WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB EM Validation Report ⓘ

Nov 16, 2022 – 12:40 PM JST

PDB ID	:	6LY8
EMDB ID	:	EMD-30014
Title	:	V/A-ATPase from Thermus thermophilus, the soluble domain, including V1, d, two EG stalks, and N-terminal domain of a-subunit.
Authors	:	Kishikawa, J.; Nakanishi, A.; Furuta, A.; Kato, T.; Namba, K.; Tamakoshi, M.; Mitsuoka, K.; Yokoyama, K.
Deposited on	:	2020-02-13
Resolution	:	3.50 Å(reported)
Based on initial model	:	5Y5Y

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1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.50 Å.

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

Metric	Percentile Ranks	Value
Clashscore		7
Ramachandran outliers		0.0%
Sidechain outliers		10.4%

Worse   *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures
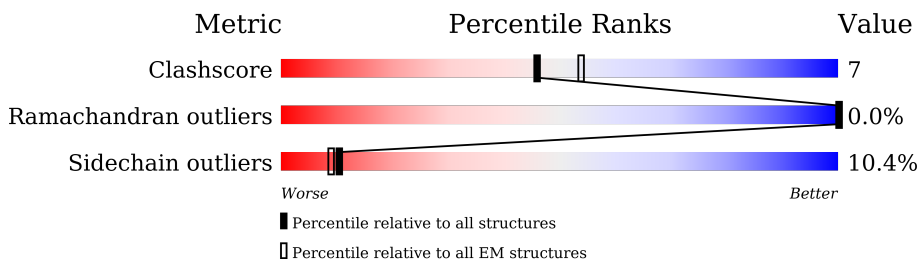
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	578	78% 19% •
1	B	578	• 78% 19% •
1	C	578	• 78% 20% •
2	D	478	• 77% 18% • •
2	E	478	• 73% 21% • •
2	F	478	• 76% 18% • •
3	G	223	20% 77% 17% • 6%
4	H	104	37% 68% 21% 7% •

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 26631 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 V-type ATP synthase alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	577	Total 4472	C 2854	N 762	O 834	S 22	0	0
1	B	577	Total 4472	C 2854	N 762	O 834	S 22	0	0
1	C	577	Total 4472	C 2854	N 762	O 834	S 22	0	0

- Molecule 2 is a protein called V-type ATP synthase beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	459	Total 3596	C 2278	N 622	O 686	S 10	0	0
2	E	459	Total 3596	C 2278	N 622	O 686	S 10	0	0
2	F	459	Total 3596	C 2278	N 622	O 686	S 10	0	0

- Molecule 3 is a protein called V-type ATP synthase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	210	Total 1642	C 1033	N 307	O 300	S 2	0	0

- Molecule 4 is a protein called V-type ATP synthase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	100	Total 758	C 479	N 131	O 145	S 3	0	0

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
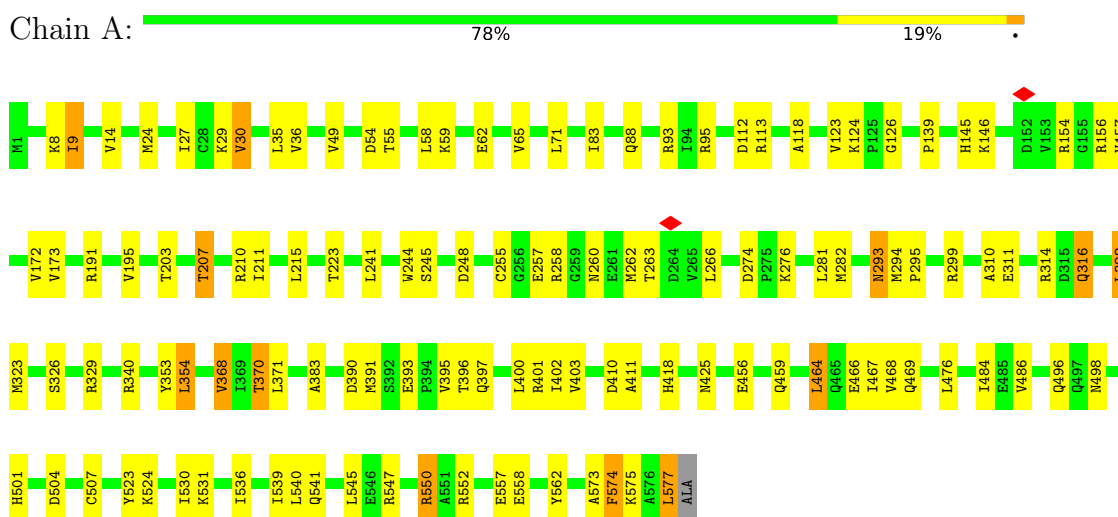
ADP
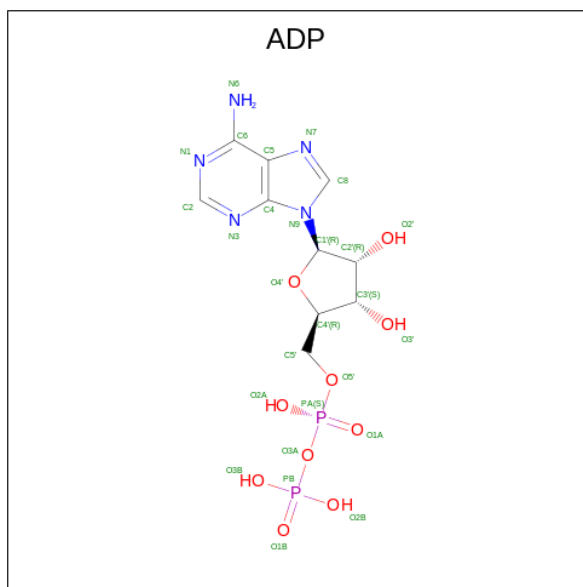
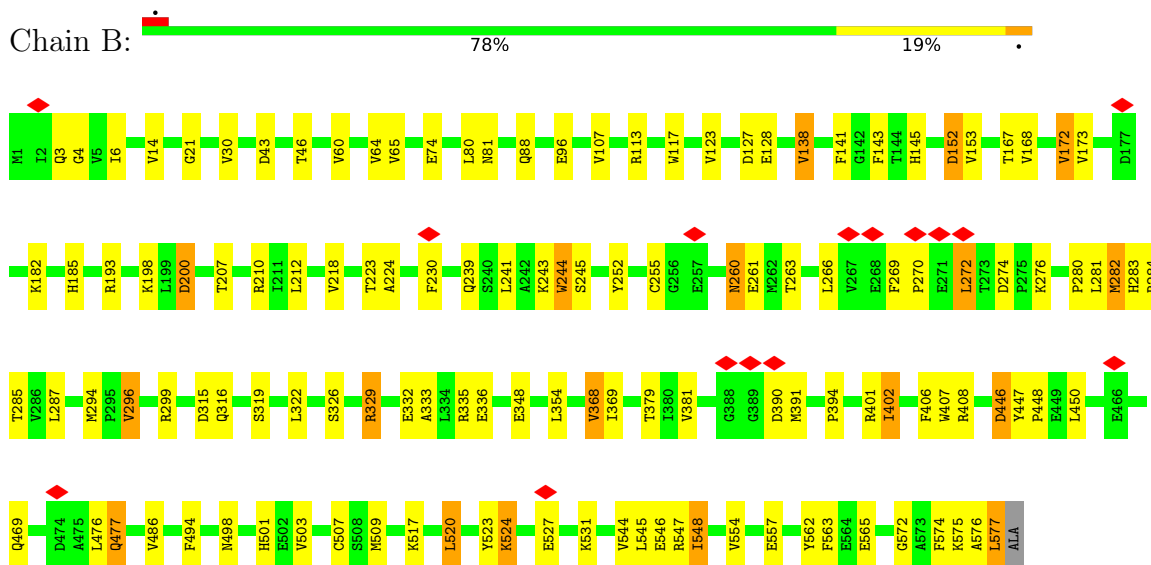| Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
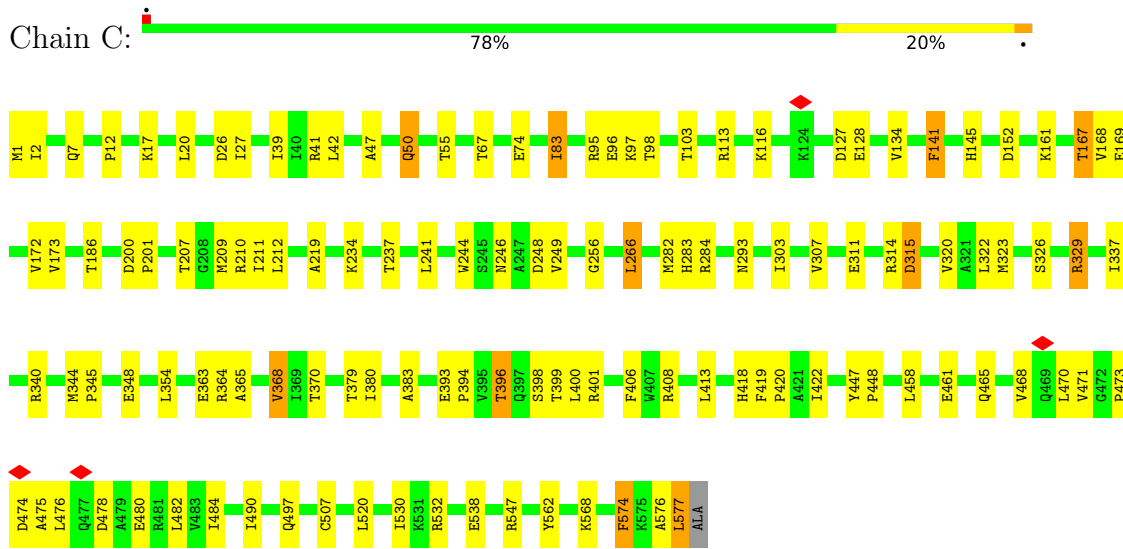
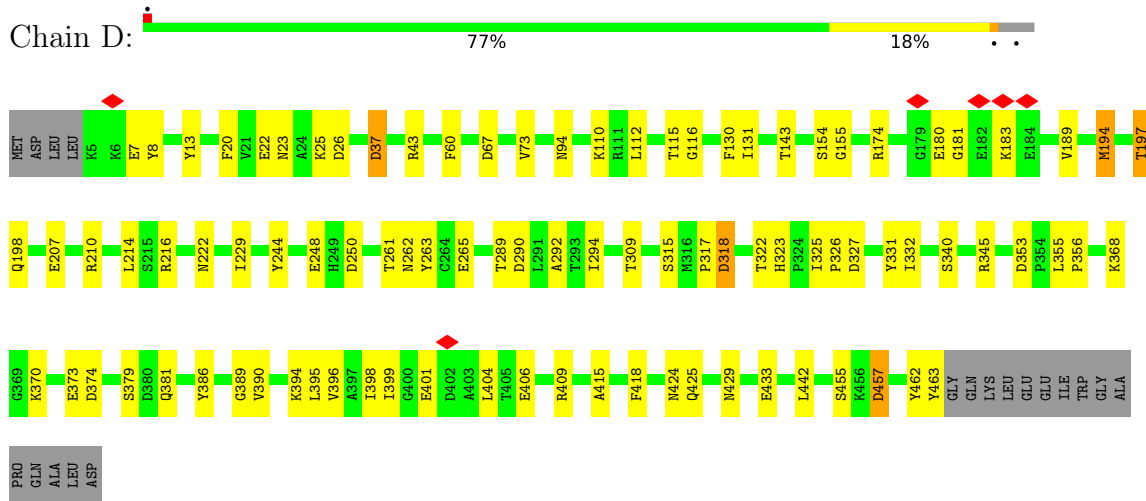- Molecule 1: V-type ATP synthase alpha chain
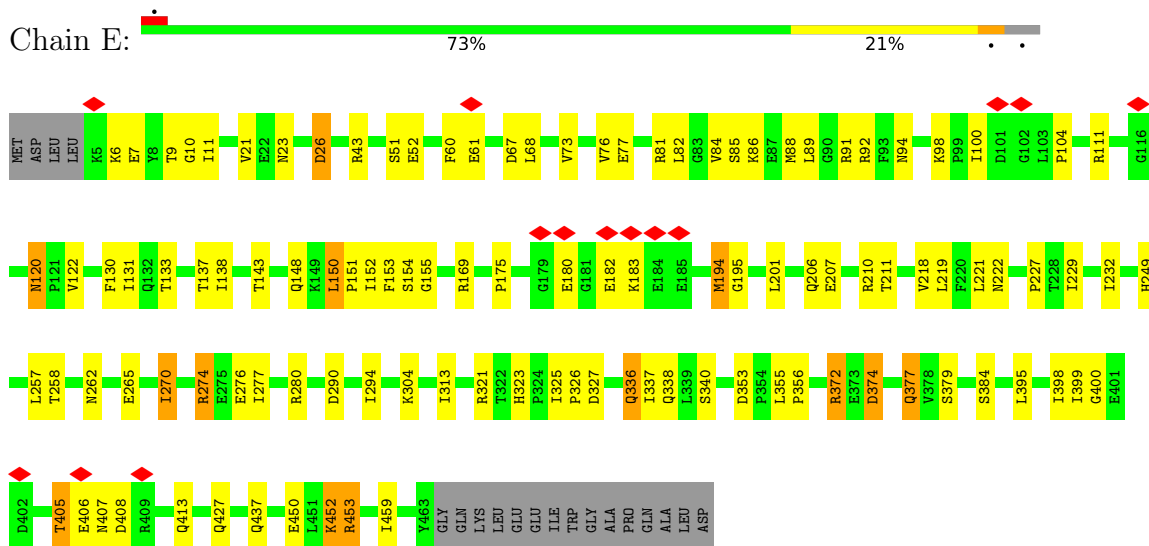
Chain A:

