Full wwPDB EM Validation Report ⓘ

Nov 30, 2024 – 01:38 PM EST

PDB ID	:	9B3I
EMDB ID	:	EMD-44141
Title	:	Cryo-EM structure of yeast (Nap1)2-H2A-H2B-Kap114-RanGTP
Authors	:	Fung, H.Y.J.; Jiou, J.; Chook, Y.M.
Deposited on	:	2024-03-19
Resolution	:	2.88 Å(reported)
Based on initial models	:	8F1E, 9B3F

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

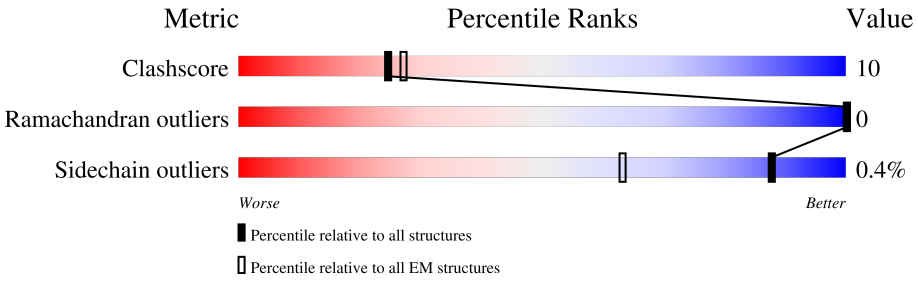
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1012	75% 19% 7%
2	B	131	18% 40% 23% 37%
3	C	130	15% 44% 25% 32%
4	D	186	78% 13% 9%
5	E	420	50% 51% 17% 33%
5	F	420	42% 49% 19% 32%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14951 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 KAP114 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	944	Total	C	N	O	S	0	0
			7531	4823	1211	1464	33		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP A0A8H4BZV8
A	-6	SER	-	expression tag	UNP A0A8H4BZV8
A	-5	PRO	-	expression tag	UNP A0A8H4BZV8
A	-4	ASN	-	expression tag	UNP A0A8H4BZV8
A	-3	SER	-	expression tag	UNP A0A8H4BZV8
A	-2	ARG	-	expression tag	UNP A0A8H4BZV8
A	-1	VAL	-	expression tag	UNP A0A8H4BZV8
A	0	ASP	-	expression tag	UNP A0A8H4BZV8

- Molecule 2 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	83	Total	C	N	O	0	0
			646	405	128	113		

- Molecule 3 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	89	Total	C	N	O	S	0	0
			693	437	119	136	1		

- Molecule 4 is a protein called GTP-binding nuclear protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	170	Total	C	N	O	S	0	0
			1384	903	236	241	4		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	initiating methionine	UNP A0A6A5PUD0
D	1	ALA	-	expression tag	UNP A0A6A5PUD0
D	71	LEU	GLN	engineered mutation	UNP A0A6A5PUD0
D	180	GLU	-	expression tag	UNP A0A6A5PUD0
D	181	ASN	-	expression tag	UNP A0A6A5PUD0
D	182	LEU	-	expression tag	UNP A0A6A5PUD0
D	183	TYR	-	expression tag	UNP A0A6A5PUD0
D	184	PHE	-	expression tag	UNP A0A6A5PUD0
D	185	GLN	-	expression tag	UNP A0A6A5PUD0

- Molecule 5 is a protein called NAP1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	283	Total	C	N	O	S	0	0
			2325	1484	373	466	2		
5	F	285	Total	C	N	O	S	0	0
			2339	1491	375	471	2		

There are 18 discrepancies between the modelled and reference sequences:

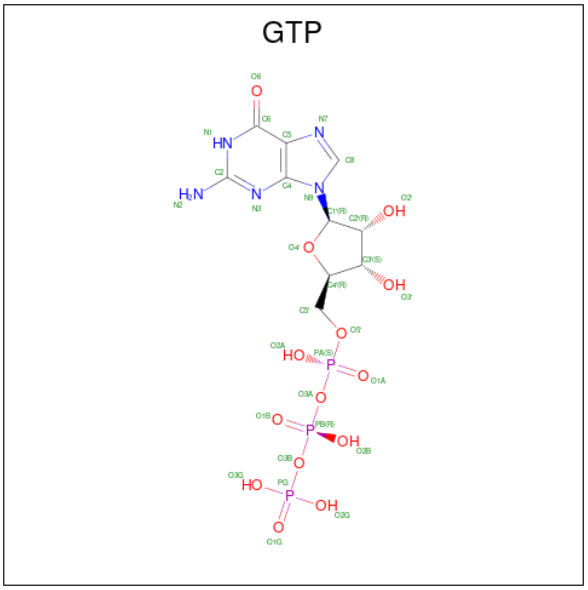
Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP A0A8H4BY55
E	-1	SER	-	expression tag	UNP A0A8H4BY55
E	0	MET	-	expression tag	UNP A0A8H4BY55
E	1	GLY	-	expression tag	UNP A0A8H4BY55
E	2	THR	-	expression tag	UNP A0A8H4BY55
E	200	ALA	CYS	engineered mutation	UNP A0A8H4BY55
E	249	ALA	CYS	engineered mutation	UNP A0A8H4BY55
E	272	ALA	CYS	engineered mutation	UNP A0A8H4BY55
E	384	ASP	GLU	conflict	UNP A0A8H4BY55
F	-2	GLY	-	expression tag	UNP A0A8H4BY55
F	-1	SER	-	expression tag	UNP A0A8H4BY55
F	0	MET	-	expression tag	UNP A0A8H4BY55
F	1	GLY	-	expression tag	UNP A0A8H4BY55
F	2	THR	-	expression tag	UNP A0A8H4BY55
F	200	ALA	CYS	engineered mutation	UNP A0A8H4BY55
F	249	ALA	CYS	engineered mutation	UNP A0A8H4BY55
F	272	ALA	CYS	engineered mutation	UNP A0A8H4BY55
F	384	ASP	GLU	conflict	UNP A0A8H4BY55

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand

of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
6	D	1	1	1	0

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



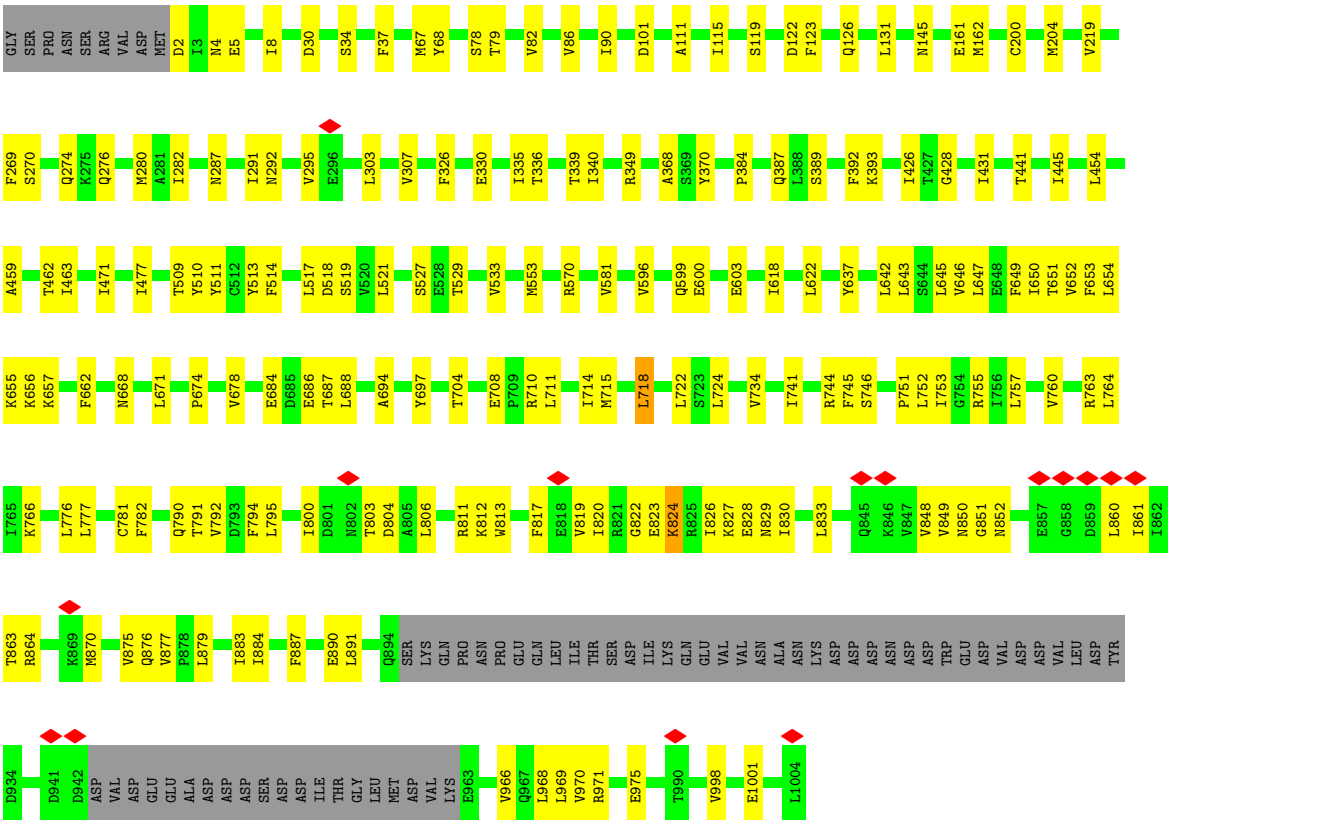
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	D	1	32	10	5	14	3	0

