



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 01:44 AM UTC

PDB ID : 8QAU / pdb_00008qau
EMDB ID : EMD-18304
Title : Outer kinetochore Ndc80-Dam1 alpha/beta-tubulin complex
Authors : Muir, K.W.; Barford, D.
Deposited on : 2023-08-23
Resolution : 3.54 Å(reported)
Based on initial model : .

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ 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:

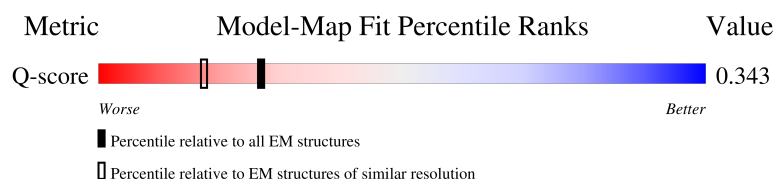
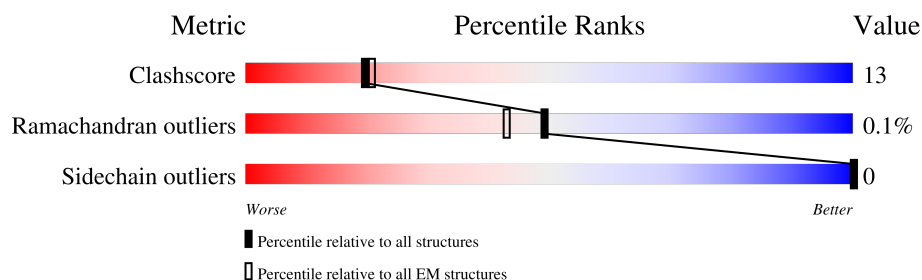
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.54 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	12891 (3.04 - 4.04)

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 $\leq 5\%$. 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	C	451	
2	D	445	
3	A	691	
4	B	451	

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Mol	Chain	Length	Quality of chain
5	E	343	 8% 92%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10137 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 Tubulin alpha-1A chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	431	Total	C	N	O	S	0	0
			3373	2136	573	642	22		

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	427	Total	C	N	O	S	0	0
			3359	2110	576	647	26		

- Molecule 3 is a protein called Kinetochore protein NDC80.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	253	Total	C	N	O	S	0	0
			1700	1076	310	310	4		

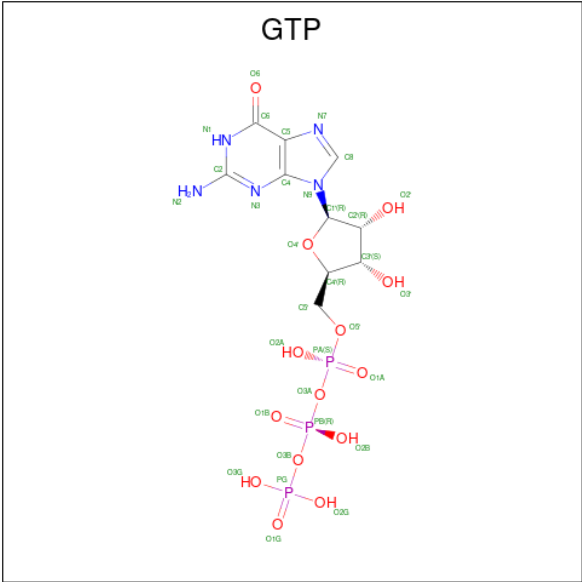
- Molecule 4 is a protein called Kinetochore protein NUF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	207	Total	C	N	O	S	0	0
			1440	897	250	286	7		

- Molecule 5 is a protein called DASH complex subunit DAM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	29	Total	C	N	O	0	0
			142	84	29	29		

- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

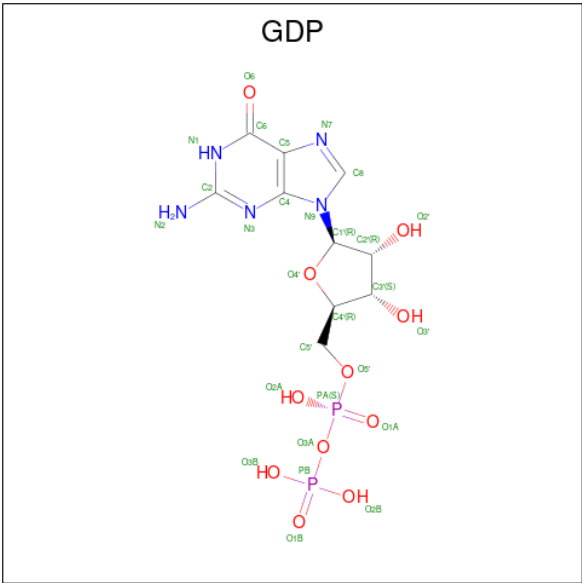


Mol	Chain	Residues	Atoms					AltConf
6	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

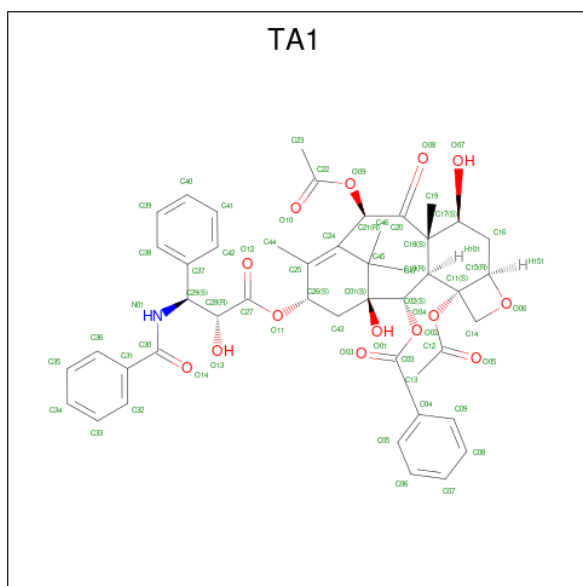
Mol	Chain	Residues	Atoms		AltConf
7	C	1	Total	Mg	0
			1	1	

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					AltConf
8	D	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 9 is TAXOL (CCD ID: TA1) (formula: $C_{47}H_{51}NO_{14}$).

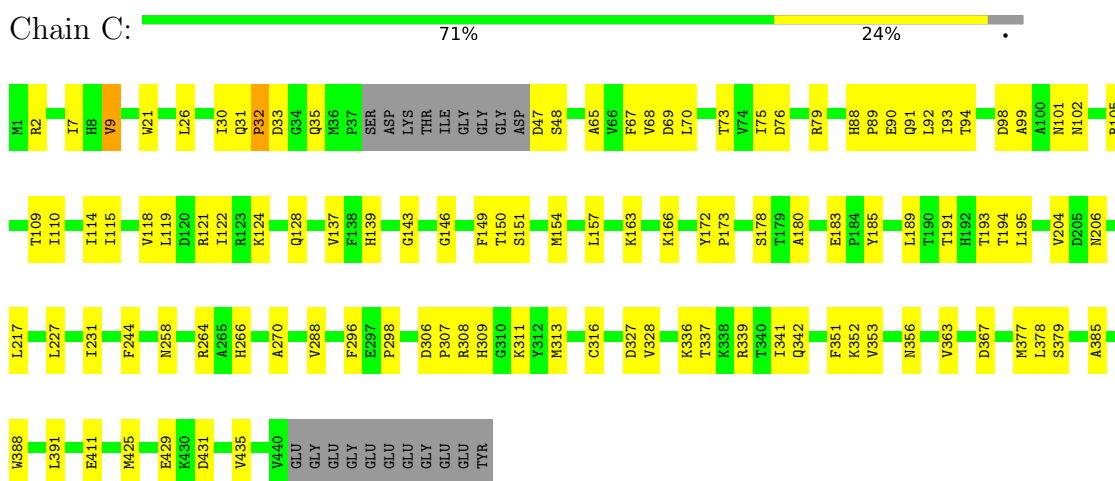


Mol	Chain	Residues	Atoms				AltConf
9	D	1	Total	C	N	O	0
			62	47	1	14	

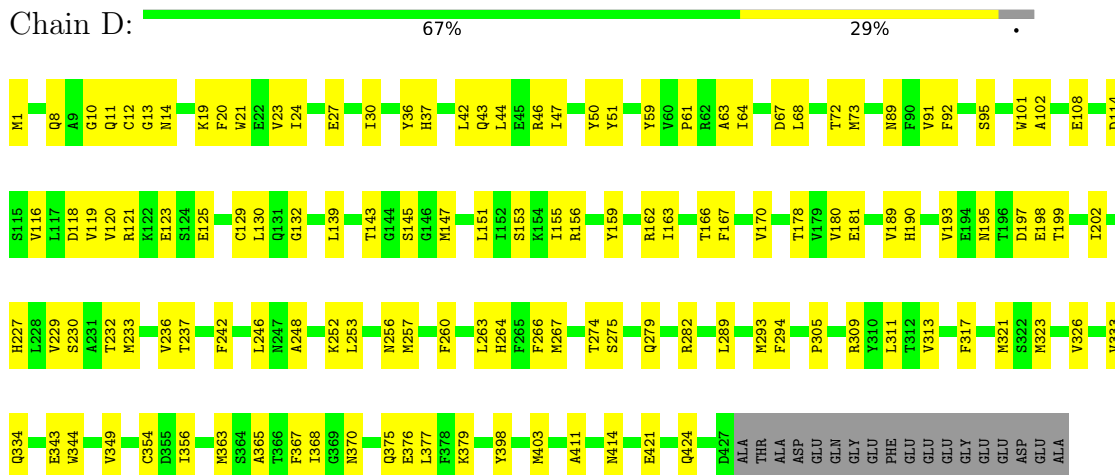
3 Residue-property plots [i](#)