- Molecule 1: V-type ATP synthase alpha chain

Chain B:

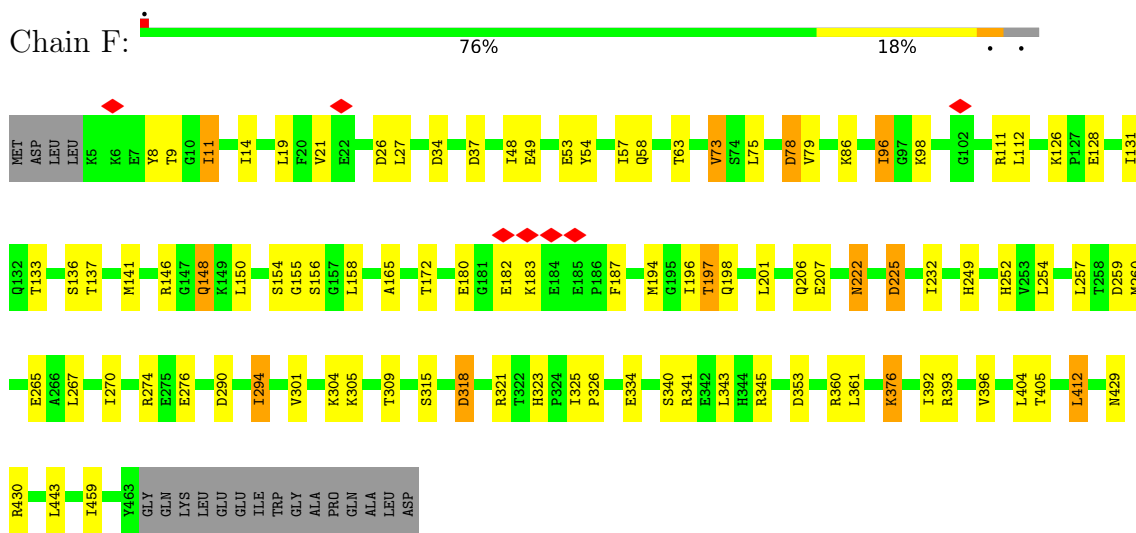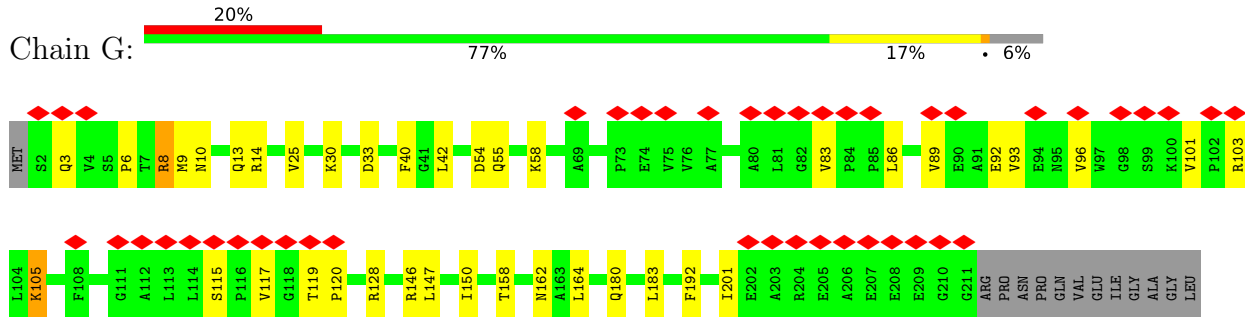- Molecule 1: V-type ATP synthase alpha chain

Chain C:

78% 20%

M1 I2 Q7 P12 K17 L20 D26 I27 I39 I40 R41 L42 A47 Q50 T55 T67 E74 I83 R95 E96 K97 T98 T103 R113 K116 K124 D127 E128 V134 F141 H145 D152 K161 T167 V168 E169

V172 V173 T186 D200 P201 T207 G208 M209 R210 I211 L212 A219 K234 T237 L241 W244 S245 N246 A247 D248 V249 G256 L266 M282 H283 R284 N293 I303 V307 E311 R314 D315 V320 A321 L322 M323 S326 R329 I337

R340 M344 P345 E348 L354 E363 R364 A365 V368 I369 T370 T379 I380 A383 E393 P394 V395 T396 Q397 S398 T399 L400 R401 F406 W407 R408 L413 H418 F419 P420 A421 I422 Y447 P448 L458 E461 Q465 V468 Q469 L470 V471 G472 P473

D474 A475 L476 Q477 D478 A479 R481 L482 V483 I484 I490 Q497 C507 L520 I530 K531 R532 E538 R547 Y562 K568 F574 K575 A576 L577 ALA

• Molecule 2: V-type ATP synthase beta chain

Chain D:

77% 18%

MET ASP LEU LEU K5 K6 E7 Y8 Y13 F20 V21 E22 N23 A24 K25 D26 D37 R43 F60 D67 V73 N94 K110 R111 L112 T115 G116 F130 I131 T143 S154 G155 R174 G179 E180 G181 E182 K183 E184 V189 M194 T197

Q198 E207 R210 L214 S215 R216 N222 I229 Y244 E248 H249 D250 T261 N262 Y263 C264 E265 T289 D290 L291 A292 T293 I294 T309 S315 M316 P317 D318 T322 H323 P324 I325 P326 D327 Y331 I332 S340 R345 D353 P354 L355 P356 K368

G369 K370 E373 D374 S379 D380 Q381 Y386 G389 V390 K394 L395 V396 A397 I398 I399 G400 E401 D402 A403 L404 T405 E406 R409 A415 F418 N424 Q425 N429 E433 L442 S455 K456 D457 Y462 V463 GLY GLN LYS LEU GLU GLU ILE TRP GLY ALA

PRO GLN ALA LEU ASP

• Molecule 2: V-type ATP synthase beta chain

Chain E:

73% 21%

MET ASP LEU LEU K5 K6 E7 Y8 T9 G10 I11 V21 E22 N23 D26 R43 S51 E52 F60 E61 D67 L68 V73 V76 E77 R81 L82 G83 V84 S85 K86 E87 M88 L89 G90 R91 R92 F93 N94 K98 P99 I100 D101 G102 L103 P104 R111 G116

N120 P121 V122 F130 I131 Q132 T133 T137 I138 T143 Q148 K149 L150 P151 I152 F153 S154 G155 R169 P175 G179 E180 G181 E182 K183 E184 E185 M194 G195 L201 Q206 E207 R210 T211 V218 L219 F220 L221 N222 P227 T228 I229 I232 H249

L257 T258 N262 E265 I270 R274 E275 E276 I277 R280 D290 I294 K304 I313 R321 T322 H323 P324 I325 P326 D327 Q336 I337 Q338 L339 S340 D353 P354 L355 P356 R372 E373 D374 Q377 V378 S379 S384 L395 I398 I399 G400 E401

D402 T405 E406 N407 D408 R409 Q413 Q427 Q437 E450 L451 K452 R463 I459 Y463 GLY GLN LYS LEU GLU GLU ILE TRP GLY ALA PRO GLN ALA LEU ASP

• Molecule 2: V-type ATP synthase beta chain

Chain F:

MET ASP LEU LEU K5 K6 E7 Y8 T9 G10 I11 I14 L19 F20 V21 E22 D26 L27 D34 D37 I48 E49 E53 Y54 I57 Q58 T63 V73 S74 L75 D78 V79 K86 I96 G97 K98 G102 R111 L112 K126 P127 E128 I131

Q132 T133 S136 T137 M141 R146 G147 Q148 K149 L150 S154 G155 S156 G157 L158 A165 T172 E180 G181 E182 K183 E184 E185 P186 F187 M194 G195 I196 T197 Q198 L201 Q206 E207 N222 D225 I232 H249 H252 V253 L254 L257 T258 D259 M260

E265 A266 L267 I270 R274 E275 E276 D290 I294 V301 K304 K305 T309 S315 D318 R321 T322 H323 P324 I325 P326 E334 S340 R341 E342 L343 H344 R345 D353 R360 L361 K376 I392 R393 V396 L404 T405 L412 N429

R430 L443 I459 Y463 GLY GLN LYS LEU GLU GLU ILE TRP GLY ALA PRO GLN ALA LEU ASP

• Molecule 3: V-type ATP synthase subunit D

Chain G:

MET S2 Q3 V4 S5 P6 T7 R8 M9 N10 Q13 R14 V25 K30 D33 F40 G41 L42 D54 Q55 K58 A69 P73 E74 V75 V76 A77 A80 L81 G82 V83 P84 P85 L86 V89 E90 A91 E92 V93 E94 N95 V96 W97 G98 S99 K100 V101 P102 R103

L104 K105 F108 G111 A112 L113 L114 S115 P116 V117 G118 T119 P120 R128 R146 L147 I150 T158 N162 A163 L164 Q180 L183 F192 I201 E202 A203 R204 E205 A206 E207 E208 E209 G210 G211 ARG PRO ASN PRO GLN VAL GLU ILE GLY ALA GLY LEU

• Molecule 4: V-type ATP synthase subunit F

Chain H:

M1 D6 A10 Q11 R14 L15 L18 E19 G20 S24 S25 A26 E27 E28 A29 Q30 L33 E34 T35 L36 V37 E38 R39 G40 G41 L44 D48 E49 A50 L51 L52 P53 D54 P55 E56 R57 A58 V59 E60 R61 L62 M63 R64 Q65 R66 D67 L68 P69 V70 L71 I74

A75 G76 L77 K78 E79 A80 F81 Q82 G83 M90 R91 E92 L93 V94 R95 K96 T97 F100 ASP ILE LYS LEU

4   Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	71196	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 $(e^-/\text{Å}^2)$	45	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.512	Depositor
Minimum map value	-0.365	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.068	Depositor
Map size (Å)	374.0, 374.0, 374.0	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5   Model quality ⓘ

5.1   Standard geometry ⓘ

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

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	0.37	0/4568	0.48	0/6198
1	B	0.35	0/4568	0.47	0/6198
1	C	0.36	0/4568	0.48	0/6198
2	D	0.36	0/3663	0.48	0/4960
2	E	0.35	0/3663	0.48	0/4960
2	F	0.37	0/3663	0.49	0/4960
3	G	0.29	0/1662	0.44	0/2235
4	H	0.26	0/769	0.50	0/1039
All	All	0.35	0/27124	0.47	0/36748

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	419	PHE	Peptide

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	4472	0	4490	61	0
1	B	4472	0	4491	62	0
1	C	4472	0	4491	60	0
2	D	3596	0	3624	42	0
2	E	3596	0	3624	56	0
2	F	3596	0	3624	46	0
3	G	1642	0	1718	24	0
4	H	758	0	764	18	0
5	A	27	0	12	0	0
All	All	26631	0	26838	354	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 7.