3 Residue-property plots (i)

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

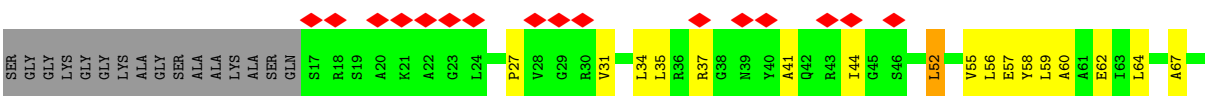
• Molecule 1: KAP114 isoform 1

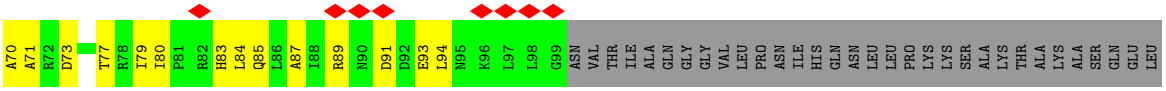
Chain A:



• Molecule 2: Histone H2A

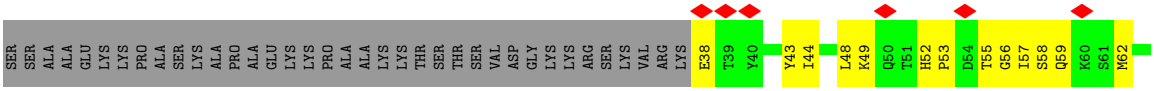
Chain B:

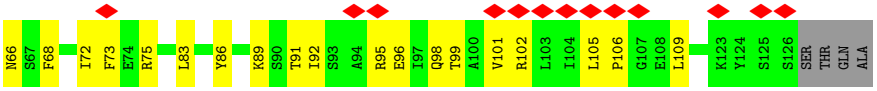




• Molecule 3: Histone H2B

Chain C:



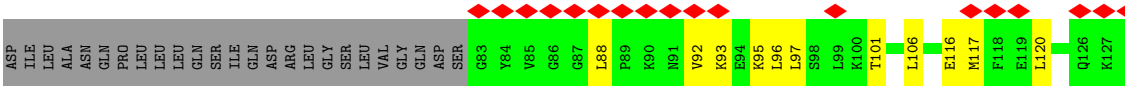


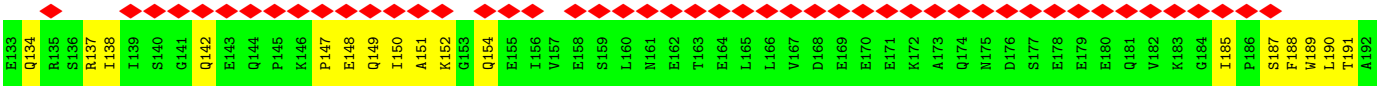
• Molecule 4: GTP-binding nuclear protein

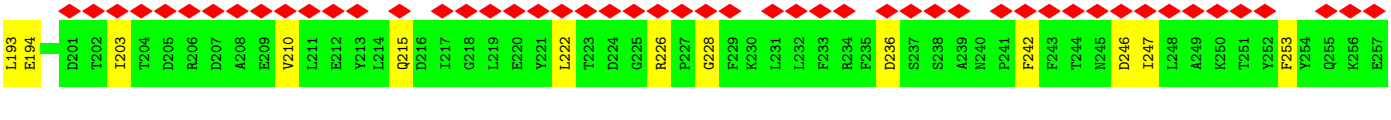
Chain D:

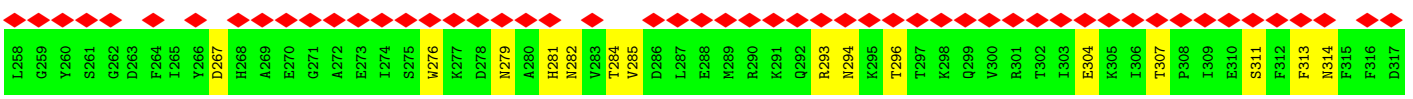
• Molecule 5: NAP1 isoform 1

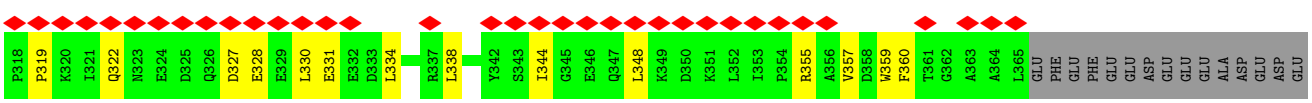
Chain E:

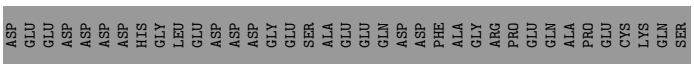








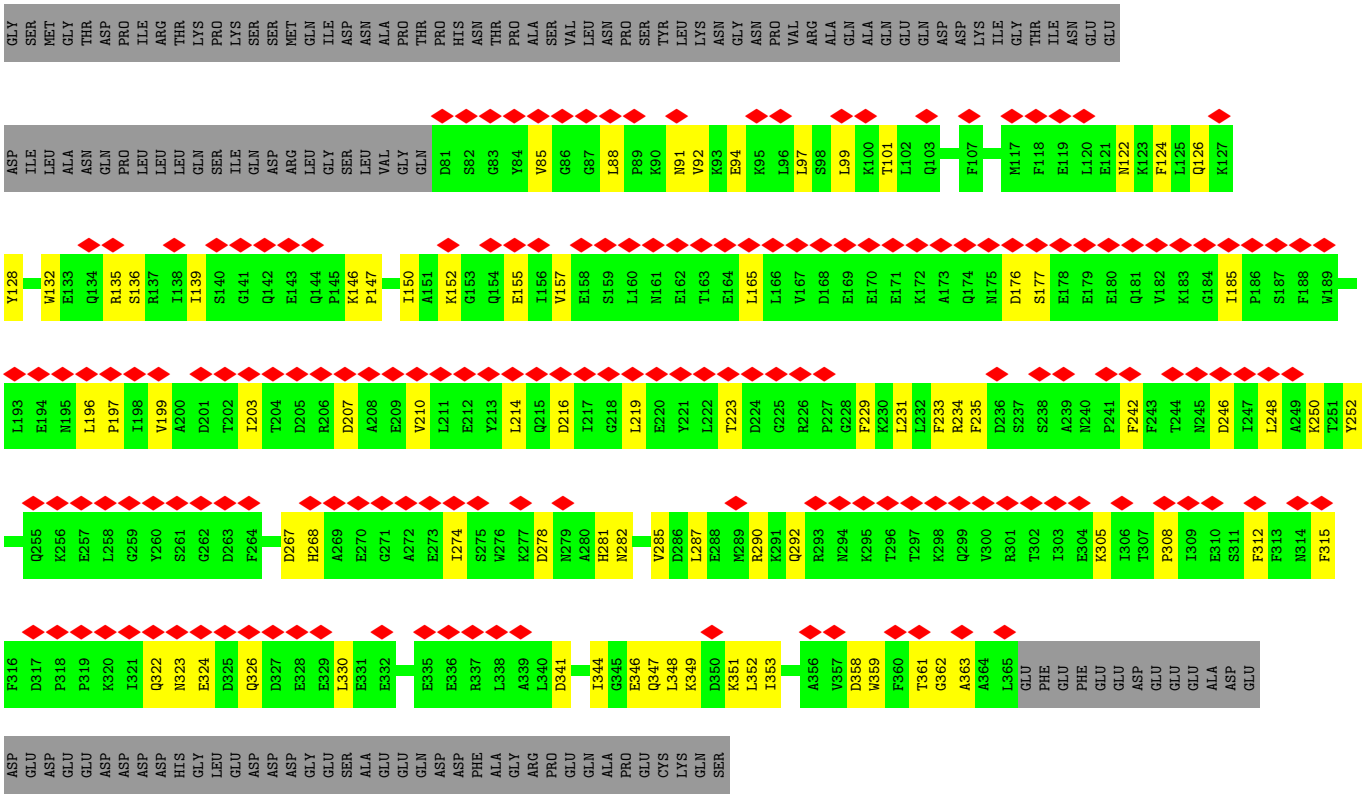




• Molecule 5: NAP1 isoform 1

Chain F:


42%
49%
19%
32%


GLY SER MET GLY THR ASP PRO ILE ARG THR LYS PRO LYS SER SER MET GLN ILE ASP ASN ALA PRO THR PRO HIS ASN THR PRO ALA SER VAL LEU ASN PRO SER TYR LEU LYS ASN GLY ASN PRO VAL ARG ALA GLN ALA GLN GLU GLN ASP ASP LYS ILE GLY THR ILE ASN GLU GLU
ASP ILE LEU ALA ASN GLN PRO LEU LEU LEU GLN SER ILE GLN ASP ARG LEU GLY SER LEU VAL GLY GLN D81 S82 G83 Y84 V85 G86 G87 L88 P89 K90 N91 V92 K93 E94 K95 L96 L97 S98 L99 K100 T101 L102 Q103 F107 M117 F118 E119 L120 E121 N122 K123 F124 L125 Q126 K127
Y128 W132 E133 Q134 R135 S136 R137 I138 I139 S140 G141 Q142 E143 Q144 P145 K146 P147 I150 A151 K152 G153 Q154 E155 I156 V157 E158 S159 L160 N161 E162 T163 E164 L165 L166 V167 D168 E169 E170 E171 K172 A173 Q174 N175 D176 S177 E178 E179 E180 Q181 V182 K183 G184 I185 P186 S187 F188 W189
L193 E194 N195 L196 P197 I198 V199 A200 D201 T202 I203 T204 D205 R206 D207 A208 E209 V210 L211 E212 Y213 L214 Q215 D216 I217 G218 L219 E220 Y221 L222 T223 D224 G225 R226 P227 G228 F229 K230 L231 L232 F233 R234 F235 D236 S237 S238 A239 N240 P241 F242 F243 T244 N245 D246 I247 L248 A249 K250 T251 Y252
Q255 K256 E257 L258 G259 Y260 S261 G262 D263 F264 D267 H268 A269 E270 G271 A272 E273 I274 S275 W276 K277 D278 N279 A280 H281 N282 V285 D286 L287 E288 M289 R290 K291 Q292 R293 N294 K295 T296 T297 K298 Q299 V300 R301 T302 I303 E304 K305 I306 T307 P308 I309 E310 S311 F312 F313 N314 F315
F316 D317 P318 P319 K320 I321 Q322 N323 E324 D325 Q326 D327 E328 E329 L330 E331 E332 E335 E336 R337 L338 A339 L340 D341 I344 G345 E346 Q347 L348 K349 D350 K351 L352 I353 A356 V357 D358 W359 F360 T361 G362 A363 A364 L365 GLU PHE GLU PHE GLU GLU ASP GLU GLU GLU ALA ASP GLU
ASP GLU ASP GLU GLU ASP ASP ASP HIS GLY LEU GLU ASP ASP ASP GLY GLU SER ALA GLU GLU GLN ASP ASP PHE ALA GLY ARG PRO GLU GLN ALA PRO GLU CYS LYS GLN SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	133516	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.700	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	381.546, 381.546, 381.546	wwPDB
Map dimensions	517, 517, 517	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.738, 0.738, 0.738	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, 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	A	0.34	0/7651	0.52	0/10371
2	B	0.34	0/654	0.64	0/881
3	C	0.29	0/703	0.49	0/948
4	D	0.39	0/1419	0.56	0/1917
5	E	0.28	0/2372	0.51	0/3204
5	F	0.26	0/2386	0.49	0/3223
All	All	0.32	0/15185	0.52	0/20544