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: Tubulin alpha-1A chain



- Molecule 2: Tubulin beta chain

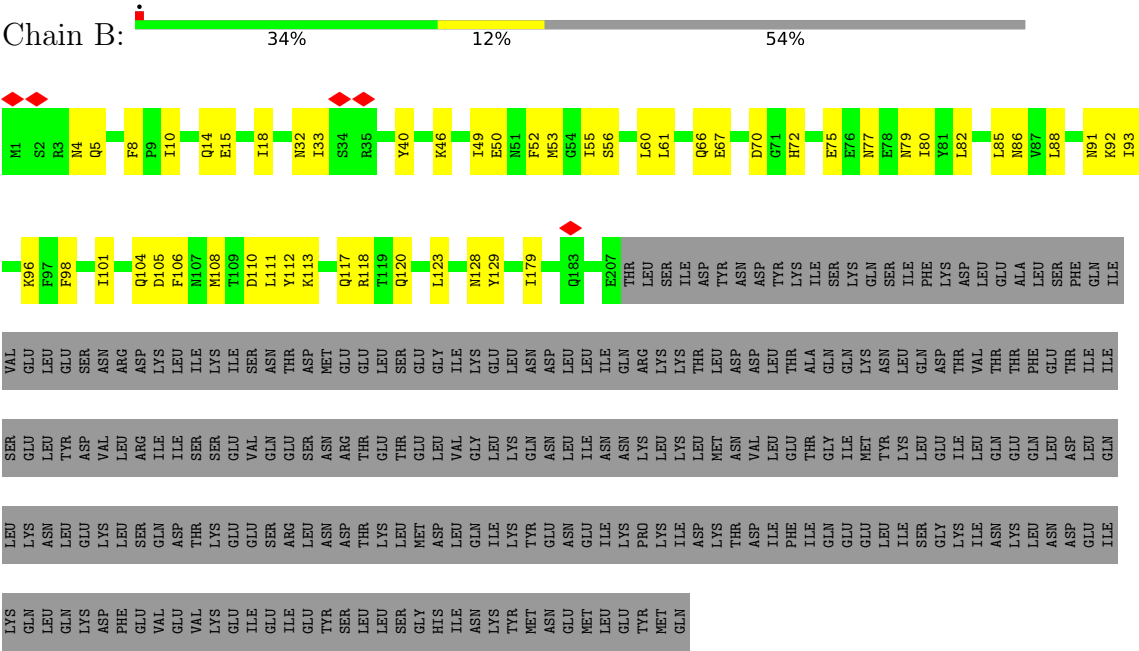


- Molecule 3: Kinetochore protein NDC80



MET	GLN	PRO	Q125	H223	LEU	ASP	GLU	VAL
SER	GLY	THR	W224	W225	ARG	SER	ARG	ILE
THR	SER	GLY	Q128	M225	LYS	SER	LYS	HIS
THR	ILE	ASN	E130	T228	GLY	ILE	VAL	ILE
THR	ASN	LYS	E131	N229	ILE	ASN	ALA	ASP
ASP	LYS	ASN	I132	T230	SER	THR	GLN	THR
GLN	ASN	LYS	K140	K231	GLU	THR	GLU	THR
HIS	ARG	THR	I143	D232	PHE	SER	ILE	THR
VAL	THR	ARG	F153	M234	GLU	SER	LYS	LYS
LEU	ARG	ARG	L154	N237	LEU	GLN	THR	ILE
HIS	SER	THR	P157	K238	GLN	LEU	ILE	THR
HIS	THR	VAL	T158	F290	ASN	GLY	GLU	GLU
MET	VAL	ALA	Q159	E294	GLN	HIS	GLN	GLN
ASP	THR	GLY	G161	N365	GLU	ASN	LYS	LYS
PRO	GLY	ASN	F162	ALA	THR	SER	THR	THR
HIS	THR	GLY	K167	LYS	ARG	LEU	LYS	ARG
ARG	THR	ASN	L171	GLN	GLU	LYS	LEU	LEU
PHE	ASN	ALA	R172	LYS	ASP	ILE	LYS	ASP
THR	ALA	LEU	D174	GLN	LYS	ILE	ASN	ILE
SER	LYS	ASP	Y188	TRP	ASN	GLU	THR	LYS
GLN	ASN	SER	K192	GLY	ILE	ASN	ASP	ILE
LEU	SER	ARG	N193	LYS	SER	LEU	LEU	ILE
ARG	ASN	ARG	Y196	GLU	ASP	ASP	GLU	GLU
ASN	VAL	ASN	F198	LYS	LYS	THR	VAL	ASN
SER	SER	LYS	L199	MET	LYS	THR	GLN	THR
THR	ARG	THR	S201	SER	THR	ILE	ILE	GLY
GLN	LEU	ASN	I202	CYS	GLU	GLY	ASN	ASN
LEU	ASN	ILE	N203	LEU	SER	THR	LYS	LYS
THR	GLN	LEU	Q206	LYS	LYS	GLU	GLN	GLU
ASP	LEU	LEU	I207	GLU	GLU	LEU	LEU	GLU
MET	GLY	GLY	S208	ILE	ALA	PHE	LEU	GLU
ILE	ASN	SER	A209	ILE	GLU	PRO	GLU	ILE
ASN	LYS	GLN	V210	LYS	LYS	LYS	GLU	LYS
SER	GLN	THR	G211	ALA	ILE	GLY	ALA	ASP
ILE	ILE	LEU	S212	LEU	PHE	SER	ASN	LEU
ALA	ALA	LEU	N213	GLN	LYS	GLY	SER	ARG
ARG	SER	SER	M214	SER	ILE	ILE	LYS	ASN
ASN	ASN	THR	W215	ASN	LEU	GLU	ARG	LYS
THR	ILE	ILE	H216	ILE	LEU	GLU	THR	THR
SER	ILE	GLY	K217	SER	ASP	SER	LYS	LYS
GLY	THR	GLY	F218	GLU	THR	ILE	GLN	GLN
THR	GLY	THR	L219	LEU	LEU	LYS	LEU	ASN
ILE	THR	GLY	M221	HIS	ARG	LYS	GLN	SER
ILE	THR	GLY	F124	ILE	TYR	ASN	ASN	ILE

● Molecule 4: Kinetochores protein NUF2



● Molecule 5: DASH complex subunit DAM1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	95730	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.042	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	317.99997, 317.99997, 317.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: GTP, TA1, GDP, 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	C	0.19	1/3450 (0.0%)	0.41	3/4684 (0.1%)
2	D	0.13	0/3434	0.31	0/4652
3	A	0.14	0/1728	0.37	0/2359
4	B	0.16	0/1456	0.44	0/1987
5	E	0.09	0/140	0.29	0/191
All	All	0.16	1/10208 (0.0%)	0.38	3/13873 (0.0%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	32	PRO	CG-CD	-7.00	1.26	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	32	PRO	CA-N-CD	-11.81	95.46	112.00
1	C	32	PRO	N-CD-CG	-9.43	89.05	103.20
1	C	32	PRO	CA-CB-CG	-5.22	94.58	104.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	9	VAL	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	C	3373	0	3281	73	0
2	D	3359	0	3239	89	0
3	A	1700	0	1343	49	0
4	B	1440	0	1197	38	0
5	E	142	0	67	1	0
6	C	32	0	12	3	0
7	C	1	0	0	0	0
8	D	28	0	12	0	0
9	D	62	0	50	4	0
All	All	10137	0	9201	242	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 13.