All (354) 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:C:576:ALA:O	1:C:577:LEU:CD2	1.80	1.29
1:C:576:ALA:O	1:C:577:LEU:HD22	1.38	1.20
1:C:576:ALA:O	1:C:577:LEU:HD23	1.62	0.98
4:H:94:VAL:HG12	4:H:100:PHE:C	1.92	0.89
1:A:577:LEU:HD23	1:A:577:LEU:H	1.42	0.85
1:C:210:ARG:NH1	1:C:507:CYS:SG	2.51	0.82
1:C:576:ALA:C	1:C:577:LEU:HD23	2.01	0.81
2:E:91:ARG:NH2	2:E:104:PRO:O	2.15	0.80
1:C:401:ARG:NH2	2:F:265:GLU:OE2	2.15	0.79
1:C:576:ALA:C	1:C:577:LEU:CD2	2.50	0.79
2:F:225:ASP:OD1	2:F:225:ASP:N	2.18	0.75
1:B:294:MET:O	1:B:299:ARG:NH1	2.20	0.74
1:A:210:ARG:NH1	1:A:507:CYS:SG	2.60	0.74
1:C:547:ARG:O	1:C:562:TYR:OH	2.04	0.74
1:C:74:GLU:OE2	1:C:113:ARG:NH2	2.22	0.73
1:B:74:GLU:OE1	1:B:113:ARG:NH2	2.23	0.72
1:B:210:ARG:NH1	1:B:494:PHE:O	2.23	0.71
1:B:224:ALA:HB3	1:B:381:VAL:HG12	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:ARG:NH1	1:C:169:GLU:OE2	2.25	0.68
2:E:274:ARG:NH1	2:E:276:GLU:OE2	2.25	0.68
2:F:318:ASP:N	2:F:318:ASP:OD1	2.25	0.68
1:A:550:ARG:NH1	1:A:562:TYR:OH	2.26	0.68
2:D:406:GLU:OE1	2:D:409:ARG:NH1	2.26	0.68
1:C:234:LYS:HD2	1:C:383:ALA:HB1	1.77	0.67
4:H:63:MET:HG2	4:H:68:LEU:HD12	1.76	0.67
1:C:1:MET:HG2	1:C:2:ILE:HG13	1.75	0.66
1:C:470:LEU:HG	1:C:471:VAL:HG13	1.76	0.66
2:E:374:ASP:OD1	2:E:374:ASP:N	2.30	0.65
1:A:29:LYS:HG2	1:A:36:VAL:HG12	1.78	0.65
1:A:340:ARG:NH2	2:F:276:GLU:OE2	2.30	0.65
2:D:318:ASP:OD1	2:D:318:ASP:N	2.29	0.65
2:F:197:THR:OG1	2:F:198:GLN:N	2.31	0.64
2:E:323:HIS:HB3	2:E:326:PRO:HD2	1.79	0.64
2:D:197:THR:OG1	2:D:198:GLN:N	2.30	0.64
2:F:11:ILE:HG22	2:F:21:VAL:HG12	1.79	0.64
2:E:407:ASN:ND2	2:E:408:ASP:OD1	2.31	0.64
1:B:326:SER:HB3	1:B:329:ARG:HB2	1.79	0.63
3:G:103:ARG:HH21	3:G:146:ARG:HD3	1.62	0.63
1:A:391:MET:O	1:A:397:GLN:NE2	2.30	0.62
1:B:200:ASP:OD1	1:B:200:ASP:N	2.31	0.62
3:G:25:VAL:HG23	3:G:164:LEU:HD23	1.81	0.61
1:B:332:GLU:OE1	1:B:335:ARG:NH1	2.32	0.61
1:A:577:LEU:HD23	1:A:577:LEU:N	2.14	0.61
1:A:467:ILE:HD11	2:D:394:LYS:HG2	1.83	0.61
1:A:370:THR:OG1	1:A:371:LEU:N	2.32	0.60
1:B:207:THR:HG23	1:B:241:LEU:HD13	1.83	0.60
1:B:401:ARG:NH2	2:E:265:GLU:OE2	2.34	0.60
2:F:325:ILE:HB	2:F:326:PRO:HD3	1.82	0.60
1:B:185:HIS:HE1	1:B:193:ARG:HH12	1.50	0.59
1:C:167:THR:OG1	1:C:168:VAL:N	2.32	0.59
1:B:4:GLY:O	1:B:64:VAL:N	2.32	0.59
2:D:325:ILE:HB	2:D:326:PRO:HD3	1.84	0.59
2:F:78:ASP:OD1	2:F:78:ASP:N	2.34	0.59
1:A:210:ARG:NH2	1:A:496:GLN:O	2.36	0.59
1:B:517:LYS:HD3	1:B:563:PHE:HZ	1.68	0.59
1:A:293:ASN:OD1	1:A:293:ASN:N	2.36	0.59
2:D:37:ASP:N	2:D:37:ASP:OD1	2.35	0.59
1:C:393:GLU:HB3	1:C:396:THR:HG22	1.85	0.59
1:A:577:LEU:H	1:A:577:LEU:CD2	2.13	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:PRO:HA	1:B:280:PRO:HA	1.85	0.58
4:H:66:ARG:HB3	4:H:68:LEU:HG	1.83	0.58
1:A:504:ASP:OD2	1:A:552:ARG:NH1	2.36	0.58
1:C:127:ASP:OD1	1:C:128:GLU:N	2.32	0.58
2:E:325:ILE:HB	2:E:326:PRO:HD3	1.84	0.58
2:E:405:THR:OG1	2:E:406:GLU:N	2.36	0.58
2:E:150:LEU:HD21	2:E:337:ILE:HD12	1.85	0.58
1:B:260:ASN:ND2	1:B:261:GLU:OE2	2.36	0.58
1:B:252:TYR:HB3	1:B:287:LEU:HD12	1.86	0.58
2:F:154:SER:OG	2:F:155:GLY:N	2.36	0.58
2:E:340:SER:HB2	2:E:353:ASP:HB2	1.85	0.57
1:C:311:GLU:OE2	1:C:364:ARG:NE	2.35	0.57
1:B:336:GLU:OE2	2:D:289:THR:OG1	2.17	0.57
1:A:393:GLU:HG2	1:A:395:VAL:H	1.70	0.57
2:D:455:SER:OG	2:D:457:ASP:OD1	2.16	0.56
2:F:27:LEU:HD23	2:F:75:LEU:HD13	1.86	0.56
2:F:49:GLU:OE1	2:F:274:ARG:NH2	2.38	0.56
4:H:100:PHE:CD2	4:H:100:PHE:N	2.73	0.56
1:A:459:GLN:HG3	2:D:345:ARG:HD2	1.87	0.56
4:H:14:ARG:NH1	4:H:20:GLY:O	2.37	0.56
1:C:315:ASP:HA	1:C:370:THR:HG21	1.86	0.56
2:E:169:ARG:NH1	2:E:207:GLU:OE2	2.38	0.56
2:F:11:ILE:HD13	2:F:11:ILE:H	1.71	0.56
2:F:136:SER:OG	2:F:430:ARG:NH1	2.39	0.56
2:E:154:SER:OG	2:E:155:GLY:N	2.39	0.56
3:G:158:THR:HG22	3:G:162:ASN:HD21	1.70	0.56
2:D:154:SER:OG	2:D:155:GLY:N	2.40	0.55
2:E:51:SER:OG	2:E:52:GLU:N	2.40	0.55
2:F:148:GLN:NE2	2:F:361:LEU:HB2	2.22	0.55
3:G:8:ARG:HD3	3:G:9:MET:H	1.72	0.55
1:A:558:GLU:OE1	1:A:558:GLU:N	2.39	0.54
2:F:318:ASP:O	3:G:3:GLN:NE2	2.35	0.54
1:B:446:ASP:OD1	1:B:446:ASP:N	2.41	0.54
1:C:473:PRO:HA	1:C:476:LEU:HD23	1.88	0.54
2:D:317:PRO:HG3	2:D:323:HIS:CD2	2.42	0.54
1:A:126:GLY:HA2	1:A:156:ARG:HH21	1.73	0.54
2:D:418:PHE:HA	2:D:442:LEU:HD21	1.90	0.53
1:C:400:LEU:O	1:C:401:ARG:HG2	2.08	0.53
2:D:13:TYR:HB3	2:D:20:PHE:HB2	1.90	0.53
2:E:210:ARG:HD2	2:E:211:THR:HG23	1.90	0.53
1:B:270:PRO:HG3	1:B:280:PRO:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:9:THR:OG1	2:E:10:GLY:N	2.42	0.53
1:A:112:ASP:OD1	1:A:113:ARG:N	2.41	0.53
1:A:118:ALA:HB3	1:A:139:PRO:HD2	1.90	0.53
4:H:67:ASP:OD1	4:H:67:ASP:N	2.36	0.53
1:A:468:VAL:HG22	1:A:476:LEU:HD11	1.91	0.52
1:B:547:ARG:O	1:B:562:TYR:OH	2.26	0.52
2:D:457:ASP:OD1	2:D:457:ASP:N	2.35	0.52
2:E:76:VAL:HG12	2:E:77:GLU:HG2	1.91	0.52
1:B:172:VAL:HG13	1:B:173:VAL:HG23	1.91	0.52
2:E:321:ARG:NH1	2:E:338:GLN:OE1	2.43	0.52
2:F:323:HIS:HD2	2:F:325:ILE:H	1.58	0.52
1:B:266:LEU:O	1:B:270:PRO:HG2	2.10	0.52
1:C:201:PRO:HB2	1:C:219:ALA:HB1	1.91	0.52
2:D:180:GLU:HG3	2:D:181:GLY:H	1.73	0.52
1:B:524:LYS:O	1:B:527:GLU:HG3	2.10	0.52
1:B:127:ASP:OD1	1:B:128:GLU:N	2.41	0.51
1:C:83:ILE:HD12	1:C:266:LEU:HD11	1.92	0.51
2:E:86:LYS:HG3	2:E:249:HIS:HD2	1.74	0.51
2:F:156:SER:OG	2:F:341:ARG:NH2	2.43	0.51
2:F:340:SER:HB2	2:F:353:ASP:HB2	1.91	0.51
2:D:115:THR:OG1	2:D:116:GLY:N	2.42	0.51
1:A:400:LEU:O	1:A:401:ARG:HG2	2.10	0.51
2:E:67:ASP:OD1	2:E:68:LEU:N	2.43	0.51
1:C:396:THR:HA	1:C:399:THR:HG22	1.92	0.51
2:F:196:ILE:HD12	2:F:201:LEU:HB2	1.93	0.51
1:A:326:SER:H	1:A:383:ALA:HB3	1.76	0.51
1:C:27:ILE:O	1:C:67:THR:OG1	2.29	0.51
1:A:390:ASP:OD1	1:A:390:ASP:N	2.44	0.51
1:A:9:ILE:HD12	1:A:58:LEU:HB2	1.93	0.51
2:F:148:GLN:HE21	2:F:361:LEU:HB2	1.76	0.51
4:H:14:ARG:HG2	4:H:20:GLY:H	1.75	0.51
1:A:310:ALA:HB2	1:A:322:LEU:HD23	1.93	0.50
1:B:527:GLU:O	1:B:531:LYS:HG2	2.11	0.50
2:E:194:MET:HA	2:E:222:ASN:HB3	1.93	0.50
1:A:172:VAL:HG23	1:A:173:VAL:HG23	1.94	0.50
1:C:474:ASP:OD1	1:C:475:ALA:N	2.43	0.50
1:B:43:ASP:N	1:B:43:ASP:OD1	2.42	0.50
2:E:377:GLN:H	2:E:377:GLN:NE2	2.09	0.50
2:F:194:MET:HA	2:F:222:ASN:HB3	1.93	0.50
1:C:7:GLN:HG3	1:C:17:LYS:HE2	1.94	0.50
1:B:145:HIS:CE1	1:B:316:GLN:HE22	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:321:ARG:NH2	2:E:336:GLN:OE1	2.45	0.50
1:C:246:ASN:O	1:C:246:ASN:ND2	2.45	0.49
1:B:576:ALA:HB3	1:B:577:LEU:HD23	1.94	0.49
1:C:482:LEU:HD22	1:C:530:ILE:HD12	1.93	0.49
2:F:96:ILE:HD13	2:F:98:LYS:HG2	1.95	0.49
1:C:212:LEU:HD21	1:C:422:ILE:HD13	1.94	0.49
1:B:210:ARG:NE	1:B:507:CYS:SG	2.83	0.49
1:B:296:VAL:HG12	1:B:333:ALA:HB1	1.95	0.48
1:B:43:ASP:OD1	1:B:46:THR:OG1	2.28	0.48
1:C:303:ILE:O	1:C:307:VAL:HG23	2.14	0.48
2:D:395:LEU:HD22	3:G:30:LYS:HG2	1.95	0.48
3:G:8:ARG:HG2	3:G:183:LEU:HD21	1.94	0.48
1:A:557:GLU:N	1:A:557:GLU:OE1	2.46	0.48
1:C:12:PRO:HA	1:C:55:THR:HG21	1.96	0.48
2:D:110:LYS:HD3	2:D:112:LEU:HD21	1.94	0.48
1:B:544:VAL:O	1:B:548:ILE:HG23	2.14	0.48
1:C:447:TYR:HB3	1:C:448:PRO:HD3	1.95	0.48
3:G:119:THR:N	3:G:120:PRO:HD3	2.29	0.48
4:H:100:PHE:N	4:H:100:PHE:HD2	2.12	0.48
1:A:257:GLU:HG2	1:A:258:ARG:H	1.79	0.48
1:A:322:LEU:HD13	1:A:323:MET:H	1.79	0.48
1:C:41:ARG:HG2	1:C:42:LEU:H	1.79	0.47
4:H:10:ALA:O	4:H:14:ARG:HG3	2.14	0.47
1:C:532:ARG:HH12	1:C:577:LEU:HA	1.79	0.47
1:B:486:VAL:HG21	1:B:523:TYR:HD1	1.79	0.47
1:A:260:ASN:HA	1:A:263:THR:HG22	1.95	0.47
2:E:120:ASN:ND2	2:E:122:VAL:HG22	2.29	0.47
1:B:239:GLN:HB3	1:B:269:PHE:HZ	1.80	0.47
1:C:97:LYS:HG3	1:C:98:THR:OG1	2.14	0.47
2:D:207:GLU:OE1	2:D:210:ARG:NH2	2.47	0.47
2:F:165:ALA:HB1	2:F:207:GLU:HG2	1.96	0.47
2:E:85:SER:OG	2:E:86:LYS:N	2.47	0.47
2:E:195:GLY:HA3	2:E:262:ASN:HD22	1.78	0.47
4:H:74:ILE:HG23	4:H:75:ALA:H	1.78	0.47
1:B:498:ASN:HD22	1:B:501:HIS:HB2	1.80	0.47
1:C:39:ILE:HG23	1:C:47:ALA:HB1	1.97	0.47
2:F:34:ASP:OD1	2:F:34:ASP:N	2.48	0.47
1:C:326:SER:HB3	1:C:329:ARG:HD2	1.95	0.47
2:E:175:PRO:HG2	2:E:182:GLU:HG3	1.97	0.47
2:D:37:ASP:OD2	2:D:43:ARG:NH1	2.48	0.47
1:C:241:LEU:HB2	1:C:323:MET:HE1	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:340:SER:HB2	2:D:353:ASP:HB2	1.98	0.46
2:E:11:ILE:HG22	2:E:21:VAL:HG22	1.97	0.46
2:F:155:GLY:HA3	2:F:158:LEU:HD12	1.96	0.46
2:D:373:GLU:OE1	2:D:373:GLU:N	2.47	0.46
1:B:117:TRP:HB3	1:B:138:VAL:HG21	1.97	0.46
1:B:391:MET:SD	1:B:391:MET:N	2.88	0.46
