



Full wwPDB EM Validation Report ⓘ

Nov 5, 2024 – 06:26 PM JST

PDB ID : 8YAJ
EMDB ID : EMD-39100
Title : ATAT-2 bound MEC-12/MEC-7 microtubule without acetyl-CoA
Authors : Lam, W.H.; Yu, D.; Zhai, Y.; Ti, S.
Deposited on : 2024-02-09
Resolution : 3.20 Å (reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ 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:

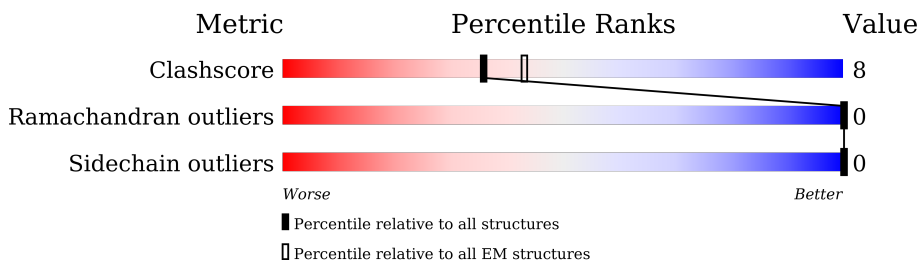
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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 3.20 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 $\leq 5\%$. 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	B	450	
1	E	450	
2	C	263	
2	I	263	
3	D	441	
3	F	441	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 15483 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-3 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	439	Total	C	N	O	S	0	0
			3429	2168	585	655	21		
1	E	431	Total	C	N	O	S	0	0
			3345	2122	566	636	21		

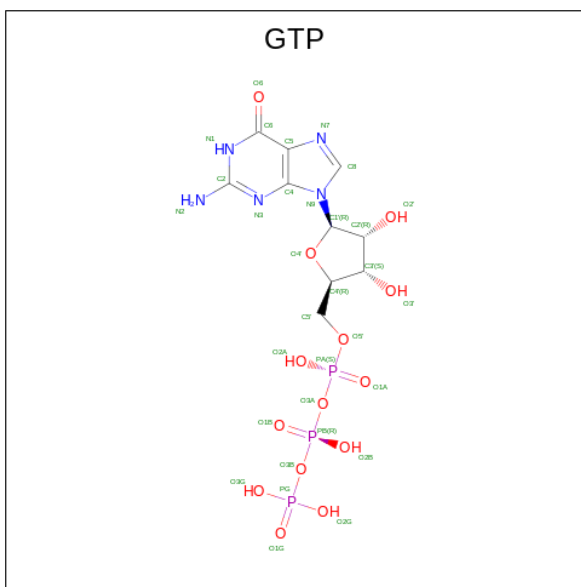
- Molecule 2 is a protein called Alpha-tubulin N-acetyltransferase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	189	Total	C	N	O	S	0	0
			1476	958	242	264	12		
2	I	50	Total	C	N	O	S	0	0
			371	224	77	69	1		

- Molecule 3 is a protein called Tubulin beta-1 chain.

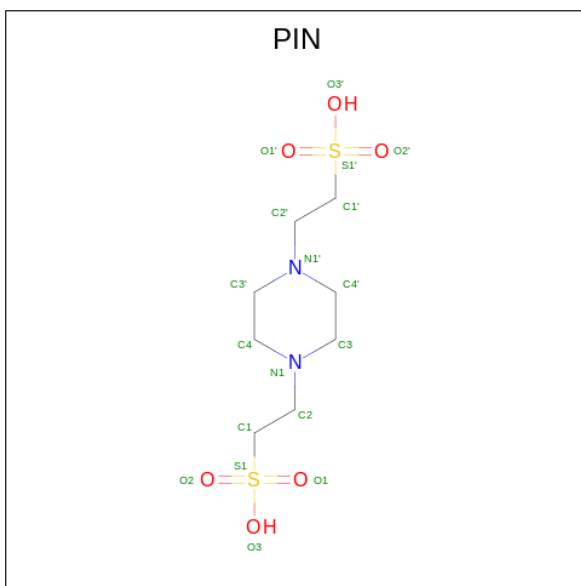
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	427	Total	C	N	O	S	0	0
			3360	2109	577	649	25		
3	F	427	Total	C	N	O	S	0	0
			3356	2107	577	647	25		

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).



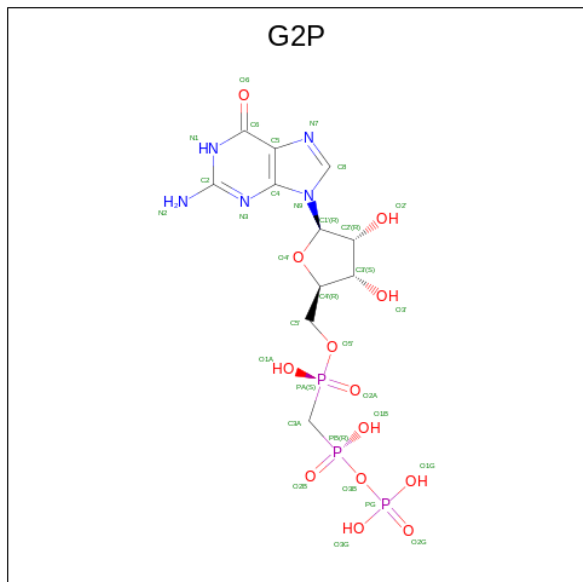
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		
4	B	1	Total	32	10	5	14	3	0
4	E	1	Total	32	10	5	14	3	0

- Molecule 5 is PIPERAZINE-N,N'-BIS(2-ETHANESULFONIC ACID) (three-letter code: PIN) (formula: $C_8H_{18}N_2O_6S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	S		
5	C	1	Total	18	8	2	6	2	0

- Molecule 6 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: G2P) (formula: $C_{11}H_{18}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

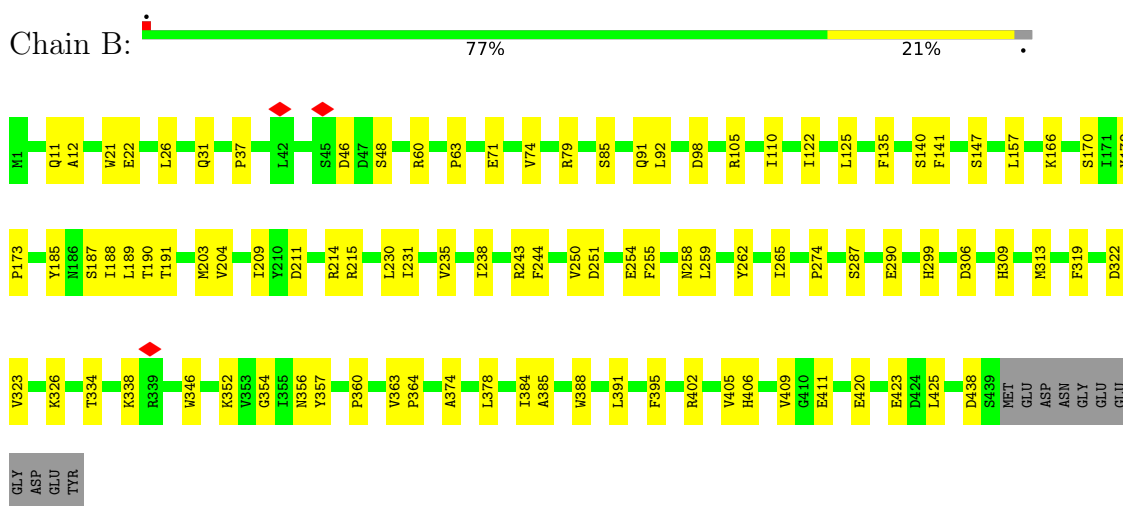


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	D	1	32	11	5	13	3	0
6	F	1	32	11	5	13	3	0

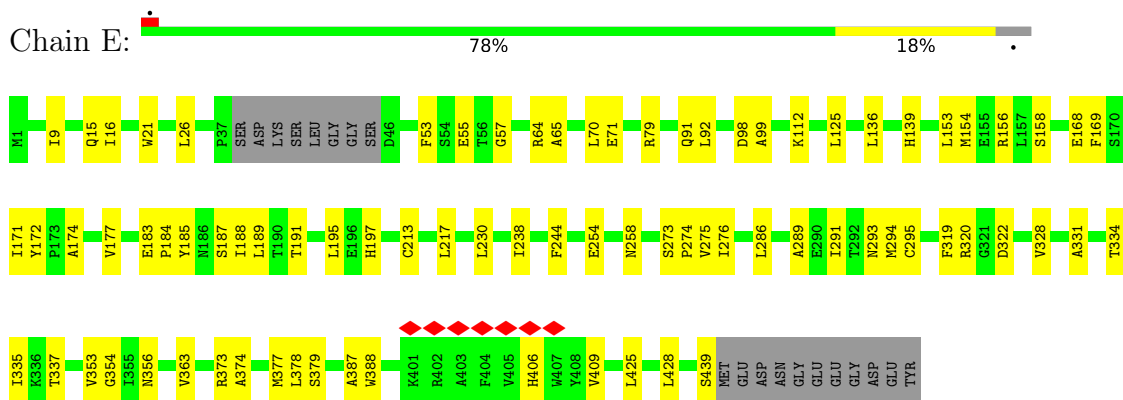
3 Residue-property plots

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.