All (242) 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)
4:B:61:LEU:HD12	4:B:86:ASN:HD22	1.28	0.98
4:B:15:GLU:HA	4:B:18:ILE:HG12	1.66	0.77
3:A:210:VAL:HG23	3:A:218:PHE:HD2	1.53	0.74
1:C:288:VAL:HG21	1:C:327:ASP:HB3	1.68	0.74
2:D:253:LEU:HG	2:D:257:MET:HE2	1.69	0.74
2:D:248:ALA:HA	2:D:252:LYS:HD3	1.69	0.73
2:D:30:ILE:HD11	2:D:47:ILE:HD11	1.70	0.72
2:D:91:VAL:HG21	2:D:116:VAL:HG12	1.72	0.71
2:D:63:ALA:O	2:D:89:ASN:ND2	2.24	0.71
2:D:190:HIS:HD2	2:D:411:ALA:HA	1.56	0.70
1:C:377:MET:HE3	1:C:379:SER:HB3	1.74	0.68
3:A:193:ASN:HD21	4:B:112:TYR:HB2	1.59	0.67
1:C:91:GLN:HG3	1:C:121:ARG:HD2	1.76	0.67
3:A:222:LEU:O	3:A:225:MET:HB2	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:128:ASN:OD1	4:B:129:TYR:N	2.28	0.66
2:D:130:LEU:HD23	2:D:162:ARG:HG3	1.76	0.66
1:C:217:LEU:HD11	1:C:367:ASP:HB3	1.78	0.66
3:A:158:THR:HG23	3:A:161:GLY:H	1.59	0.66
2:D:143:THR:O	2:D:147:MET:HB2	1.96	0.66
2:D:170:VAL:HG11	2:D:377:LEU:HD21	1.79	0.65
3:A:230:ILE:HG22	3:A:234:MET:HE1	1.76	0.65
3:A:231:LYS:HA	3:A:234:MET:HE2	1.76	0.65
2:D:421:GLU:HG3	3:A:203:ASN:HD21	1.62	0.65
2:D:64:ILE:HG13	2:D:120:VAL:HG12	1.80	0.64
2:D:8:GLN:HE21	2:D:14:ASN:HA	1.62	0.64
2:D:227:HIS:NE2	9:D:502:TA1:O14	2.26	0.64
1:C:191:THR:HA	1:C:194:THR:HG22	1.79	0.64
4:B:53:MET:SD	4:B:55:ILE:HG12	2.38	0.63
2:D:11:GLN:HA	2:D:72:THR:HG21	1.81	0.63
1:C:328:VAL:HG11	1:C:353:VAL:HG11	1.81	0.63
2:D:190:HIS:NE2	2:D:414:ASN:OD1	2.31	0.63
2:D:424:GLN:NE2	3:A:206:GLN:OE1	2.32	0.62
3:A:213:SER:O	3:A:216:HIS:ND1	2.32	0.62
2:D:198:GLU:HA	2:D:264:HIS:HB2	1.82	0.62
4:B:91:ASN:ND2	4:B:108:MET:HB2	2.14	0.62
2:D:51:TYR:HB3	2:D:59:TYR:HB3	1.80	0.61
1:C:178:SER:OG	1:C:183:GLU:OE1	2.18	0.61
1:C:180:ALA:HB3	1:C:183:GLU:HB2	1.81	0.61
2:D:50:TYR:HH	2:D:237:THR:HG1	1.48	0.61
1:C:124:LYS:O	1:C:128:GLN:NE2	2.33	0.60
1:C:102:ASN:HB3	1:C:105:ARG:HB2	1.83	0.60
3:A:119:LEU:HD11	3:A:220:GLY:HA3	1.83	0.59
1:C:316:CYS:SG	1:C:378:LEU:HB2	2.42	0.59
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.83	0.59
4:B:79:ASN:OD1	4:B:80:ILE:HD12	2.03	0.59
3:A:157:PRO:HG3	3:A:215:TRP:CD2	2.38	0.58
1:C:258:ASN:HB3	1:C:352:LYS:HG3	1.85	0.58
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.39	0.58
3:A:124:PHE:O	3:A:128:ILE:HG12	2.03	0.58
4:B:105:ASP:O	4:B:118:ARG:NH2	2.37	0.58
2:D:20:PHE:HA	2:D:230:SER:HB2	1.85	0.58
2:D:275:SER:O	2:D:279:GLN:HB2	2.03	0.57
2:D:309:ARG:NH1	2:D:343:GLU:OE1	2.37	0.57
1:C:7:ILE:HD12	1:C:137:VAL:HG22	1.87	0.57
2:D:178:THR:HB	2:D:181:GLU:HG3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:151:LEU:O	2:D:155:ILE:HG12	2.04	0.57
3:A:125:GLN:NE2	3:A:129:GLN:HE21	2.02	0.57
3:A:231:LYS:HB3	4:B:85:LEU:HD21	1.87	0.57
1:C:298:PRO:HB3	1:C:307:PRO:HD2	1.87	0.56
4:B:93:ILE:HA	4:B:96:LYS:HG3	1.88	0.56
4:B:5:GLN:HG2	5:E:305:VAL:HA	1.88	0.56
3:A:140:LYS:HG3	3:A:143:ILE:HB	1.86	0.56
1:C:425:MET:O	1:C:429:GLU:HG2	2.05	0.55
2:D:102:ALA:HB2	2:D:403:MET:HG3	1.88	0.55
2:D:267:MET:HE1	2:D:305:PRO:HG3	1.88	0.55
2:D:236:VAL:HG22	2:D:368:ILE:HD11	1.89	0.55
3:A:125:GLN:HE21	3:A:129:GLN:HE21	1.54	0.55
3:A:196:TYR:OH	3:A:221:MET:SD	2.54	0.55
1:C:296:PHE:HZ	1:C:351:PHE:HE2	1.55	0.54
1:C:336:LYS:O	1:C:339:ARG:NH2	2.40	0.54
1:C:98:ASP:OD1	1:C:99:ALA:N	2.39	0.54
2:D:10:GLY:O	2:D:14:ASN:ND2	2.34	0.54
1:C:313:MET:HE1	1:C:435:VAL:HG13	1.90	0.54
3:A:132:ILE:HD11	3:A:223:HIS:HA	1.89	0.54
2:D:260:PHE:HB2	2:D:263:LEU:HD13	1.91	0.53
4:B:32:ASN:HB3	4:B:40:TYR:CZ	2.43	0.53
1:C:9:VAL:HG11	1:C:146:GLY:HA2	1.90	0.53
2:D:266:PHE:HE1	2:D:370:ASN:HD22	1.56	0.53
4:B:108:MET:HA	4:B:111:LEU:HD13	1.90	0.53
1:C:298:PRO:HG2	1:C:308:ARG:CZ	2.39	0.53
2:D:64:ILE:HD11	2:D:123:GLU:HG3	1.90	0.53
2:D:279:GLN:NE2	9:D:502:TA1:O07	2.41	0.53
1:C:69:ASP:OD1	1:C:70:LEU:N	2.41	0.53
4:B:55:ILE:HD12	4:B:60:LEU:HD21	1.89	0.53
4:B:117:GLN:O	4:B:120:GLN:HG3	2.08	0.53
2:D:323:MET:HA	2:D:326:VAL:HG12	1.92	0.52
3:A:121:ASP:OD1	3:A:122:LYS:N	2.43	0.52
3:A:225:MET:O	3:A:228:THR:OG1	2.27	0.52
1:C:306:ASP:HB2	1:C:309:HIS:CD2	2.45	0.52
4:B:14:GLN:OE1	4:B:14:GLN:N	2.35	0.52
2:D:252:LYS:O	2:D:256:ASN:ND2	2.40	0.51
4:B:4:ASN:ND2	4:B:104:GLN:H	2.08	0.51
1:C:151:SER:HB3	1:C:193:THR:HG21	1.91	0.51
2:D:313:VAL:HB	2:D:349:VAL:HG22	1.93	0.51
3:A:140:LYS:HD2	3:A:143:ILE:HD12	1.93	0.51
1:C:75:ILE:O	1:C:79:ARG:N	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:178:THR:HG22	2:D:180:VAL:H	1.76	0.51
4:B:98:PHE:HD2	4:B:106:PHE:CG	2.29	0.51
2:D:21:TRP:CZ3	2:D:61:PRO:HB3	2.46	0.50
2:D:36:TYR:CD1	2:D:44:LEU:HD21	2.47	0.50
2:D:118:ASP:OD1	2:D:119:VAL:N	2.43	0.50
2:D:153:SER:HA	2:D:195:ASN:HD22	1.76	0.50
2:D:21:TRP:CZ3	2:D:24:ILE:HD11	2.47	0.50
1:C:311:LYS:HD2	1:C:342:GLN:HG2	1.94	0.50
2:D:27:GLU:O	2:D:43:GLN:NE2	2.42	0.50
1:C:26:LEU:HD12	1:C:363:VAL:HG22	1.94	0.49
3:A:196:TYR:CE1	3:A:198:PHE:HB2	2.47	0.49
4:B:110:ASP:OD2	4:B:118:ARG:NH2	2.45	0.49
4:B:66:GLN:NE2	4:B:67:GLU:OE2	2.46	0.49
4:B:70:ASP:OD1	4:B:72:HIS:ND1	2.44	0.49
1:C:76:ASP:HA	1:C:79:ARG:HB2	1.94	0.49
4:B:33:ILE:HG12	4:B:123:LEU:HD11	1.94	0.48
1:C:163:LYS:HE2	1:C:163:LYS:HA	1.95	0.48
3:A:200:GLU:N	3:A:200:GLU:OE2	2.45	0.48
3:A:159:GLN:NE2	3:A:208:SER:O	2.46	0.48
4:B:98:PHE:HA	4:B:101:ILE:HG12	1.94	0.48
1:C:172:TYR:CD1	1:C:173:PRO:HD2	2.49	0.48
1:C:67:PHE:HB2	1:C:92:LEU:HD23	1.96	0.48
3:A:233:ASP:OD1	3:A:234:MET:N	2.46	0.48
1:C:2:ARG:HD3	1:C:2:ARG:H	1.78	0.48
2:D:274:THR:HG21	2:D:282:ARG:HE	1.78	0.48
1:C:90:GLU:OE1	1:C:121:ARG:NH2	2.47	0.48
1:C:206:ASN:OD1	6:C:501:GTP:O2'	2.27	0.48
2:D:232:THR:O	2:D:236:VAL:HG23	2.14	0.47
1:C:204:VAL:HG11	1:C:231:ILE:HD11	1.96	0.47
1:C:195:LEU:O	1:C:266:HIS:NE2	2.41	0.47
1:C:70:LEU:HD12	1:C:99:ALA:HB2	1.94	0.47
1:C:244:PHE:HB2	1:C:356:ASN:HD21	1.79	0.47
2:D:67:ASP:OD1	2:D:68:LEU:N	2.48	0.47
9:D:502:TA1:O12	9:D:502:TA1:N01	2.45	0.47
3:A:222:LEU:HA	3:A:225:MET:HG2	1.97	0.47
1:C:109:THR:HG22	1:C:110:ILE:HD13	1.97	0.47
1:C:298:PRO:HG2	1:C:308:ARG:NH1	2.29	0.47
3:A:196:TYR:HE1	3:A:198:PHE:HB2	1.78	0.47
1:C:21:TRP:CZ2	1:C:65:ALA:HB2	2.49	0.47
2:D:21:TRP:CE3	2:D:24:ILE:HD11	2.50	0.46
3:A:193:ASN:ND2	4:B:108:MET:HE1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:ASN:HD22	1:C:227:LEU:HD22	1.80	0.46
2:D:73:MET:HE1	2:D:92:PHE:CD1	2.51	0.46
2:D:42:LEU:HD22	2:D:356:ILE:HD11	1.97	0.46
2:D:167:PHE:CE2	2:D:233:MET:HG2	2.51	0.46
1:C:101:ASN:CG	2:D:252:LYS:HZ2	2.23	0.46
1:C:88:HIS:HD2	1:C:89:PRO:HD2	1.81	0.45
1:C:337:THR:O	1:C:339:ARG:NH1	2.49	0.45
2:D:95:SER:OG	2:D:108:GLU:OE1	2.35	0.45
2:D:189:VAL:O	2:D:193:VAL:HG23	2.17	0.45
2:D:323:MET:HE2	2:D:323:MET:HB3	1.91	0.45
3:A:157:PRO:HG2	3:A:211:GLY:HA2	1.99	0.45
2:D:166:THR:HG23	2:D:199:THR:HG23	1.98	0.45
1:C:31:GLN:HB2	1:C:35:GLN:O	2.17	0.45
1:C:139:HIS:CG	1:C:150:THR:HG21	2.52	0.45
1:C:115:ILE:HA	1:C:118:VAL:HG12	1.98	0.45
2:D:334:GLN:HE21	2:D:349:VAL:HG23	1.81	0.45
2:D:132:GLY:HA3	2:D:163:ILE:HG22	1.99	0.45
2:D:229:VAL:HG12	2:D:233:MET:HE3	1.99	0.45
1:C:119:LEU:HA	1:C:122:ILE:HG22	1.98	0.45
1:C:143:GLY:HA3	6:C:501:GTP:O2B	2.17	0.45
2:D:139:LEU:HA	2:D:145:SER:HB3	1.99	0.45
2:D:293:MET:SD	2:D:367:PHE:HB2	2.57	0.44
4:B:10:ILE:HG23	4:B:120:GLN:HE22	1.82	0.44
4:B:77:ASN:OD1	4:B:80:ILE:HB	2.17	0.44
1:C:73:THR:OG1	2:D:46:ARG:NH1	2.51	0.44
2:D:294:PHE:CE1	2:D:333:VAL:HG11	2.52	0.44
3:A:153:PHE:HZ	3:A:161:GLY:HA3	1.83	0.44
3:A:220:GLY:O	3:A:223:HIS:HB3	2.18	0.44
4:B:92:LYS:NZ	4:B:96:LYS:HE3	2.33	0.44
2:D:317:PHE:HB3	2:D:321:MET:HE1	1.99	0.44
4:B:14:GLN:NE2	4:B:15:GLU:OE1	2.51	0.44
1:C:115:ILE:O	1:C:119:LEU:HD23	2.18	0.44
2:D:246:LEU:HD23	2:D:246:LEU:HA	1.86	0.44
1:C:32:PRO:HD2	1:C:33:ASP:N	2.32	0.43
1:C:122:ILE:HD13	1:C:157:LEU:HD21	2.00	0.43
1:C:385:ALA:HA	1:C:388:TRP:HD1	1.80	0.43
2:D:64:ILE:HD12	2:D:119:VAL:HG12	1.99	0.43
2:D:170:VAL:N	2:D:202:ILE:O	2.51	0.43
2:D:190:HIS:CD2	2:D:411:ALA:HA	2.46	0.43
2:D:311:LEU:HD23	2:D:311:LEU:HA	1.89	0.43
3:A:174:ASP:CG	4:B:91:ASN:HD21	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:216:HIS:CE1	3:A:217:LYS:HG3	2.53	0.43
4:B:50:GLU:HG3	4:B:56:SER:HA	2.00	0.43
4:B:79:ASN:O	4:B:82:LEU:HG	2.18	0.43
1:C:88:HIS:HB3	1:C:91:GLN:OE1	2.19	0.43
2:D:44:LEU:HA	2:D:47:ILE:HB	1.99	0.43
3:A:290:PHE:HA	3:A:294:GLU:O	2.18	0.43
1:C:30:ILE:HG22	1:C:31:GLN:O	2.18	0.43
1:C:270:ALA:HA	1:C:378:LEU:HD23	2.00	0.43
3:A:159:GLN:OE1	3:A:210:VAL:HG12	2.18	0.43
2:D:36:TYR:O	2:D:37:HIS:ND1	2.51	0.43
3:A:237:ASN:OD1	3:A:238:LYS:N	2.51	0.43
1:C:75:ILE:HG13	1:C:94:THR:HG22	2.01	0.43
3:A:162:PHE:HE1	3:A:222:LEU:HD11	1.83	0.43
3:A:192:LYS:NZ	3:A:199:LEU:HD13	2.34	0.43
1:C:105:ARG:HG3	1:C:411:GLU:HG2	2.01	0.42
1:C:173:PRO:HG2	1:C:391:LEU:HD11	2.01	0.42
3:A:199:LEU:O	3:A:202:ILE:HG22	2.19	0.42
3:A:218:PHE:O	3:A:221:MET:HB2	2.19	0.42
1:C:264:ARG:NE	1:C:431:ASP:OD2	2.30	0.42
2:D:1:MET:O	2:D:129:CYS:HB3	2.19	0.42
2:D:344:TRP:CD1	2:D:344:TRP:H	2.37	0.42
1:C:185:TYR:O	1:C:189:LEU:HG	2.19	0.42
2:D:375:GLN:HG2	2:D:379:LYS:NZ	2.35	0.42
3:A:173:LEU:HD12	4:B:88:LEU:HG	2.01	0.42
3:A:199:LEU:O	3:A:199:LEU:HD23	2.19	0.42
3:A:210:VAL:O	3:A:215:TRP:HB2	2.19	0.42
2:D:12:CYS:SG	2:D:13:GLY:N	2.93	0.42
2:D:101:TRP:H	2:D:398:TYR:HE1	1.67	0.42
2:D:114:ASP:N	2:D:114:ASP:OD1	2.51	0.42
2:D:293:MET:HE2	2:D:365:ALA:HB1	2.02	0.42
2:D:242:PHE:HB2	2:D:354:CYS:SG	2.60	0.42
2:D:19:LYS:O	2:D:23:VAL:HG23	2.19	0.42
2:D:73:MET:HE1	2:D:92:PHE:CG	2.55	0.42
9:D:502:TA1:H432	9:D:502:TA1:H101	1.76	0.42
3:A:128:ILE:HA	3:A:131:GLU:OE2	2.20	0.42
1:C:172:TYR:OH	1:C:391:LEU:HD12	2.20	0.41
1:C:316:CYS:HA	1:C:352:LYS:O	2.20	0.41
3:A:123:ASN:OD1	3:A:124:PHE:N	2.53	0.41
4:B:46:LYS:O	4:B:49:ILE:HG22	2.20	0.41
1:C:313:MET:HE1	1:C:435:VAL:CG1	2.49	0.41
2:D:121:ARG:O	2:D:125:GLU:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:376:GLU:HA	2:D:379:LYS:NZ	2.36	0.41
3:A:167:LYS:O	3:A:171:LEU:HD23	2.20	0.41
3:A:215:TRP:CZ2	3:A:219:LEU:HB3	2.55	0.41
1:C:341:ILE:HD12	1:C:341:ILE:H	1.85	0.41
2:D:293:MET:CE	2:D:365:ALA:HB1	2.50	0.41
6:C:501:GTP:O1A	2:D:252:LYS:NZ	2.52	0.41
2:D:73:MET:HE2	2:D:73:MET:HB3	1.90	0.41
4:B:92:LYS:O	4:B:96:LYS:HG3	2.20	0.41
2:D:155:ILE:O	2:D:159:TYR:N	2.36	0.41
2:D:376:GLU:HA	2:D:379:LYS:HZ3	1.85	0.41
3:A:129:GLN:HG2	3:A:154:LEU:HD22	2.03	0.41
3:A:188:TYR:CE1	3:A:199:LEU:HD21	2.56	0.41
4:B:75:GLU:OE1	4:B:77:ASN:N	2.54	0.41
1:C:47:ASP:HB3	1:C:48:SER:H	1.61	0.41
2:D:253:LEU:HD21	2:D:368:ILE:HD12	2.04	0.41
4:B:8:PHE:HB3	4:B:128:ASN:HD22	1.86	0.41
4:B:49:ILE:HD12	4:B:52:PHE:CZ	2.55	0.40
4:B:112:TYR:C	4:B:113:LYS:HD2	2.46	0.40
2:D:156:ARG:NH1	2:D:197:ASP:OD1	2.54	0.40
1:C:150:THR:O	1:C:154:MET:HG2	2.21	0.40
1:C:154:MET:HE1	1:C:166:LYS:HD2	2.02	0.40
2:D:289:LEU:HD11	2:D:363:MET:HG2	2.02	0.40
1:C:68:VAL:HG11	1:C:149:PHE:CE2	2.57	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	C	427/451 (95%)	410 (96%)	17 (4%)	0	100	100
2	D	425/445 (96%)	411 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	251/691 (36%)	244 (97%)	7 (3%)	0	100	100
4	B	205/451 (46%)	197 (96%)	7 (3%)	1 (0%)	24	58
5	E	25/343 (7%)	24 (96%)	1 (4%)	0	100	100
All	All	1333/2381 (56%)	1286 (96%)	46 (4%)	1 (0%)	49	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	179	ILE