4:H:90:MET:O	4:H:94:VAL:HG22	2.16	0.46
3:G:42:LEU:HD22	3:G:150:ILE:HD12	1.96	0.46
1:B:269:PHE:CD2	1:B:281:LEU:HD23	2.50	0.46
1:C:41:ARG:HG2	1:C:42:LEU:N	2.31	0.46
2:D:229:ILE:H	2:D:229:ILE:HD12	1.80	0.46
2:D:60:PHE:HD1	2:D:229:ILE:HD13	1.80	0.46
4:H:1:MET:SD	4:H:1:MET:N	2.70	0.46
2:D:263:TYR:OH	2:D:290:ASP:OD1	2.30	0.46
1:B:390:ASP:OD1	1:B:390:ASP:N	2.49	0.45
2:E:353:ASP:O	2:E:356:PRO:HD2	2.16	0.45
2:F:392:ILE:HG22	2:F:412:LEU:HD23	1.98	0.45
1:A:464:LEU:HB3	1:A:484:ILE:HD11	1.98	0.45
1:C:172:VAL:HG23	1:C:173:VAL:HG23	1.98	0.45
1:C:322:LEU:HD23	1:C:323:MET:N	2.31	0.45
2:D:8:TYR:OH	2:D:26:ASP:HB3	2.16	0.45
2:D:250:ASP:N	2:D:250:ASP:OD1	2.50	0.45
1:A:418:HIS:CD2	1:A:496:GLN:HE21	2.34	0.45
1:B:185:HIS:CE1	1:B:193:ARG:HH12	2.32	0.45
2:E:450:GLU:O	2:E:452:LYS:HD3	2.16	0.45
2:F:222:ASN:O	2:F:222:ASN:ND2	2.43	0.45
2:F:318:ASP:HB2	3:G:3:GLN:NE2	2.32	0.45
1:A:154:ARG:HE	1:A:154:ARG:HB3	1.59	0.45
1:B:274:ASP:O	1:B:276:LYS:N	2.50	0.45
2:E:399:ILE:HG13	2:E:400:GLY:H	1.80	0.45
4:H:77:LEU:HD13	4:H:78:LYS:H	1.81	0.45
2:F:334:GLU:HA	2:F:360:ARG:HH11	1.82	0.45
2:F:396:VAL:HG22	2:F:404:LEU:HD11	1.99	0.45
3:G:93:VAL:HG13	3:G:103:ARG:H	1.82	0.45
3:G:105:LYS:HE2	3:G:105:LYS:HB3	1.73	0.45
2:E:60:PHE:CE1	2:E:229:ILE:HG12	2.53	0.44
2:E:372:ARG:NH1	2:E:374:ASP:OD2	2.50	0.44
3:G:8:ARG:C	3:G:10:ASN:H	2.20	0.44
4:H:58:ALA:HA	4:H:61:ARG:HD2	1.99	0.44
1:A:8:LYS:NZ	2:F:49:GLU:OE2	2.40	0.44
1:A:30:VAL:HG22	1:A:35:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:480:GLU:O	1:C:484:ILE:HG12	2.17	0.44
2:E:61:GLU:HG3	2:E:227:PRO:HG3	1.99	0.44
1:B:402:ILE:HD13	1:B:402:ILE:HA	1.80	0.44
1:B:520:LEU:HD12	1:B:520:LEU:HA	1.69	0.44
3:G:158:THR:O	3:G:162:ASN:ND2	2.51	0.44
1:A:486:VAL:HG21	1:A:523:TYR:HD1	1.82	0.44
2:D:244:TYR:O	2:D:248:GLU:HB2	2.17	0.44
1:A:316:GLN:HE21	1:A:316:GLN:HB2	1.54	0.44
1:B:576:ALA:C	1:B:577:LEU:HD23	2.39	0.44
1:C:413:LEU:HD22	1:C:418:HIS:CD2	2.53	0.43
1:C:413:LEU:HD22	1:C:418:HIS:HD2	1.83	0.43
2:E:84:VAL:HA	2:E:88:MET:HE1	2.00	0.43
2:E:138:ILE:HG12	2:E:337:ILE:HD13	1.99	0.43
1:A:248:ASP:OD1	1:A:276:LYS:NZ	2.51	0.43
1:B:81:ASN:HD22	1:B:282:MET:HB3	1.83	0.43
1:B:152:ASP:OD1	1:B:152:ASP:N	2.51	0.43
2:E:91:ARG:HG3	2:E:92:ARG:H	1.83	0.43
1:A:294:MET:HB3	1:A:295:PRO:HD2	2.00	0.43
1:B:198:LYS:HA	1:B:368:VAL:HG23	2.00	0.43
1:B:241:LEU:O	1:B:245:SER:HB3	2.18	0.43
1:C:161:LYS:HG2	1:C:172:VAL:HA	2.00	0.43
2:D:174:ARG:NH2	2:D:433:GLU:OE1	2.46	0.43
3:G:58:LYS:HG2	4:H:78:LYS:HG3	2.00	0.43
1:B:212:LEU:HD22	1:B:407:TRP:CE2	2.53	0.43
2:E:151:PRO:HG2	2:E:336:GLN:HB2	2.00	0.43
2:F:301:VAL:HG23	2:F:304:LYS:HB2	2.01	0.43
1:A:59:LYS:N	1:A:62:GLU:OE2	2.51	0.43
1:A:464:LEU:HD13	1:A:464:LEU:HA	1.71	0.43
1:C:348:GLU:OE2	2:E:280:ARG:NH2	2.34	0.43
1:C:465:GLN:HA	1:C:468:VAL:HB	2.00	0.43
2:E:152:ILE:HB	2:E:313:ILE:HG13	2.01	0.43
2:E:232:ILE:HD12	2:E:270:ILE:HD12	2.00	0.43
2:D:292:ALA:HB2	2:D:332:ILE:HD13	2.01	0.43
2:E:26:ASP:N	2:E:26:ASP:OD1	2.52	0.43
2:F:341:ARG:O	2:F:345:ARG:HG2	2.19	0.43
4:H:96:LYS:HD3	4:H:96:LYS:HA	1.83	0.43
1:C:209:MET:HA	1:C:497:GLN:HE22	1.83	0.43
2:F:305:LYS:HE2	2:F:305:LYS:HB3	1.69	0.43
3:G:96:VAL:HG12	3:G:101:VAL:O	2.19	0.43
1:A:14:VAL:HG22	1:A:49:VAL:HB	2.01	0.43
2:E:218:VAL:HG12	2:E:219:LEU:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:14:ILE:HG12	2:F:19:LEU:HD13	2.01	0.43
1:A:393:GLU:OE1	1:A:396:THR:OG1	2.37	0.42
2:D:355:LEU:HD21	2:D:386:TYR:HD2	1.83	0.42
2:E:6:LYS:O	2:E:6:LYS:HG2	2.18	0.42
3:G:40:PHE:HD1	3:G:40:PHE:HA	1.72	0.42
1:A:498:ASN:ND2	1:A:501:HIS:HB2	2.34	0.42
1:B:406:PHE:CE2	1:B:408:ARG:HG2	2.54	0.42
4:H:95:ARG:HD3	4:H:95:ARG:HA	1.62	0.42
1:C:314:ARG:HD2	1:C:368:VAL:HG12	2.02	0.42
2:D:8:TYR:HB2	2:D:73:VAL:O	2.19	0.42
2:F:260:MET:HE1	2:F:294:ILE:HD11	2.01	0.42
1:B:3:GLN:HG2	1:B:65:VAL:HG22	2.01	0.42
2:D:396:VAL:CG2	2:D:404:LEU:HD11	2.50	0.42
2:E:120:ASN:HD22	2:E:122:VAL:H	1.66	0.42
2:D:194:MET:HA	2:D:222:ASN:HB3	2.00	0.42
1:A:311:GLU:HG2	1:A:314:ARG:NH1	2.35	0.42
1:A:354:LEU:HD23	1:A:354:LEU:HA	1.78	0.42
1:A:573:ALA:O	1:A:577:LEU:CD2	2.67	0.42
2:E:175:PRO:HB2	2:E:182:GLU:HA	2.00	0.42
1:A:27:ILE:HD11	1:A:71:LEU:HB2	2.00	0.42
1:A:401:ARG:HD3	2:D:262:ASN:ND2	2.34	0.42
1:B:167:THR:OG1	1:B:168:VAL:N	2.52	0.42
1:B:272:LEU:HD23	1:B:272:LEU:HA	1.86	0.42
1:C:141:PHE:CG	1:C:283:HIS:HD2	2.38	0.42
2:E:399:ILE:HG13	2:E:400:GLY:N	2.35	0.42
1:B:477:GLN:HE21	1:B:477:GLN:HB2	1.59	0.42
2:D:22:GLU:HG2	2:D:23:ASN:H	1.84	0.42
3:G:6:PRO:O	3:G:10:ASN:ND2	2.53	0.42
1:A:207:THR:O	1:A:207:THR:OG1	2.35	0.41
1:A:574:PHE:HA	1:A:577:LEU:HD21	2.01	0.41
1:C:406:PHE:CE2	1:C:408:ARG:HB2	2.56	0.41
3:G:42:LEU:HB3	3:G:147:LEU:HD13	2.01	0.41
1:A:241:LEU:O	1:A:245:SER:HB3	2.19	0.41
1:C:394:PRO:O	1:C:398:SER:OG	2.32	0.41
2:D:389:GLY:HA3	2:D:415:ALA:HB2	2.02	0.41
3:G:103:ARG:NH2	3:G:146:ARG:HB2	2.35	0.41
1:A:410:ASP:OD1	1:A:411:ALA:N	2.53	0.41
2:D:261:THR:O	2:D:265:GLU:HG2	2.20	0.41
2:F:86:LYS:HD2	2:F:249:HIS:CD2	2.55	0.41
1:C:256:GLY:HA3	1:C:329:ARG:HG2	2.03	0.41
2:E:377:GLN:H	2:E:377:GLN:HE21	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:96:ILE:H	2:F:96:ILE:HG13	1.43	0.41
2:F:267:LEU:HD12	2:F:267:LEU:HA	1.82	0.41
3:G:14:ARG:HD3	3:G:14:ARG:HA	1.80	0.41
2:D:374:ASP:OD1	2:D:374:ASP:N	2.33	0.41
3:G:180:GLN:HE21	3:G:180:GLN:HB2	1.69	0.41
1:B:447:TYR:HB3	1:B:448:PRO:HD3	2.03	0.41
1:B:545:LEU:HD23	1:B:545:LEU:HA	1.81	0.41
1:C:576:ALA:C	1:C:577:LEU:HD22	2.21	0.41
2:F:146:ARG:HD2	2:F:252:HIS:HD2	1.86	0.41
1:A:145:HIS:ND1	1:A:146:LYS:O	2.53	0.41
1:A:539:ILE:HG23	1:A:574:PHE:HZ	1.84	0.41
1:B:182:LYS:HE3	1:B:182:LYS:HB2	1.93	0.41
1:C:50:GLN:O	1:C:50:GLN:HG3	2.21	0.41
2:F:8:TYR:HB2	2:F:73:VAL:O	2.21	0.41
1:C:574:PHE:HD1	1:C:574:PHE:HA	1.72	0.41
2:E:23:ASN:ND2	2:E:23:ASN:O	2.54	0.41
2:E:453:ARG:HH11	2:E:453:ARG:HB2	1.86	0.41
1:A:402:ILE:HG23	1:A:403:VAL:HG13	2.03	0.41
1:B:6:ILE:HG23	1:B:14:VAL:HG13	2.03	0.41
2:E:201:LEU:HD11	2:E:221:LEU:HD13	2.02	0.41
2:E:207:GLU:CD	2:E:210:ARG:HH12	2.24	0.41
2:E:277:ILE:HG12	3:G:192:PHE:CZ	2.55	0.41
2:F:48:ILE:HD11	2:F:58:GLN:NE2	2.36	0.41
2:F:57:ILE:HG22	2:F:58:GLN:H	1.86	0.41
1:A:54:ASP:O	1:A:55:THR:OG1	2.30	0.41
1:A:195:VAL:HG11	1:A:368:VAL:HG21	2.03	0.41
1:B:21:GLY:HA2	2:E:67:ASP:OD2	2.21	0.40
2:D:355:LEU:HB2	2:D:356:PRO:HD3	2.03	0.40
2:D:462:TYR:O	2:D:463:TYR:HB3	2.21	0.40
1:B:348:GLU:HG3	1:B:394:PRO:HD3	2.04	0.40
2:F:376:LYS:H	2:F:376:LYS:HG2	1.70	0.40
4:H:91:ARG:HA	4:H:91:ARG:HD3	1.74	0.40
1:A:262:MET:HE2	1:A:262:MET:HB2	1.96	0.40
2:D:67:ASP:OD1	2:D:67:ASP:N	2.54	0.40
2:E:395:LEU:O	2:E:399:ILE:HG12	2.21	0.40
2:F:443:LEU:HD23	2:F:443:LEU:HA	1.91	0.40
3:G:158:THR:HG22	3:G:162:ASN:ND2	2.36	0.40
1:A:255:CYS:SG	1:A:299:ARG:HB3	2.62	0.40
1:B:243:LYS:HD2	1:B:244:TRP:CZ3	2.57	0.40
1:B:572:GLY:O	1:B:575:LYS:HG2	2.21	0.40
1:C:344:MET:HG2	1:C:345:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:398:ILE:HD13	2:E:398:ILE:HA	1.90	0.40
1:A:9:ILE:CD1	1:A:58:LEU:HB2	2.51	0.40
1:B:141:PHE:HE2	1:B:283:HIS:CD2	2.39	0.40
1:C:237:THR:O	1:C:241:LEU:HG	2.21	0.40
1:C:365:ALA:HB2	1:C:380:ILE:HD12	2.03	0.40
1:C:458:LEU:HD21	1:C:490:ILE:HG21	2.02	0.40
2:E:153:PHE:CE2	2:E:336:GLN:HG3	2.56	0.40
2:F:321:ARG:HE	2:F:321:ARG:HB3	1.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	575/578 (100%)	515 (90%)	60 (10%)	0	100	100
1	B	575/578 (100%)	517 (90%)	58 (10%)	0	100	100
1	C	575/578 (100%)	516 (90%)	58 (10%)	1 (0%)	47	81
2	D	457/478 (96%)	407 (89%)	50 (11%)	0	100	100
2	E	457/478 (96%)	401 (88%)	56 (12%)	0	100	100
2	F	457/478 (96%)	400 (88%)	57 (12%)	0	100	100
3	G	208/223 (93%)	190 (91%)	18 (9%)	0	100	100
4	H	98/104 (94%)	78 (80%)	20 (20%)	0	100	100
All	All	3402/3495 (97%)	3024 (89%)	377 (11%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	420	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	468/468 (100%)	421 (90%)	47 (10%)	7	32
1	B	468/468 (100%)	418 (89%)	50 (11%)	6	30
1	C	468/468 (100%)	427 (91%)	41 (9%)	10	38
2	D	386/401 (96%)	354 (92%)	32 (8%)	11	40
2	E	386/401 (96%)	341 (88%)	45 (12%)	5	26
2	F	386/401 (96%)	339 (88%)	47 (12%)	5	23
3	G	166/176 (94%)	152 (92%)	14 (8%)	11	40
4	H	76/80 (95%)	60 (79%)	16 (21%)	1	5
All	All	2804/2863 (98%)	2512 (90%)	292 (10%)	10	31