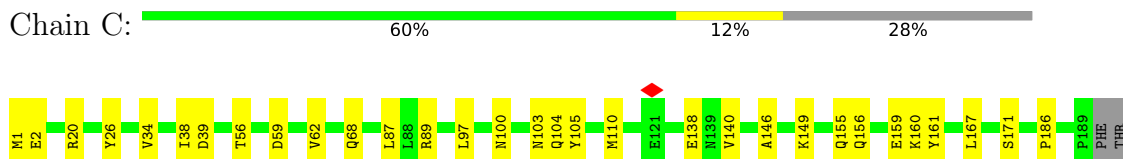
- Molecule 1: Tubulin alpha-3 chain



- Molecule 1: Tubulin alpha-3 chain



- Molecule 2: Alpha-tubulin N-acetyltransferase 2



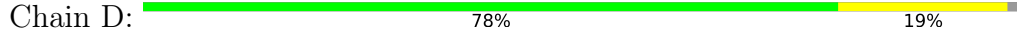
PRO	ARG	GLN	THR	ARG	GLY	ALA	SER	SER	VAL	SER	SER	SER	HIS	ALA	ALA	SER	SER	ARG	ARG	PRO	ILE	GLY
LYS	ASN	ALA	ARG	ASP	PHE	GLY	HIS	ARG	ILE	TRP												

● Molecule 2: Alpha-tubulin N-acetyltransferase 2



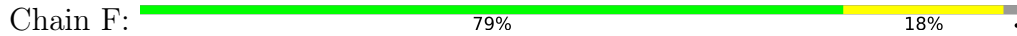
MET	GLU	ILE	ASP	ALA	PHE	ASP	GLU	SER	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ILE	VAL	ASP	HIS	ARG	GLY	ASN	GLU	PHE	GLN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
GLU	GLN	ARG	SER	GLY	ASN	GLY	PHE	GLU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
PHE	ILE	GLY	ARG	HIS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
T214	R219	M220	H224	V227	R232	Q233	D234	M235	L236	A237	G238	D244	S247	L251	K252	M253	A254	R255				

● Molecule 3: Tubulin beta-1 chain



M1	H6	K19	F20	M21	I24	S33	M48	A54	K58	P61	R62	L84	V91	G98	H99	N100	W101	K103	G104	Y106	V116	L117	R121	Q131	G132	L139	G140	G141	M147	G148	L151	I152	S153	K154	E158	R162	F167	
V170	P173	K174	V179	V180	E181	P182	A185	V189	N204	A206	L207	F212	P220	L225	N226	S230	M233	D249	K252	L253	N256	M257	A271	R276	T285	V286	P287	E288	L289	T290	Q291	Q292	C293	N298	A302	C303	H307	
Y310	F317	R318	G319	F341	M348	P357	I368	S371	L377	M388	R391	L395	M403	D404	E405	Q426	E427	ALA	ALA	ASP	ASP	ALA	ALA	GLU	ALA	PHE	ASP	GLY	GLU									

● Molecule 3: Tubulin beta-1 chain



M1	F20	W21	E27	N52	E53	A54	K58	P61	R62	M73	F81	L84	F92	G98	N99	M100	W101	A102	K103	G109	L112	V113	V116	L139	G140	G141	S145	T149	L150	L151	I152	R156	M164	M165	V170	P171	S188	V189	H190				
Q191	L192	T196	D197	L202	L207	L215	L225	S230	A231	T232	N233	S234	G235	V236	T237	L250	L253	A254	M257	V258	P268	G269	F270	A271	P272	L273	Q279	Q280	Y281	R282	A283	Q292	C293	N298	L311	T312	A313	I316	G319	V342	V349		
P357	P358	R359	S364	F367	I368	L377	R391	E401	A411	M415	E427	ALA	ALA	ALA	ASP	GLU	ASP	ALA	ALA	ALA	PHE	ASP	ASP	GLU																			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	110097	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	47170	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.359	Depositor
Minimum map value	-0.384	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.3	Depositor
Map size (\AA)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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, PIN, G2P

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	B	0.26	0/3508	0.47	0/4762
1	E	0.27	0/3423	0.47	0/4653
2	C	0.25	0/1512	0.47	0/2050
2	I	0.24	0/379	0.55	0/513
3	D	0.27	0/3434	0.48	0/4653
3	F	0.26	0/3430	0.47	0/4648
All	All	0.26	0/15686	0.48	0/21279

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3429	0	3336	67	0
1	E	3345	0	3232	48	0
2	C	1476	0	1414	20	0
2	I	371	0	337	11	0
3	D	3360	0	3243	56	0
3	F	3356	0	3239	50	0
4	B	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	32	0	12	1	0
5	C	18	0	16	0	0
6	D	32	0	14	3	0
6	F	32	0	14	2	0
All	All	15483	0	14869	231	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 8.