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

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	7531	0	7624	146	0
2	B	646	0	680	30	0
3	C	693	0	710	34	0
4	D	1384	0	1402	20	0
5	E	2325	0	2260	58	0
5	F	2339	0	2269	68	0
6	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	32	0	12	4	0
All	All	14951	0	14957	312	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 10.

All (312) 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)
5:E:106:LEU:HD22	5:F:132:TRP:CH2	1.86	1.10
5:F:282:ASN:HD22	5:F:285:VAL:HG22	1.32	0.93
1:A:752:LEU:HD23	1:A:755:ARG:HH21	1.32	0.93
5:E:150:ILE:HG12	5:F:94:GLU:HB2	1.55	0.88
5:E:96:LEU:HD23	5:F:165:LEU:HD21	1.62	0.81
1:A:968:LEU:HD23	1:A:971:ARG:HH12	1.46	0.81
1:A:724:LEU:HD21	1:A:766:LYS:HG2	1.63	0.80
5:E:92:VAL:HA	5:E:95:LYS:HE3	1.62	0.80
1:A:823:GLU:HG2	1:A:827:LYS:HE3	1.64	0.78
1:A:850:ASN:HA	1:A:876:GLN:HA	1.63	0.78
5:E:106:LEU:CD2	5:F:132:TRP:CH2	2.67	0.77
1:A:777:LEU:HD22	1:A:813:TRP:CD1	2.21	0.75
5:E:327:ASP:O	5:E:331:GLU:N	2.21	0.74
1:A:527:SER:HB2	1:A:570:ARG:HH12	1.53	0.73
5:E:253:PHE:CD2	5:E:267:ASP:HB3	2.24	0.73
5:E:106:LEU:CD2	5:F:132:TRP:CZ3	2.72	0.72
4:D:24:GLY:HA2	7:D:202:GTP:H5”	1.69	0.72
1:A:864:ARG:NH1	2:B:93:GLU:OE2	2.24	0.71
5:F:199:VAL:HG22	5:F:344:ILE:HG23	1.72	0.71
1:A:852:ASN:O	1:A:875:VAL:N	2.21	0.70
2:B:84:LEU:HD21	3:C:68:PHE:HE2	1.54	0.70
3:C:89:LYS:HD2	3:C:91:THR:H	1.57	0.70
5:E:137:ARG:NH1	5:E:142:GLN:OE1	2.22	0.69
3:C:38:GLU:HG3	3:C:66:ASN:HD21	1.58	0.69
4:D:47:VAL:HG12	4:D:68:THR:HA	1.73	0.69
1:A:852:ASN:HB2	1:A:875:VAL:HB	1.74	0.68
4:D:97:ARG:HH12	4:D:137:THR:HG21	1.59	0.67
5:F:128:TYR:HB3	5:F:132:TRP:CZ3	2.29	0.67
1:A:757:LEU:HD11	1:A:795:LEU:HG	1.77	0.66
2:B:80:ILE:HG12	2:B:83:HIS:CE1	2.31	0.66
1:A:819:VAL:HA	3:C:99:THR:HG22	1.77	0.66
1:A:777:LEU:HD22	1:A:813:TRP:HD1	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:MET:HG3	1:A:68:TYR:CD1	2.31	0.66
1:A:751:PRO:O	1:A:755:ARG:NH2	2.29	0.66
2:B:35:LEU:HD21	3:C:92:ILE:HD11	1.76	0.66
3:C:59:GLN:HA	3:C:62:MET:HE2	1.78	0.65
5:F:346:GLU:HA	5:F:349:LYS:HE2	1.77	0.65
4:D:125:LYS:HG2	7:D:202:GTP:C5	2.31	0.65
5:E:106:LEU:HD22	5:F:132:TRP:CZ3	2.31	0.65
5:E:226:ARG:HD2	5:E:253:PHE:HZ	1.60	0.65
1:A:441:THR:O	1:A:445:ILE:HG12	1.97	0.65
1:A:687:THR:HG23	1:A:688:LEU:HD12	1.77	0.64
1:A:101:ASP:OD1	1:A:145:ASN:ND2	2.29	0.64
5:F:322:GLN:O	5:F:326:GLN:N	2.31	0.63
1:A:811:ARG:HA	1:A:849:VAL:HG13	1.79	0.63
3:C:89:LYS:NZ	3:C:91:THR:O	2.29	0.63
1:A:655:LYS:HG2	1:A:697:TYR:CZ	2.35	0.62
1:A:864:ARG:NH1	2:B:91:ASP:OD2	2.30	0.62
5:F:235:PHE:N	5:F:246:ASP:O	2.26	0.62
3:C:48:LEU:HD21	3:C:55:THR:HB	1.82	0.61
5:E:279:ASN:ND2	5:E:304:GLU:OE2	2.31	0.61
1:A:459:ALA:O	1:A:463:ILE:HG13	2.00	0.61
1:A:518:ASP:OD1	1:A:519:SER:N	2.33	0.61
5:E:253:PHE:HD2	5:E:267:ASP:HB3	1.62	0.61
1:A:817:PHE:HA	1:A:820:ILE:HD12	1.83	0.61
1:A:78:SER:O	1:A:79:THR:OG1	2.19	0.61
5:F:278:ASP:OD1	5:F:281:HIS:N	2.31	0.60
1:A:647:LEU:O	1:A:651:THR:HG23	2.01	0.60
1:A:968:LEU:HA	1:A:971:ARG:NH1	2.17	0.60
1:A:599:GLN:HG3	1:A:649:PHE:HE2	1.66	0.60
1:A:668:ASN:OD1	1:A:710:ARG:NH1	2.34	0.59
1:A:781:CYS:SG	1:A:829:ASN:ND2	2.75	0.59
1:A:848:VAL:HB	1:A:876:GLN:HB3	1.84	0.59
1:A:704:THR:O	1:A:708:GLU:HG2	2.02	0.59
3:C:48:LEU:O	3:C:52:HIS:N	2.31	0.59
5:E:95:LYS:NZ	5:F:185:ILE:HG12	2.18	0.59
5:F:248:LEU:HD22	5:F:274:ILE:HG12	1.85	0.59
1:A:122:ASP:OD1	1:A:126:GLN:NE2	2.35	0.58
1:A:864:ARG:HG3	2:B:58:TYR:OH	2.02	0.58
1:A:426:ILE:HG22	1:A:431:ILE:HD13	1.84	0.58
5:F:94:GLU:HA	5:F:97:LEU:HD12	1.86	0.58
5:F:351:LYS:O	5:F:359:TRP:NE1	2.36	0.58
5:F:326:GLN:HA	5:F:330:LEU:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:147:PRO:HA	5:E:150:ILE:HD12	1.84	0.58
1:A:851:GLY:H	1:A:877:VAL:HG22	1.69	0.58
5:E:226:ARG:HD2	5:E:253:PHE:CZ	2.37	0.58
2:B:35:LEU:HD21	2:B:44:ILE:HD12	1.83	0.58
5:F:282:ASN:ND2	5:F:285:VAL:HG22	2.11	0.58
5:F:252:TYR:OH	5:F:341:ASP:O	2.22	0.58
5:F:88:LEU:HD12	5:F:92:VAL:HG11	1.86	0.57
5:F:351:LYS:HB3	5:F:359:TRP:CZ2	2.40	0.57
1:A:887:PHE:O	1:A:890:GLU:HG3	2.04	0.57
2:B:27:PRO:HD3	3:C:43:TYR:HD2	1.68	0.57
4:D:139:THR:O	4:D:142:ARG:HG2	2.05	0.57
5:F:146:LYS:HG2	5:F:147:PRO:HD2	1.86	0.57
1:A:715:MET:HG3	1:A:752:LEU:HD13	1.87	0.56
2:B:94:LEU:HD12	3:C:109:LEU:HD11	1.87	0.56
1:A:804:ASP:OD1	1:A:806:LEU:N	2.35	0.56
3:C:95:ARG:O	3:C:99:THR:HG23	2.04	0.56
5:E:311:SER:N	5:E:314:ASN:OD1	2.38	0.56
5:E:185:ILE:HG12	5:F:92:VAL:HG13	1.88	0.56
1:A:811:ARG:HD2	1:A:812:LYS:N	2.21	0.55
3:C:92:ILE:HG22	3:C:96:GLU:OE1	2.06	0.55
2:B:55:VAL:O	2:B:59:LEU:HG	2.06	0.55
1:A:370:TYR:HB2	4:D:142:ARG:HH11	1.72	0.55
1:A:459:ALA:HA	1:A:462:THR:HG22	1.89	0.55
2:B:41:ALA:HB2	3:C:92:ILE:HG23	1.88	0.55
2:B:93:GLU:HB2	3:C:106:PRO:HG2	1.89	0.55
1:A:652:VAL:O	1:A:656:LYS:HG3	2.07	0.55
1:A:336:THR:O	1:A:340:ILE:HG12	2.06	0.55
1:A:971:ARG:O	1:A:975:GLU:N	2.31	0.55
5:E:117:MET:O	5:E:120:LEU:N	2.40	0.55
1:A:650:ILE:O	1:A:654:LEU:HD13	2.06	0.54