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	C	363/377 (96%)	363 (100%)	0	100	100
2	D	368/381 (97%)	368 (100%)	0	100	100
3	A	118/652 (18%)	118 (100%)	0	100	100
4	B	123/433 (28%)	123 (100%)	0	100	100
All	All	972/1843 (53%)	972 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	88	HIS
1	C	226	ASN
2	D	57	ASN
2	D	191	GLN
2	D	329	GLN
2	D	426	GLN
3	A	129	GLN
3	A	189	GLN

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Mol	Chain	Res	Type
3	A	193	ASN
4	B	91	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\# Z > 2$
9	TA1	D	502	-	68,68,68	0.66	1 (1%)	105,105,105	1.55	17 (16%)
8	GDP	D	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
6	GTP	C	501	7	33,34,34	0.97	1 (3%)	50,54,54	1.60	9 (18%)

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
9	TA1	D	502	-	-	14/41/127/127	0/7/7/7
8	GDP	D	501	-	-	2/16/32/32	0/3/3/3
6	GTP	C	501	7	-	3/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	501	GDP	C5-C4	3.10	1.47	1.38
8	D	501	GDP	C6-N1	-2.40	1.34	1.38
9	D	502	TA1	C18-C10	2.39	1.62	1.57
6	C	501	GTP	C2-N3	2.14	1.38	1.33
8	D	501	GDP	C5-N7	-2.08	1.34	1.39

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	501	GDP	C5-C4-N3	-6.15	118.61	128.39
6	C	501	GTP	C5-C4-N3	-5.11	120.25	128.39
8	D	501	GDP	C2-N3-C4	5.06	121.02	112.30
9	D	502	TA1	C21-C24-C25	-4.97	113.24	120.29
6	C	501	GTP	C2-N3-C4	4.64	120.29	112.30
9	D	502	TA1	O08-C20-C21	-4.54	113.82	119.28
8	D	501	GDP	N9-C4-N3	4.50	134.95	125.95
9	D	502	TA1	O04-C11-C14	4.47	117.60	108.13
9	D	502	TA1	C19-C18-C17	-3.81	102.29	109.61
9	D	502	TA1	C10-C18-C20	-3.77	110.07	116.30
9	D	502	TA1	C18-C20-C21	3.57	129.02	121.38
9	D	502	TA1	C02-O02-C03	3.47	124.15	117.80
9	D	502	TA1	C47-C45-C46	-3.32	96.86	106.29
9	D	502	TA1	C45-C24-C21	3.31	129.47	119.08
8	D	501	GDP	C6-C5-N7	3.29	136.27	130.29
9	D	502	TA1	C45-C24-C25	-3.27	115.20	119.60
6	C	501	GTP	N9-C4-N3	3.23	132.42	125.95
6	C	501	GTP	C2-N1-C6	-3.03	119.61	125.11
9	D	502	TA1	C01-C43-C26	2.99	120.48	114.98
9	D	502	TA1	O09-C21-C20	2.94	115.32	108.66
9	D	502	TA1	C47-C45-C24	2.72	123.62	112.78
6	C	501	GTP	N9-C8-N7	-2.69	108.42	113.40
8	D	501	GDP	C4-C5-N7	-2.64	106.49	110.67
9	D	502	TA1	C11-O04-C12	2.59	125.73	119.17
6	C	501	GTP	C8-N7-C5	2.59	108.87	104.26
6	C	501	GTP	C5-C6-N1	2.55	119.75	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	502	TA1	C17-C18-C20	2.38	107.93	102.58
6	C	501	GTP	O6-C6-C5	-2.25	120.59	126.53
8	D	501	GDP	C3'-C2'-C1'	2.23	105.69	101.46
9	D	502	TA1	C19-C18-C10	2.16	119.86	113.26
9	D	502	TA1	O04-C11-C10	-2.11	105.97	109.24
6	C	501	GTP	C3'-C2'-C1'	2.10	105.43	101.46
8	D	501	GDP	O6-C6-C5	-2.09	121.02	126.53

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	501	GTP	C5'-O5'-PA-O3A
6	C	501	GTP	C5'-O5'-PA-O1A
6	C	501	GTP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O1A
9	D	502	TA1	C20-C21-O09-C22
9	D	502	TA1	O02-C03-C04-C05
9	D	502	TA1	O02-C03-C04-C09
9	D	502	TA1	O03-C03-C04-C09
9	D	502	TA1	O03-C03-C04-C05
9	D	502	TA1	O13-C28-C29-C37
9	D	502	TA1	C23-C22-O09-C21
9	D	502	TA1	C27-C28-C29-N01
8	D	501	GDP	C5'-O5'-PA-O3A
9	D	502	TA1	O11-C27-C28-O13
9	D	502	TA1	O12-C27-C28-O13
9	D	502	TA1	O10-C22-O09-C21
9	D	502	TA1	N01-C29-C37-C42
9	D	502	TA1	N01-C29-C37-C38
9	D	502	TA1	O11-C27-C28-C29

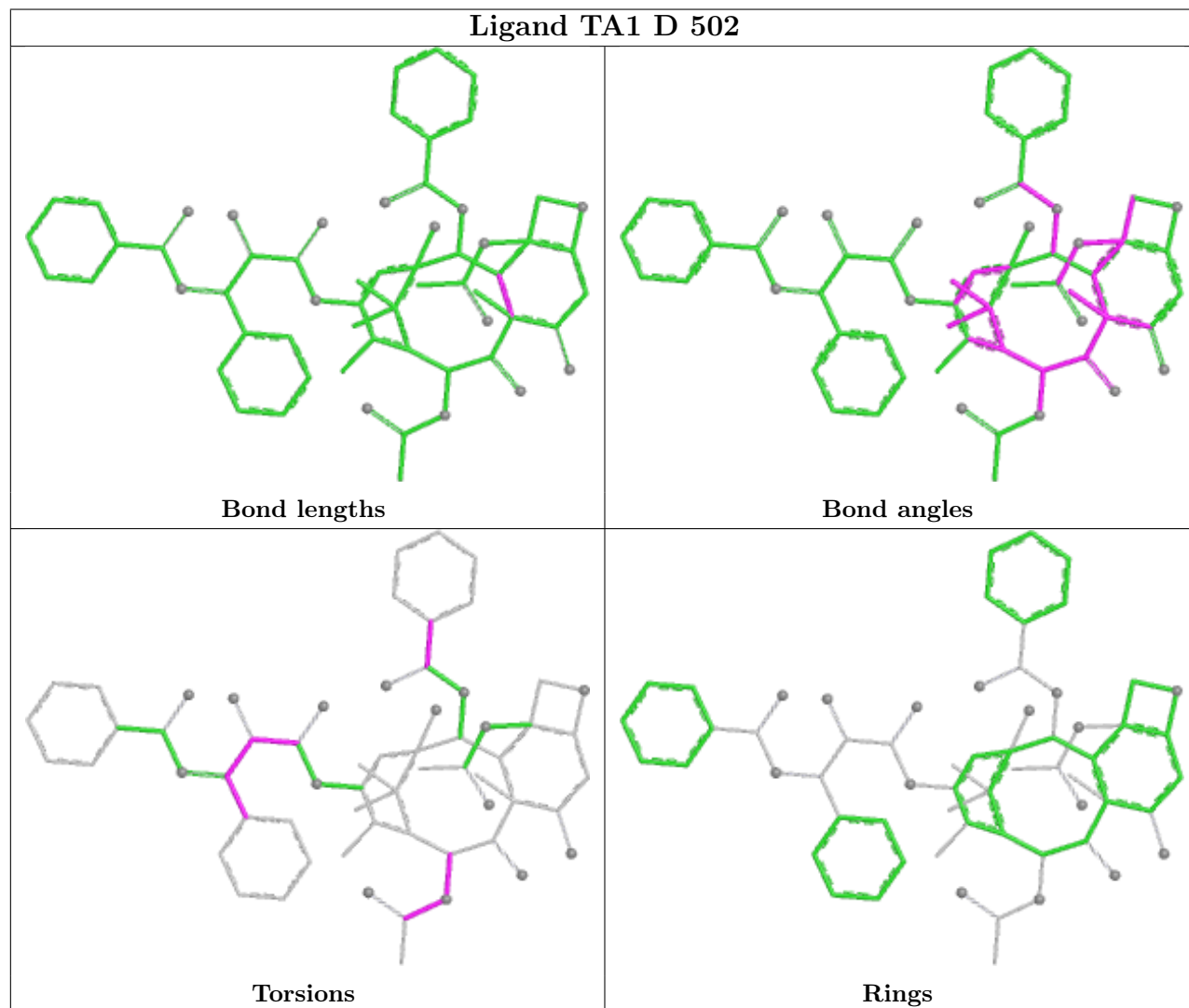
There are no ring outliers.