All (292) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	24	MET
1	A	30	VAL
1	A	65	VAL
1	A	83	ILE
1	A	88	GLN
1	A	93	ARG
1	A	95	ARG
1	A	123	VAL
1	A	124	LYS
1	A	157	VAL
1	A	191	ARG
1	A	203	THR
1	A	207	THR
1	A	211	ILE
1	A	215	LEU
1	A	223	THR
1	A	244	TRP
1	A	266	LEU

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Mol	Chain	Res	Type
1	A	274	ASP
1	A	281	LEU
1	A	282	MET
1	A	293	ASN
1	A	316	GLN
1	A	322	LEU
1	A	329	ARG
1	A	353	TYR
1	A	354	LEU
1	A	368	VAL
1	A	370	THR
1	A	425	ASN
1	A	456	GLU
1	A	464	LEU
1	A	466	GLU
1	A	469	GLN
1	A	524	LYS
1	A	530	ILE
1	A	531	LYS
1	A	536	ILE
1	A	540	LEU
1	A	541	GLN
1	A	545	LEU
1	A	547	ARG
1	A	550	ARG
1	A	574	PHE
1	A	575	LYS
1	A	577	LEU
1	B	30	VAL
1	B	60	VAL
1	B	80	LEU
1	B	88	GLN
1	B	96	GLU
1	B	107	VAL
1	B	123	VAL
1	B	138	VAL
1	B	143	PHE
1	B	152	ASP
1	B	153	VAL
1	B	172	VAL
1	B	200	ASP
1	B	218	VAL

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Mol	Chain	Res	Type
1	B	223	THR
1	B	230	PHE
1	B	244	TRP
1	B	255	CYS
1	B	260	ASN
1	B	263	THR
1	B	272	LEU
1	B	282	MET
1	B	284	ARG
1	B	285	THR
1	B	296	VAL
1	B	315	ASP
1	B	319	SER
1	B	322	LEU
1	B	329	ARG
1	B	354	LEU
1	B	368	VAL
1	B	369	ILE
1	B	379	THR
1	B	402	ILE
1	B	446	ASP
1	B	450	LEU
1	B	469	GLN
1	B	476	LEU
1	B	477	GLN
1	B	503	VAL
1	B	509	MET
1	B	520	LEU
1	B	524	LYS
1	B	546	GLU
1	B	548	ILE
1	B	554	VAL
1	B	557	GLU
1	B	565	GLU
1	B	574	PHE
1	B	577	LEU
1	C	20	LEU
1	C	26	ASP
1	C	50	GLN
1	C	83	ILE
1	C	95	ARG
1	C	96	GLU

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Mol	Chain	Res	Type
1	C	103	THR
1	C	116	LYS
1	C	134	VAL
1	C	141	PHE
1	C	145	HIS
1	C	152	ASP
1	C	167	THR
1	C	186	THR
1	C	200	ASP
1	C	207	THR
1	C	211	ILE
1	C	244	TRP
1	C	248	ASP
1	C	249	VAL
1	C	266	LEU
1	C	282	MET
1	C	284	ARG
1	C	293	ASN
1	C	315	ASP
1	C	320	VAL
1	C	329	ARG
1	C	337	ILE
1	C	340	ARG
1	C	354	LEU
1	C	363	GLU
1	C	368	VAL
1	C	379	THR
1	C	396	THR
1	C	461	GLU
1	C	478	ASP
1	C	520	LEU
1	C	538	GLU
1	C	568	LYS
1	C	574	PHE
1	C	577	LEU
2	D	7	GLU
2	D	25	LYS
2	D	37	ASP
2	D	94	ASN
2	D	130	PHE
2	D	131	ILE
2	D	143	THR

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Mol	Chain	Res	Type
2	D	183	LYS
2	D	189	VAL
2	D	194	MET
2	D	197	THR
2	D	214	LEU
2	D	216	ARG
2	D	294	ILE
2	D	309	THR
2	D	315	SER
2	D	318	ASP
2	D	322	THR
2	D	327	ASP
2	D	331	TYR
2	D	368	LYS
2	D	370	LYS
2	D	379	SER
2	D	381	GLN
2	D	390	VAL
2	D	398	ILE
2	D	399	ILE
2	D	401	GLU
2	D	424	ASN
2	D	425	GLN
2	D	429	ASN
2	D	457	ASP
2	E	7	GLU
2	E	26	ASP
2	E	43	ARG
2	E	73	VAL
2	E	81	ARG
2	E	82	LEU
2	E	89	LEU
2	E	94	ASN
2	E	98	LYS
2	E	100	ILE
2	E	111	ARG
2	E	120	ASN
2	E	130	PHE
2	E	131	ILE
2	E	133	THR
2	E	137	THR
2	E	143	THR

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Mol	Chain	Res	Type
2	E	148	GLN
2	E	150	LEU
2	E	180	GLU
2	E	183	LYS
2	E	194	MET
2	E	206	GLN
2	E	257	LEU
2	E	258	THR
2	E	270	ILE
2	E	274	ARG
2	E	290	ASP
2	E	294	ILE
2	E	304	LYS
2	E	327	ASP
2	E	336	GLN
2	E	355	LEU
2	E	372	ARG
2	E	374	ASP
2	E	377	GLN
2	E	379	SER
2	E	384	SER
2	E	405	THR
2	E	413	GLN
2	E	427	GLN
2	E	437	GLN
2	E	452	LYS
2	E	453	ARG
2	E	459	ILE
2	F	9	THR
2	F	11	ILE
2	F	26	ASP
2	F	37	ASP
2	F	53	GLU
2	F	54	TYR
2	F	63	THR
2	F	73	VAL
2	F	78	ASP
2	F	79	VAL
2	F	96	ILE
2	F	111	ARG
2	F	112	LEU
2	F	126	LYS