All (231) 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:B:254:GLU:HG2	3:D:98:GLY:HA2	1.60	0.82
1:B:364:PRO:HB2	2:C:104:GLN:HE21	1.50	0.77
1:E:172:TYR:HE2	1:E:387:ALA:HB1	1.51	0.73
1:E:71:GLU:HB3	1:E:98:ASP:HB3	1.72	0.71
3:F:279:GLN:NE2	2:I:232:ARG:O	2.24	0.70
3:D:58:LYS:HE2	3:F:280:GLN:HB3	1.74	0.69
3:D:181:GLU:HG3	3:D:182:PRO:HD3	1.73	0.68
3:F:113:VAL:HG21	3:F:150:LEU:HD23	1.75	0.68
3:F:52:ASN:OD1	3:F:62:ARG:NH1	2.28	0.67
1:B:244:PHE:HB2	1:B:356:ASN:HD21	1.60	0.66
1:B:326:LYS:HD3	3:D:220:PRO:HD2	1.78	0.65
1:B:274:PRO:HG3	1:B:374:ALA:HA	1.79	0.65
3:D:48:ASN:O	3:D:62:ARG:NH2	2.30	0.64
1:E:439:SER:HB3	3:F:391:ARG:HD2	1.79	0.64
3:F:237:THR:HG22	3:F:250:LEU:HD21	1.80	0.63
3:D:100:ASN:HB3	3:D:103:LYS:HB2	1.79	0.63
3:F:282:ARG:NH2	3:F:292:GLN:OE1	2.32	0.63
3:D:33:SER:O	3:D:58:LYS:NZ	2.32	0.62
1:B:191:THR:HG21	1:B:425:LEU:HD13	1.80	0.62
1:B:11:GLN:HG3	1:B:74:VAL:HG21	1.81	0.62
1:B:211:ASP:OD1	1:B:214:ARG:NH1	2.31	0.62
1:B:26:LEU:HD22	1:B:363:VAL:HG12	1.83	0.60
3:D:307:HIS:O	3:D:426:GLN:NE2	2.34	0.60
3:F:99:ASN:ND2	6:F:501:G2P:O2G	2.34	0.60
1:E:26:LEU:HD22	1:E:363:VAL:HG12	1.84	0.60
3:D:91:VAL:HG21	3:D:116:VAL:HG22	1.84	0.60
3:D:395:LEU:HD21	3:D:405:GLU:HG2	1.84	0.60
1:E:139:HIS:NE2	1:E:168:GLU:OE2	2.36	0.59
3:F:359:ARG:O	2:I:232:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:254:GLU:O	1:E:258:ASN:ND2	2.29	0.59
3:D:116:VAL:HG11	3:D:151:LEU:HD11	1.86	0.58
1:B:105:ARG:NH1	1:B:411:GLU:OE2	2.37	0.57
3:D:102:ALA:HB2	3:D:403:MET:HG3	1.87	0.57
3:D:139:LEU:HD12	3:D:170:VAL:HG12	1.87	0.57
1:E:15:GLN:NE2	4:E:501:GTP:O6	2.37	0.57
3:F:109:GLY:O	3:F:113:VAL:HG23	2.05	0.56
1:B:388:TRP:CD1	1:B:425:LEU:HD11	2.39	0.56
1:B:385:ALA:HA	1:B:388:TRP:HE3	1.69	0.56
2:C:160:LYS:HE3	2:C:161:TYR:HE2	1.70	0.56
3:F:271:ALA:HB2	3:F:293:CYS:SG	2.46	0.56
3:D:141:GLY:HA3	6:D:501:G2P:H3A1	1.88	0.56
2:I:262:ILE:HG13	2:I:263:TRP:CD1	2.41	0.56
3:D:132:GLY:HA2	3:D:162:ARG:HB3	1.89	0.56
1:B:262:TYR:HB2	1:B:265:ILE:HG12	1.88	0.55
1:E:273:SER:HB2	1:E:295:CYS:SG	2.47	0.55
2:C:97:LEU:HB2	2:C:105:TYR:HB2	1.89	0.55
2:C:156:GLN:HA	2:C:159:GLU:HG2	1.88	0.55
3:F:156:ARG:NH2	3:F:197:ASP:OD1	2.40	0.55
3:D:252:LYS:O	3:D:256:ASN:ND2	2.34	0.54
3:F:54:ALA:HB3	3:F:58:LYS:HB3	1.88	0.54
1:B:250:VAL:HG22	1:B:352:LYS:HE3	1.89	0.54
3:D:310:TYR:HA	3:D:371:SER:HA	1.90	0.54
1:B:406:HIS:HA	1:B:409:VAL:HG22	1.90	0.54
3:D:207:LEU:HB3	3:D:225:LEU:HD22	1.89	0.54
2:C:100:ASN:O	2:C:103:ASN:ND2	2.41	0.54
1:B:71:GLU:HB3	1:B:98:ASP:HB3	1.90	0.54
1:B:215:ARG:NH2	1:B:299:HIS:O	2.38	0.54
1:B:79:ARG:NH2	1:B:92:LEU:O	2.41	0.54
1:E:276:ILE:HD11	1:E:286:LEU:HD11	1.87	0.54
2:C:138:GLU:O	2:C:140:VAL:HG23	2.07	0.53
1:E:136:LEU:HD22	1:E:169:PHE:HE2	1.72	0.53
2:C:68:GLN:OE1	2:C:89:ARG:NH1	2.40	0.53
3:D:204:ASN:OD1	6:D:501:G2P:N2	2.41	0.53
1:E:291:ILE:HA	1:E:294:MET:HG2	1.90	0.53
1:B:364:PRO:HB2	2:C:104:GLN:NE2	2.23	0.53
3:F:319:GLY:HA2	3:F:357:PRO:HG3	1.90	0.52
1:E:187:SER:O	1:E:191:THR:HG23	2.08	0.52
1:E:286:LEU:O	1:E:373:ARG:NH1	2.39	0.52
1:E:9:ILE:HD11	1:E:153:LEU:HD23	1.91	0.52
3:D:117:LEU:HD11	3:D:154:LYS:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:73:MET:SD	3:F:92:PHE:HB3	2.49	0.52
2:C:105:TYR:HA	2:C:186:PRO:HD2	1.92	0.51
1:B:384:ILE:HG23	1:B:388:TRP:HZ3	1.75	0.51
3:F:270:PHE:O	3:F:298:ASN:ND2	2.33	0.51
3:D:117:LEU:HD21	3:D:154:LYS:HB3	1.93	0.51
1:E:183:GLU:HG2	1:E:184:PRO:HD3	1.92	0.51
1:B:188:ILE:HD12	1:B:395:PHE:HB2	1.92	0.51
3:D:253:LEU:HD12	3:D:368:ILE:HD11	1.92	0.51
1:B:238:ILE:HD11	1:B:378:LEU:HD21	1.93	0.51
1:E:406:HIS:HA	1:E:409:VAL:HG22	1.93	0.51
1:E:188:ILE:HD13	1:E:425:LEU:HD13	1.93	0.50
1:B:60:ARG:HH12	1:B:85:SER:HB3	1.76	0.50
1:E:238:ILE:HG12	1:E:378:LEU:HD11	1.92	0.50
3:F:207:LEU:HB3	3:F:225:LEU:HG	1.94	0.50
1:B:185:TYR:O	1:B:189:LEU:HD23	2.11	0.50
1:B:322:ASP:OD1	2:I:255:ARG:NH2	2.36	0.50
1:E:195:LEU:HD11	1:E:428:LEU:HD22	1.93	0.50
1:E:55:GLU:HG3	1:E:57:GLY:H	1.77	0.50
3:D:20:PHE:HA	3:D:230:SER:OG	2.12	0.50
3:D:173:PRO:HG2	3:D:174:LYS:NZ	2.26	0.49
3:D:104:GLY:O	3:D:147:MET:HB2	2.12	0.49
3:D:170:VAL:HG21	3:D:377:LEU:HD21	1.93	0.49
3:D:276:ARG:O	3:D:276:ARG:NH1	2.45	0.49
1:E:254:GLU:HB3	3:F:98:GLY:HA2	1.94	0.49
1:E:322:ASP:HB2	2:I:219:ARG:HH21	1.77	0.49
3:F:253:LEU:HD11	3:F:316:ILE:HD11	1.94	0.49
1:B:135:PHE:HB2	1:B:166:LYS:HG2	1.94	0.49
1:B:172:TYR:N	1:B:204:VAL:O	2.45	0.49
3:D:292:GLN:HG2	3:D:298:ASN:ND2	2.26	0.49
1:E:154:MET:HG2	1:E:197:HIS:HB2	1.95	0.49
3:D:207:LEU:HD13	3:D:225:LEU:HB3	1.94	0.49
3:F:27:GLU:OE2	3:F:234:SER:OG	2.28	0.49
1:B:319:PHE:N	1:B:354:GLY:O	2.45	0.49
1:B:306:ASP:HB3	1:B:309:HIS:CE1	2.49	0.48
1:B:402:ARG:HG3	1:B:405:VAL:HG21	1.94	0.48
3:F:20:PHE:HA	3:F:230:SER:HB3	1.95	0.48
3:D:185:ALA:O	3:D:189:VAL:HG23	2.13	0.48
3:F:272:PRO:HG3	3:F:364:SER:HA	1.95	0.48
1:B:360:PRO:HG3	1:B:374:ALA:HB2	1.94	0.48
1:B:251:ASP:HB3	1:B:254:GLU:HG3	1.94	0.48
3:D:19:LYS:HZ1	2:I:259:HIS:CE1	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:145:SER:OG	3:F:188:SER:HB2	2.13	0.48
1:E:53:PHE:O	1:E:64:ARG:NH2	2.43	0.48
2:C:39:ASP:OD2	2:I:220:ASN:ND2	2.44	0.48
3:D:121:ARG:NE	3:D:158:GLU:OE2	2.34	0.48
1:E:79:ARG:HH21	1:E:92:LEU:HB2	1.77	0.48
1:E:319:PHE:N	1:E:354:GLY:O	2.46	0.48
1:B:187:SER:HB3	1:B:391:LEU:HD21	1.95	0.47
1:B:420:GLU:O	1:B:423:GLU:HG3	2.14	0.47
3:F:141:GLY:HA3	6:F:501:G2P:H3A1	1.95	0.47
3:F:313:ALA:HB3	3:F:349:VAL:HG23	1.96	0.47
1:E:16:ILE:HD11	1:E:171:ILE:HD11	1.96	0.47
3:D:303:CYS:SG	3:D:377:LEU:HB2	2.55	0.47
1:B:48:SER:HB2	1:B:243:ARG:HB2	1.96	0.47
1:B:352:LYS:HB2	3:D:179:VAL:HG23	1.96	0.47
3:F:149:THR:HG21	3:F:188:SER:HA	1.95	0.47
2:C:34:VAL:O	2:C:38:ILE:HG12	2.15	0.47
3:F:170:VAL:HG11	3:F:377:LEU:HD23	1.97	0.47
1:B:172:TYR:HB2	1:B:203:MET:HB3	1.97	0.47
1:B:254:GLU:O	1:B:258:ASN:ND2	2.36	0.46
2:C:56:THR:HG21	2:C:87:LEU:HD21	1.96	0.46
1:B:287:SER:H	1:B:290:GLU:CD	2.19	0.46
1:B:334:THR:O	1:B:338:LYS:HG2	2.16	0.46
3:D:257:MET:HE1	3:D:368:ILE:O	2.16	0.46
1:E:174:ALA:HB3	1:E:177:VAL:O	2.15	0.46
3:D:286:VAL:O	3:D:290:THR:HG23	2.15	0.46
1:E:21:TRP:CZ2	1:E:65:ALA:HB2	2.50	0.46
1:E:377:MET:SD	1:E:379:SER:HB3	2.56	0.46
3:F:189:VAL:HG11	3:F:415:MET:SD	2.56	0.46
2:C:20:ARG:NH1	2:C:62:VAL:O	2.49	0.46
1:E:388:TRP:HB3	1:E:425:LEU:HD21	1.98	0.46
3:F:165:ASN:HD21	3:F:250:LEU:HD22	1.80	0.46
2:I:244:ASP:HB3	2:I:247:SER:HB3	1.98	0.46
1:B:46:ASP:OD2	2:C:149:LYS:NZ	2.38	0.46
1:E:112:LYS:HE3	1:E:156:ARG:HH21	1.81	0.46
1:E:158:SER:HB2	1:E:197:HIS:HB3	1.97	0.46
3:F:232:THR:HG21	3:F:268:PRO:HB2	1.98	0.46
3:D:106:TYR:HE2	3:D:403:MET:HG2	1.80	0.45
1:B:122:ILE:HG21	1:B:157:LEU:HD21	1.98	0.45
1:B:211:ASP:HB3	1:B:215:ARG:HH12	1.80	0.45
1:B:287:SER:N	1:B:290:GLU:OE2	2.41	0.45
3:F:311:LEU:HD23	3:F:342:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ARG:NH2	1:B:110:ILE:HD11	2.32	0.45
2:C:26:TYR:HB3	2:C:34:VAL:HG21	1.99	0.45
3:F:103:LYS:HB3	3:F:103:LYS:HE2	1.76	0.45
1:E:217:LEU:HG	1:E:275:VAL:HG12	1.99	0.45
3:F:215:LEU:HD13	2:I:227:VAL:HG22	1.98	0.45
3:F:254:ALA:O	3:F:258:VAL:HG22	2.16	0.45
1:E:244:PHE:O	1:E:356:ASN:ND2	2.49	0.45
1:B:147:SER:OG	1:B:190:THR:HB	2.17	0.44
3:F:100:ASN:HB3	3:F:103:LYS:HB2	1.98	0.44
1:B:384:ILE:HG12	1:B:388:TRP:CZ3	2.52	0.44
2:I:253:ASN:HA	2:I:257:PHE:HB2	2.00	0.44
1:B:21:TRP:CZ3	1:B:63:PRO:HB3	2.53	0.44
1:B:141:PHE:HB2	1:B:170:SER:HB3	2.00	0.44
1:B:438:ASP:OD1	1:B:438:ASP:N	2.46	0.44
3:D:206:ALA:HB2	3:D:302:ALA:N	2.33	0.44
1:B:12:ALA:HB3	1:B:140:SER:HB3	1.99	0.44
1:B:255:PHE:CZ	1:B:259:LEU:HD13	2.52	0.44
3:D:167:PHE:CE2	3:D:233:MET:HG2	2.53	0.44
3:F:253:LEU:O	3:F:257:MET:HG2	2.16	0.44
1:E:320:ARG:N	1:E:374:ALA:O	2.47	0.44
1:E:172:TYR:CE2	1:E:387:ALA:HB1	2.42	0.44
2:C:155:GLN:HE22	2:C:167:LEU:HB2	1.83	0.44
1:E:70:LEU:HD12	1:E:99:ALA:HB2	1.99	0.44
3:D:54:ALA:HA	3:F:283:ALA:HB2	1.99	0.43
1:E:112:LYS:HD2	1:E:112:LYS:HA	1.78	0.43
1:B:209:ILE:HG23	1:B:230:LEU:HD12	2.00	0.43
1:E:273:SER:HB3	1:E:274:PRO:HD3	2.00	0.43
1:B:231:ILE:O	1:B:235:VAL:HG23	2.18	0.43
3:D:285:THR:N	3:D:288:GLU:OE2	2.50	0.43
1:B:326:LYS:HD2	3:D:212:PHE:HZ	1.83	0.43
1:B:357:TYR:HB3	2:I:251:LEU:HD12	2.01	0.43
1:B:172:TYR:CD1	1:B:173:PRO:HD2	2.54	0.43
1:B:319:PHE:HB3	1:B:323:VAL:HG21	2.01	0.43
1:E:334:THR:O	1:E:337:THR:OG1	2.36	0.43
3:F:273:LEU:O	3:F:292:GLN:NE2	2.51	0.43
1:B:26:LEU:O	2:C:171:SER:OG	2.37	0.43
3:D:6:HIS:CD2	3:D:21:TRP:HE1	2.37	0.43
3:F:192:LEU:O	3:F:196:THR:HG22	2.19	0.43
3:F:189:VAL:HA	3:F:192:LEU:HB2	2.01	0.42
1:B:31:GLN:HG3	1:B:37:PRO:HD3	1.99	0.42
1:E:328:VAL:HG11	1:E:353:VAL:HG11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:ASN:OD1	1:B:357:TYR:N	2.52	0.42
3:D:318:ARG:HB3	3:D:357:PRO:HA	2.01	0.42
1:B:384:ILE:HG23	1:B:388:TRP:CZ3	2.53	0.42
3:D:20:PHE:O	3:D:24:ILE:HG12	2.19	0.42
3:D:271:ALA:HB2	3:D:293:CYS:SG	2.59	0.42
3:D:148:GLY:O	3:D:152:ILE:HG12	2.20	0.42
3:D:290:THR:HG22	3:D:317:PHE:HZ	1.84	0.42
1:E:289:ALA:O	1:E:293:ASN:ND2	2.41	0.42
1:B:346:TRP:CD1	3:D:391:ARG:HD3	2.55	0.42
3:F:21:TRP:CZ3	3:F:61:PRO:HB3	2.55	0.42
2:C:59:ASP:HA	2:C:62:VAL:HG22	2.00	0.41
3:F:152:ILE:HG12	3:F:164:MET:HE1	2.01	0.41
1:B:91:GLN:NE2	1:B:125:LEU:HD21	2.34	0.41
3:D:131:GLN:HE22	3:D:249:ASP:HB2	1.85	0.41
2:C:110:MET:O	2:C:146:ALA:N	2.48	0.41
3:F:190:HIS:HD2	3:F:411:ALA:HA	1.85	0.41
3:D:226:ASN:OD1	6:D:501:G2P:N1	2.51	0.41
1:E:91:GLN:NE2	1:E:125:LEU:HD21	2.36	0.41
1:E:213:CYS:HA	1:E:217:LEU:HB2	2.03	0.41
1:B:313:MET:HE3	1:B:346:TRP:HH2	1.86	0.41
3:F:170:VAL:N	3:F:202:ILE:O	2.54	0.41
3:D:61:PRO:HD3	3:D:84:LEU:HG	2.03	0.41
3:F:81:PHE:HD2	3:F:84:LEU:HD22	1.85	0.41
3:F:236:VAL:HG22	3:F:368:ILE:HD11	2.03	0.41
1:B:22:GLU:O	1:B:26:LEU:HD13	2.21	0.40
1:B:166:LYS:HB2	1:B:166:LYS:HE2	1.89	0.40
2:C:1:MET:HB3	2:C:2:GLU:H	1.70	0.40
3:D:341:PHE:HB3	3:D:348:ASN:ND2	2.36	0.40
1:E:185:TYR:O	1:E:189:LEU:HG	2.22	0.40
3:F:102:ALA:HB1	3:F:401:GLU:HB2	2.03	0.40
3:F:112:LEU:O	3:F:116:VAL:HG23	2.21	0.40
3:D:105:HIS:HD2	3:D:106:TYR:CE1	2.39	0.40
3:D:179:VAL:O	3:D:388:MET:HE1	2.22	0.40
1:E:230:LEU:HD23	1:E:230:LEU:HA	1.92	0.40
3:F:293:CYS:HB3	3:F:367:PHE:HB2	2.03	0.40
3:D:319:GLY:HA2	3:D:357:PRO:HD3	2.04	0.40
1:E:331:ALA:O	1:E:335:ILE:HG12	2.21	0.40
3:F:139:LEU:HB2	3:F:171:PRO:HD3	2.04	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	B	437/450 (97%)	419 (96%)	18 (4%)	0	100	100
1	E	427/450 (95%)	412 (96%)	15 (4%)	0	100	100
2	C	187/263 (71%)	180 (96%)	7 (4%)	0	100	100
2	I	48/263 (18%)	46 (96%)	2 (4%)	0	100	100
3	D	425/441 (96%)	411 (97%)	14 (3%)	0	100	100
3	F	425/441 (96%)	410 (96%)	15 (4%)	0	100	100
All	All	1949/2308 (84%)	1878 (96%)	71 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	373/383 (97%)	373 (100%)	0	100	100
1	E	360/383 (94%)	360 (100%)	0	100	100
2	C	151/233 (65%)	151 (100%)	0	100	100
2	I	35/233 (15%)	35 (100%)	0	100	100
3	D	369/376 (98%)	369 (100%)	0	100	100
3	F	368/376 (98%)	368 (100%)	0	100	100
All	All	1656/1984 (84%)	1656 (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 (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	104	GLN
1	E	285	GLN
3	F	8	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](#)