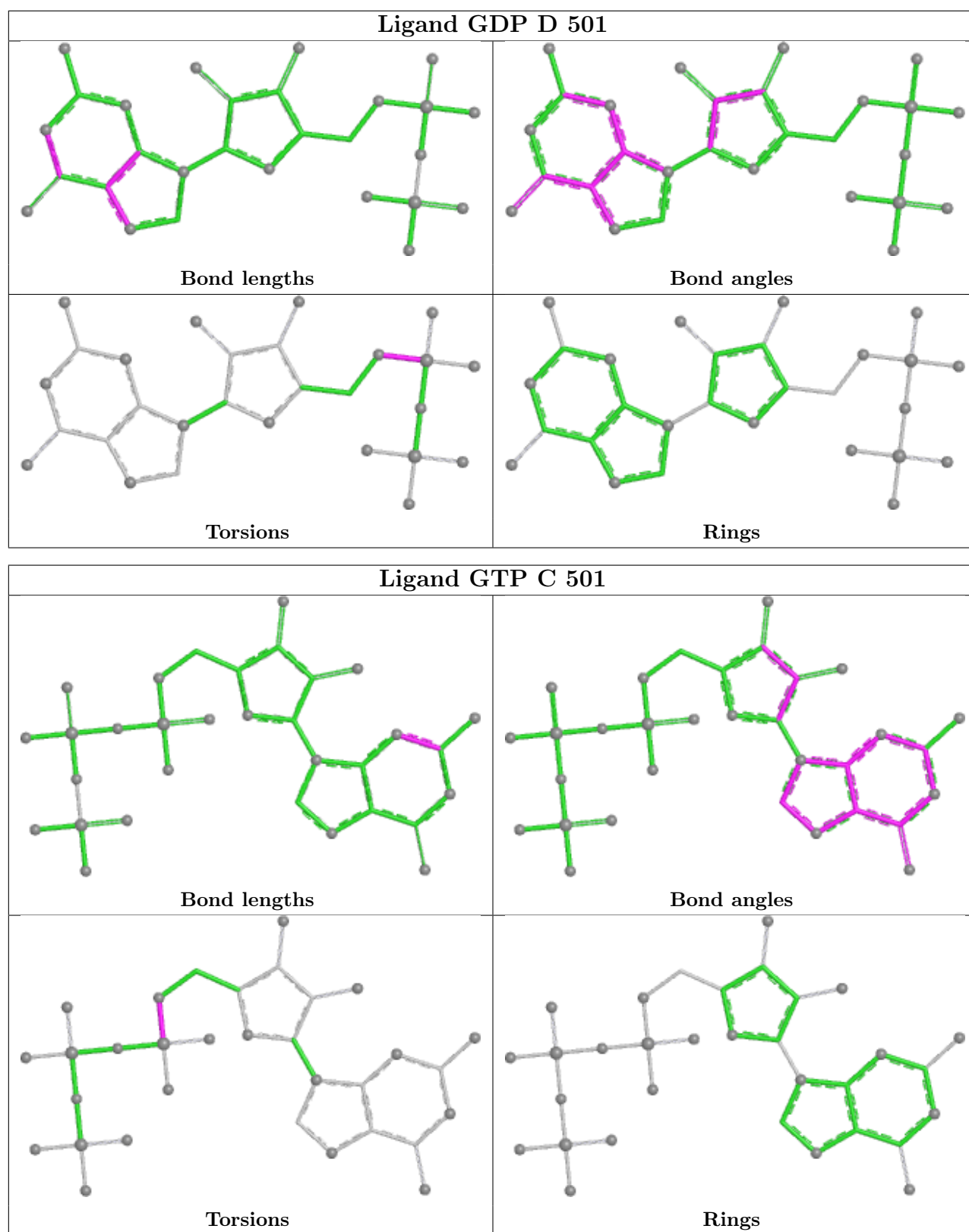
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	502	TA1	4	0
6	C	501	GTP	3	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 than 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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

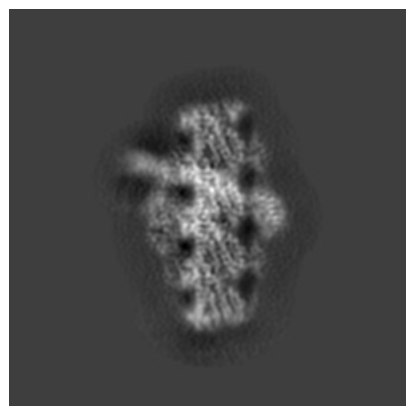
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18304. These allow visual inspection of the internal detail of the map and identification of artifacts.

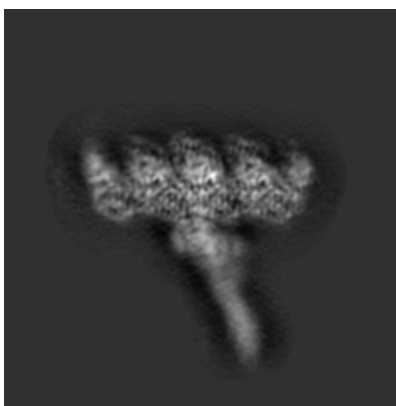
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

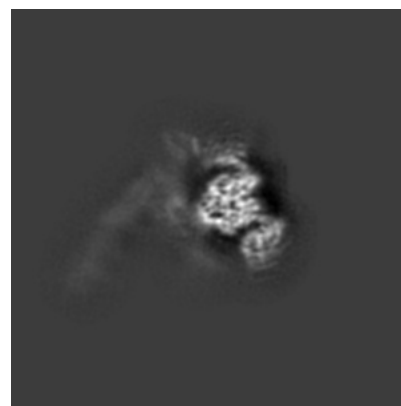
6.1.1 Primary map



X

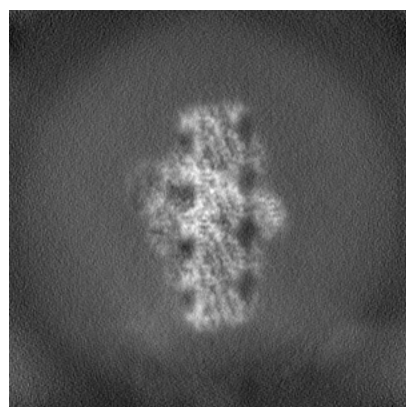


Y

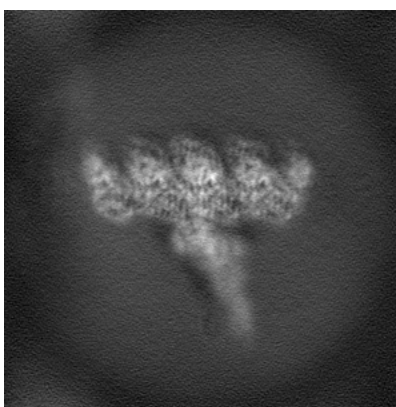


Z

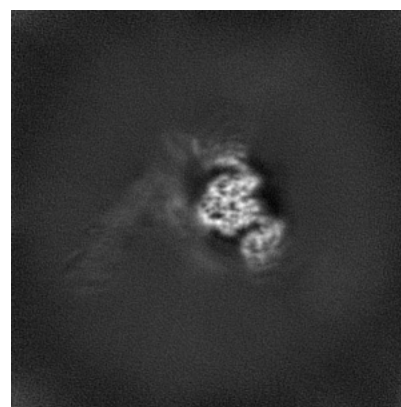
6.1.2 Raw map



X



Y

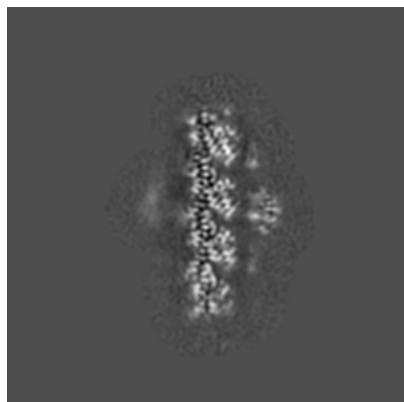


Z

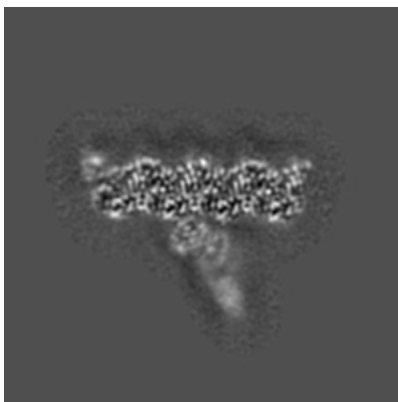
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