5:F:285:VAL:HG12	5:F:308:PRO:HA	1.90	0.54
1:A:335:ILE:O	1:A:339:THR:HG23	2.08	0.54
1:A:760:VAL:O	1:A:776:LEU:HD23	2.08	0.54
1:A:764:LEU:HD21	1:A:777:LEU:HD21	1.90	0.54
5:E:210:VAL:HG22	5:E:242:PHE:CD2	2.43	0.54
1:A:722:LEU:HD21	1:A:734:VAL:HG21	1.90	0.53
1:A:684:GLU:HB3	1:A:687:THR:HG22	1.90	0.53
5:F:122:ASN:ND2	5:F:223:THR:OG1	2.42	0.53
4:D:31:ARG:NH1	4:D:153:ALA:O	2.32	0.53
5:E:188:PHE:HA	5:E:360:PHE:CE1	2.44	0.53
1:A:887:PHE:HB3	1:A:969:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:357:VAL:HG21	5:F:99:LEU:HB3	1.91	0.53
1:A:295:VAL:HA	1:A:303:LEU:HD23	1.90	0.52
1:A:822:GLY:O	1:A:826:ILE:HG13	2.09	0.52
2:B:52:LEU:HD13	2:B:56:LEU:HD23	1.92	0.52
5:E:328:GLU:HA	5:E:331:GLU:HB2	1.92	0.52
5:E:215:GLN:OE1	5:E:236:ASP:HB3	2.10	0.52
5:F:252:TYR:OH	5:F:341:ASP:OD1	2.20	0.52
1:A:370:TYR:HB2	4:D:142:ARG:NH1	2.25	0.51
1:A:599:GLN:HG3	1:A:649:PHE:CE2	2.45	0.51
5:F:229:PHE:CZ	5:F:349:LYS:HD3	2.45	0.51
1:A:622:LEU:HD21	1:A:653:PHE:CE2	2.46	0.51
5:E:293:ARG:NH1	5:E:294:ASN:O	2.44	0.51
1:A:833:LEU:HD12	1:A:883:ILE:HD13	1.93	0.51
2:B:27:PRO:HD3	3:C:43:TYR:CD2	2.45	0.51
2:B:77:THR:O	3:C:56:GLY:N	2.24	0.51
1:A:119:SER:HB2	1:A:123:PHE:HB2	1.93	0.51
4:D:31:ARG:NH1	4:D:154:LYS:O	2.32	0.51
5:F:210:VAL:HG22	5:F:242:PHE:CD2	2.46	0.51
1:A:830:ILE:HG23	1:A:969:LEU:HD13	1.93	0.50
5:F:147:PRO:HA	5:F:150:ILE:HB	1.93	0.50
5:F:323:ASN:OD1	5:F:324:GLU:N	2.44	0.50
5:F:132:TRP:HA	5:F:135:ARG:HG2	1.92	0.50
1:A:883:ILE:HG13	1:A:884:ILE:N	2.27	0.50
5:E:151:ALA:O	5:E:154:GLN:HB3	2.12	0.50
1:A:823:GLU:O	1:A:827:LYS:HG3	2.12	0.50
5:E:152:LYS:HD2	5:F:101:THR:HG21	1.94	0.49
1:A:2:ASP:HA	1:A:5:GLU:OE2	2.13	0.49
1:A:656:LYS:O	1:A:657:LYS:HE2	2.13	0.49
1:A:817:PHE:O	3:C:95:ARG:NH2	2.45	0.49
5:F:85:VAL:HA	5:F:88:LEU:HD23	1.95	0.49
1:A:37:PHE:HB3	1:A:90:ILE:HD11	1.95	0.49
1:A:511:TYR:HA	1:A:514:PHE:CE1	2.47	0.49
1:A:711:LEU:O	1:A:714:ILE:HG22	2.13	0.49
5:E:246:ASP:OD1	5:E:247:ILE:N	2.45	0.49
5:F:361:THR:HG23	5:F:363:ALA:H	1.77	0.49
1:A:792:VAL:HA	1:A:795:LEU:HD12	1.94	0.49
5:E:222:LEU:HD12	5:E:228:GLY:HA3	1.94	0.49
1:A:850:ASN:HA	1:A:875:VAL:O	2.12	0.48
1:A:34:SER:HB3	1:A:86:VAL:HG21	1.93	0.48
1:A:303:LEU:O	1:A:307:VAL:HG23	2.13	0.48
1:A:368:ALA:HB1	4:D:141:HIS:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:152:LYS:O	5:F:155:GLU:HG3	2.14	0.48
2:B:41:ALA:HB3	3:C:92:ILE:HG12	1.95	0.48
1:A:161:GLU:HG2	1:A:162:MET:N	2.29	0.48
1:A:269:PHE:CE2	1:A:274:GLN:HG2	2.48	0.48
1:A:111:ALA:O	1:A:115:ILE:HG13	2.14	0.48
1:A:204:MET:CE	1:A:219:VAL:HA	2.44	0.48
1:A:800:ILE:O	1:A:803:THR:HG22	2.13	0.48
1:A:200:CYS:O	1:A:204:MET:HG3	2.13	0.48
1:A:790:GLN:NE2	1:A:791:THR:OG1	2.47	0.48
2:B:79:ILE:HB	3:C:57:ILE:HD12	1.96	0.48
1:A:428:GLY:N	1:A:431:ILE:HD12	2.29	0.47
5:F:196:LEU:HD21	5:F:347:GLN:HG2	1.95	0.47
1:A:792:VAL:HA	1:A:795:LEU:HB2	1.95	0.47
5:E:267:ASP:HA	5:E:322:GLN:NE2	2.29	0.47
5:F:132:TRP:CD1	5:F:135:ARG:NH2	2.82	0.47
1:A:763:ARG:HB3	1:A:776:LEU:HD21	1.96	0.47
2:B:67:ALA:HA	2:B:87:ALA:HB2	1.95	0.47
1:A:646:VAL:O	1:A:650:ILE:HG13	2.15	0.47
1:A:753:ILE:O	1:A:757:LEU:N	2.39	0.47
3:C:72:ILE:HA	3:C:75:ARG:HG2	1.97	0.47
4:D:18:VAL:HG11	4:D:110:LEU:HD11	1.97	0.47
5:E:357:VAL:CG2	5:F:99:LEU:HB3	2.45	0.47
1:A:270:SER:O	1:A:274:GLN:HG3	2.15	0.47
4:D:56:THR:HG22	4:D:178:PHE:CD1	2.49	0.47
1:A:510:TYR:O	1:A:513:TYR:HB2	2.15	0.47
1:A:998:VAL:HA	1:A:1001:GLU:HG2	1.97	0.47
4:D:141:HIS:HA	4:D:146:LEU:HD23	1.96	0.47
5:F:358:ASP:HA	5:F:361:THR:HG22	1.97	0.46
1:A:82:VAL:HG13	1:A:82:VAL:O	2.15	0.46
5:F:122:ASN:O	5:F:126:GLN:HG2	2.16	0.46
1:A:890:GLU:OE2	1:A:891:LEU:HD12	2.16	0.46
3:C:49:LYS:NZ	3:C:53:PRO:O	2.26	0.46
1:A:637:TYR:CE1	1:A:678:VAL:HG22	2.50	0.46
1:A:643:LEU:O	1:A:647:LEU:HG	2.16	0.46
3:C:89:LYS:NZ	3:C:96:GLU:OE2	2.36	0.46
1:A:819:VAL:HG12	3:C:98:GLN:HG2	1.98	0.46
5:F:128:TYR:O	5:F:132:TRP:HE3	1.98	0.46
5:F:157:VAL:HG21	5:F:165:LEU:HB2	1.98	0.46
4:D:27:THR:HG21	7:D:202:GTP:C8	2.51	0.46
4:D:97:ARG:NH1	4:D:97:ARG:HG3	2.31	0.46
1:A:509:THR:HG22	1:A:513:TYR:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:LEU:HD12	1:A:521:LEU:HD11	1.98	0.45
1:A:741:ILE:HG13	1:A:745:PHE:HD2	1.80	0.45
1:A:850:ASN:CA	1:A:876:GLN:HA	2.42	0.45
5:F:233:PHE:O	5:F:248:LEU:N	2.41	0.45
1:A:674:PRO:O	1:A:678:VAL:HG23	2.17	0.45
1:A:820:ILE:O	3:C:95:ARG:NH2	2.41	0.45
1:A:824:LYS:HA	1:A:824:LYS:HD3	1.63	0.45
3:C:83:LEU:HG	3:C:96:GLU:OE2	2.17	0.45
5:E:319:PRO:HG2	5:E:338:LEU:HG	1.97	0.45
2:B:80:ILE:HG22	3:C:58:SER:OG	2.15	0.45
5:F:136:SER:HB2	5:F:216:ASP:OD1	2.16	0.45
1:A:527:SER:HB2	1:A:570:ARG:NH1	2.27	0.45
2:B:34:LEU:O	2:B:37:ARG:HG2	2.16	0.45
5:F:139:ILE:HG12	5:F:185:ILE:HD12	1.97	0.45
1:A:849:VAL:HG21	1:A:879:LEU:HA	1.98	0.45
5:F:290:ARG:CG	5:F:292:GLN:HE22	2.30	0.45
1:A:642:LEU:O	1:A:646:VAL:HG23	2.17	0.45
1:A:757:LEU:HD13	1:A:794:PHE:HB2	1.99	0.44
5:E:282:ASN:OD1	5:E:284:THR:OG1	2.20	0.44