5 ligands are 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
6	G2P	D	501	-	27,34,34	3.13	11 (40%)	33,54,54	2.58	7 (21%)
5	PIN	C	301	-	18,18,18	0.73	0	22,26,26	0.97	0
4	GTP	B	501	-	26,34,34	1.76	5 (19%)	32,54,54	1.54	7 (21%)
4	GTP	E	501	-	26,34,34	1.82	5 (19%)	32,54,54	1.59	8 (25%)
6	G2P	F	501	-	27,34,34	3.12	9 (33%)	33,54,54	2.63	7 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	G2P	D	501	-	-	3/15/38/38	0/3/3/3
5	PIN	C	301	-	-	3/12/22/22	0/1/1/1
4	GTP	B	501	-	-	4/18/38/38	0/3/3/3
4	GTP	E	501	-	-	8/18/38/38	0/3/3/3
6	G2P	F	501	-	-	6/15/38/38	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	501	G2P	PA-O5'	12.60	1.76	1.57
6	D	501	G2P	PA-O5'	12.49	1.75	1.57
4	E	501	GTP	PA-O5'	6.05	1.83	1.59
4	B	501	GTP	PA-O5'	5.95	1.83	1.59
6	F	501	G2P	C6-N1	5.62	1.42	1.33
6	D	501	G2P	C6-N1	5.48	1.42	1.33
4	E	501	GTP	C6-N1	3.25	1.42	1.37
6	D	501	G2P	PB-O3B	-3.17	1.54	1.58
6	F	501	G2P	PB-O3B	-3.14	1.54	1.58
6	D	501	G2P	C4-N3	3.10	1.40	1.35
6	F	501	G2P	C4-N3	3.09	1.40	1.35
4	B	501	GTP	C6-N1	3.05	1.42	1.37
4	B	501	GTP	O5'-C5'	-2.92	1.33	1.44
4	E	501	GTP	O5'-C5'	-2.91	1.33	1.44
6	D	501	G2P	O5'-C5'	-2.81	1.34	1.44
6	F	501	G2P	O5'-C5'	-2.79	1.34	1.44
6	D	501	G2P	C2-N2	2.71	1.39	1.33
4	E	501	GTP	C5-C6	-2.67	1.42	1.47
6	F	501	G2P	C2-N2	2.66	1.39	1.33
4	B	501	GTP	C5-C6	-2.64	1.42	1.47
6	F	501	G2P	PA-O1A	-2.42	1.50	1.56
6	D	501	G2P	PA-O1A	-2.40	1.50	1.56
6	D	501	G2P	PB-O1B	-2.28	1.51	1.56
6	D	501	G2P	O4'-C1'	-2.22	1.38	1.41
6	D	501	G2P	C2-N1	2.22	1.39	1.35
6	F	501	G2P	C2-N1	2.22	1.39	1.35
6	F	501	G2P	PB-O1B	-2.18	1.51	1.56
6	D	501	G2P	O4'-C4'	-2.12	1.40	1.45
4	B	501	GTP	C2-N2	2.06	1.39	1.34
4	E	501	GTP	C2-N2	2.02	1.39	1.34

