:C	2.56	0.48
2:C:36:SER:HB2	3:E:43:GLN:HG2	1.95	0.47
3:E:76:VAL:HG11	3:E:221:THR:HG23	1.96	0.47
4:g:81:VAL:HG22	4:g:237:ASN:HD22	1.79	0.47
3:F:153:GLY:O	3:F:157:ASN:ND2	2.46	0.47
3:D:160:GLU:OE2	3:D:164:ASN:ND2	2.47	0.47
2:C:39:ILE:HD12	2:C:277:LEU:HB3	1.96	0.47
3:E:397:ARG:NH2	3:E:438:GLY:HA2	2.30	0.47
2:B:126:LEU:HD23	2:B:126:LEU:H	1.80	0.47
2:B:158:ILE:HG23	2:B:376:SER:HB2	1.95	0.47
2:C:169:ILE:CG1	2:C:331:ILE:HG23	2.44	0.47
2:C:469:ASP:OD1	2:C:470:ALA:N	2.47	0.47
2:A:444:ASP:OD1	2:A:477:ARG:NH2	2.48	0.47
2:C:31:THR:CG2	2:C:32:ILE:N	2.78	0.47
2:C:409:GLN:OE1	2:C:409:GLN:N	2.44	0.47
3:E:140:LYS:NZ	3:E:241:ASP:OD2	2.48	0.47
3:E:255:ALA:O	3:E:259:VAL:HG23	2.15	0.47
3:D:153:GLY:N	7:D:501:ADP:O1B	2.40	0.47
4:g:227:GLU:HA	4:g:230:VAL:HG22	1.95	0.47
3:D:289:SER:HB2	3:D:294:SER:HA	1.97	0.46
4:g:26:MET:HE2	4:g:26:MET:HA	1.97	0.46
2:A:144:ASP:N	2:A:144:ASP:OD1	2.48	0.46
2:C:416:GLU:HG2	2:C:419:ARG:HH21	1.80	0.46
4:g:53:ILE:HG13	4:g:54:ALA:N	2.29	0.46
2:A:276:LEU:HD13	3:F:268:SER:HA	1.96	0.46
4:g:65:HIS:CE1	4:g:68:MET:HE1	2.50	0.46
2:B:467:ASP:C	2:B:469:ASP:H	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:272:TYR:HD2	3:F:276:LEU:HD13	1.79	0.46
3:E:289:SER:HB2	3:E:294:SER:HA	1.97	0.46
4:g:49:MET:HG3	4:g:225:TYR:CD2	2.51	0.46
3:F:58:THR:HA	3:F:61:LEU:HD12	1.98	0.46
4:g:60:ASN:HD21	4:g:63:TYR:HD1	1.64	0.46
2:C:35:VAL:O	2:C:35:VAL:HG13	2.16	0.45
2:C:398:LEU:O	2:C:402:ARG:HG3	2.15	0.45
3:D:14:ILE:O	3:D:52:THR:OG1	2.30	0.45
2:A:144:ASP:OD1	2:A:304:ARG:NH1	2.48	0.45
2:C:400:GLN:HE22	2:C:421:GLN:CD	2.24	0.45
3:F:247:ASP:OD1	3:F:248:ASN:N	2.49	0.45
4:g:62:GLU:HG2	4:g:63:TYR:HD1	1.81	0.45
2:C:271:TYR:HA	2:C:274:ILE:HG22	1.97	0.45
4:g:75:ARG:NH1	4:g:112:GLU:HG2	2.31	0.45
3:D:131:VAL:HG22	3:D:405:PHE:CD1	2.51	0.45
3:D:403:ARG:HB3	3:D:448:PHE:O	2.17	0.45
3:F:151:GLY:N	7:F:501:ADP:O1B	2.49	0.45
2:A:218:ALA:O	2:A:222:THR:OG1	2.30	0.45
2:C:403:GLU:OE1	2:C:403:GLU:HA	2.16	0.45
3:D:426:LYS:HZ2	3:D:427:GLU:N	2.15	0.45
2:B:443:ALA:HB1	2:B:484:MET:SD	2.57	0.45
2:A:360:LEU:HB2	2:A:368:ALA:HB1	1.98	0.45
3:F:375:LEU:HD21	3:F:391:ASP:HB3	1.98	0.45
3:F:450:MET:HE3	3:F:450:MET:HB2	1.76	0.44
4:g:117:LEU:HD13	4:g:122:ALA:HB1	1.98	0.44
2:B:67:LEU:HD23	3:F:63:ARG:HG3	1.99	0.44
3:D:403:ARG:HG3	3:D:403:ARG:NH1	2.30	0.44
3:D:464:LEU:HD23	3:D:464:LEU:HA	1.86	0.44
2:A:415:ASP:OD1	2:A:416:GLU:N	2.50	0.44
2:B:148:GLN:O	2:B:187:GLN:NE2	2.51	0.44
3:F:41:VAL:HG13	3:F:50:VAL:HG13	2.00	0.44
4:g:65:HIS:CD2	4:g:67:TYR:H	2.36	0.44
4:g:76:VAL:HG22	4:g:77:GLY:N	2.32	0.44
2:A:230:ALA:HB2	3:F:285:GLU:HG3	1.98	0.44
2:A:282:PRO:HD3	3:F:266:MET:HE1	1.99	0.44
2:C:117:ASP:OD1	2:C:117:ASP:N	2.49	0.44
2:A:36:SER:HB3	3:F:43:GLN:HG3	2.00	0.44
2:C:494:ASN:OD1	2:C:497:ILE:HG12	2.17	0.44
3:E:424:PRO:HG2	3:E:427:GLU:HG2	1.99	0.44
3:F:22:SER:O	3:F:22:SER:OG	2.31	0.44
3:F:103:GLU:OE2	3:F:103:GLU:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:g:218:LEU:O	4:g:221:LEU:HG	2.18	0.44
2:A:147:VAL:HG23	2:A:162:ARG:HG2	1.99	0.44
3:F:453:GLY:N	3:F:456:GLU:OE1	2.41	0.44
4:g:229:MET:HA	4:g:232:GLN:HG3	1.98	0.43
3:E:5:ARG:HA	3:E:5:ARG:HD3	1.82	0.43
2:A:117:ASP:OD1	2:A:117:ASP:N	2.39	0.43
3:F:57:SER:OG	3:F:59:GLU:OE1	2.24	0.43
3:F:381:ILE:HG13	4:g:26:MET:HE1	2.00	0.43
4:g:262:ASP:N	4:g:262:ASP:OD1	2.51	0.43
3:E:240:ARG:HD3	3:E:240:ARG:HA	1.87	0.43
3:F:381:ILE:CG1	4:g:26:MET:HE1	2.49	0.43
3:E:14:ILE:O	3:E:52:THR:OG1	2.23	0.43
3:F:399:ARG:O	3:F:403:ARG:HG2	2.19	0.43
4:g:221:LEU:HA	4:g:224:ARG:HD2	1.99	0.43
2:A:171:ASP:O	2:A:176:LYS:NZ	2.50	0.43
4:g:69:VAL:HG12	4:g:71:ARG:HG2	1.99	0.43
3:E:365:VAL:HG23	3:E:436:LEU:HD11	1.99	0.43
3:D:230:ARG:HG2	3:D:231:ASP:OD1	2.18	0.43
2:B:241:TYR:OH	2:B:294:LEU:HD12	2.19	0.42
3:E:122:THR:HG22	3:E:123:ASP:H	1.84	0.42
2:A:485:LYS:O	2:A:489:GLU:HG2	2.19	0.42
4:g:101:GLN:HA	4:g:104:LYS:HE3	2.01	0.42
4:g:103:VAL:HG23	4:g:113:VAL:HG11	2.01	0.42
2:A:173:GLN:HE22	3:F:347:ARG:NE	2.17	0.42
1:e:53:LEU:HA	1:e:58:THR:O	2.20	0.42
3:E:122:THR:HG22	3:E:123:ASP:N	2.34	0.42
2:B:404:LEU:HD12	2:B:422:LEU:HD13	2.00	0.42
3:D:55:MET:HE1	3:D:217:ARG:HG3	2.01	0.42
3:E:140:LYS:HE3	3:E:140:LYS:HB3	1.68	0.42
2:C:100:VAL:HG12	2:C:246:MET:HA	2.02	0.42
4:g:73:VAL:HG12	4:g:167:ARG:HH11	1.85	0.42
2:B:117:ASP:OD1	2:B:117:ASP:N	2.52	0.42
2:B:468:PHE:HB2	2:B:514:TYR:CD2	2.54	0.42
2:C:52:GLU:OE2	2:C:91:CYS:HB2	2.20	0.42
2:C:399:ALA:HA	2:C:402:ARG:NE	2.35	0.42
2:C:459:ASP:OD1	2:C:459:ASP:N	2.51	0.42
3:E:203:MET:HE3	3:E:203:MET:HB2	1.91	0.42
3:F:207:GLN:HB2	3:F:210:GLU:HG2	2.02	0.42
4:g:15:LYS:O	4:g:19:LYS:HG3	2.20	0.42
2:C:148:GLN:O	2:C:187:GLN:NE2	2.51	0.42
3:D:87:MET:HB2	3:D:87:MET:HE3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:g:259:LEU:HD12	4:g:259:LEU:HA	1.91	0.41
2:A:353:GLN:NE2	2:A:373:ILE:O	2.51	0.41
3:F:21:THR:OG1	3:F:22:SER:N	2.53	0.41
3:F:50:VAL:HG12	3:F:52:THR:HG23	2.01	0.41
3:F:254:LEU:HD13	3:F:254:LEU:HA	1.88	0.41
2:A:94:ARG:HB2	2:A:94:ARG:NH1	2.35	0.41
2:B:148:GLN:HG3	2:B:442:ILE:HD11	2.03	0.41
3:D:363:ARG:HD2	3:D:363:ARG:HA	1.92	0.41
3:D:214:ASN:O	3:D:218:VAL:CG2	2.60	0.41
2:A:65:LEU:HD12	2:A:65:LEU:HA	1.84	0.41
3:D:375:LEU:HD22	3:D:378:ILE:HD11	2.02	0.41
3:E:221:THR:HG22	3:E:225:MET:HE3	2.03	0.41
3:F:167:LYS:HD3	3:F:422:LEU:HD22	2.03	0.41
3:F:86:ILE:HD11	3:F:189:TYR:CD1	2.56	0.41
3:F:421:LYS:HD3	3:F:421:LYS:HA	1.80	0.41
2:C:444:ASP:OD2	2:C:473:ILE:HG23	2.21	0.41
2:A:284:ARG:NH1	3:E:310:ASP:OD1	2.47	0.41
2:B:398:LEU:HD23	2:B:398:LEU:HA	1.75	0.41
3:E:13:VAL:HG21	3:E:262:LEU:HB3	2.03	0.41
3:E:229:PHE:HD1	3:E:229:PHE:HA	1.79	0.41
3:E:349:LEU:HD12	3:E:349:LEU:HA	1.83	0.41
3:E:363:ARG:NH1	3:E:366:GLN:OE1	2.53	0.41
3:F:103:GLU:CD	3:F:103:GLU:H	2.29	0.41
3:F:379:ILE:HD12	3:F:384:MET:SD	2.61	0.41
3:D:216:LEU:HD13	3:D:255:ALA:HB3	2.02	0.41
3:E:86:ILE:HD11	3:E:189:TYR:CD1	2.56	0.41
3:E:234:ASP:OD1	3:E:234:ASP:N	2.53	0.41
3:E:384:MET:HE1	3:E:395:VAL:HG11	2.02	0.41
3:F:192:MET:HB3	3:F:198:LEU:HB2	2.02	0.41
4:g:79:ILE:HD13	4:g:79:ILE:HA	1.96	0.40
4:g:210:TYR:HB3	4:g:213:GLU:O	2.21	0.40
2:C:241:TYR:O	2:C:245:THR:HG23	2.21	0.40
2:C:366:ARG:HB2	2:C:367:PRO:HD3	2.03	0.40
3:E:363:ARG:HA	3:E:363:ARG:HD3	1.75	0.40
4:g:43:ARG:N	4:g:44:PRO:HD2	2.36	0.40
2:A:32:ILE:HG23	2:A:40:VAL:HG13	2.03	0.40
2:A:350:THR:O	2:A:377:ARG:NH1	2.54	0.40
2:C:299:LEU:HD21	2:C:329:PRO:HG3	2.03	0.40
3:D:28:ASP:O	3:D:41:VAL:HG23	2.21	0.40
3:D:81:ALA:HB3	3:D:102:THR:OG1	2.21	0.40
3:E:95:ASP:OD1	3:E:95:ASP:N	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:g:98:LYS:HD2	4:g:183:PRO:HB2	2.03	0.40
2:B:32:ILE:HD12	2:B:87:GLN:HB2	2.03	0.40
2:B:151:TYR:HB2	2:B:154:VAL:HG12	2.03	0.40
3:D:280:MET:HE2	3:D:280:MET:HB2	1.85	0.40
3:D:378:ILE:CG2	4:g:20:ILE:HD12	2.51	0.40
3:F:29:ALA:O	3:F:70:THR:OG1	2.30	0.40
2:B:42:ILE:HG21	2:B:45:LEU:HD12	2.03	0.40
3:D:134:LEU:HD22	3:D:432:PHE:CE2	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	e	80/139 (58%)	70 (88%)	10 (12%)	0	100	100
2	A	487/514 (95%)	475 (98%)	12 (2%)	0	100	100
2	B	487/514 (95%)	472 (97%)	15 (3%)	0	100	100
2	C	487/514 (95%)	476 (98%)	11 (2%)	0	100	100
3	D	461/464 (99%)	445 (96%)	16 (4%)	0	100	100
3	E	461/464 (99%)	432 (94%)	29 (6%)	0	100	100
3	F	461/464 (99%)	448 (97%)	13 (3%)	0	100	100
4	g	286/289 (99%)	274 (96%)	12 (4%)	0	100	100
All	All	3210/3362 (96%)	3092 (96%)	118 (4%)	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	
2	A	384/406 (95%)	384 (100%)	0	100	100
2	B	384/406 (95%)	382 (100%)	2 (0%)	81	93
2	C	384/406 (95%)	381 (99%)	3 (1%)	73	89
3	D	378/379 (100%)	377 (100%)	1 (0%)	86	95
3	E	378/379 (100%)	378 (100%)	0	100	100
3	F	378/379 (100%)	378 (100%)	0	100	100
4	g	235/236 (100%)	235 (100%)	0	100	100
All	All	2521/2591 (97%)	2515 (100%)	6 (0%)	85	96