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Mol	Chain	Res	Type
2	F	128	GLU
2	F	131	ILE
2	F	133	THR
2	F	137	THR
2	F	141	MET
2	F	148	GLN
2	F	150	LEU
2	F	172	THR
2	F	180	GLU
2	F	182	GLU
2	F	183	LYS
2	F	187	PHE
2	F	197	THR
2	F	206	GLN
2	F	222	ASN
2	F	225	ASP
2	F	232	ILE
2	F	254	LEU
2	F	257	LEU
2	F	259	ASP
2	F	270	ILE
2	F	290	ASP
2	F	294	ILE
2	F	309	THR
2	F	315	SER
2	F	318	ASP
2	F	343	LEU
2	F	376	LYS
2	F	393	ARG
2	F	405	THR
2	F	412	LEU
2	F	429	ASN
2	F	459	ILE
3	G	8	ARG
3	G	13	GLN
3	G	33	ASP
3	G	54	ASP
3	G	55	GLN
3	G	83	VAL
3	G	86	LEU
3	G	89	VAL
3	G	92	GLU

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Mol	Chain	Res	Type
3	G	105	LYS
3	G	115	SER
3	G	117	VAL
3	G	128	ARG
3	G	201	ILE
4	H	1	MET
4	H	6	ASP
4	H	28	GLU
4	H	35	THR
4	H	36	LEU
4	H	44	LEU
4	H	70	VAL
4	H	71	LEU
4	H	74	ILE
4	H	77	LEU
4	H	81	PHE
4	H	90	MET
4	H	93	LEU
4	H	95	ARG
4	H	96	LYS
4	H	100	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	81	ASN
1	A	88	GLN
1	A	196	GLN
1	A	425	ASN
1	A	469	GLN
1	A	496	GLN
1	A	571	GLN
1	B	3	GLN
1	B	7	GLN
1	B	50	GLN
1	B	81	ASN
1	B	88	GLN
1	B	185	HIS
1	B	202	ASN
1	B	316	GLN
1	B	418	HIS

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Mol	Chain	Res	Type
1	B	477	GLN
1	B	496	GLN
1	B	498	ASN
1	C	50	GLN
1	C	238	GLN
1	C	283	HIS
1	C	316	GLN
1	C	469	GLN
1	C	496	GLN
1	C	497	GLN
2	D	94	ASN
2	D	142	ASN
2	D	148	GLN
2	D	170	GLN
2	D	206	GLN
2	D	249	HIS
2	D	252	HIS
2	D	262	ASN
2	D	310	GLN
2	D	407	ASN
2	D	413	GLN
2	D	424	ASN
2	D	425	GLN
2	E	23	ASN
2	E	120	ASN
2	E	142	ASN
2	E	148	GLN
2	E	252	HIS
2	E	323	HIS
2	E	363	ASN
2	E	377	GLN
2	E	407	ASN
2	E	427	GLN
2	E	437	GLN
2	E	448	GLN
2	F	46	GLN
2	F	58	GLN
2	F	129	GLN
2	F	142	ASN
2	F	148	GLN
2	F	166	GLN
2	F	252	HIS

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Mol	Chain	Res	Type
2	F	310	GLN
2	F	323	HIS
2	F	363	ASN
2	F	388	ASN
2	F	413	GLN
2	F	429	ASN
2	F	448	GLN
3	G	10	ASN
3	G	13	GLN
3	G	17	GLN
3	G	55	GLN
3	G	95	ASN
3	G	162	ASN
3	G	180	GLN
4	H	11	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

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	$\#\|Z\| > 2$
5	ADP	A	600	1	24,29,29	0.95	1 (4%)	29,45,45	1.45	5 (17%)

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
5	ADP	A	600	1	-	5/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	600	ADP	C5-C4	2.40	1.47	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(º)	Ideal(º)
5	A	600	ADP	C3'-C2'-C1'	3.37	106.05	100.98
5	A	600	ADP	N3-C2-N1	-3.19	123.69	128.68
5	A	600	ADP	PA-O3A-PB	-3.05	122.35	132.83
5	A	600	ADP	C4-C5-N7	-2.24	107.07	109.40
5	A	600	ADP	C2'-C3'-C4'	2.05	106.62	102.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	600	ADP	O4'-C4'-C5'-O5'
5	A	600	ADP	C3'-C4'-C5'-O5'
5	A	600	ADP	PB-O3A-PA-O1A
5	A	600	ADP	PB-O3A-PA-O2A
5	A	600	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

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 ADP A 600

Bond lengths

Bond angles

Torsions

Rings
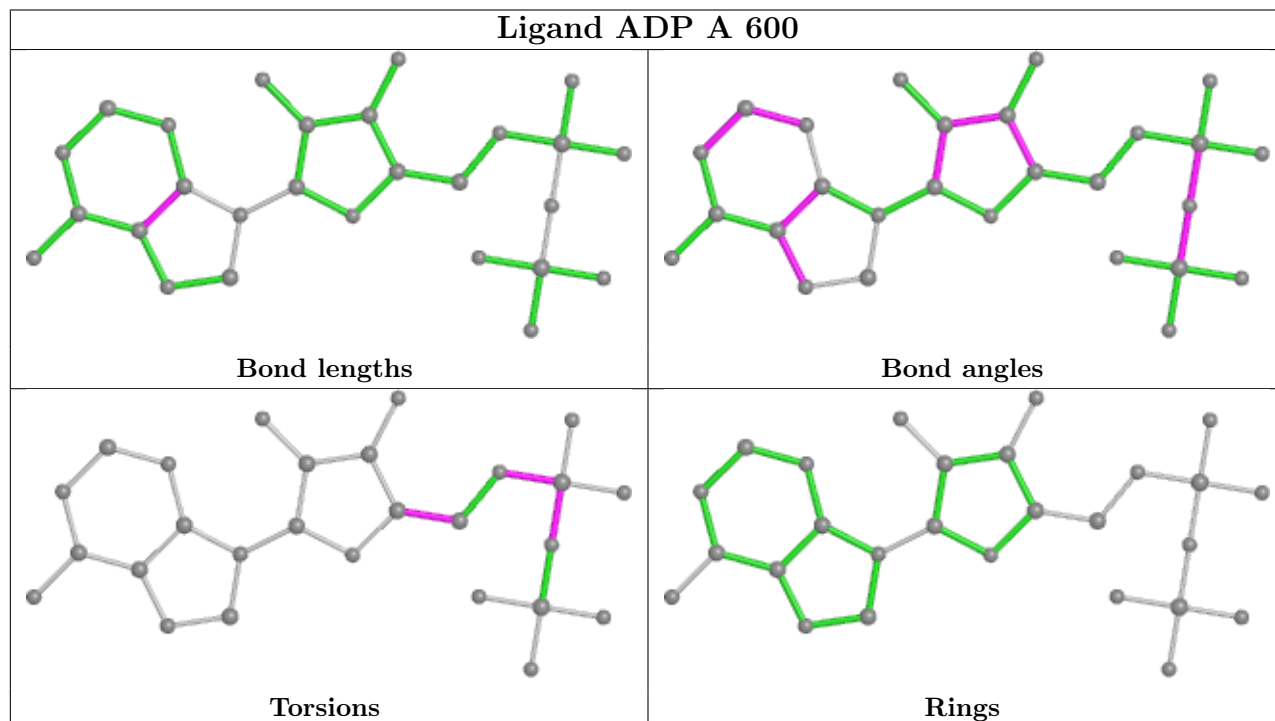
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-30014. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections ⓘ

6.1.1 Primary map

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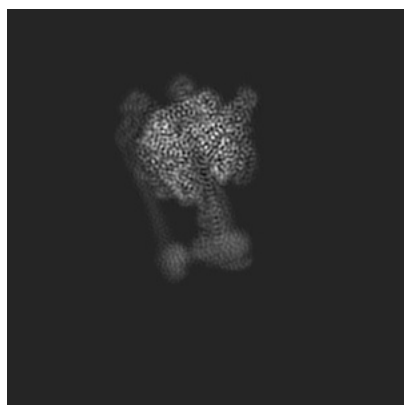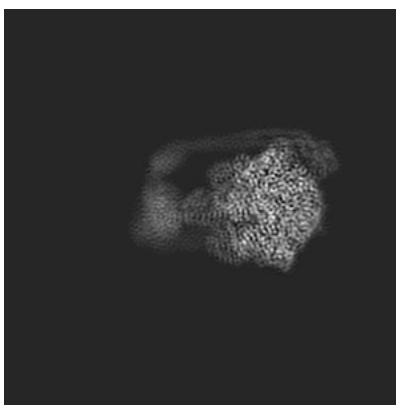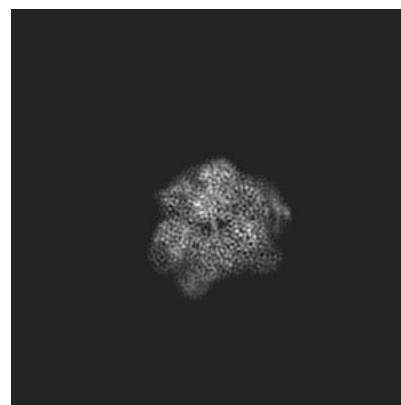
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
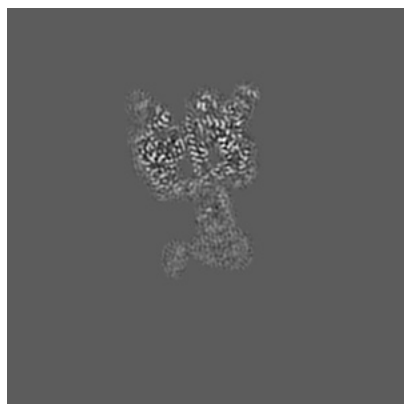
6.2.1 Primary map
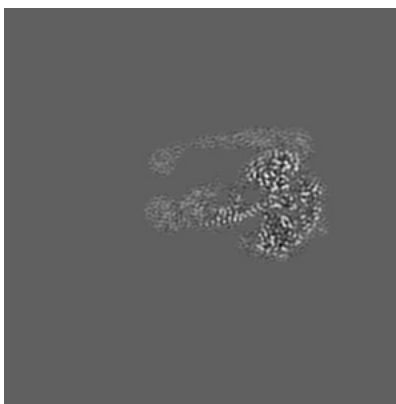
X Index: 170   Y Index: 170   Z Index: 170

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

6.3 Largest variance slices ⓘ
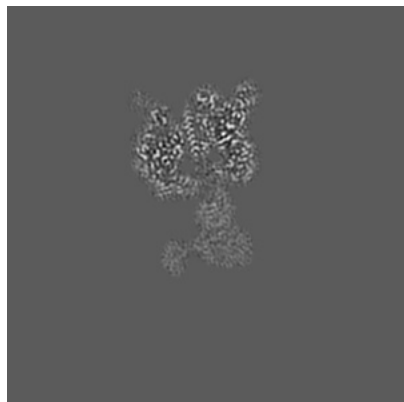
6.3.1 Primary map
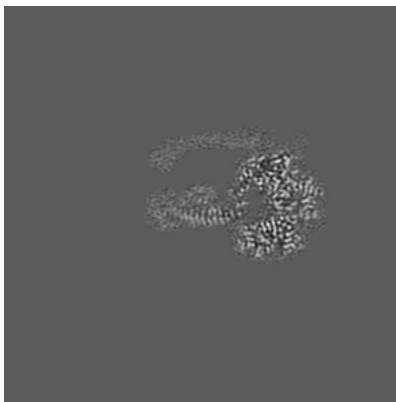
| X Index: 173 | Y Index: 175 | Z Index: 224 |
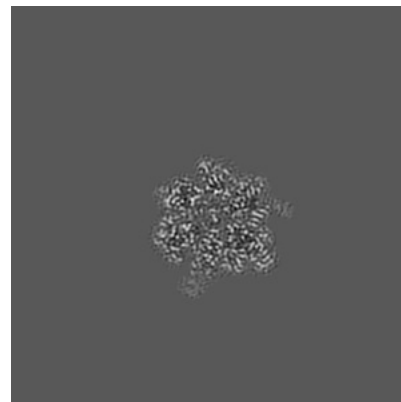
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views ⓘ
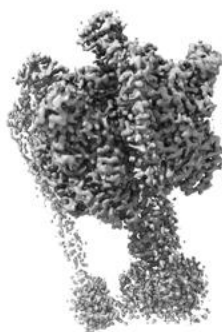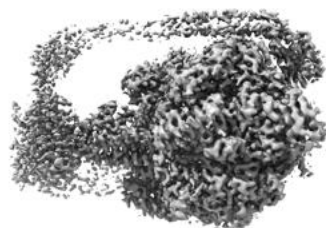
6.4.1 Primary map

| X | Y | Z |
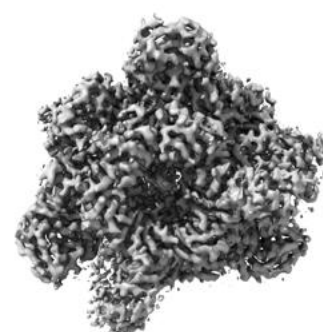
The images above show the 3D surface view of the map at the recommended contour level 0.068. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