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	501	G2P	C5-C6-N1	-10.86	108.58	123.43
6	D	501	G2P	C5-C6-N1	-10.70	108.80	123.43
6	F	501	G2P	C2-N1-C6	5.49	124.65	115.93
6	D	501	G2P	C2-N1-C6	5.43	124.56	115.93
6	F	501	G2P	C2-N3-C4	-4.79	109.89	115.36
6	D	501	G2P	C2-N3-C4	-4.72	109.97	115.36
4	E	501	GTP	O5'-PA-O1A	-3.71	94.58	109.07
4	B	501	GTP	O5'-PA-O1A	-3.63	94.88	109.07
4	B	501	GTP	O6-C6-N1	-3.22	116.84	120.65
4	E	501	GTP	O6-C6-N1	-3.22	116.85	120.65
6	D	501	G2P	O1A-PA-C3A	3.20	119.69	106.58
6	F	501	G2P	O1A-PA-C3A	3.20	119.69	106.58
4	E	501	GTP	O6-C6-C5	3.18	130.59	124.37
4	B	501	GTP	O6-C6-C5	3.14	130.50	124.37
6	F	501	G2P	C4-C5-N7	2.71	112.22	109.40
6	F	501	G2P	C4-C5-C6	2.64	123.31	120.80
6	F	501	G2P	O2A-PA-C3A	2.60	115.95	109.07
4	E	501	GTP	O4'-C1'-C2'	-2.54	103.21	106.93
6	D	501	G2P	C4-C5-N7	2.53	112.03	109.40
6	D	501	G2P	O2A-PA-C3A	2.50	115.69	109.07
6	D	501	G2P	C4-C5-C6	2.45	123.14	120.80
4	E	501	GTP	O2A-PA-O5'	-2.35	96.83	107.75
4	B	501	GTP	O2A-PA-O5'	-2.35	96.84	107.75
4	B	501	GTP	N1-C2-N3	2.15	127.33	123.32
4	E	501	GTP	N1-C2-N3	2.11	127.25	123.32
4	B	501	GTP	C2-N1-C6	-2.06	121.31	125.10
4	E	501	GTP	C2-N1-C6	-2.04	121.34	125.10
4	E	501	GTP	N2-C2-N3	-2.04	115.77	119.74
4	B	501	GTP	N2-C2-N3	-2.02	115.80	119.74

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	GTP	O4'-C4'-C5'-O5'
4	B	501	GTP	C3'-C4'-C5'-O5'
4	E	501	GTP	C5'-O5'-PA-O1A
4	E	501	GTP	C5'-O5'-PA-O2A
6	D	501	G2P	PB-C3A-PA-O1A
6	D	501	G2P	PB-C3A-PA-O5'
6	F	501	G2P	PB-C3A-PA-O1A