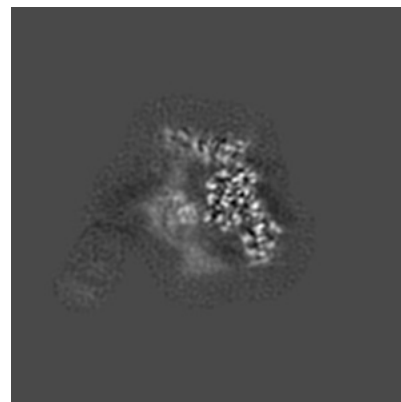
6.2.1 Primary map



X Index: 150

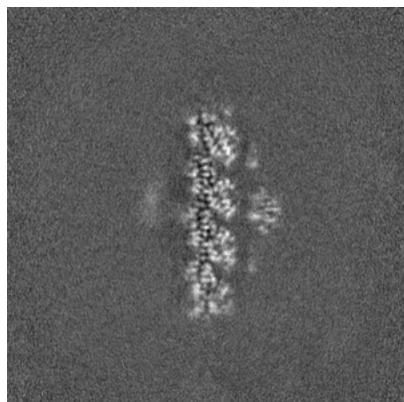


Y Index: 150

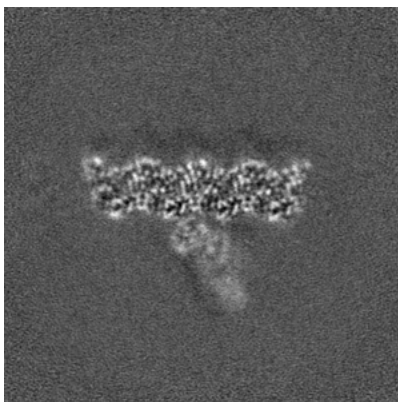


Z Index: 150

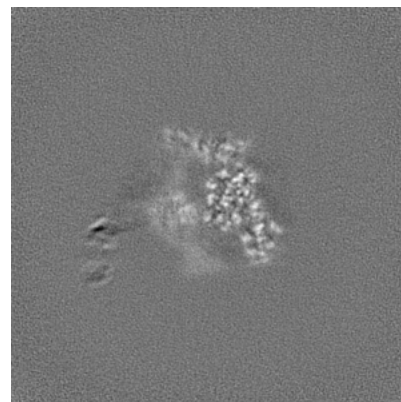
6.2.2 Raw map



X Index: 150



Y Index: 150

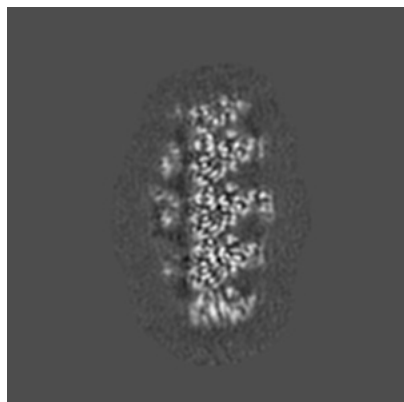


Z Index: 150

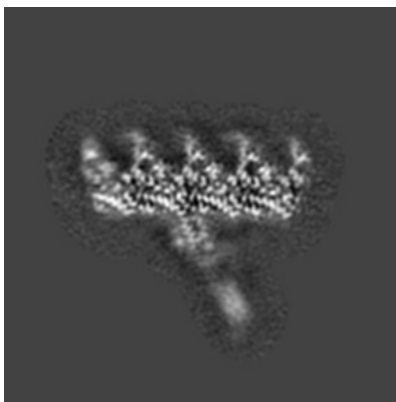
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

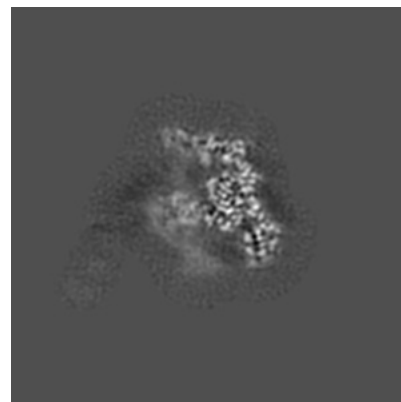
6.3.1 Primary map



X Index: 173

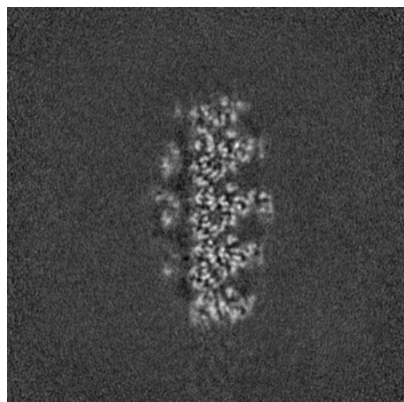


Y Index: 141

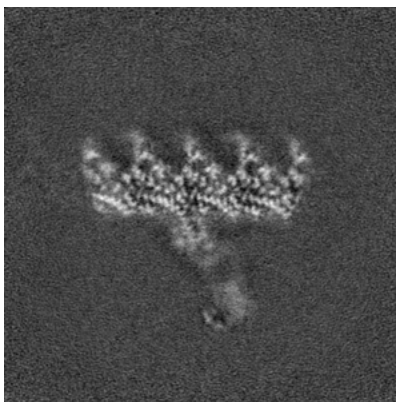


Z Index: 148

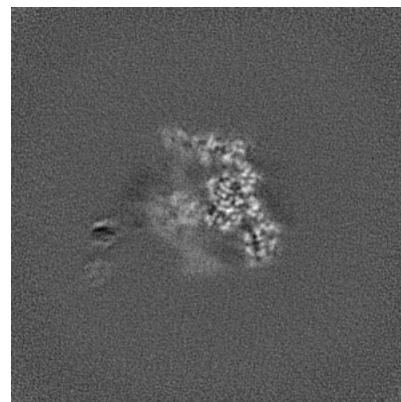
6.3.2 Raw map



X Index: 173



Y Index: 141



Z Index: 148

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

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

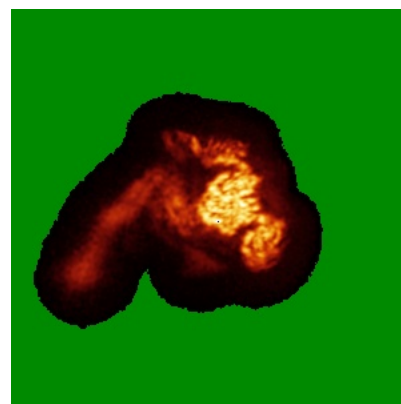
6.4.1 Primary map



X

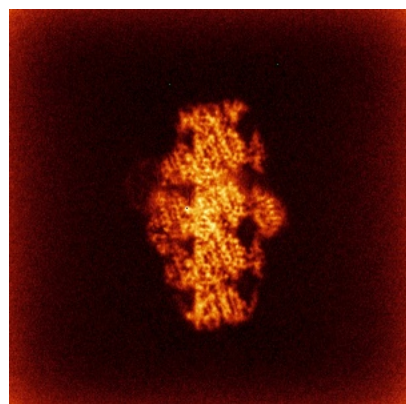


Y

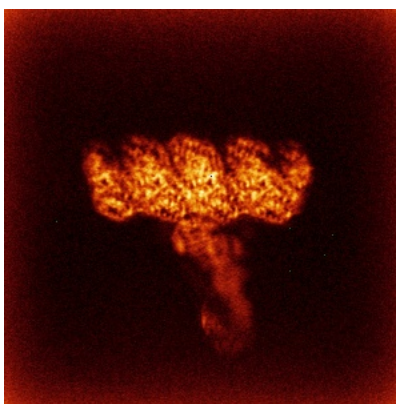


Z

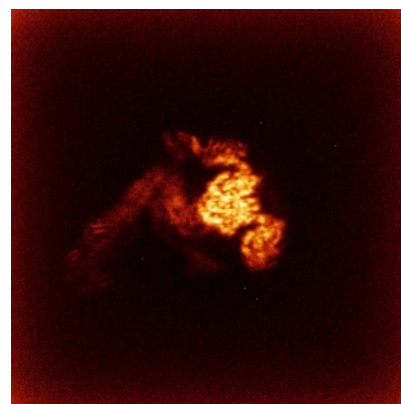
6.4.2 Raw map



X



Y



Z

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

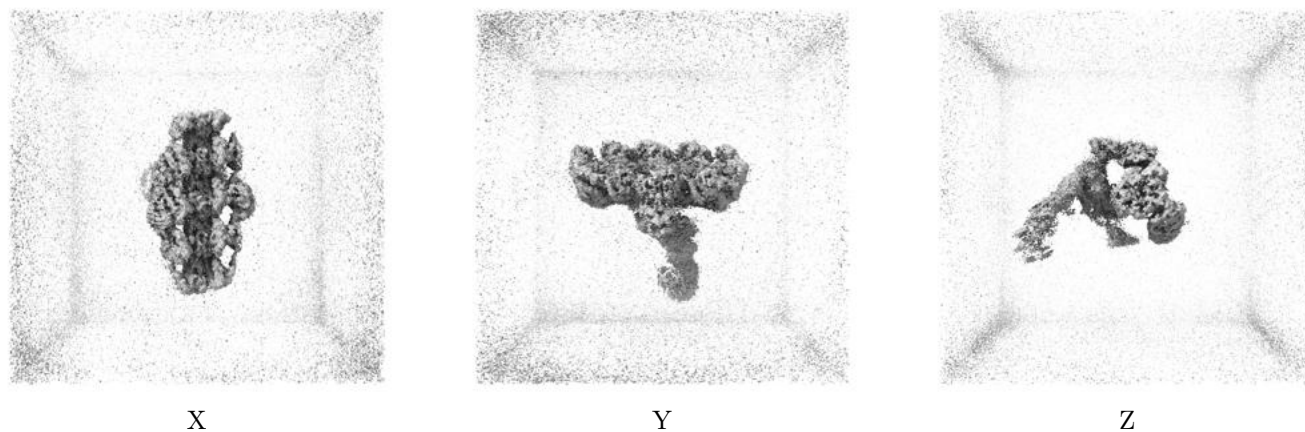
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.004. 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



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

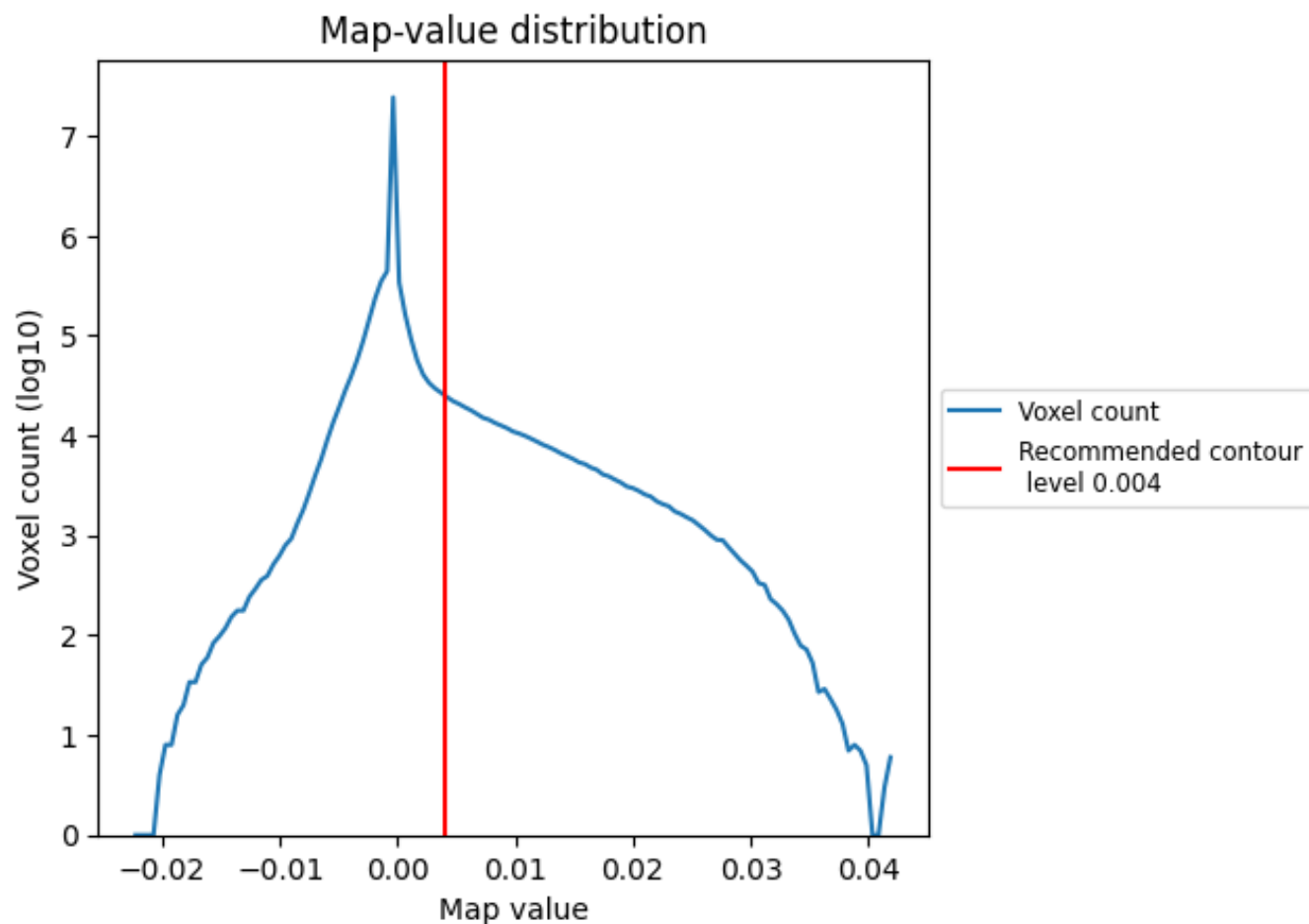
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