1:A:596:VAL:O	1:A:599:GLN:HB3	2.18	0.44
3:C:101:VAL:HG13	3:C:105:LEU:HD12	1.98	0.44
4:D:125:LYS:HG2	7:D:202:GTP:C6	2.52	0.44
1:A:861:ILE:HG13	2:B:57:GLU:HG2	1.97	0.44
4:D:97:ARG:HG3	4:D:97:ARG:HH11	1.82	0.44
1:A:645:LEU:HD11	1:A:649:PHE:HE2	1.82	0.44
1:A:123:PHE:HZ	1:A:131:LEU:HD21	1.83	0.44
1:A:471:ILE:HG13	1:A:477:ILE:HG12	1.99	0.44
1:A:819:VAL:HG11	3:C:102:ARG:HG3	1.99	0.44
1:A:4:ASN:O	1:A:8:ILE:HG12	2.17	0.44
5:E:276:TRP:HH2	5:E:313:PHE:HD2	1.66	0.44
1:A:384:PRO:HG2	1:A:387:GLN:HG2	1.99	0.43
1:A:757:LEU:HA	1:A:760:VAL:HG12	2.00	0.43
2:B:71:ALA:HB2	2:B:79:ILE:HG12	2.00	0.43
1:A:860:LEU:HD21	1:A:870:MET:HE1	1.99	0.43
1:A:741:ILE:O	1:A:745:PHE:N	2.50	0.43
1:A:718:LEU:HD13	1:A:718:LEU:HA	1.80	0.43
1:A:718:LEU:O	1:A:722:LEU:HD23	2.19	0.43
1:A:819:VAL:CG1	3:C:98:GLN:HG2	2.48	0.43
5:F:267:ASP:OD1	5:F:268:HIS:N	2.48	0.43
5:E:106:LEU:HD21	5:F:132:TRP:CZ3	2.50	0.43
1:A:752:LEU:CD2	1:A:755:ARG:HH21	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:101:THR:HG23	5:F:152:LYS:HG2	2.01	0.43
5:E:294:ASN:OD1	5:E:296:THR:N	2.47	0.43
5:F:348:LEU:HG	5:F:352:LEU:HD23	1.99	0.43
5:E:95:LYS:CE	5:F:185:ILE:HG12	2.49	0.43
5:E:330:LEU:O	5:E:334:LEU:HG	2.18	0.43
5:E:88:LEU:HB3	5:E:92:VAL:HG21	2.01	0.43
5:E:189:TRP:O	5:E:193:LEU:HD23	2.19	0.43
5:E:285:VAL:HG13	5:E:307:THR:H	1.84	0.43
1:A:282:ILE:HD13	1:A:330:GLU:HB2	2.01	0.43
1:A:392:PHE:CE2	1:A:431:ILE:HG23	2.53	0.43
1:A:618:ILE:HA	1:A:622:LEU:HD23	2.01	0.43
1:A:662:PHE:HE1	1:A:744:ARG:NH1	2.17	0.43
1:A:752:LEU:HD23	1:A:755:ARG:NH2	2.15	0.43
5:F:91:ASN:HA	5:F:94:GLU:OE2	2.19	0.42
5:E:93:LYS:O	5:E:97:LEU:HG	2.19	0.42
5:E:193:LEU:HB3	5:E:203:ILE:HD11	2.00	0.42
1:A:123:PHE:CZ	1:A:131:LEU:HD21	2.55	0.42
1:A:651:THR:HG22	1:A:694:ALA:HB2	2.01	0.42
1:A:287:ASN:O	1:A:291:ILE:HD12	2.20	0.42
1:A:553:MET:HE1	1:A:581:VAL:HG23	2.01	0.42
2:B:85:GLN:O	2:B:89:ARG:HG2	2.20	0.42
5:F:250:LYS:HG2	5:F:315:PHE:CE2	2.55	0.42
1:A:349:ARG:HG3	1:A:454:LEU:HD12	2.00	0.42
2:B:31:VAL:HG13	3:C:73:PHE:HE2	1.83	0.42
2:B:70:ALA:O	2:B:73:ASP:HB2	2.20	0.42
1:A:654:LEU:HD11	1:A:671:LEU:CD1	2.50	0.42
5:E:187:SER:HB3	5:E:190:LEU:HD23	2.01	0.42
5:E:355:ARG:O	5:E:359:TRP:HD1	2.03	0.42
1:A:529:THR:O	1:A:533:VAL:HG23	2.19	0.41
1:A:655:LYS:HG2	1:A:697:TYR:CE1	2.55	0.41
1:A:864:ARG:HE	2:B:62:GLU:CD	2.23	0.41
4:D:126:VAL:HG12	4:D:152:SER:HB3	2.02	0.41
5:E:116:GLU:HG3	5:F:124:PHE:HZ	1.84	0.41
5:E:134:GLN:O	5:E:138:ILE:HG12	2.20	0.41
2:B:83:HIS:CD2	2:B:83:HIS:N	2.88	0.41
5:F:176:ASP:OD1	5:F:177:SER:N	2.53	0.41
1:A:596:VAL:O	1:A:600:GLU:OE1	2.38	0.41
3:C:44:ILE:HG21	3:C:62:MET:HG3	2.01	0.41
4:D:134:LYS:O	4:D:138:ILE:HG12	2.19	0.41
1:A:389:SER:O	1:A:393:LYS:HG3	2.20	0.41
1:A:966:VAL:O	1:A:970:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:148:GLU:O	5:E:152:LYS:HG2	2.20	0.41
5:F:290:ARG:HD2	5:F:292:GLN:HE22	1.86	0.41
1:A:863:THR:HA	2:B:58:TYR:CE1	2.55	0.41
4:D:127:ASP:OD2	4:D:154:LYS:HB3	2.20	0.41
5:E:187:SER:HB3	5:E:190:LEU:HB3	2.02	0.41
5:E:210:VAL:HG22	5:E:242:PHE:CE2	2.55	0.41
1:A:684:GLU:CD	1:A:686:GLU:H	2.24	0.41
1:A:782:PHE:HB2	1:A:828:GLU:OE2	2.19	0.41
2:B:60:ALA:O	2:B:64:LEU:HB2	2.20	0.41
5:F:358:ASP:O	5:F:362:GLY:N	2.54	0.41
1:A:276:GLN:HG2	1:A:280:MET:HE2	2.03	0.41
1:A:292:ASN:HA	1:A:295:VAL:HG23	2.03	0.41
1:A:326:PHE:HA	1:A:330:GLU:OE2	2.21	0.41
1:A:757:LEU:O	1:A:760:VAL:HG12	2.20	0.41
1:A:813:TRP:CH2	1:A:833:LEU:HD22	2.56	0.41
5:E:149:GLN:HA	5:E:152:LYS:HG2	2.03	0.41
5:F:219:LEU:HD11	5:F:353:ILE:HG13	2.03	0.41
1:A:600:GLU:O	1:A:603:GLU:HG3	2.21	0.41
1:A:822:GLY:HA2	3:C:86:TYR:CD2	2.56	0.41
5:E:92:VAL:HA	5:E:95:LYS:HG2	2.02	0.41
5:E:242:PHE:HA	5:E:281:HIS:HB3	2.02	0.41
5:E:344:ILE:O	5:E:348:LEU:HD23	2.21	0.41
5:F:231:LEU:HD13	5:F:348:LEU:HD13	2.03	0.41
5:E:191:THR:HB	5:E:360:PHE:CD1	2.56	0.41
5:F:146:LYS:CG	5:F:147:PRO:HD2	2.51	0.41
5:F:207:ASP:CG	5:F:312:PHE:H	2.23	0.41
2:B:52:LEU:HD12	3:C:73:PHE:CD2	2.56	0.40
5:E:284:THR:HG22	5:E:311:SER:OG	2.20	0.40
5:F:214:LEU:HD12	5:F:234:ARG:O	2.21	0.40
5:E:190:LEU:O	5:E:194:GLU:HG2	2.21	0.40
5:F:203:ILE:HA	5:F:312:PHE:HB2	2.03	0.40
5:F:128:TYR:HB3	5:F:132:TRP:CE3	2.55	0.40
5:F:196:LEU:HA	5:F:197:PRO:HD3	1.98	0.40
5:F:287:LEU:HA	5:F:305:LYS:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	938/1012 (93%)	925 (99%)	13 (1%)	0	100	100
2	B	81/131 (62%)	80 (99%)	1 (1%)	0	100	100
3	C	87/130 (67%)	86 (99%)	1 (1%)	0	100	100
4	D	168/186 (90%)	164 (98%)	4 (2%)	0	100	100
5	E	281/420 (67%)	274 (98%)	7 (2%)	0	100	100
5	F	283/420 (67%)	276 (98%)	7 (2%)	0	100	100
All	All	1838/2299 (80%)	1805 (98%)	33 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	871/935 (93%)	867 (100%)	4 (0%)	86	95
2	B	65/98 (66%)	64 (98%)	1 (2%)	60	84
3	C	77/109 (71%)	77 (100%)	0	100	100
4	D	149/160 (93%)	148 (99%)	1 (1%)	81	93
5	E	255/374 (68%)	255 (100%)	0	100	100
5	F	257/374 (69%)	257 (100%)	0	100	100
All	All	1674/2050 (82%)	1668 (100%)	6 (0%)	88	96