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

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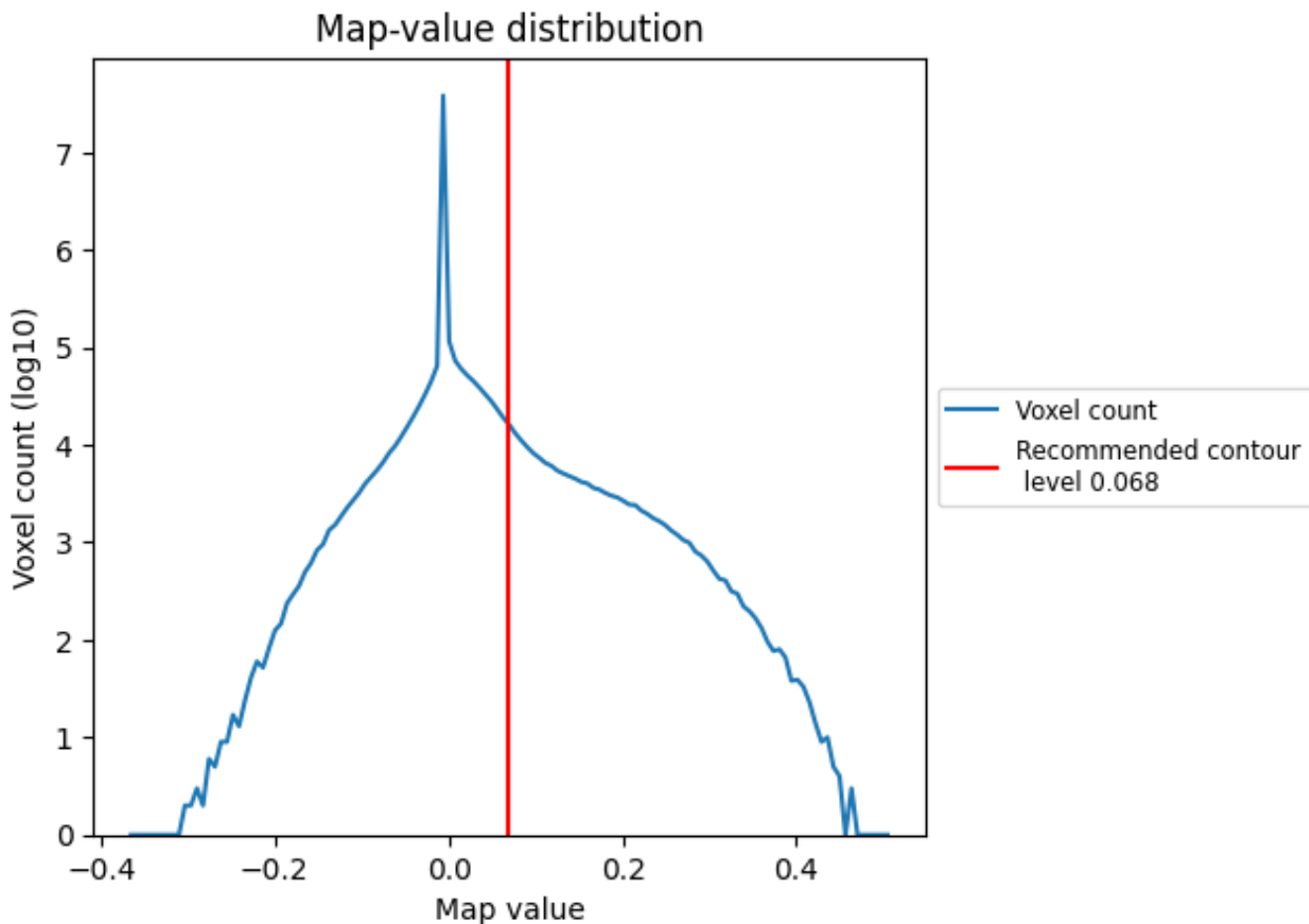
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ
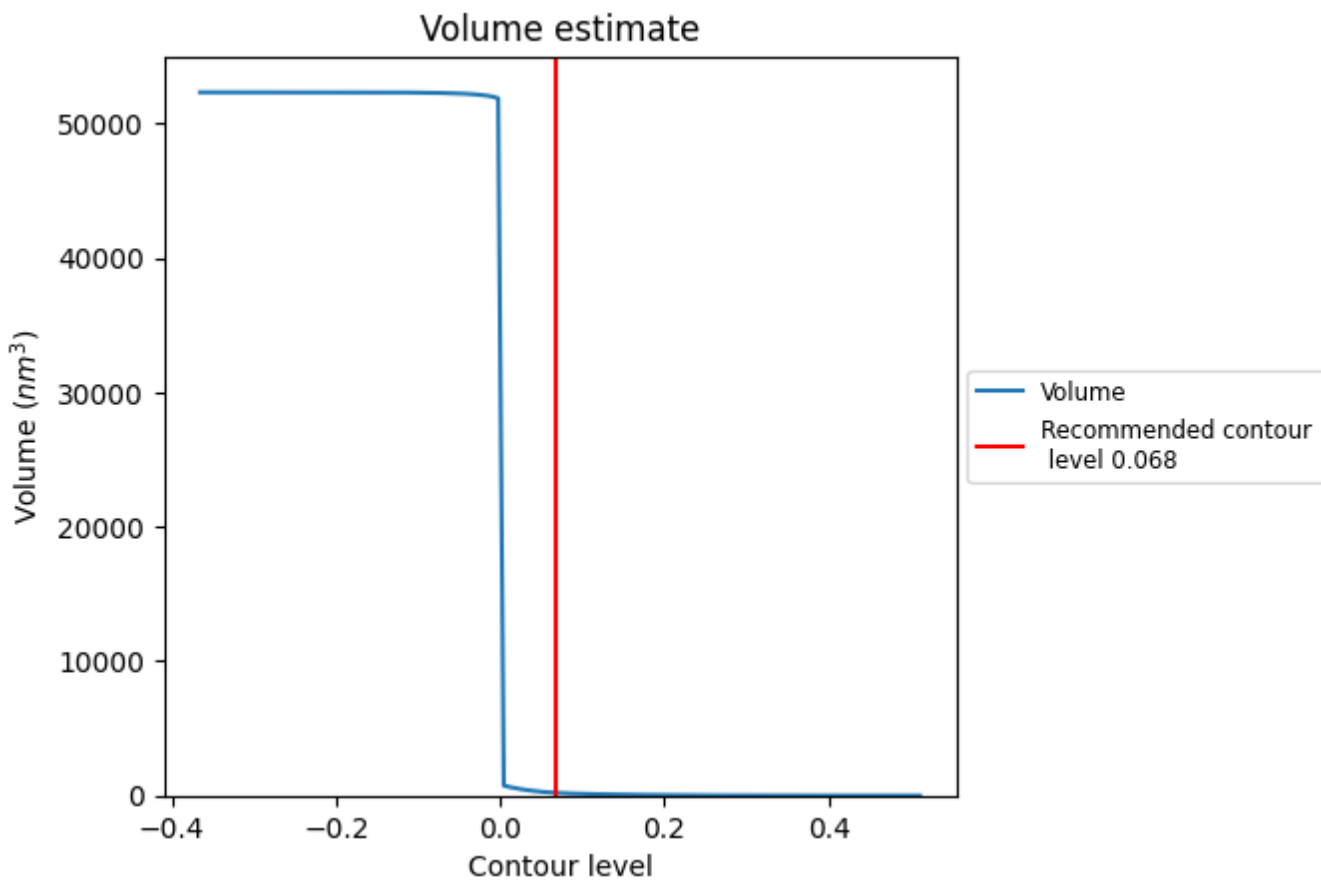
The volume at the recommended contour level is 204 nm^3; this corresponds to an approximate mass of 184 kDa.

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)
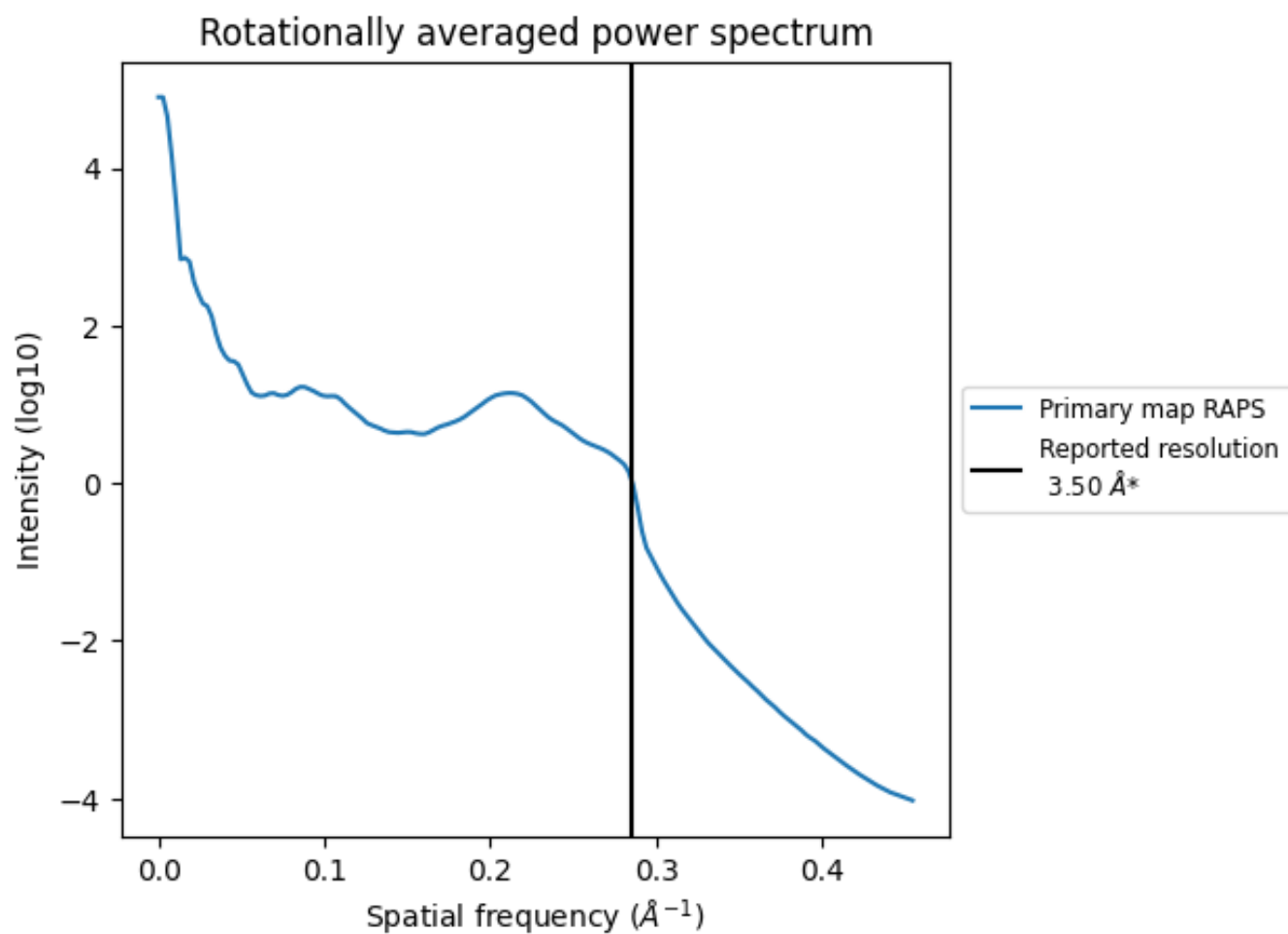
*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8　Fourier-Shell correlation ⓘ