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	263	ASP
2	B	444	ASP
2	C	263	ASP
2	C	469	ASP
2	C	493	TYR
3	D	172	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	69	GLN
2	A	295	HIS
2	B	145	GLN
2	B	295	HIS
2	B	400	GLN
2	C	87	GLN
2	C	362	ASN
2	C	400	GLN
2	C	421	GLN

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Mol	Chain	Res	Type
3	D	8	GLN
3	D	410	HIS
3	E	42	GLN
3	F	157	ASN
3	F	163	ASN
3	F	358	HIS
4	g	60	ASN
4	g	102	HIS
4	g	106	GLN
4	g	107	GLN
4	g	109	GLN
4	g	139	GLN
4	g	237	ASN
4	g	258	GLN
4	g	264	GLN
4	g	268	ASN
4	g	272	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 11 ligands modelled in this entry, 5 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	$\#\|Z\| > 2$
6	ATP	E	502	5	29,33,33	0.33	0	44,52,52	0.51	1 (2%)
6	ATP	A	602	5	29,33,33	0.33	0	44,52,52	0.45	1 (2%)
6	ATP	B	601	5	29,33,33	0.32	0	44,52,52	0.45	1 (2%)
7	ADP	F	501	-	27,29,29	1.35	4 (14%)	42,45,45	1.96	10 (23%)
6	ATP	C	602	5	29,33,33	0.32	0	44,52,52	0.44	0
7	ADP	D	501	5	27,29,29	1.36	4 (14%)	42,45,45	1.95	10 (23%)

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
6	ATP	E	502	5	-	8/22/38/38	0/3/3/3
6	ATP	A	602	5	-	2/22/38/38	0/3/3/3
6	ATP	B	601	5	-	6/22/38/38	0/3/3/3
7	ADP	F	501	-	-	11/16/32/32	0/3/3/3
6	ATP	C	602	5	-	7/22/38/38	0/3/3/3
7	ADP	D	501	5	-	3/16/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	501	ADP	C5-C4	4.47	1.47	1.39
7	D	501	ADP	C5-C4	4.41	1.47	1.39
7	F	501	ADP	C5-C6	2.67	1.48	1.41
7	D	501	ADP	C5-C6	2.60	1.48	1.41
7	F	501	ADP	C8-N7	2.45	1.36	1.31
7	D	501	ADP	C5-N7	-2.33	1.34	1.39
7	D	501	ADP	C8-N7	2.30	1.36	1.31
7	F	501	ADP	C5-N7	-2.11	1.35	1.39

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	501	ADP	C5-C4-N3	-6.14	118.74	126.75
7	F	501	ADP	C5-C4-N3	-6.05	118.86	126.75
7	D	501	ADP	N3-C4-N9	4.73	134.87	127.08
7	F	501	ADP	N3-C4-N9	4.70	134.83	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	F	501	ADP	PA-O3A-PB	-3.90	119.45	132.83
7	F	501	ADP	C2-N3-C4	3.79	120.71	111.75
7	D	501	ADP	C2-N3-C4	3.75	120.60	111.75
7	D	501	ADP	PA-O3A-PB	-3.47	120.91	132.83
7	F	501	ADP	C4-C5-N7	-3.31	106.58	110.62
7	D	501	ADP	C4-C5-N7	-3.25	106.66	110.62
7	F	501	ADP	N3-C2-N1	-3.10	123.75	128.60
7	D	501	ADP	N3-C2-N1	-2.96	123.98	128.60
7	F	501	ADP	C5-N7-C8	2.78	107.46	103.51
7	F	501	ADP	C4-N9-C8	2.69	108.64	105.73
7	D	501	ADP	C5-N7-C8	2.66	107.29	103.51
7	D	501	ADP	C3'-C2'-C1'	2.58	106.33	101.43
7	D	501	ADP	C4-N9-C8	2.43	108.37	105.73
7	F	501	ADP	C6-C5-N7	2.23	136.17	132.02
7	F	501	ADP	N9-C8-N7	-2.13	111.00	113.91
7	D	501	ADP	C6-C5-N7	2.09	135.92	132.02
6	A	602	ATP	PB-O3B-PG	2.04	139.83	132.83
6	E	502	ATP	PB-O3B-PG	2.04	139.83	132.83
6	B	601	ATP	PB-O3B-PG	2.04	139.82	132.83

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	601	ATP	PB-O3B-PG-O2G
6	C	602	ATP	PB-O3B-PG-O3G
6	E	502	ATP	PB-O3B-PG-O3G
6	E	502	ATP	C5'-O5'-PA-O2A
6	E	502	ATP	O4'-C1'-N9-C8
6	E	502	ATP	O4'-C1'-N9-C4
7	F	501	ADP	PA-O3A-PB-O3B
7	F	501	ADP	C5'-O5'-PA-O1A
7	F	501	ADP	C5'-O5'-PA-O2A
6	A	602	ATP	O4'-C4'-C5'-O5'
6	B	601	ATP	O4'-C4'-C5'-O5'
6	C	602	ATP	O4'-C4'-C5'-O5'
7	D	501	ADP	O4'-C4'-C5'-O5'
7	F	501	ADP	O4'-C4'-C5'-O5'
7	F	501	ADP	C3'-C4'-C5'-O5'
6	C	602	ATP	C3'-C4'-C5'-O5'
7	F	501	ADP	C2'-C1'-N9-C8
6	A	602	ATP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
6	C	602	ATP	PA-O3A-PB-O1B
7	F	501	ADP	C4'-C5'-O5'-PA
6	B	601	ATP	PG-O3B-PB-O1B
6	B	601	ATP	PA-O3A-PB-O1B
7	D	501	ADP	PB-O3A-PA-O1A
6	E	502	ATP	C5'-O5'-PA-O1A
7	D	501	ADP	PB-O3A-PA-O2A
7	F	501	ADP	C2'-C1'-N9-C4
7	F	501	ADP	O4'-C1'-N9-C8
6	C	602	ATP	PB-O3B-PG-O1G
6	E	502	ATP	PB-O3B-PG-O1G
7	F	501	ADP	PA-O3A-PB-O1B
6	B	601	ATP	PB-O3B-PG-O3G
6	C	602	ATP	PB-O3B-PG-O2G
6	E	502	ATP	C5'-O5'-PA-O3A
7	F	501	ADP	C5'-O5'-PA-O3A
6	C	602	ATP	PA-O3A-PB-O2B
6	E	502	ATP	O4'-C4'-C5'-O5'
6	B	601	ATP	PB-O3B-PG-O1G