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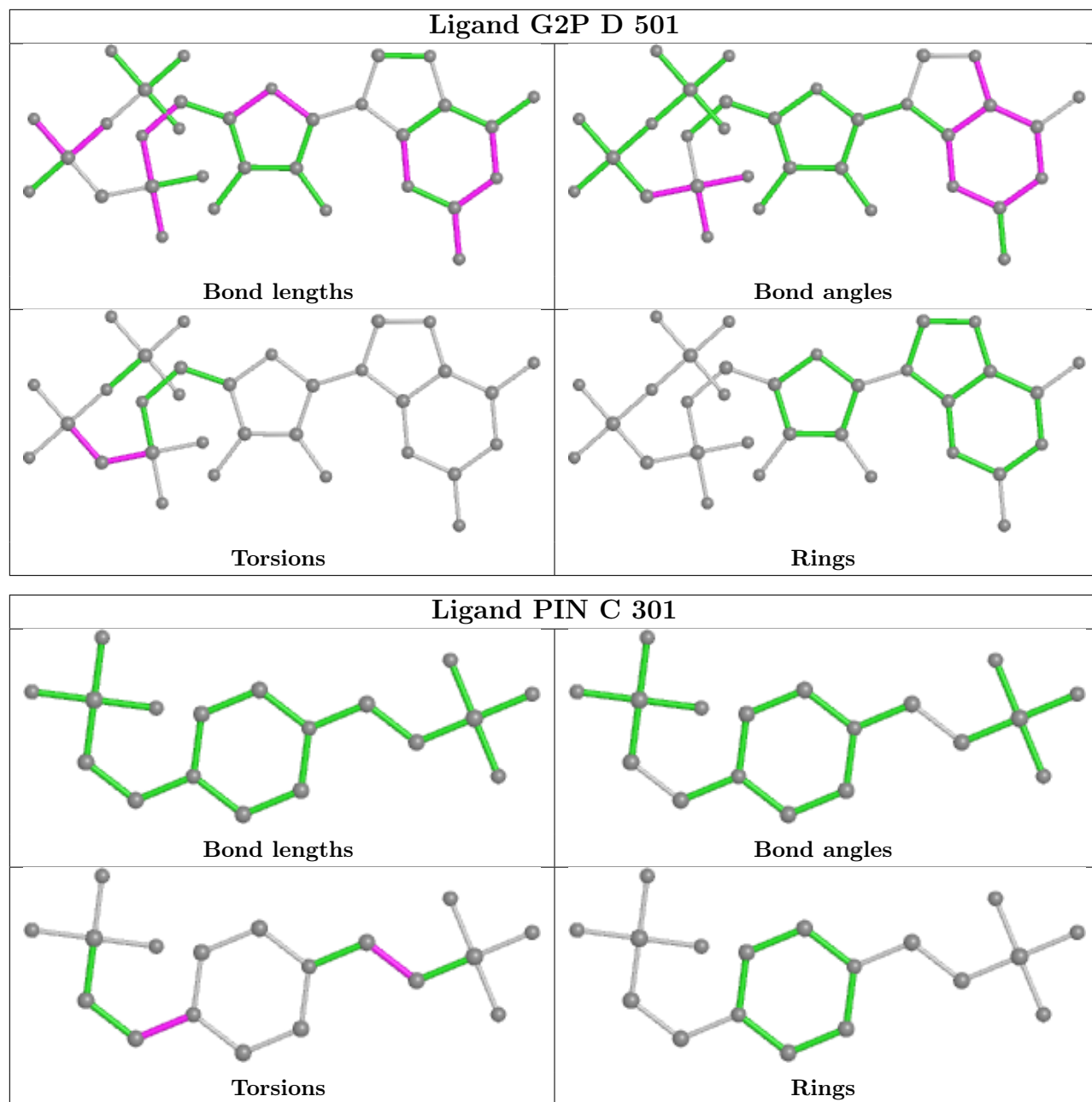
Mol	Chain	Res	Type	Atoms
6	F	501	G2P	PB-C3A-PA-O2A
6	F	501	G2P	PB-C3A-PA-O5'
6	F	501	G2P	O4'-C4'-C5'-O5'
6	F	501	G2P	C3'-C4'-C5'-O5'
4	E	501	GTP	C3'-C4'-C5'-O5'
5	C	301	PIN	C1'-C2'-N1'-C3'
5	C	301	PIN	C1'-C2'-N1'-C4'
4	E	501	GTP	O4'-C4'-C5'-O5'
4	B	501	GTP	C5'-O5'-PA-O3A
4	E	501	GTP	C5'-O5'-PA-O3A
4	B	501	GTP	C5'-O5'-PA-O1A
4	E	501	GTP	PG-O3B-PB-O2B
4	E	501	GTP	C4'-C5'-O5'-PA
6	D	501	G2P	PA-C3A-PB-O2B
6	F	501	G2P	PB-O3B-PG-O1G
4	E	501	GTP	PB-O3A-PA-O2A
5	C	301	PIN	S1-C1-C2-N1

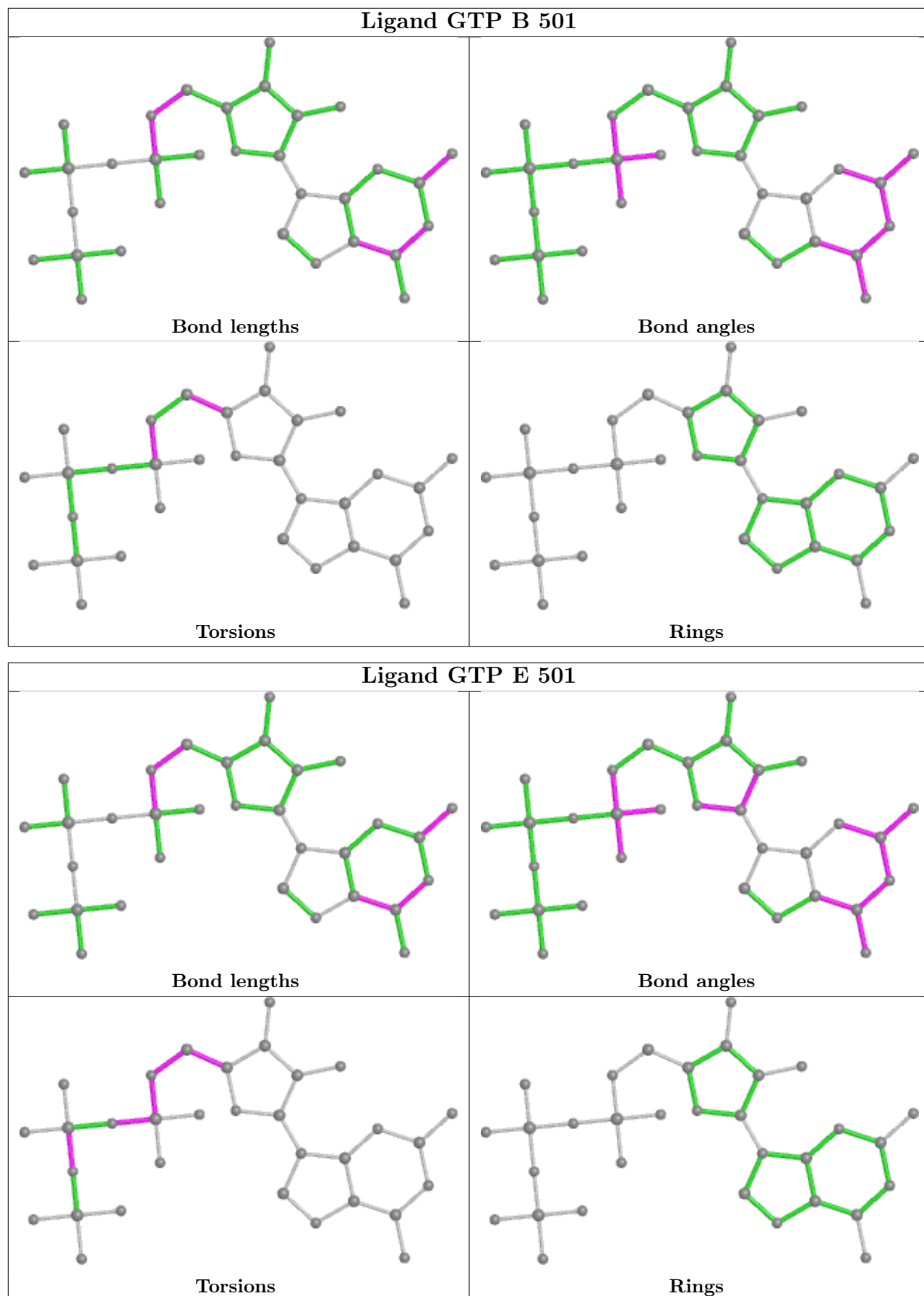
There are no ring outliers.

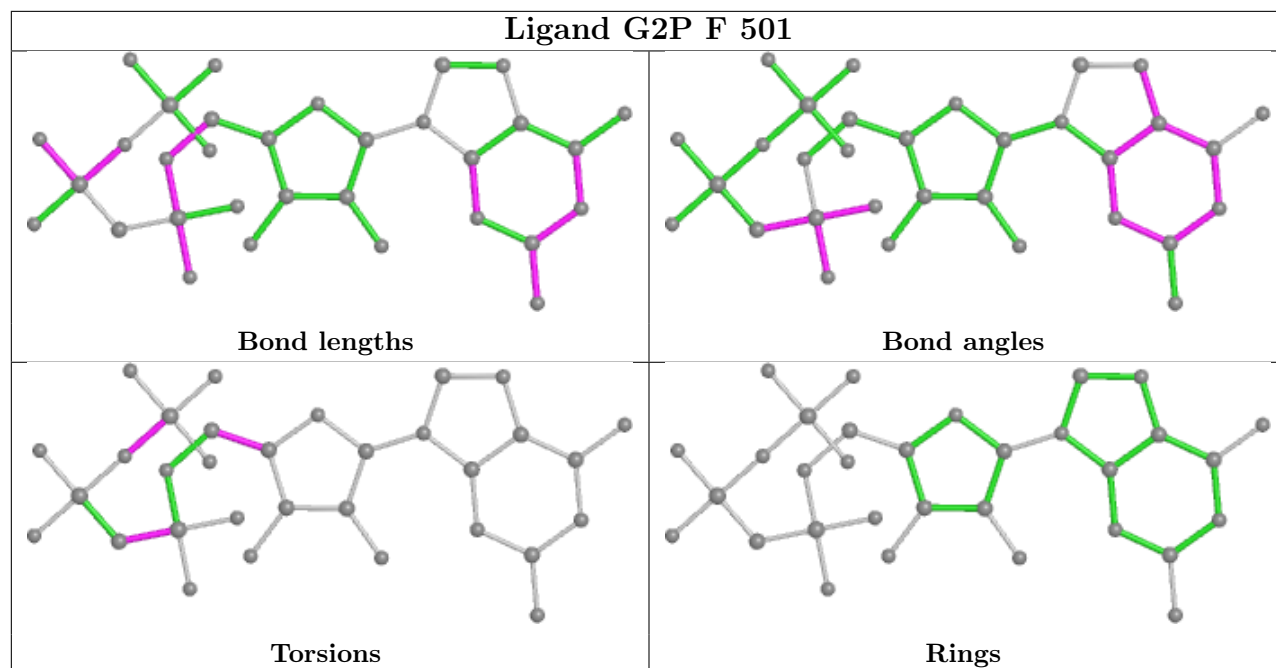
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	501	G2P	3	0
4	E	501	GTP	1	0
6	F	501	G2P	2	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 [i](#)

There are no chain breaks in this entry.