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

Mol	Chain	Res	Type
1	A	30	ASP
1	A	718	LEU
1	A	746	SER
1	A	824	LYS
2	B	52	LEU
4	D	150	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	GLN
1	A	790	GLN
2	B	69	ASN
2	B	83	HIS
3	C	66	ASN
5	F	282	ASN
5	F	292	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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\#\|Z\| > 2$
7	GTP	D	202	6	29,34,34	1.00	2 (6%)	35,54,54	0.72	0

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
7	GTP	D	202	6	-	4/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	202	GTP	C5-C6	-2.76	1.42	1.47
7	D	202	GTP	C8-N7	-2.14	1.31	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	202	GTP	C3'-C4'-C5'-O5'
7	D	202	GTP	O4'-C4'-C5'-O5'
7	D	202	GTP	PB-O3A-PA-O1A
7	D	202	GTP	PB-O3A-PA-O2A

There are no ring outliers.

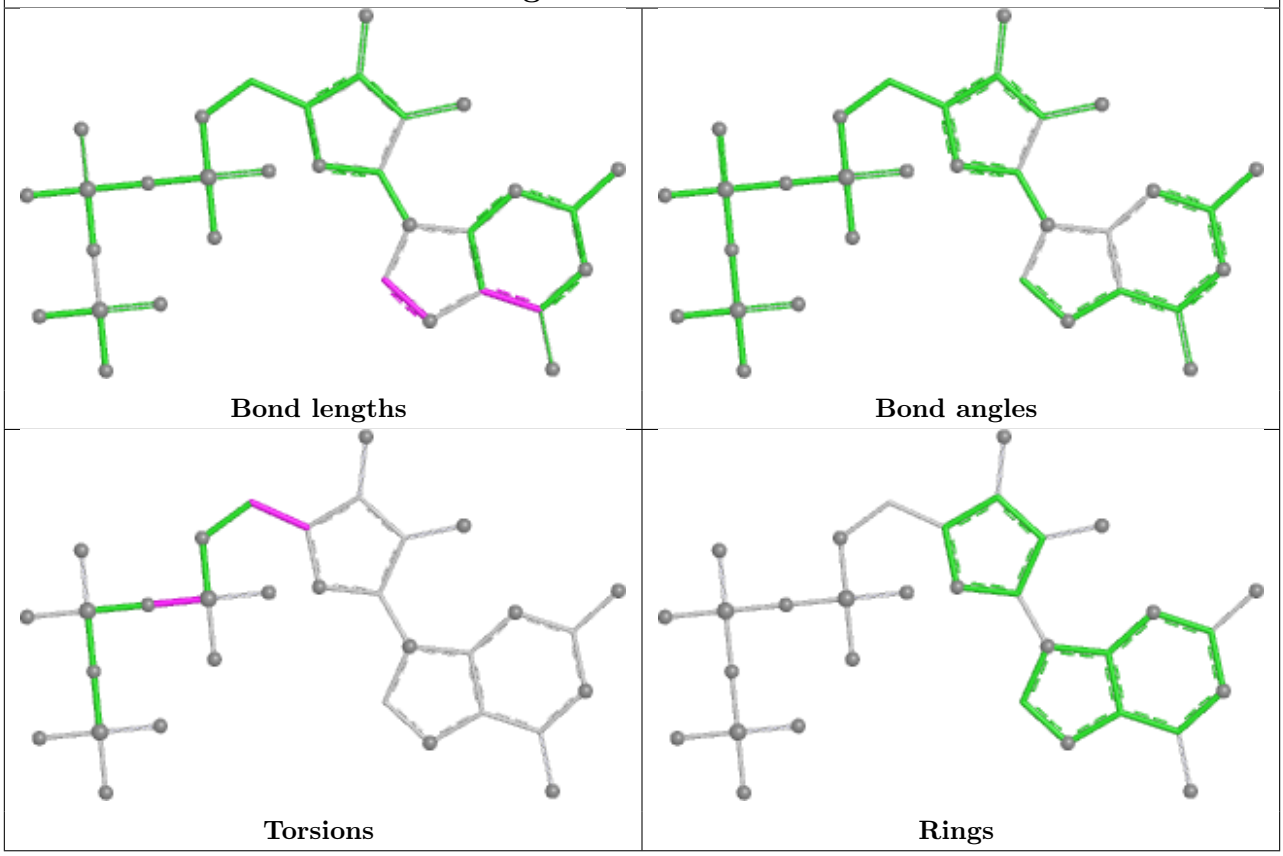
1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	202	GTP	4	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 GTP D 202



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.

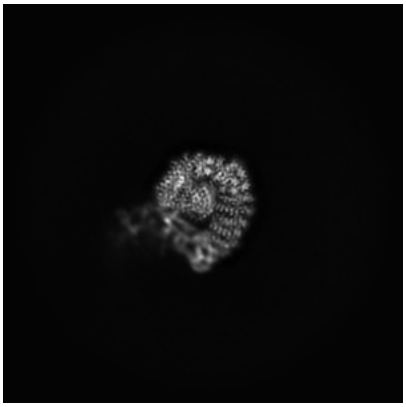
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44141. These allow visual inspection of the internal detail of the map and identification of artifacts.

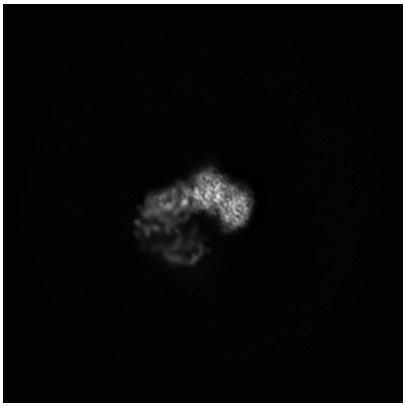
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

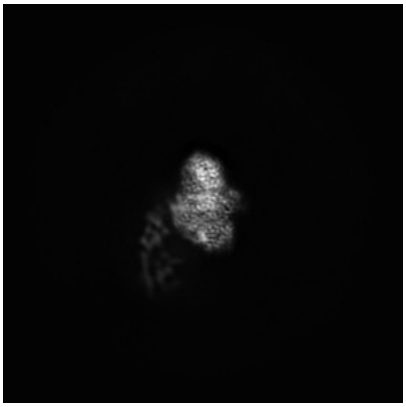
6.1.1 Primary map



X



Y



Z

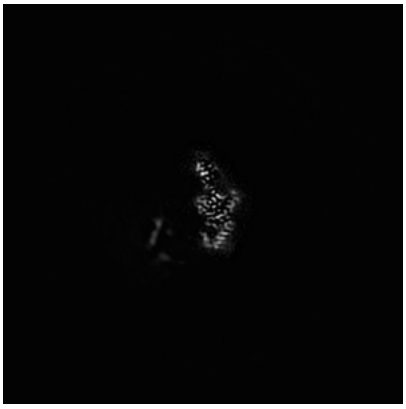
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 258

Y Index: 258



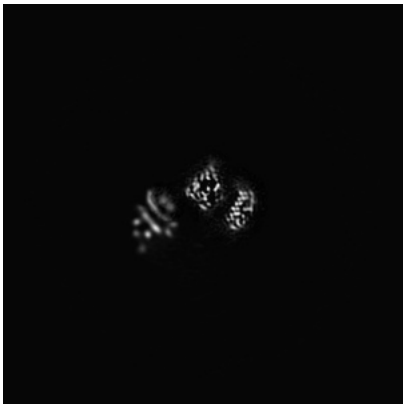
Z Index: 258

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: 259



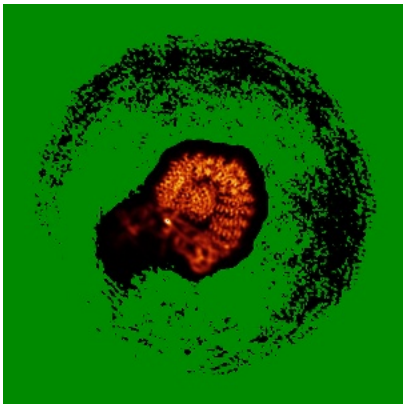
Y Index: 254

Z Index: 298

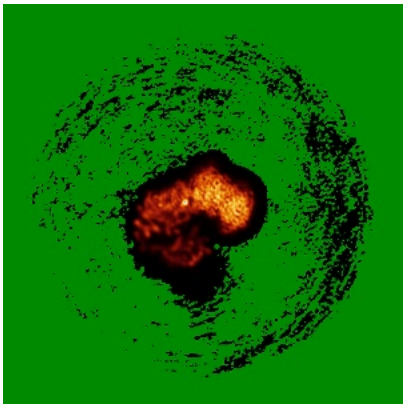
The images above show the largest variance slices of the map in three orthogonal directions.

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

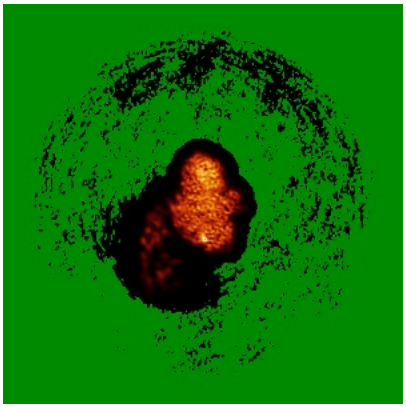
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