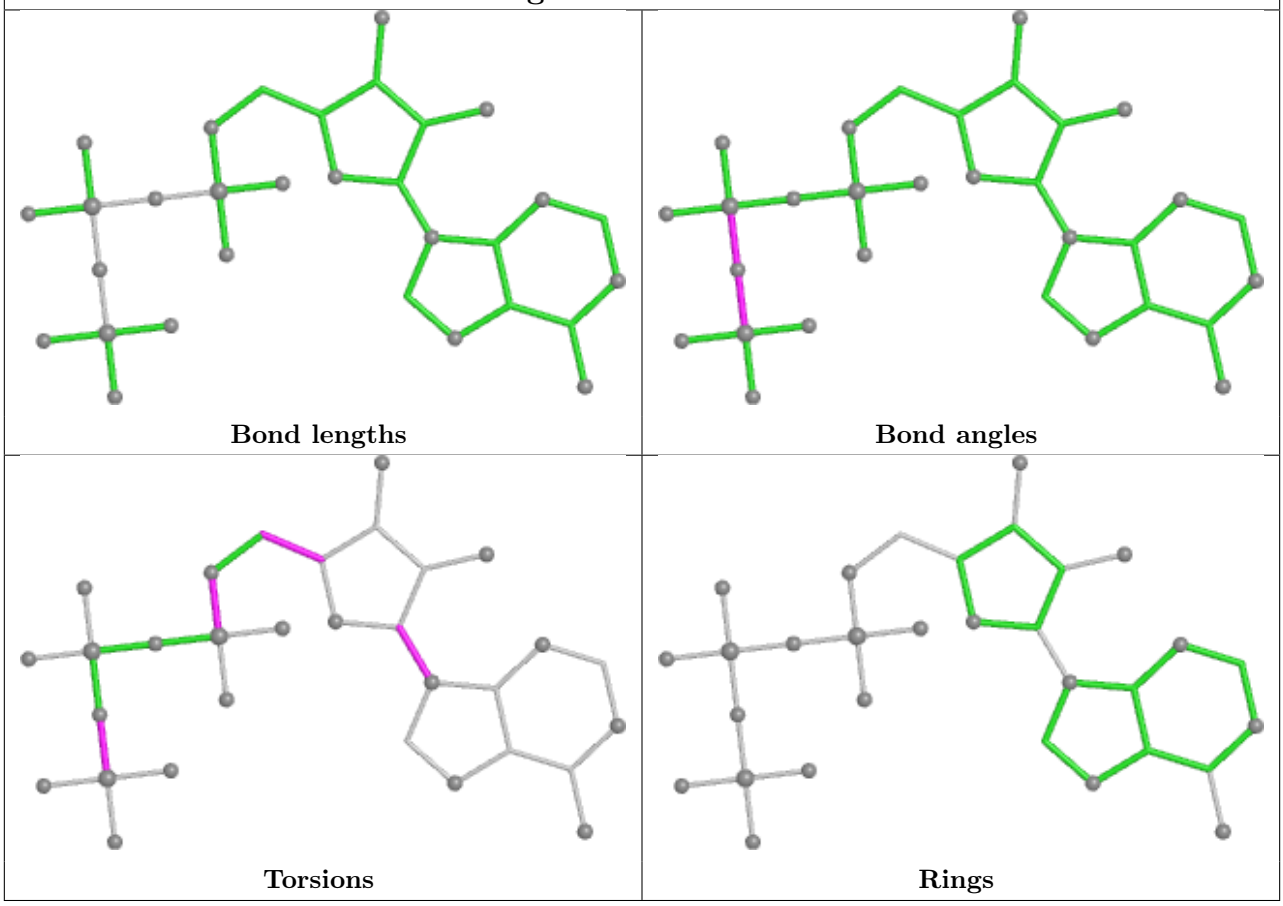
There are no ring outliers.

4 monomers are involved in 10 short contacts:

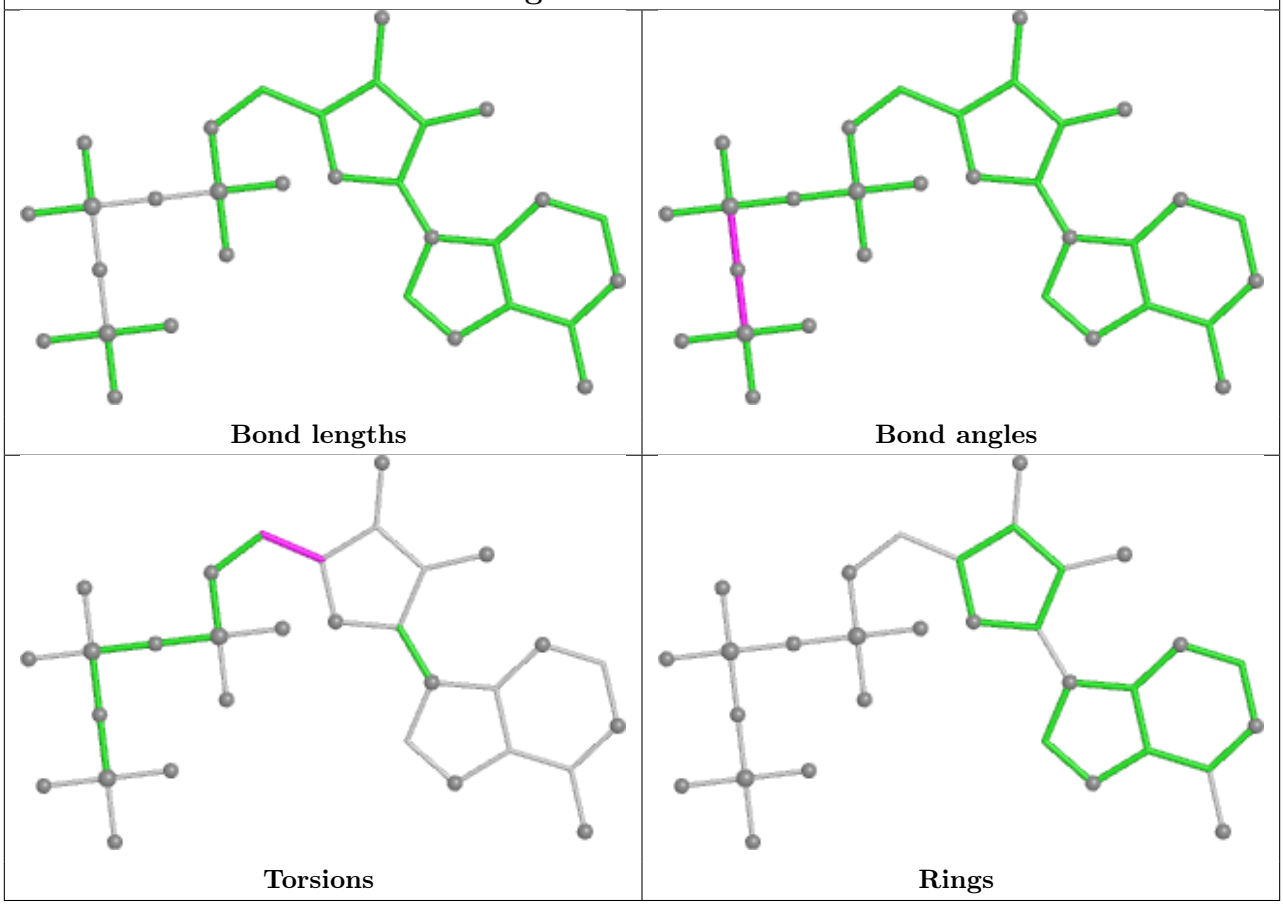
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	502	ATP	1	0
6	B	601	ATP	1	0
7	F	501	ADP	7	0
7	D	501	ADP	1	0

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.