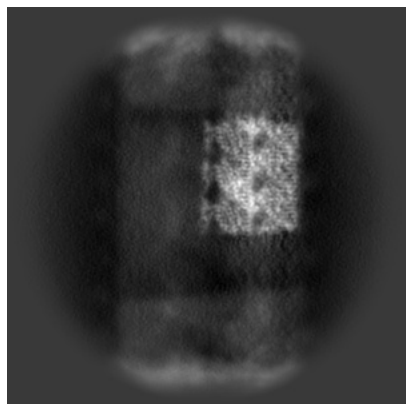
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39100. These allow visual inspection of the internal detail of the map and identification of artifacts.

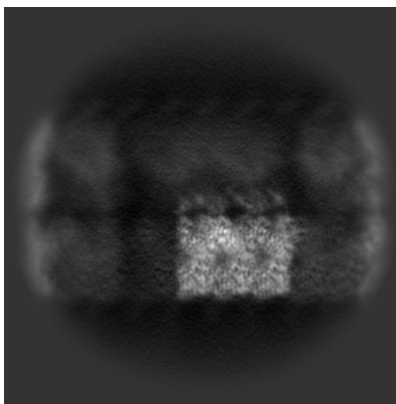
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

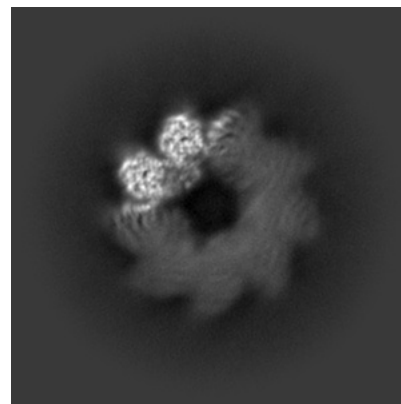
6.1.1 Primary map



X

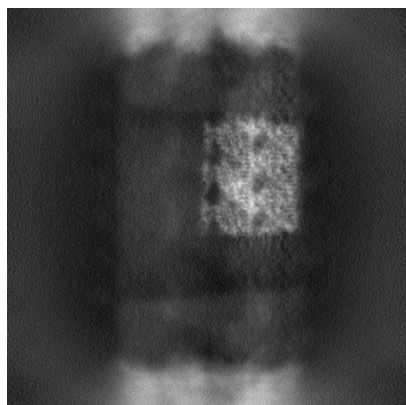


Y

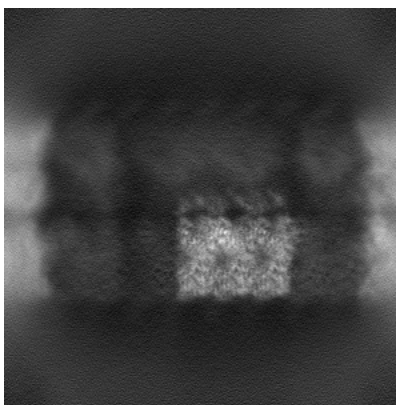


Z

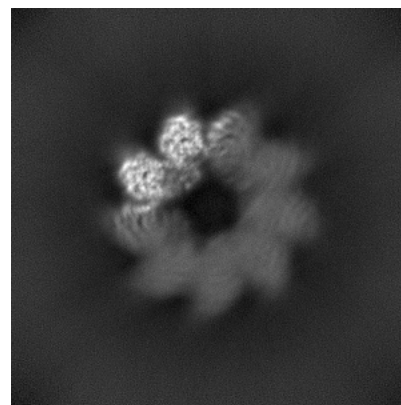
6.1.2 Raw map



X



Y

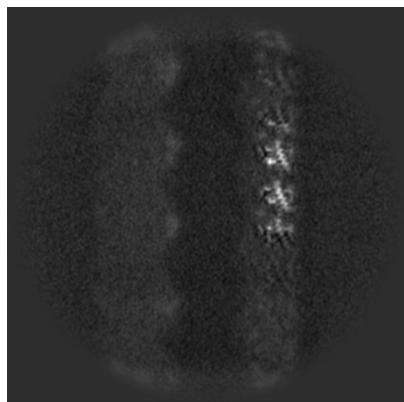


Z

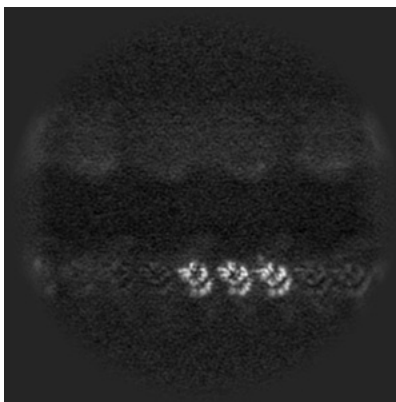
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

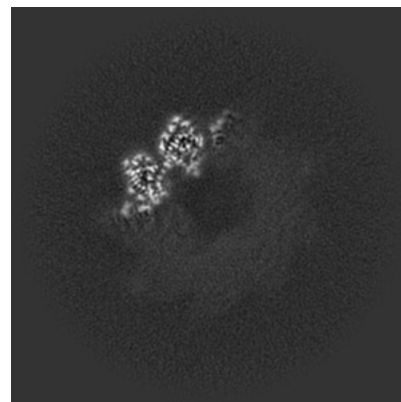
6.2.1 Primary map



X Index: 200

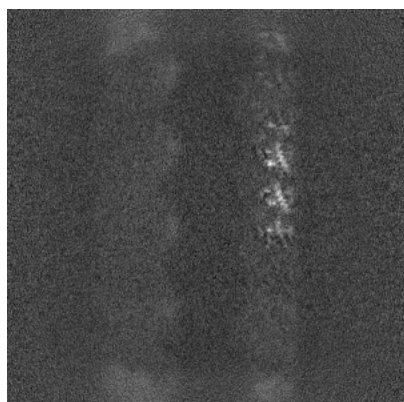


Y Index: 200

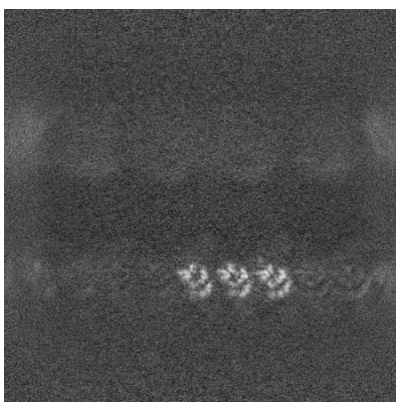


Z Index: 200

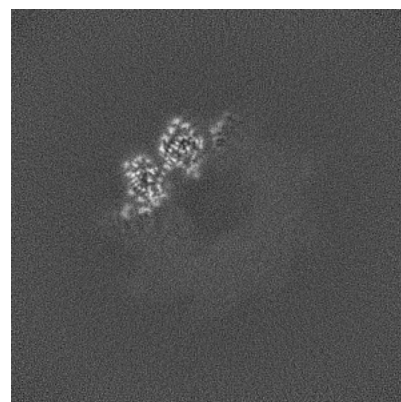
6.2.2 Raw map



X Index: 200



Y Index: 200

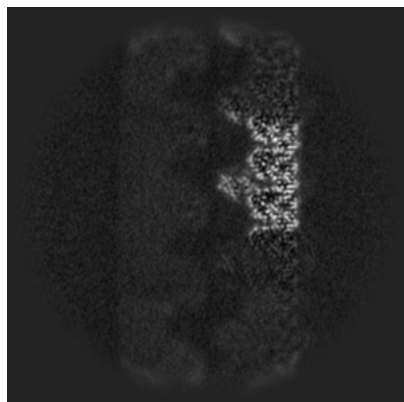


Z Index: 200

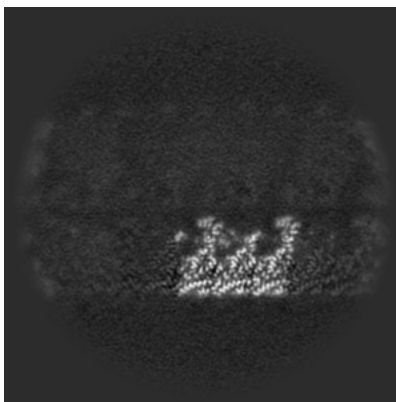
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