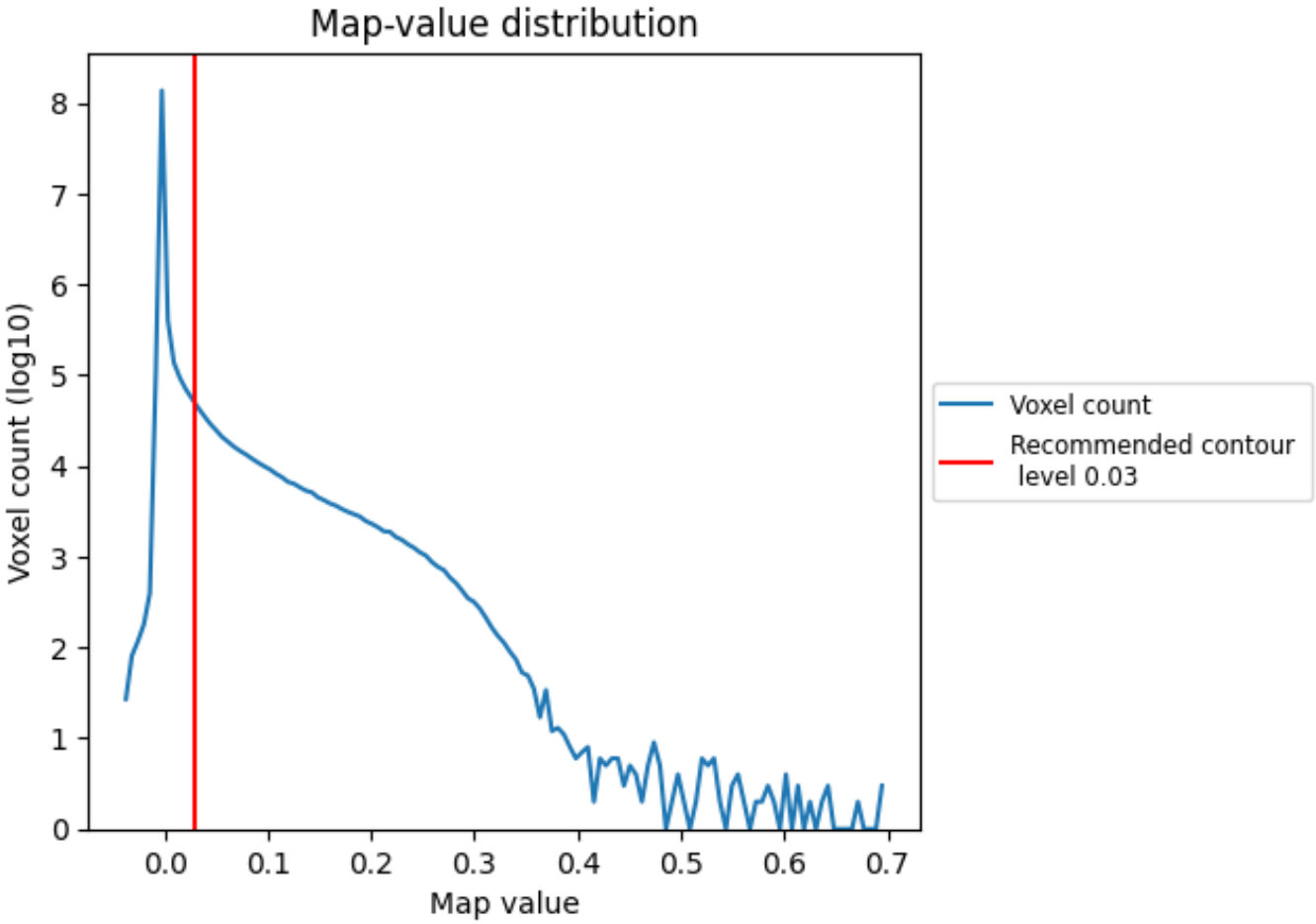
6.6 Mask visualisation (i)

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

7 Map analysis

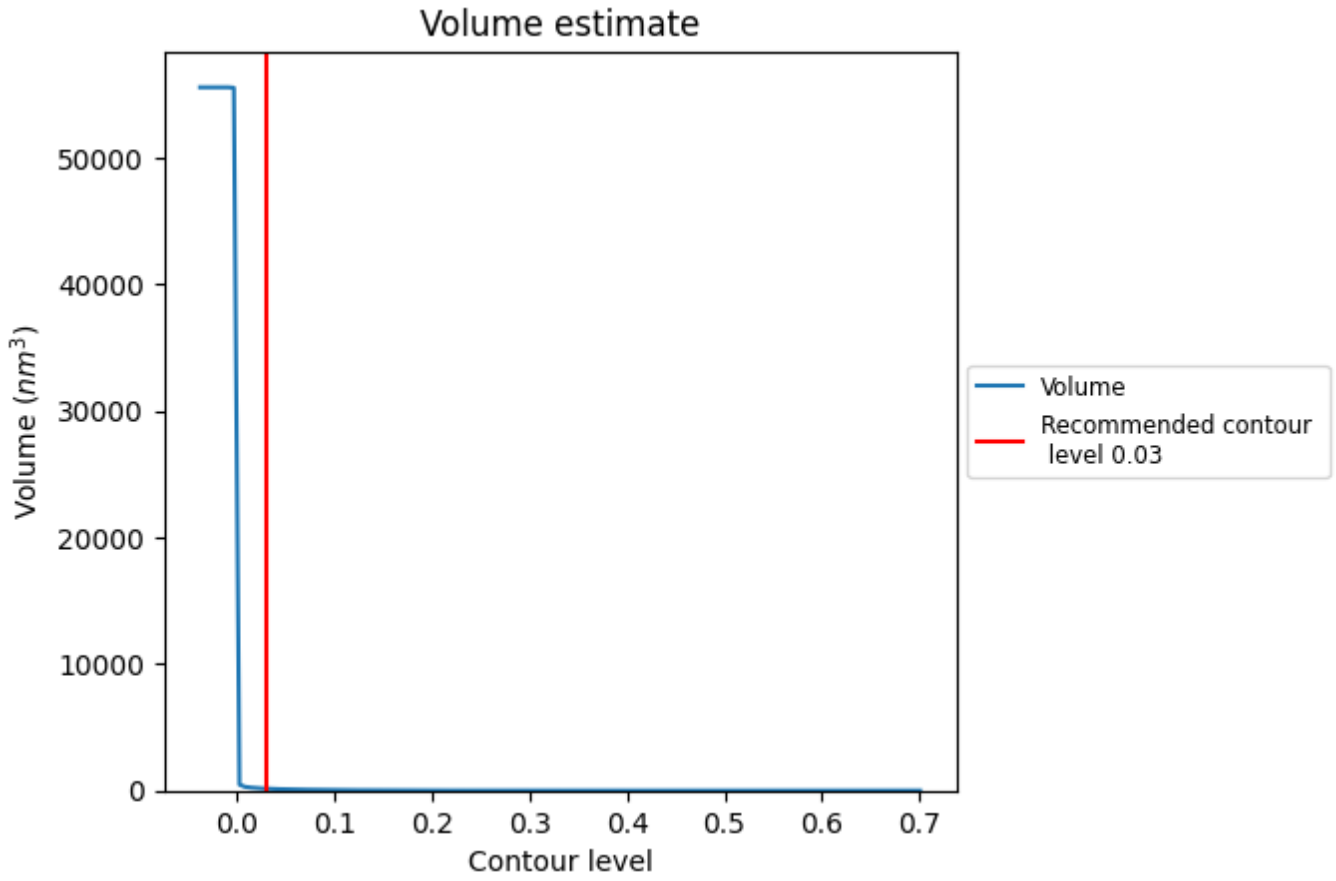
This section contains the results of statistical analysis of the map.

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.

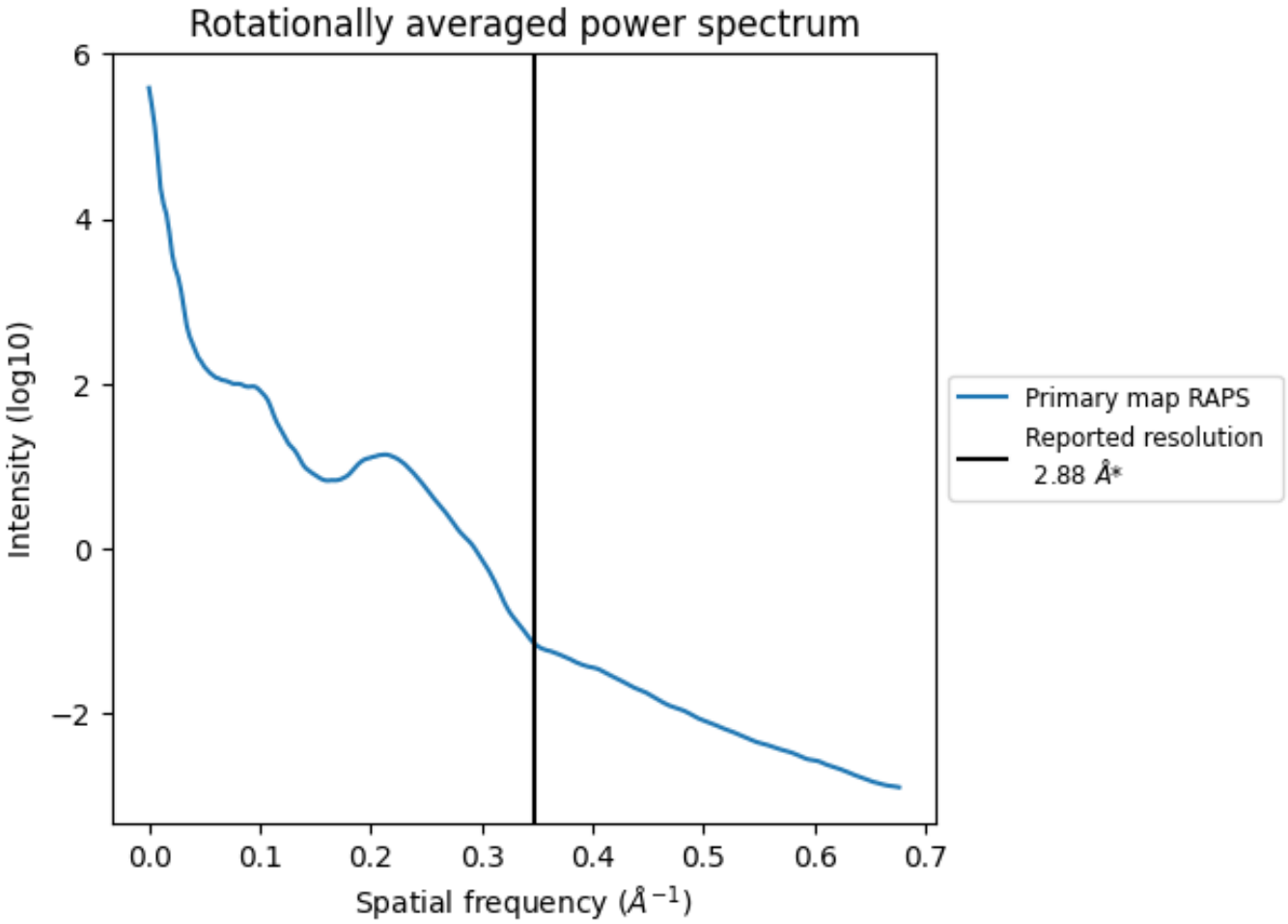
7.2 Volume estimate (i)