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 ⓘ
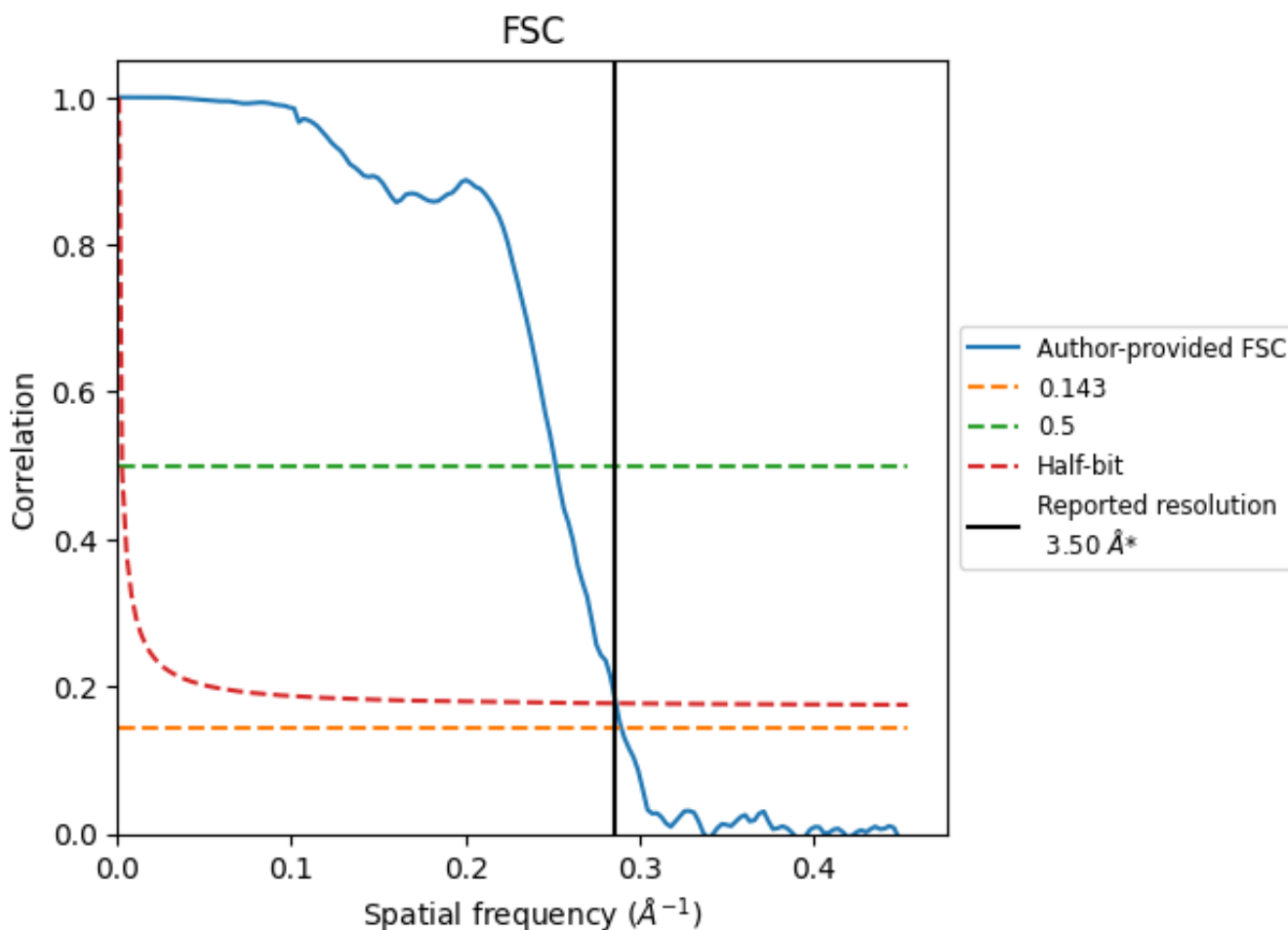
*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8.2   Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.45	3.97	3.49
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9   Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-30014 and PDB model 6LY8. Per-residue inclusion information can be found in section 3 on page 5.

9.1   Map-model overlay ⓘ

X   Y   Z

The images above show the 3D surface view of the map at the recommended contour level 0.068 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 ⓘ

X　　　　　　　　　　Y　　　　　　　　　　Z
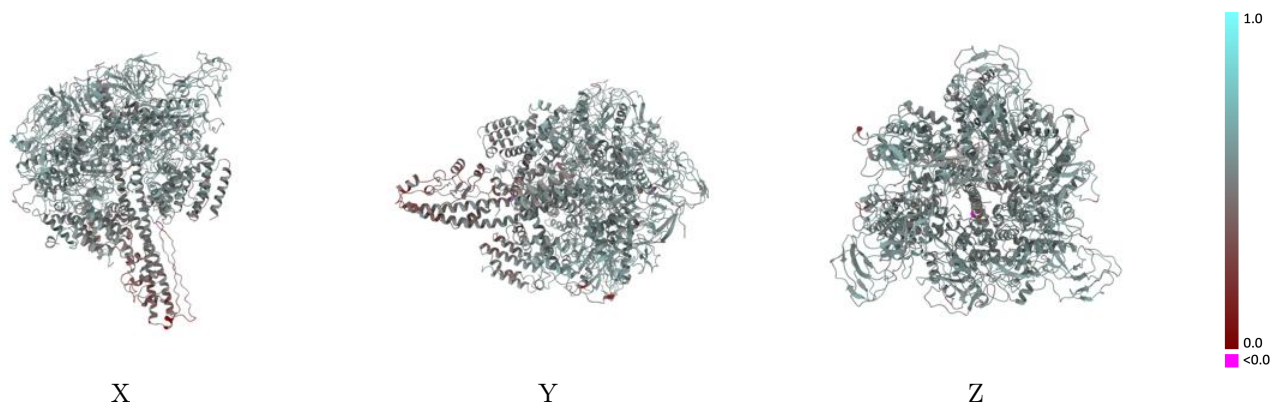
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ

X　　　　　　　　　　Y　　　　　　　　　　Z
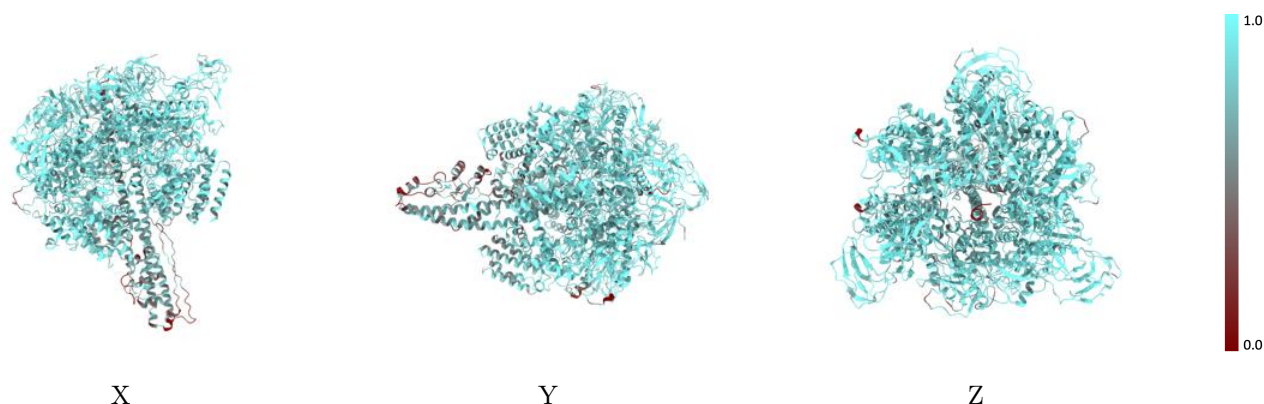
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.068).

9.4   Atom inclusion ⓘ
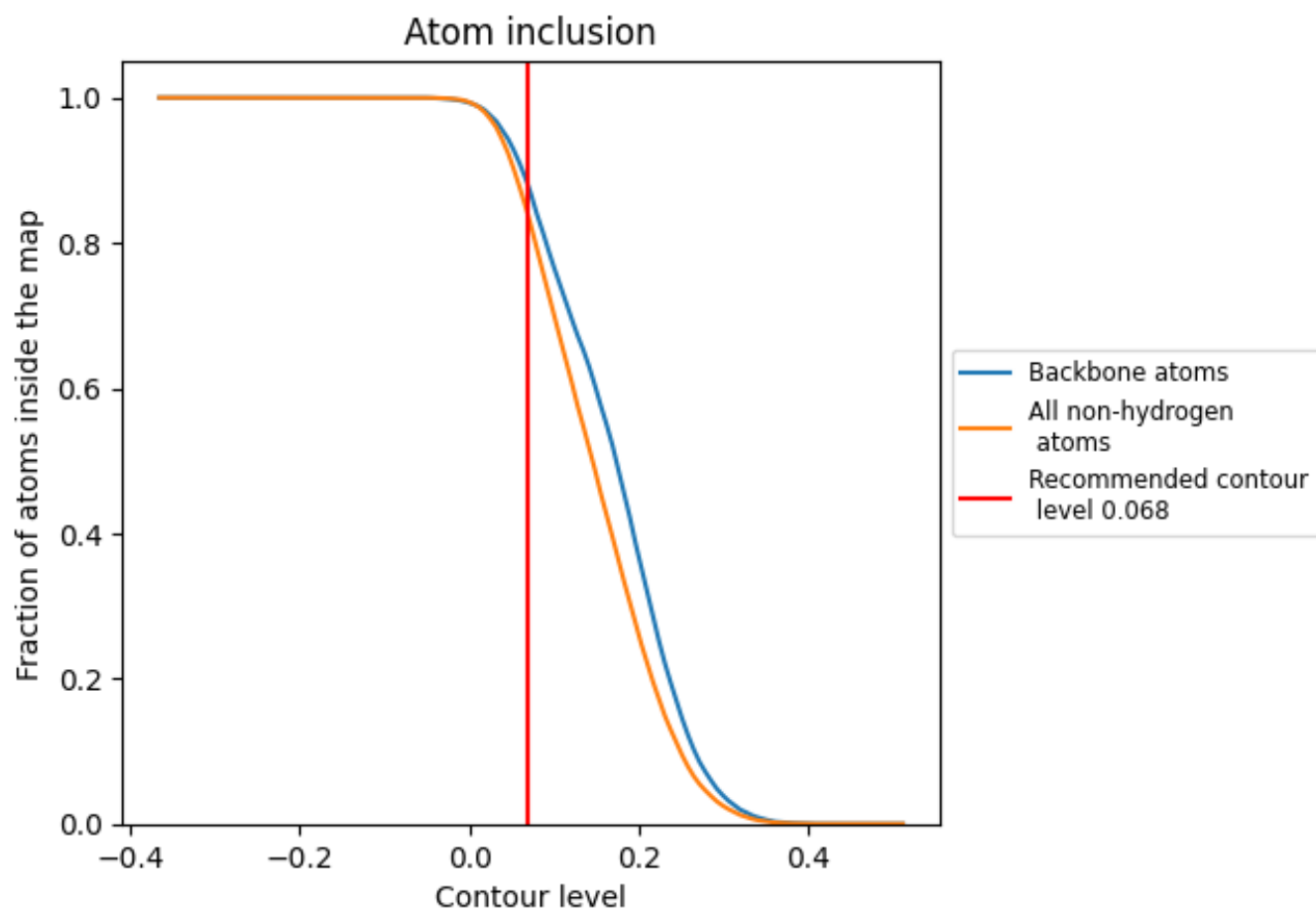
At the recommended contour level, 88% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.068) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8444	0.5290
A	0.8746	0.5390
B	0.8525	0.5280
C	0.8786	0.5430
D	0.8870	0.5470
E	0.8431	0.5300
F	0.8796	0.5460
G	0.6386	0.4500
H	0.4953	0.3820

1.0

0.0
<0.0