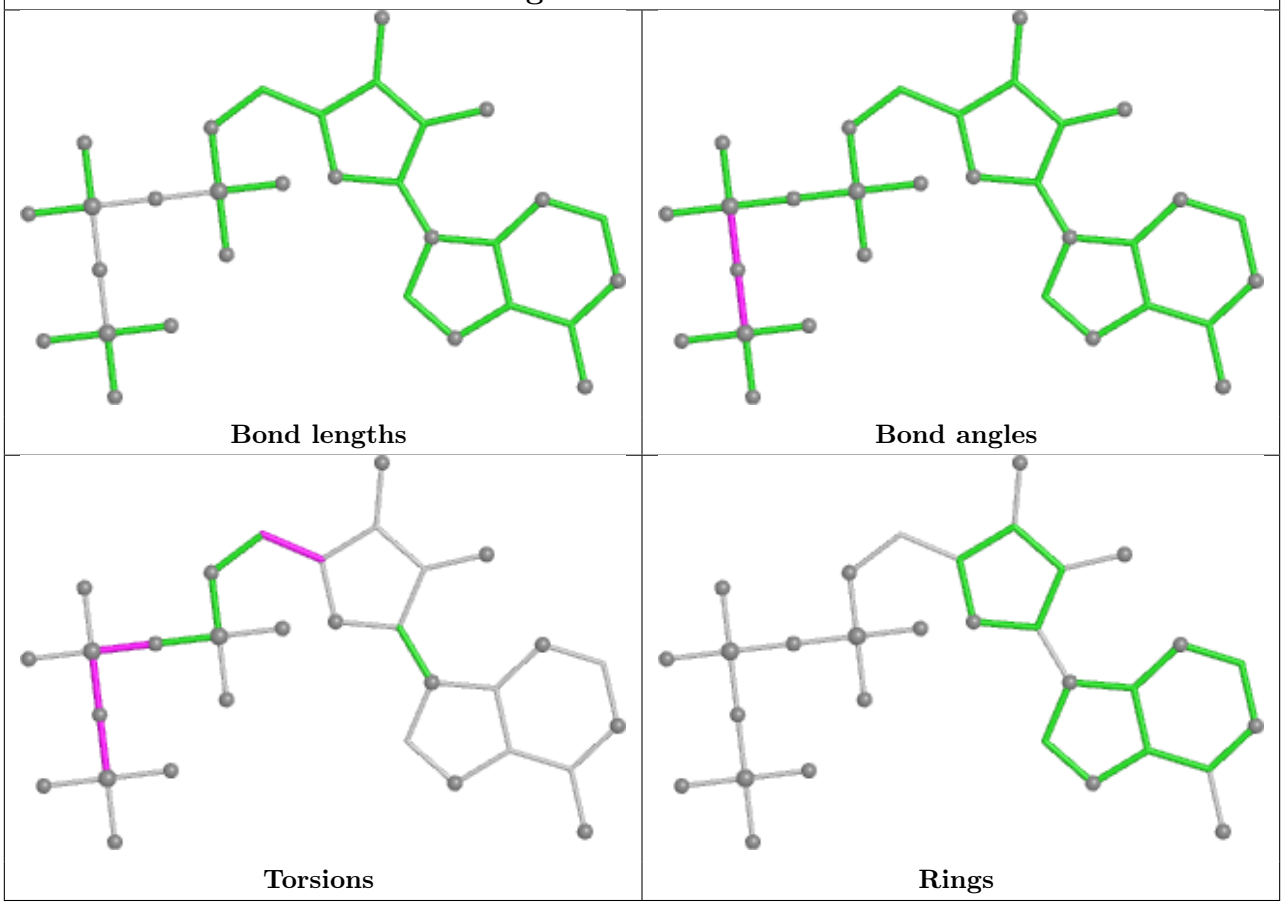
Ligand ATP E 502



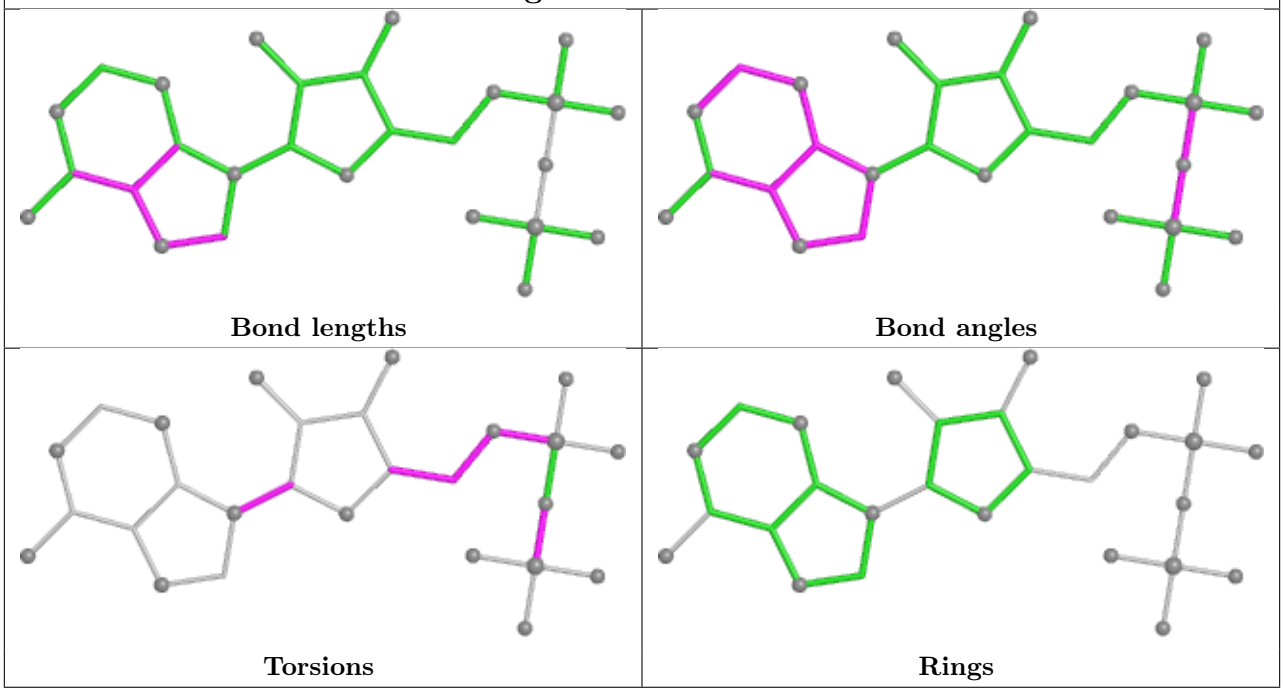
Ligand ATP A 602



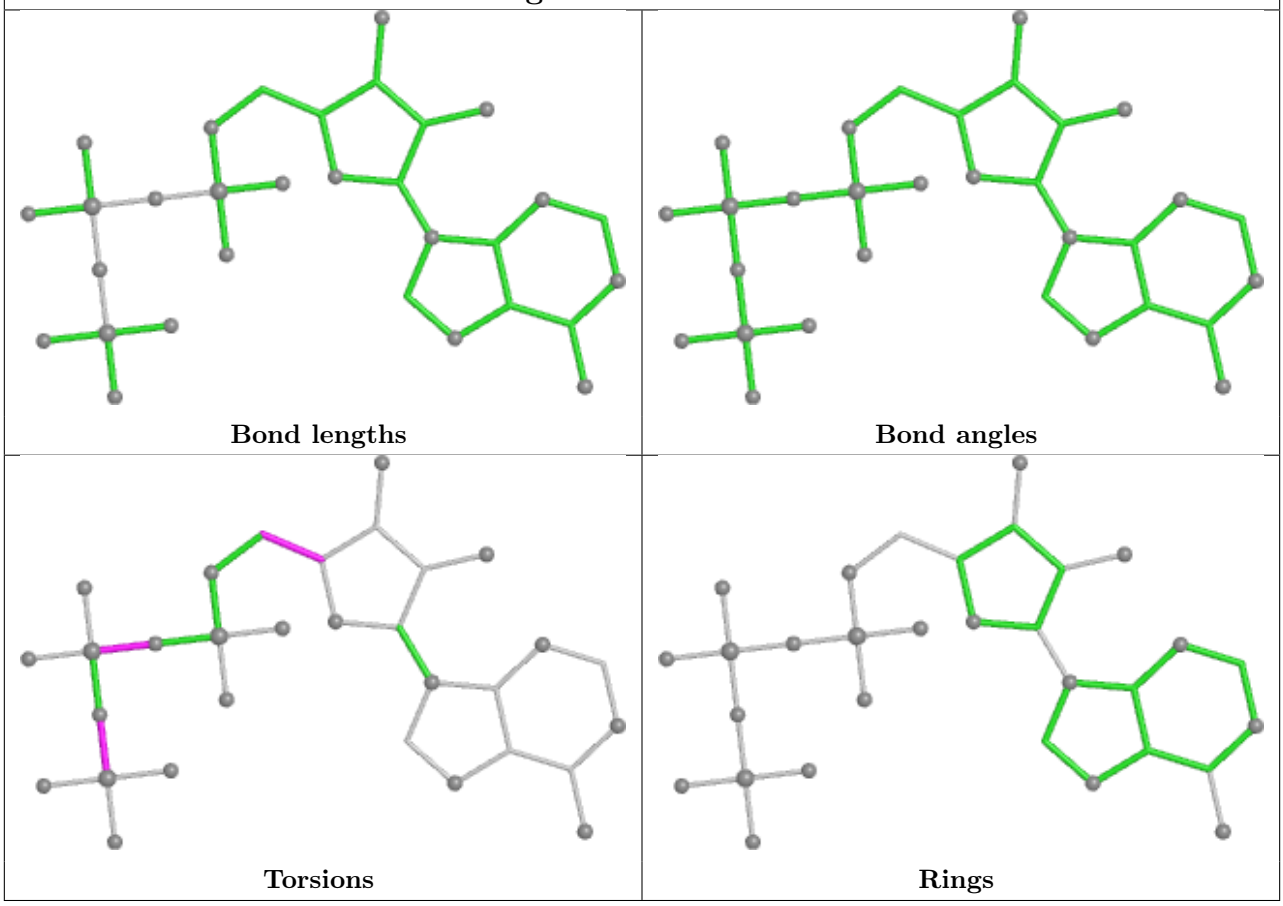
Ligand ATP B 601



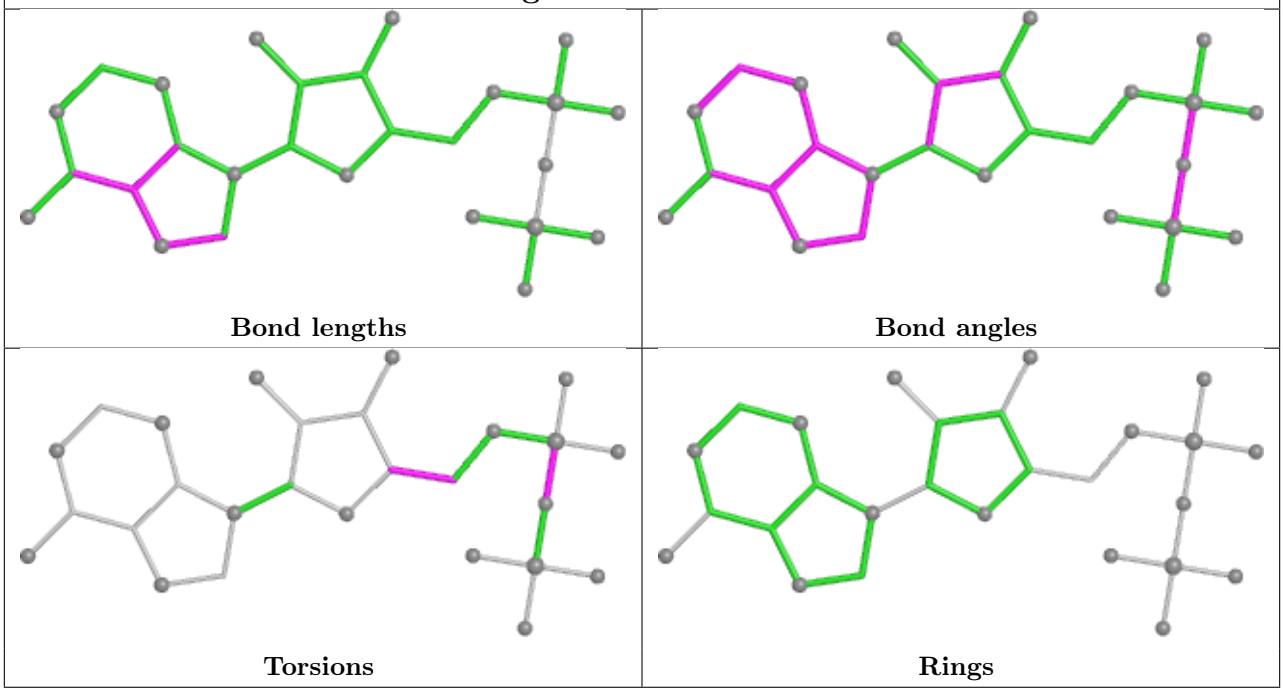
Ligand ADP F 501



Ligand ATP C 602



Ligand ADP D 501



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.