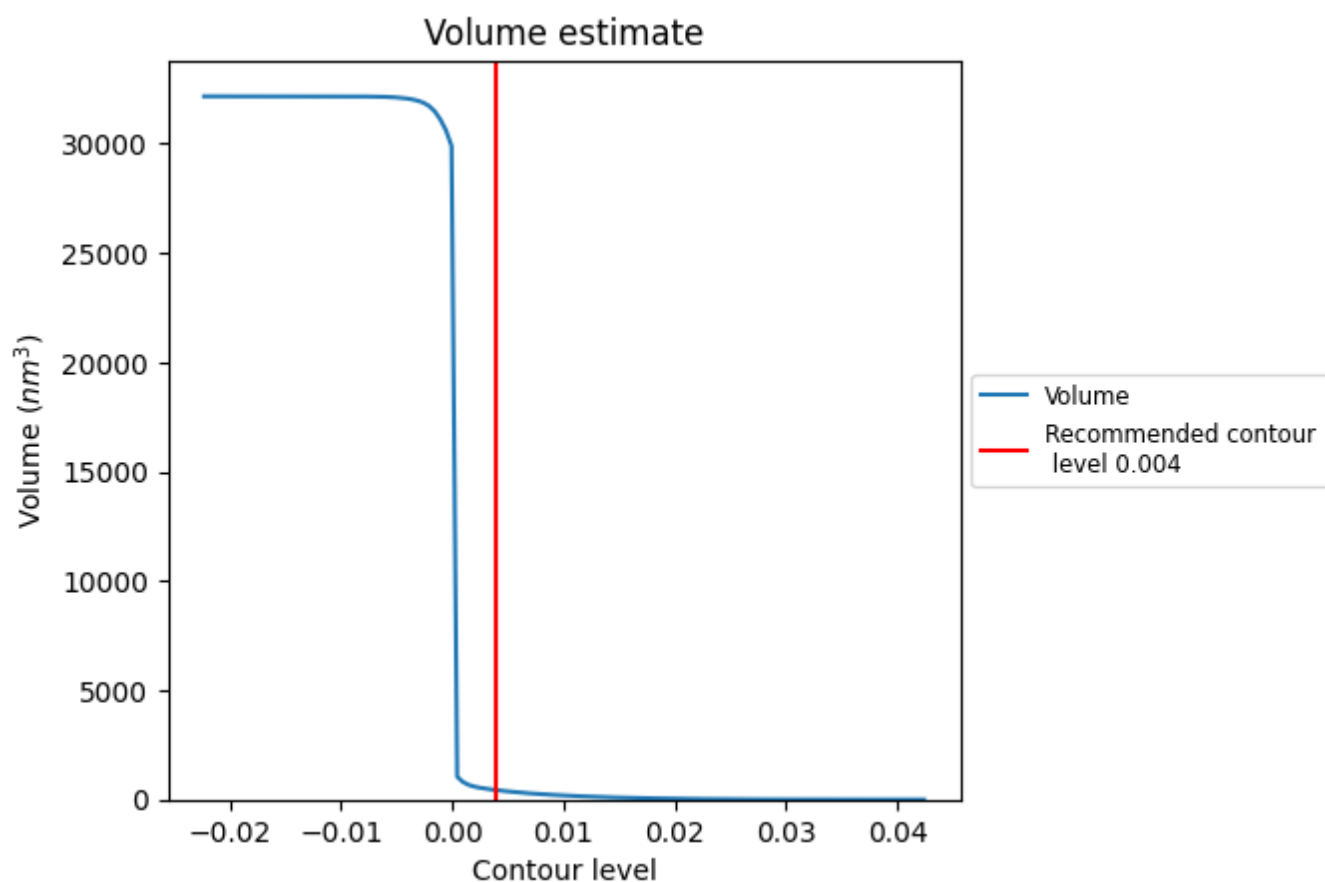
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

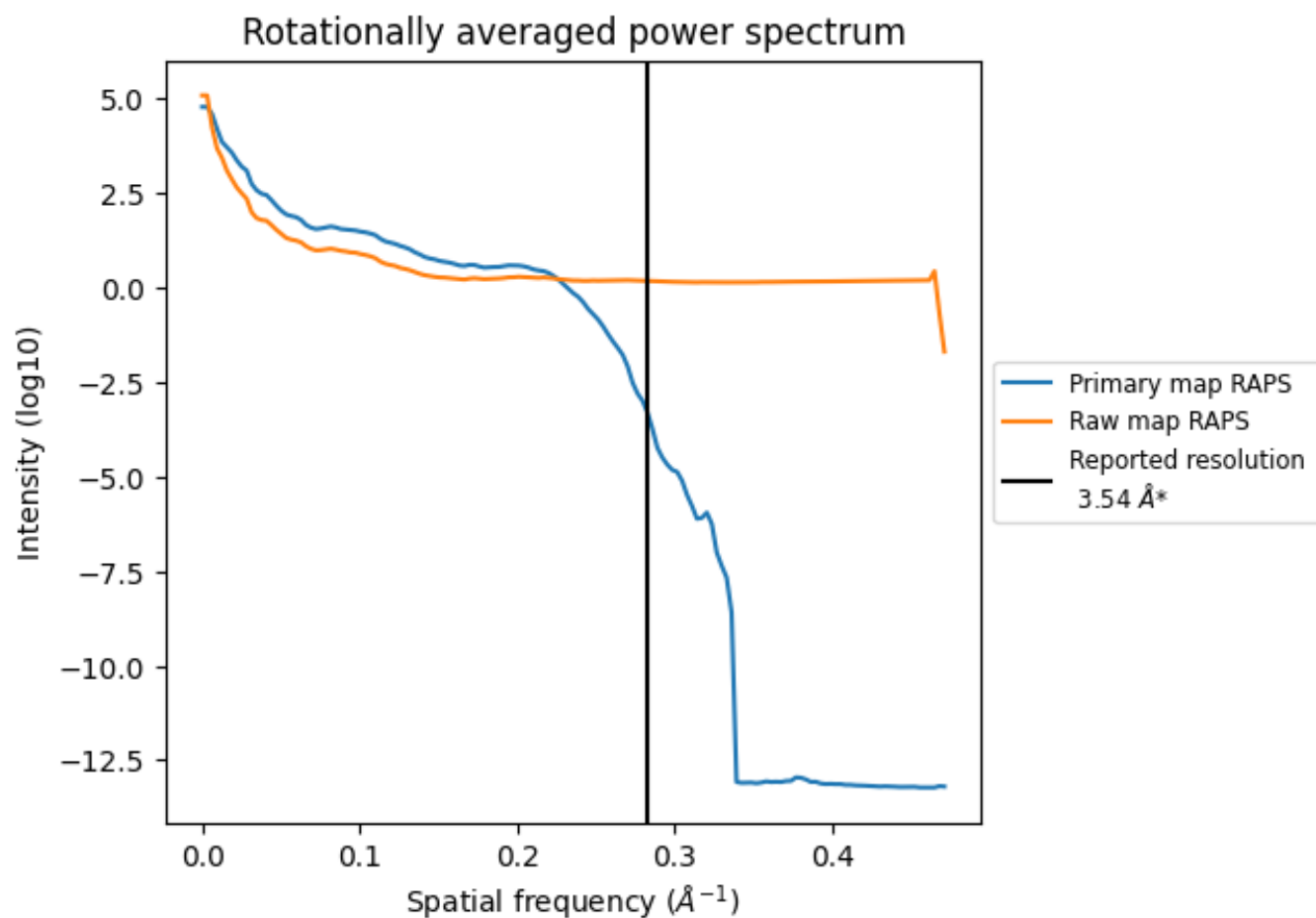
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 430 nm^3 ; this corresponds to an approximate mass of 388 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