The volume at the recommended contour level is 153 nm^3; this corresponds to an approximate mass of 138 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}

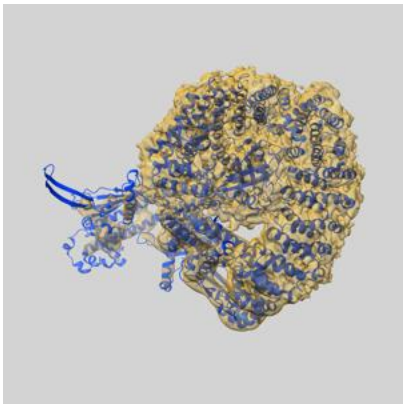
8 Fourier-Shell correlation (i)

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

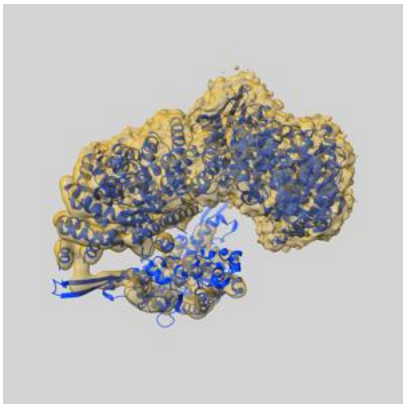
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44141 and PDB model 9B3I. Per-residue inclusion information can be found in section 3 on page 6.

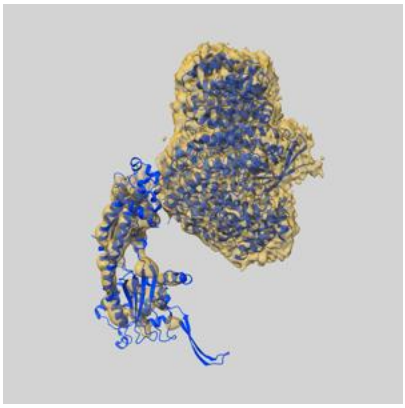
9.1 Map-model overlay



X



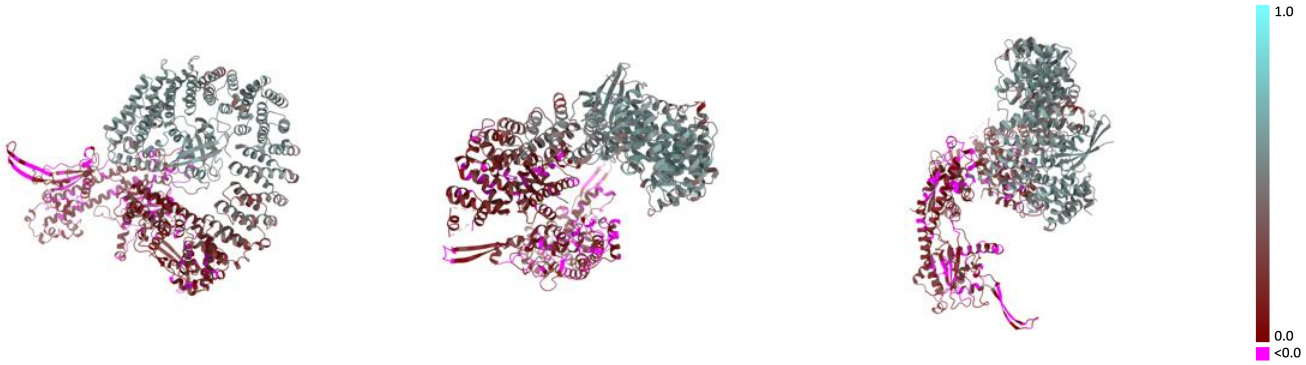
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

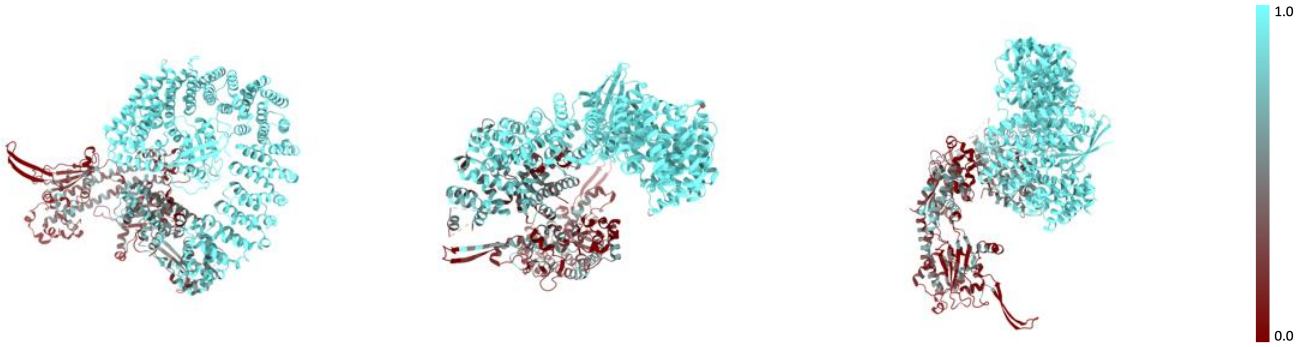
9.2 Q-score mapped to coordinate model



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.

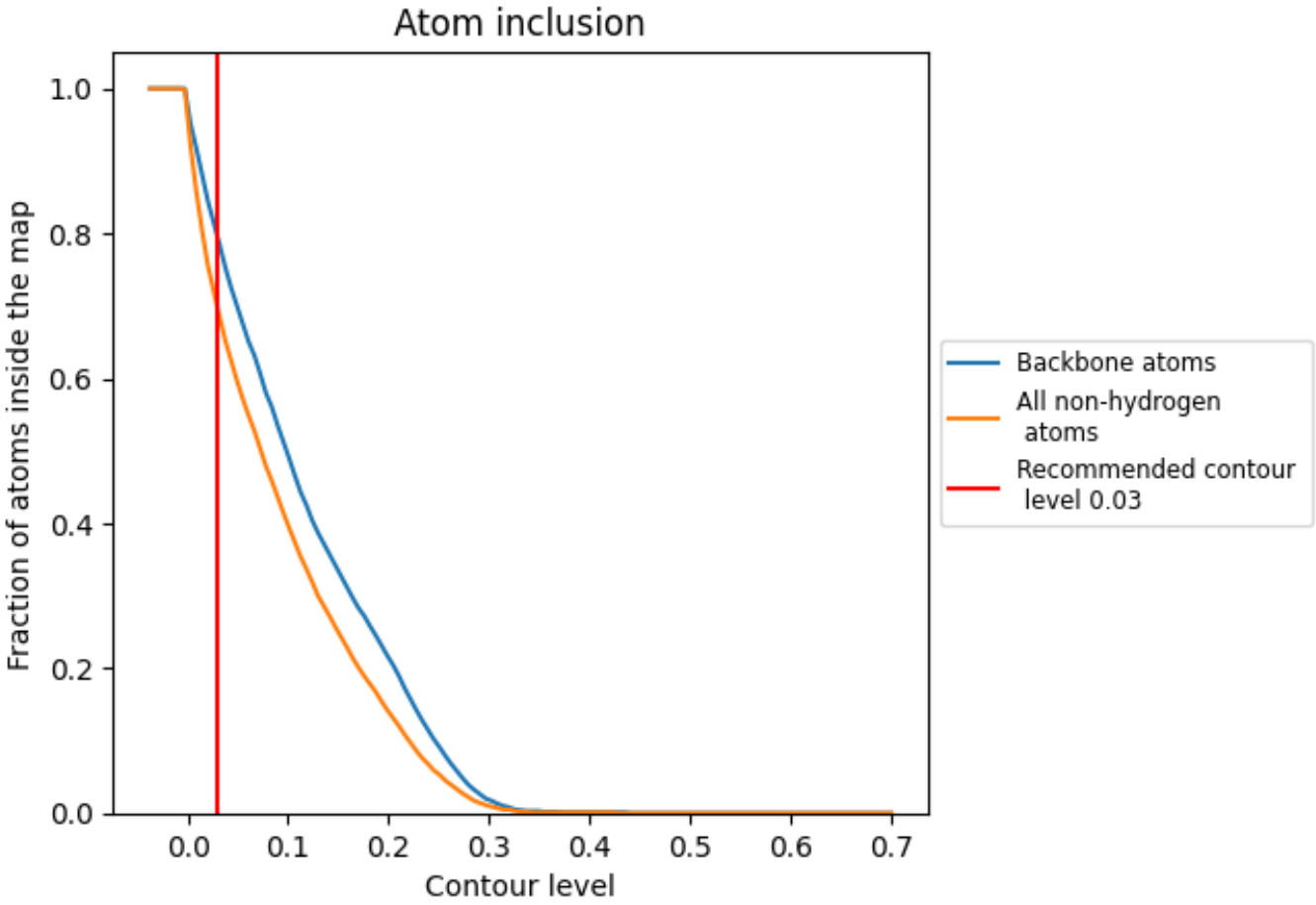
9.3 Atom inclusion mapped to coordinate model



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 (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6950	0.2930
A	0.9370	0.4180
B	0.5250	0.1040
C	0.5790	0.1110
D	0.9870	0.5320
E	0.2030	0.0600
F	0.3070	0.0800