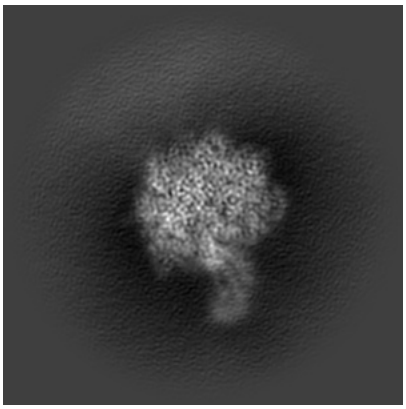
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-69450. These allow visual inspection of the internal detail of the map and identification of artifacts.

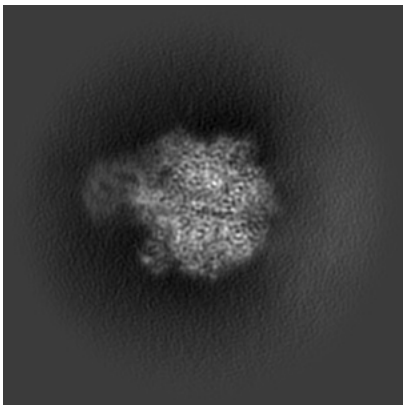
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

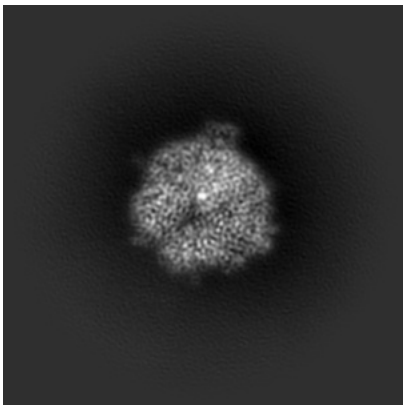
6.1.1 Primary map



X

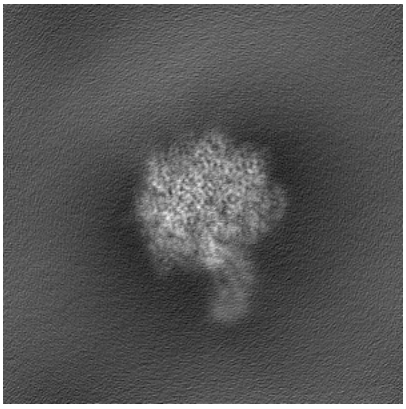


Y

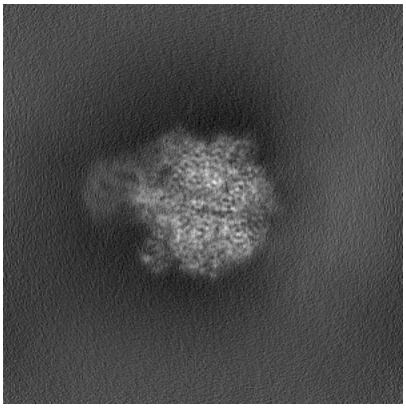


Z

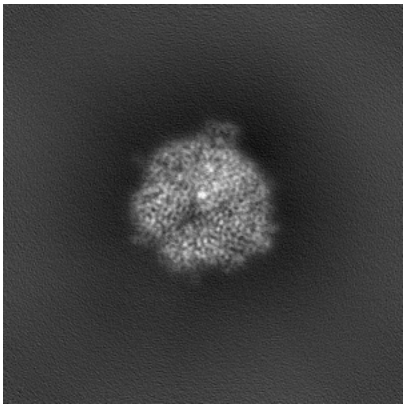
6.1.2 Raw map



X



Y

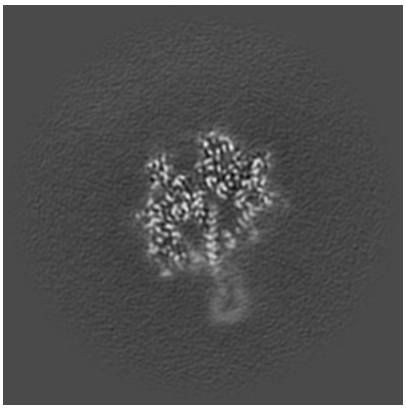


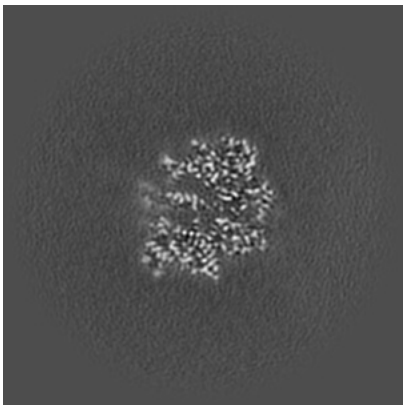
Z

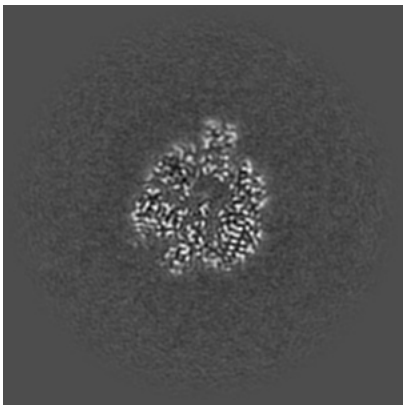
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

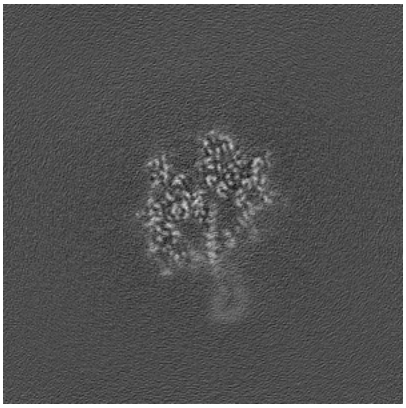
6.2.1 Primary map

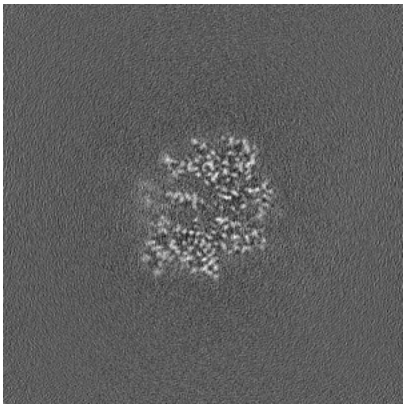

X Index: 175

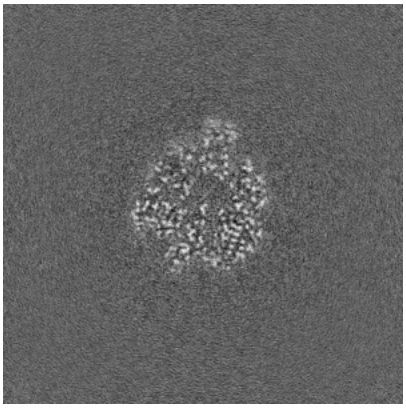

Y Index: 175


Z Index: 175

6.2.2 Raw map


X Index: 175

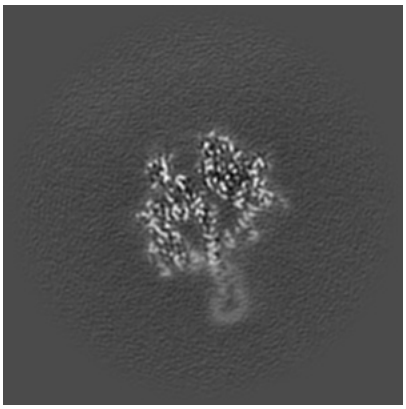

Y Index: 175

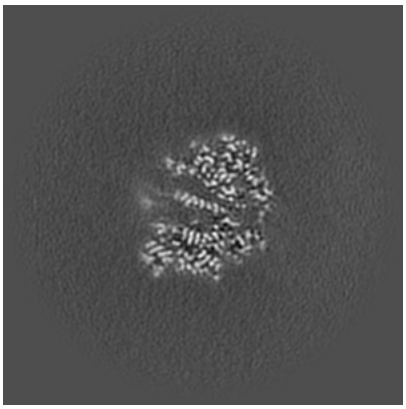

Z Index: 175

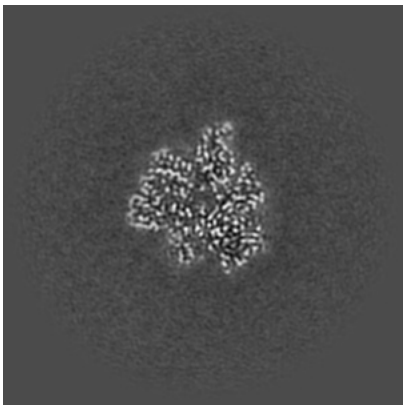
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