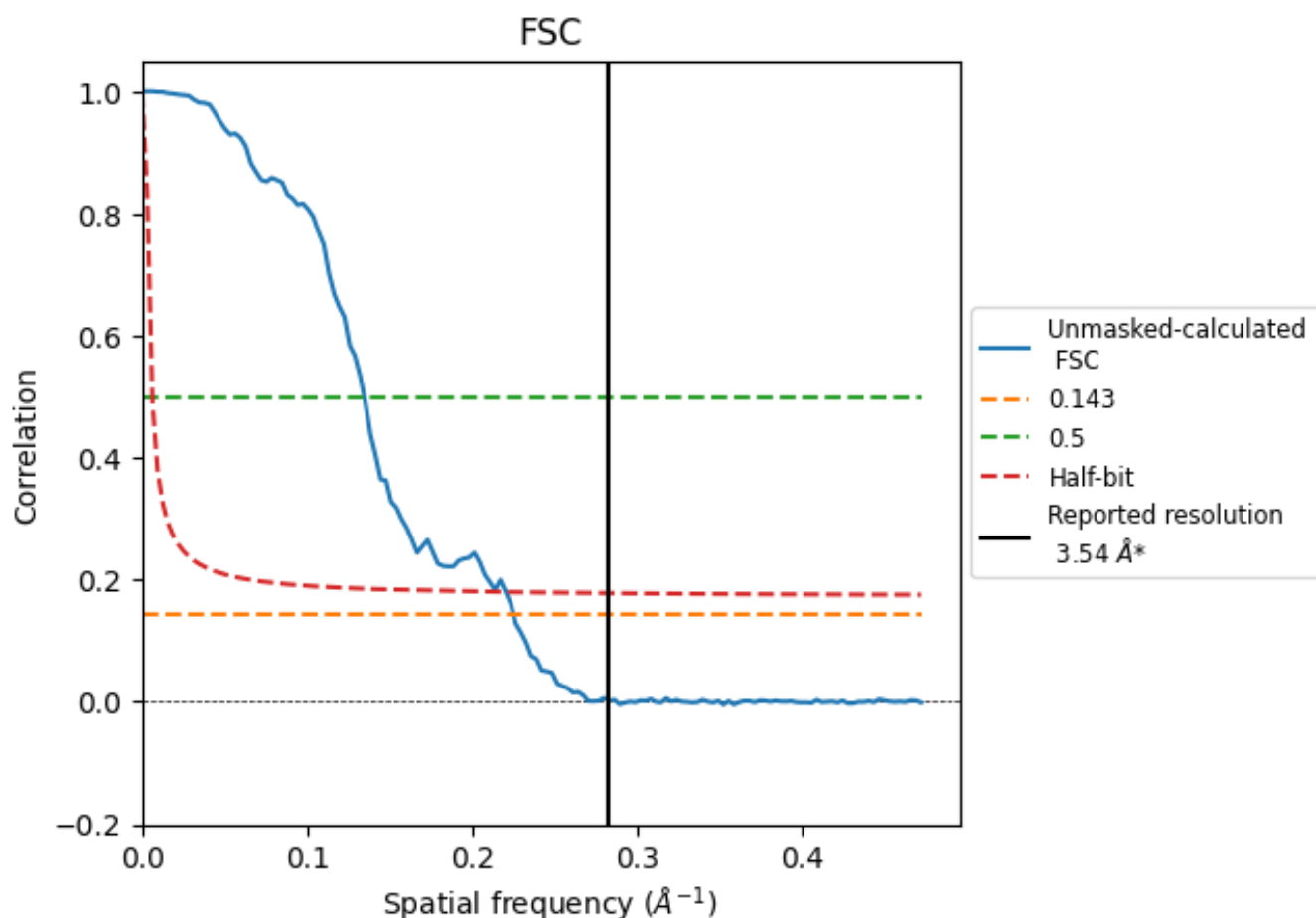


*Reported resolution corresponds to spatial frequency of 0.282 Å⁻¹

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 $0.282 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

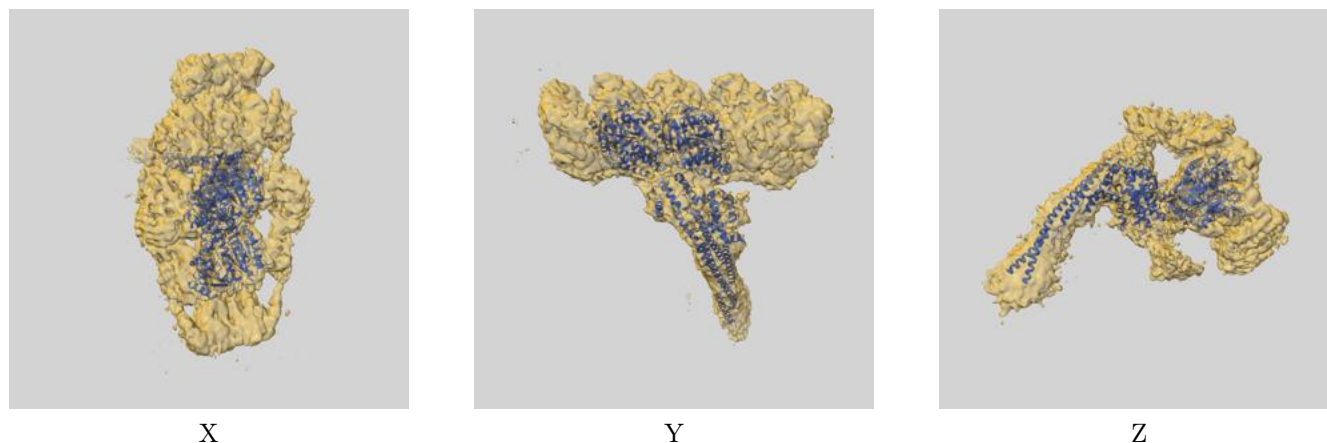
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.54	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.44	7.42	4.54

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.44 differs from the reported value 3.54 by more than 10 %

9 Map-model fit [i](#)

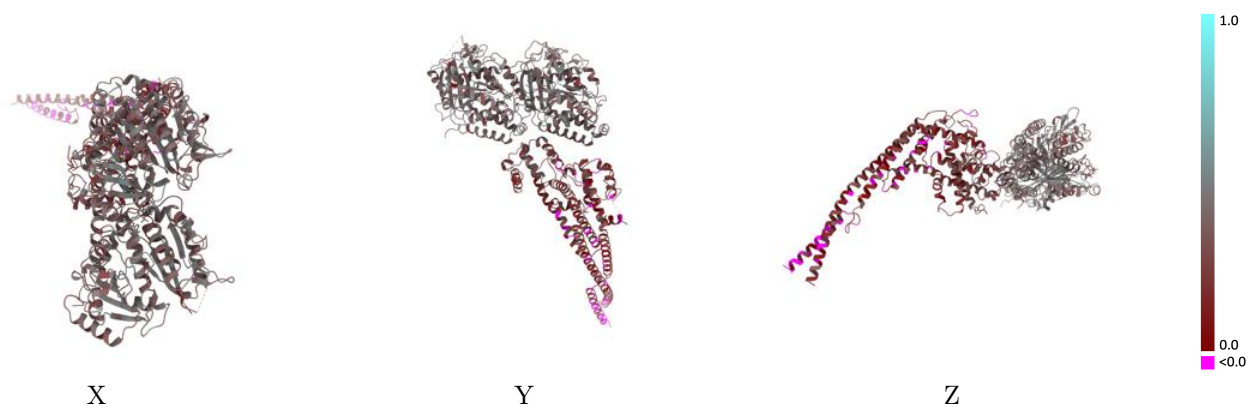
This section contains information regarding the fit between EMDB map EMD-18304 and PDB model 8QAU. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



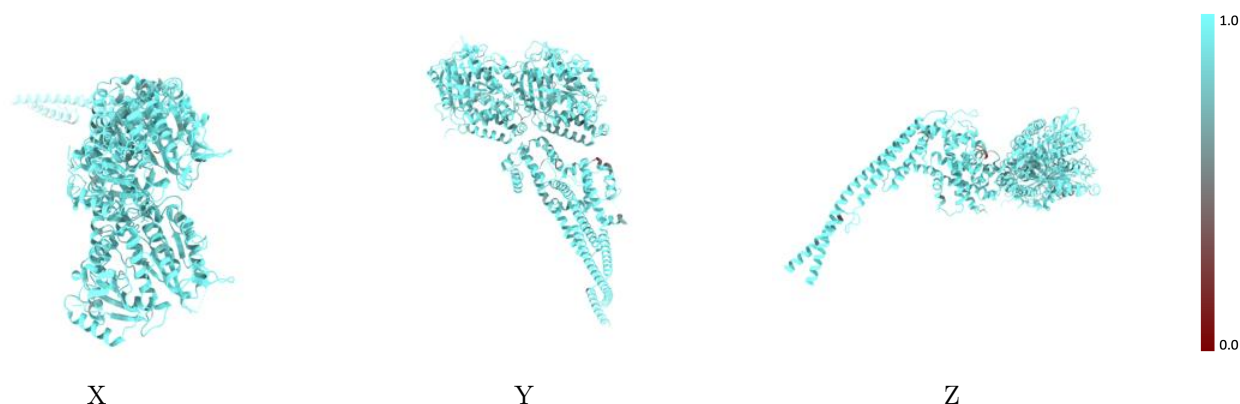
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



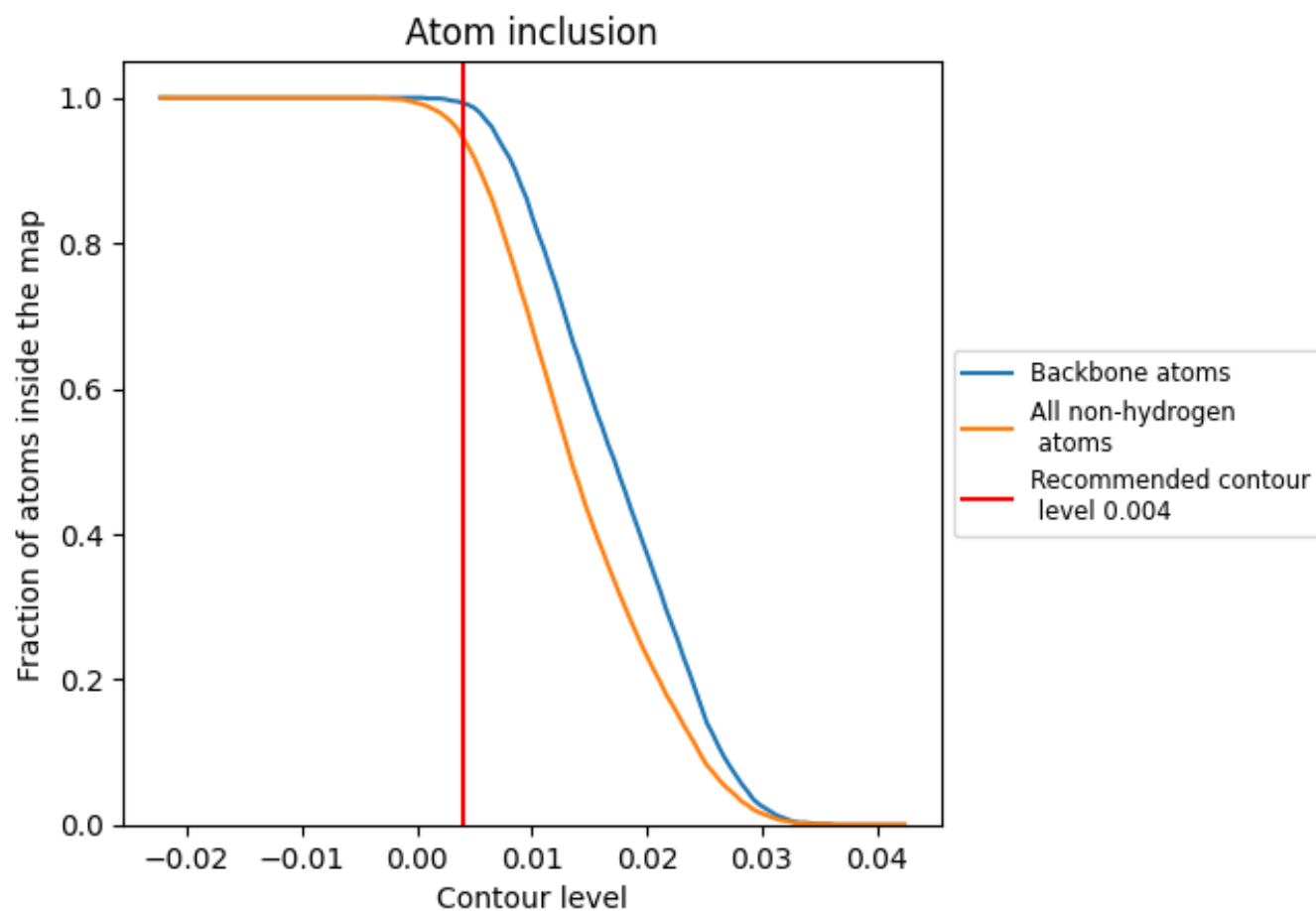
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.004).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 94% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9450	0.3430
A	0.9700	0.2380
B	0.9430	0.1690
C	0.9420	0.4060
D	0.9360	0.4120
E	0.9370	0.1800