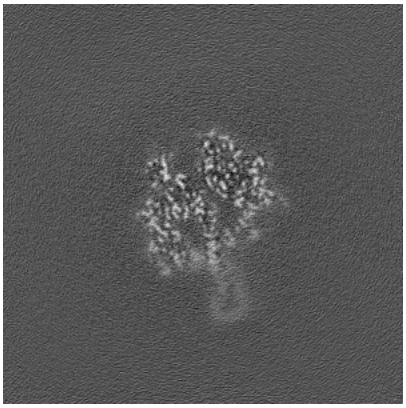
6.3.1 Primary map

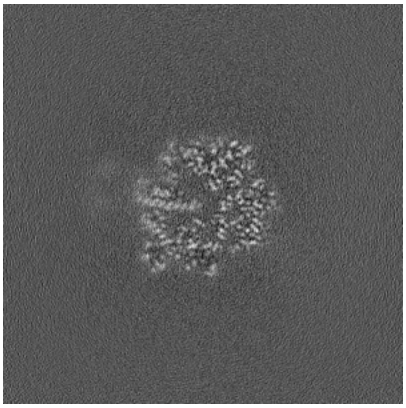

X Index: 176

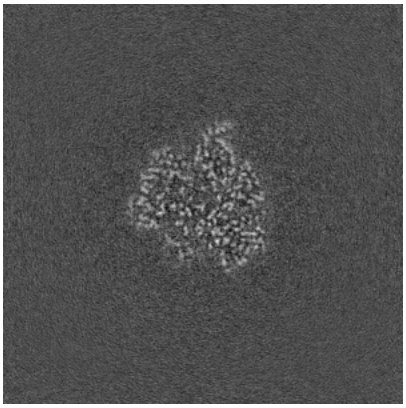

Y Index: 173


Z Index: 184

6.3.2 Raw map


X Index: 176

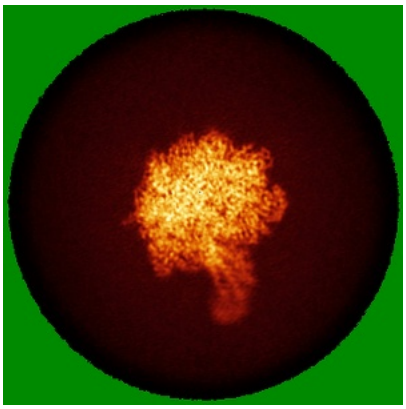

Y Index: 181


Z Index: 185

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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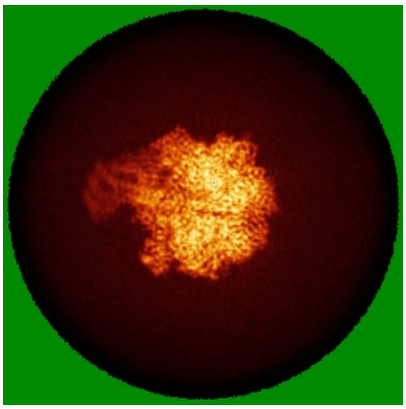
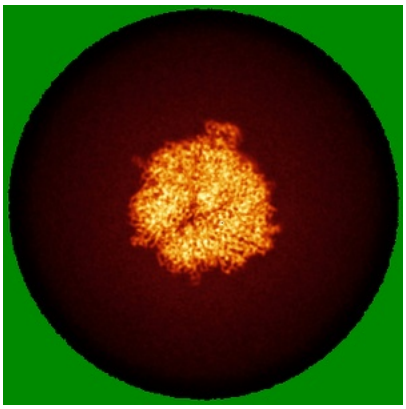
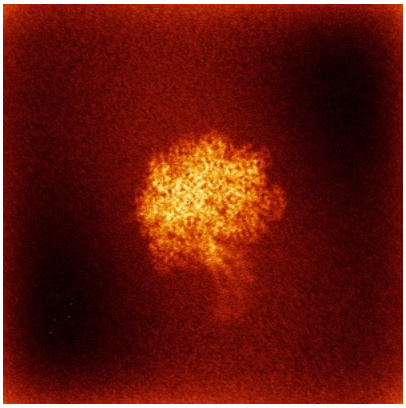
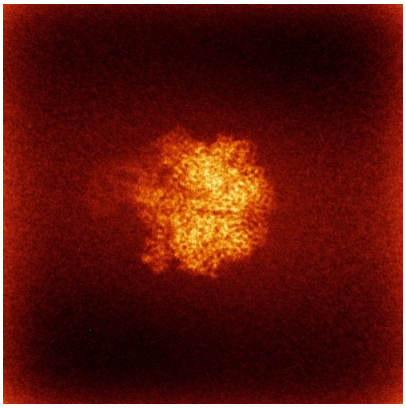
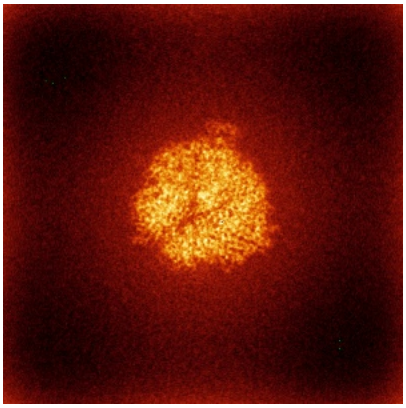

Y


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.

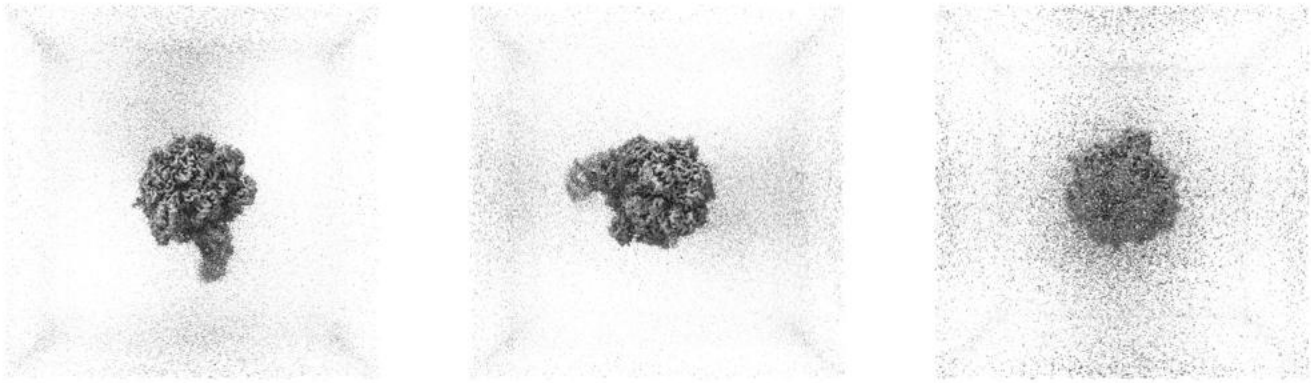
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0712. 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.

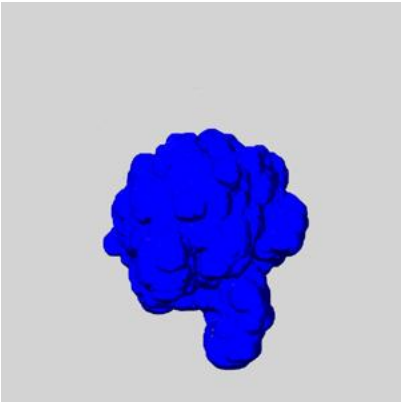
6.6 Mask visualisation (i)

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

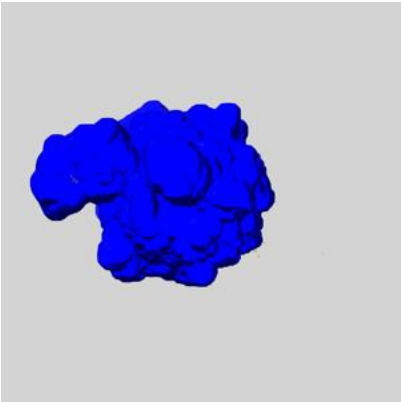
A mask typically either:

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

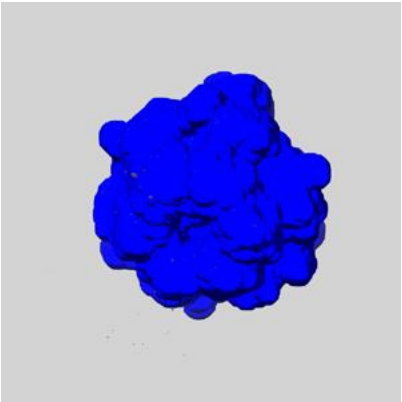
6.6.1 emd_69450_msk_1.map (i)



X



Y

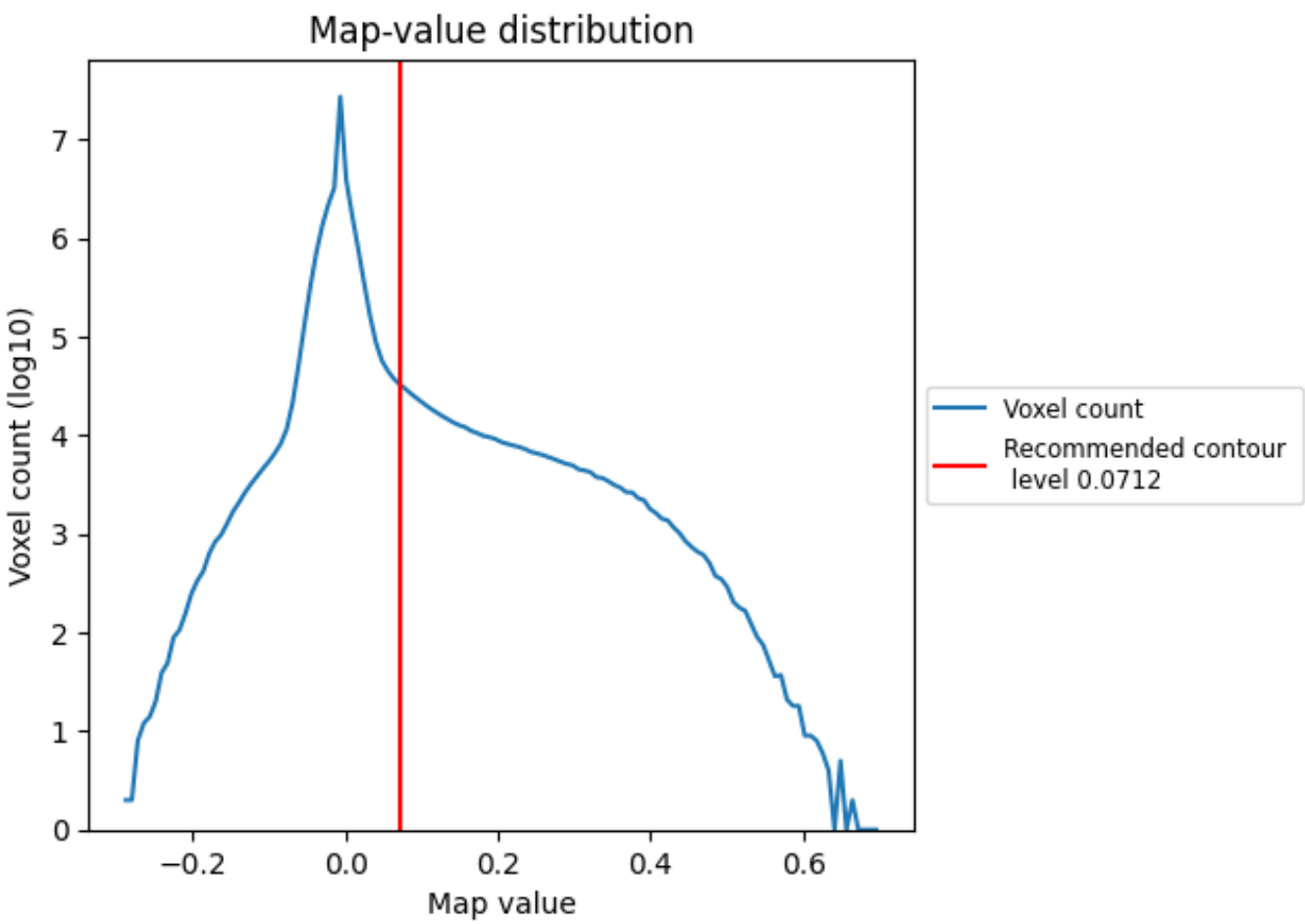


Z

7 Map analysis (i)

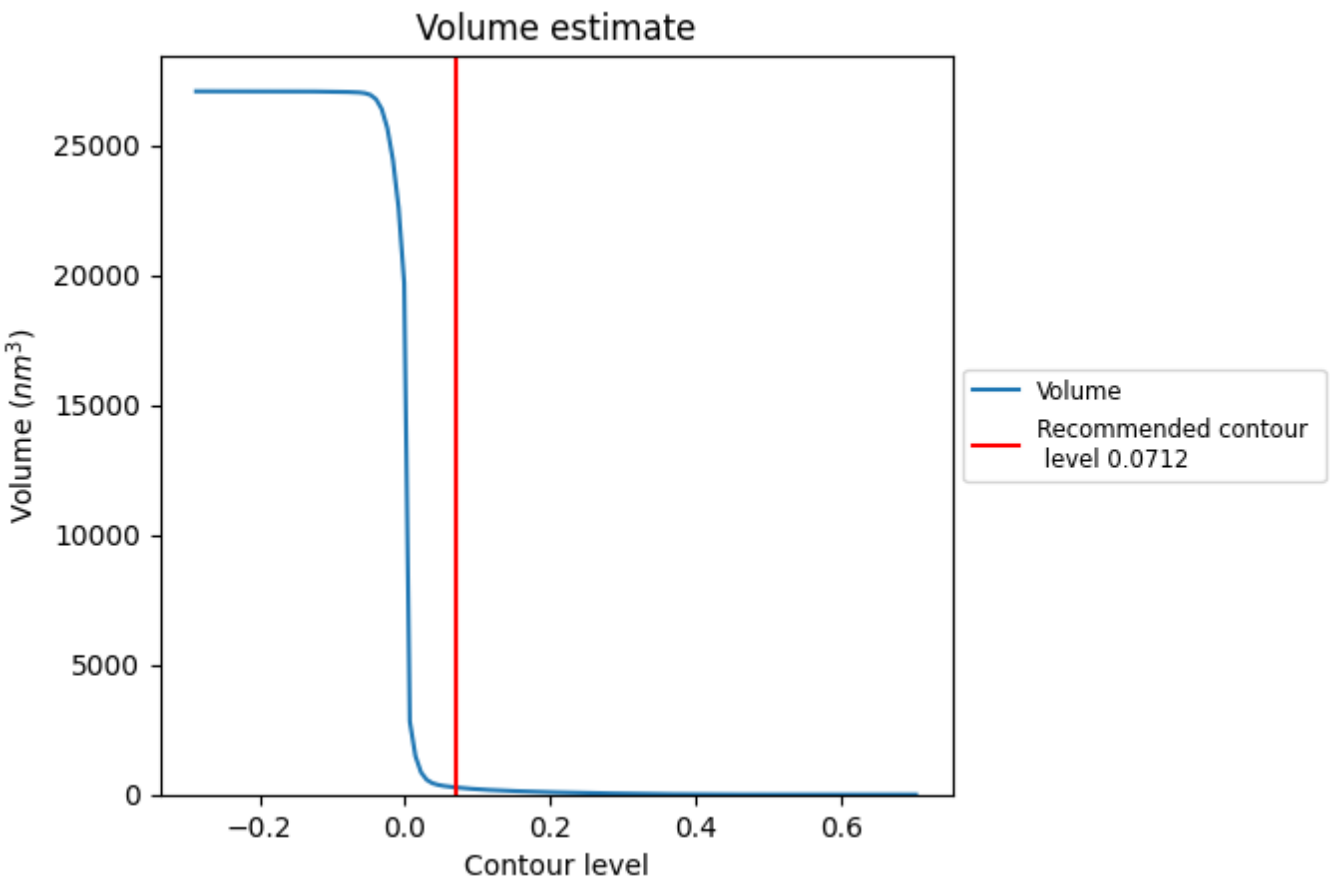
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

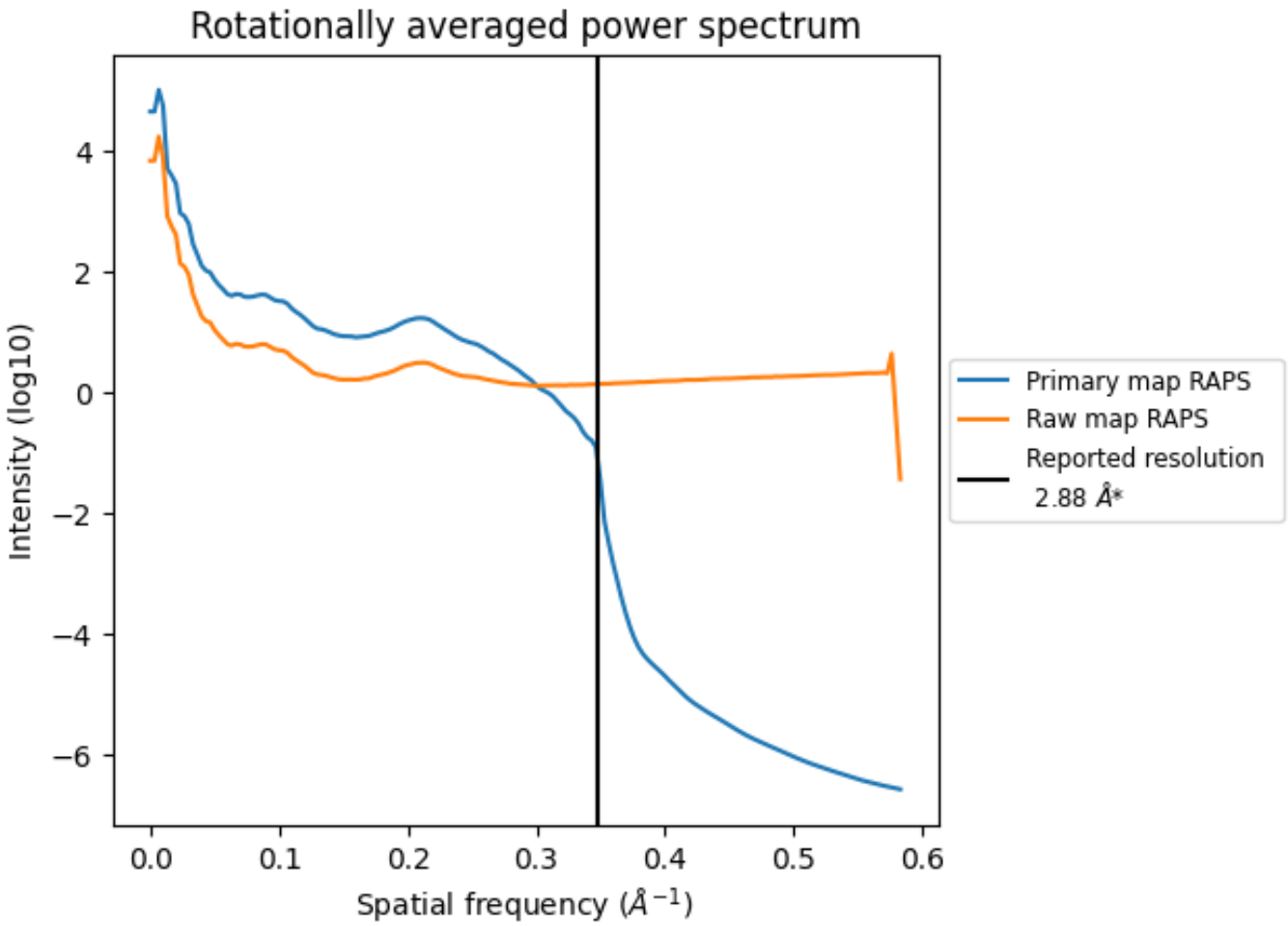
7.2 Volume estimate (i)



The volume at the recommended contour level is 271 nm^3; this corresponds to an approximate mass of 245 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)

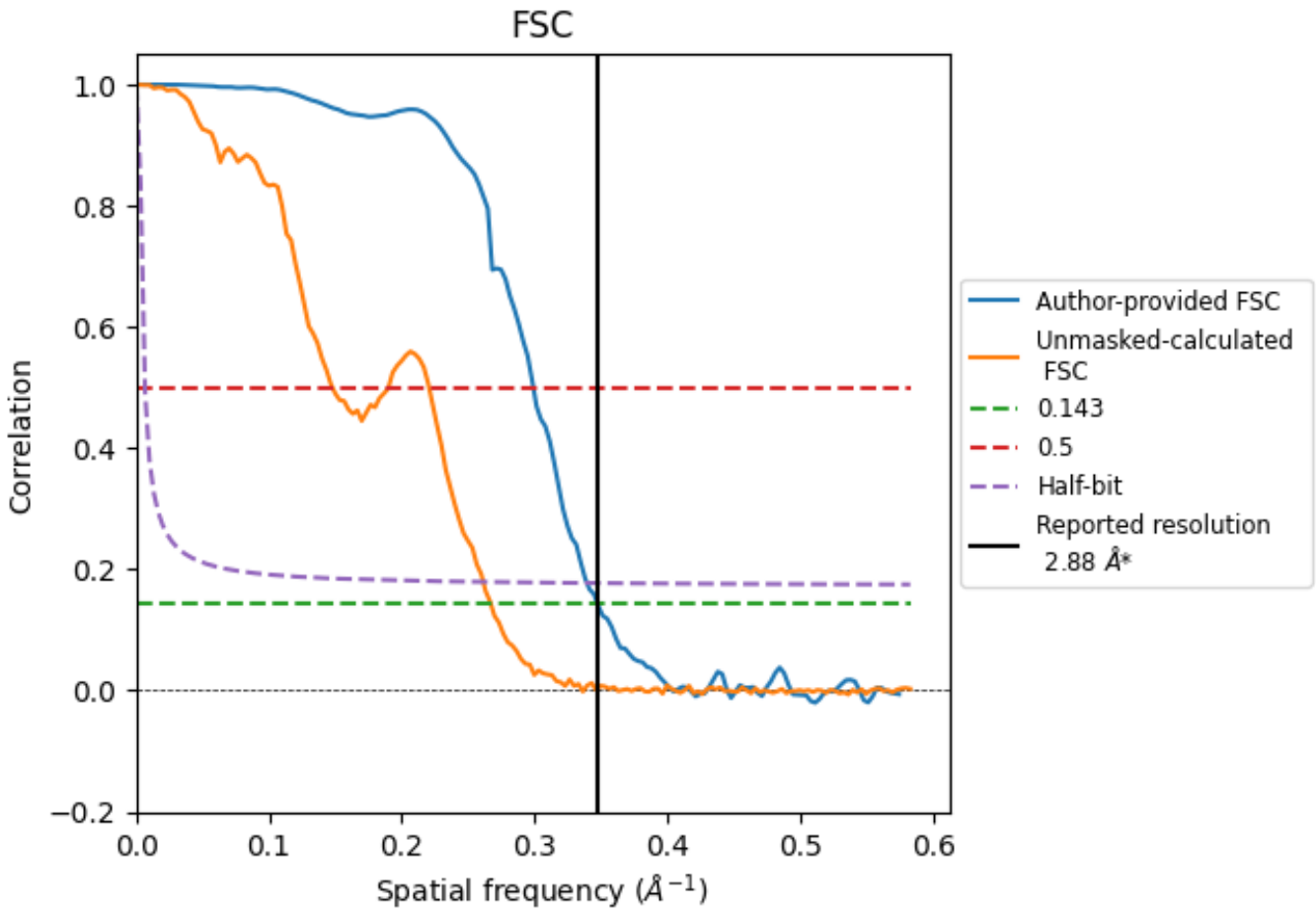


*Reported resolution corresponds to spatial frequency of 0.347 Å^{-1}

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 0.347 Å^{-1}

8.2 Resolution estimates (i)

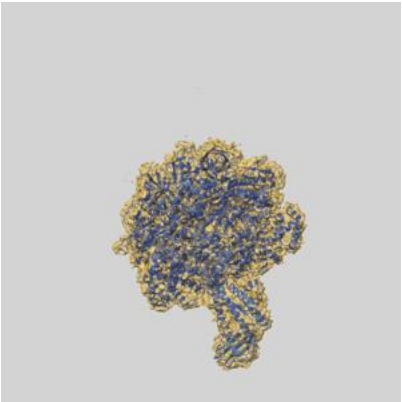
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	2.88	3.34	2.95
Unmasked-calculated*	3.75	6.77	3.83

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.75 differs from the reported value 2.88 by more than 10 %

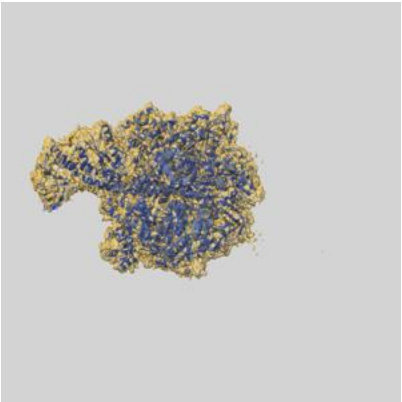
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-69450 and PDB model 24DN. Per-residue inclusion information can be found in section 3 on page 7.

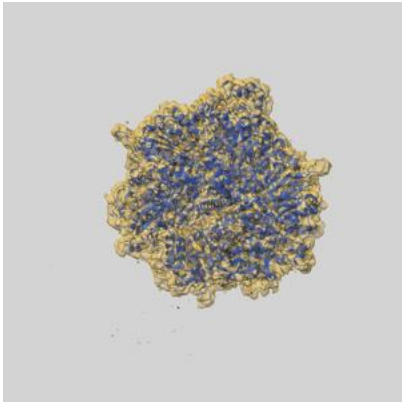
9.1 Map-model overlay (i)



X



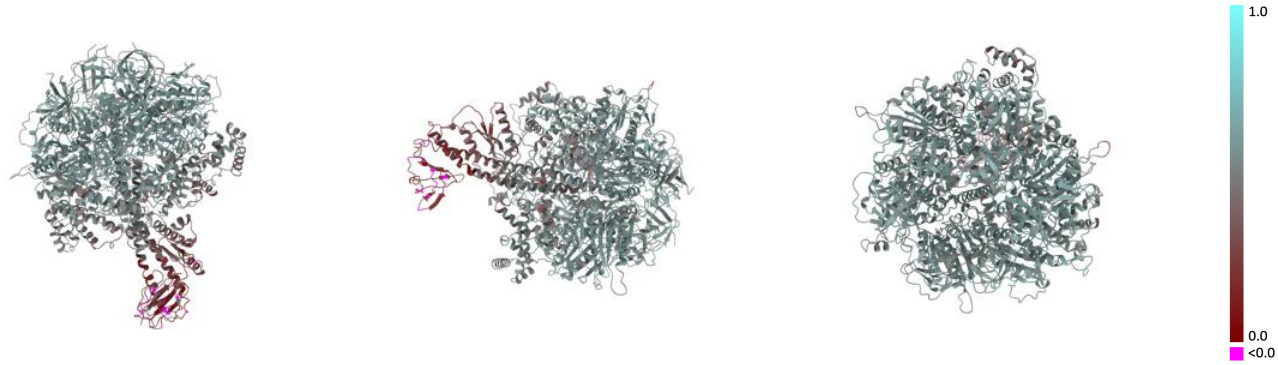
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0712 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.

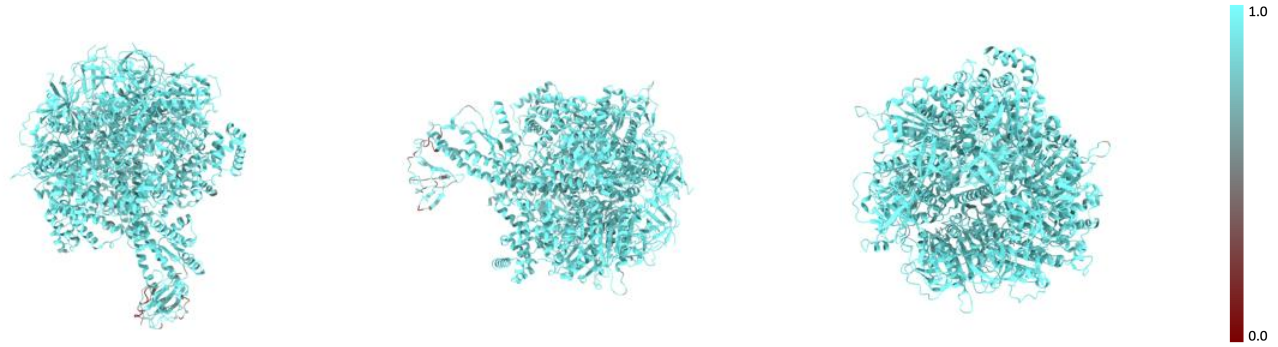
9.2 Q-score mapped to coordinate model (i)



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.

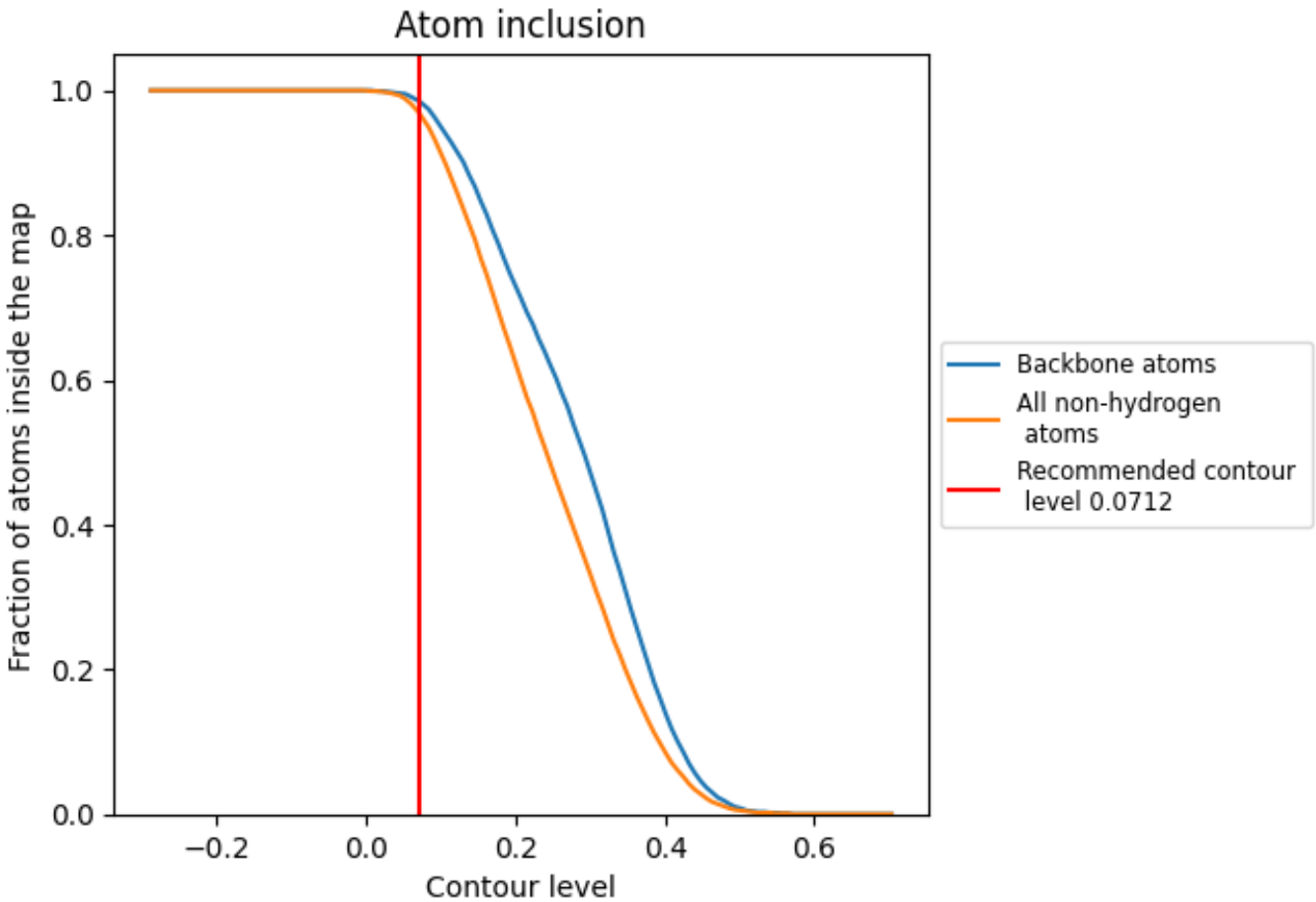
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0712).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (0.0712) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9690	0.5260
A	0.9830	0.5550
B	0.9830	0.5510
C	0.9800	0.5450
D	0.9780	0.5450
E	0.9810	0.5590
F	0.9750	0.5400
e	0.7670	0.1570
g	0.9050	0.3650