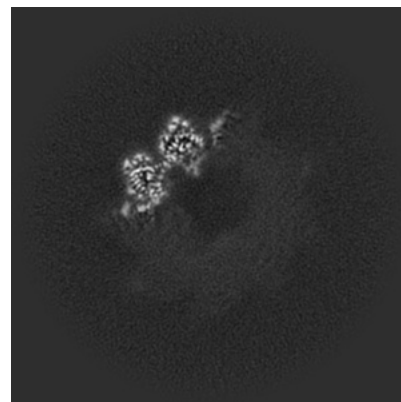
6.3.1 Primary map



X Index: 166

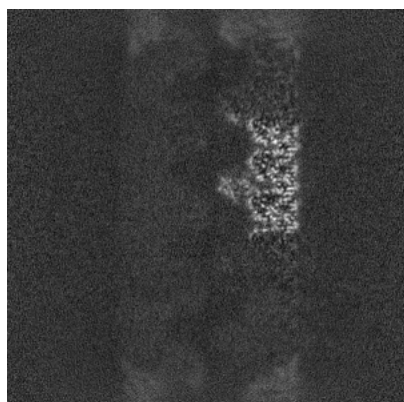


Y Index: 243

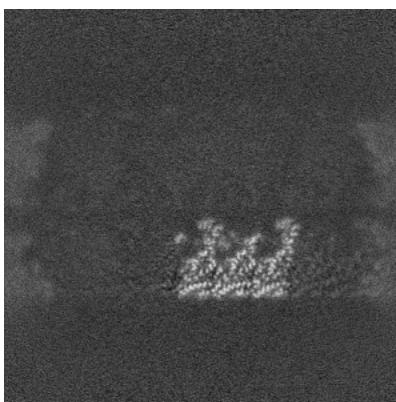


Z Index: 199

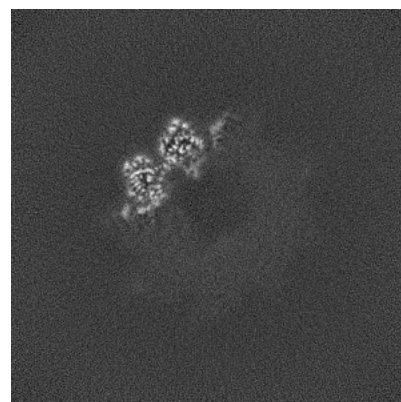
6.3.2 Raw map



X Index: 166



Y Index: 243

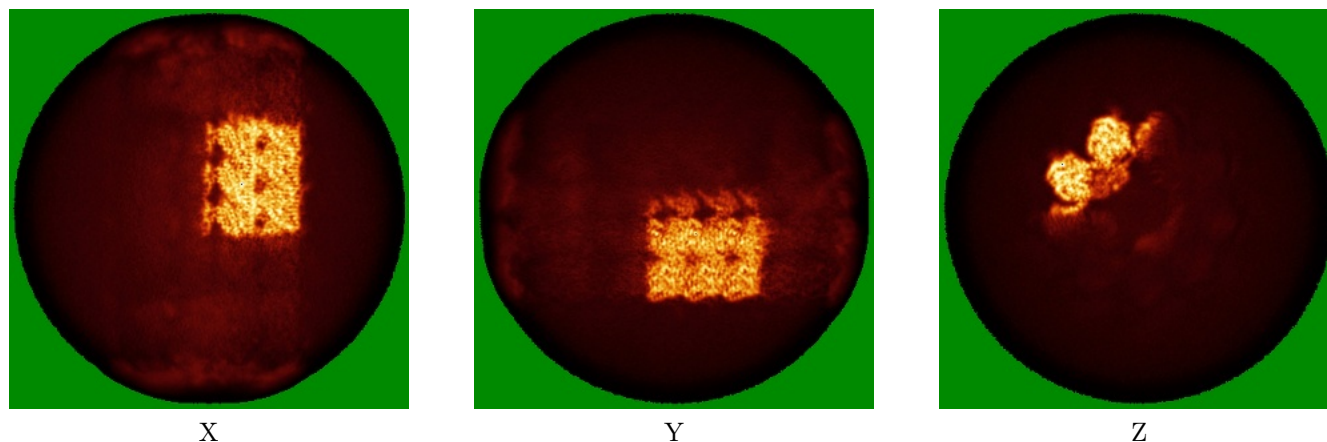


Z Index: 199

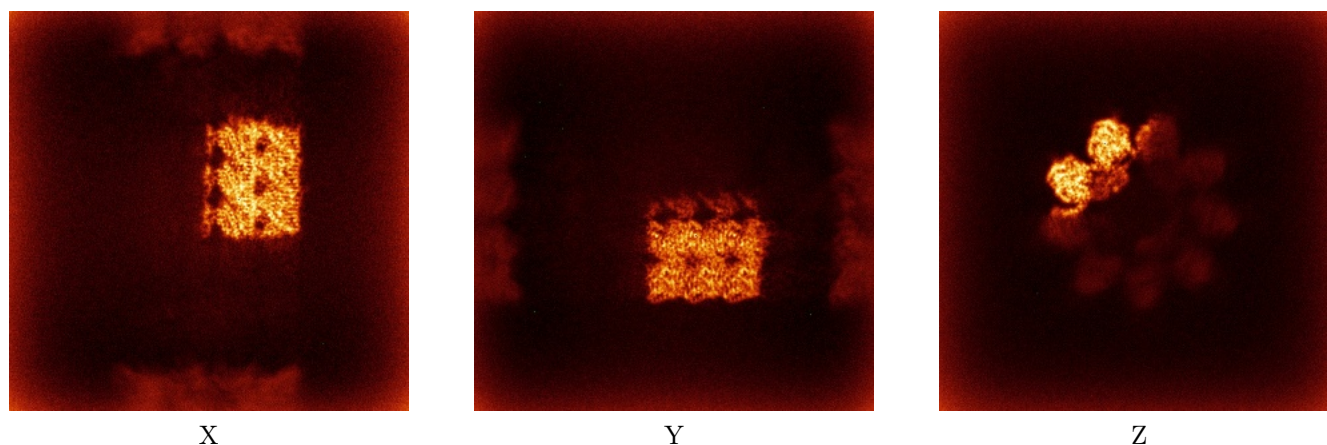
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



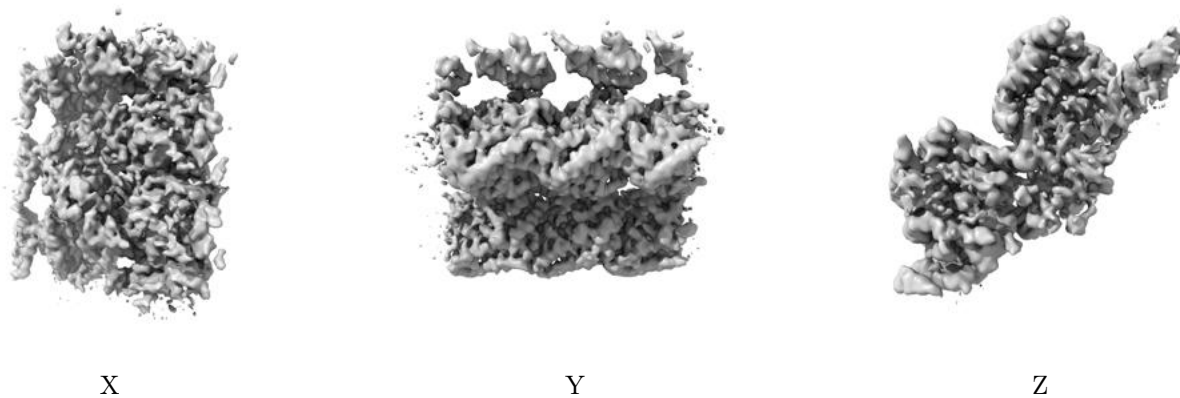
6.4.2 Raw map



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 0.3. 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.

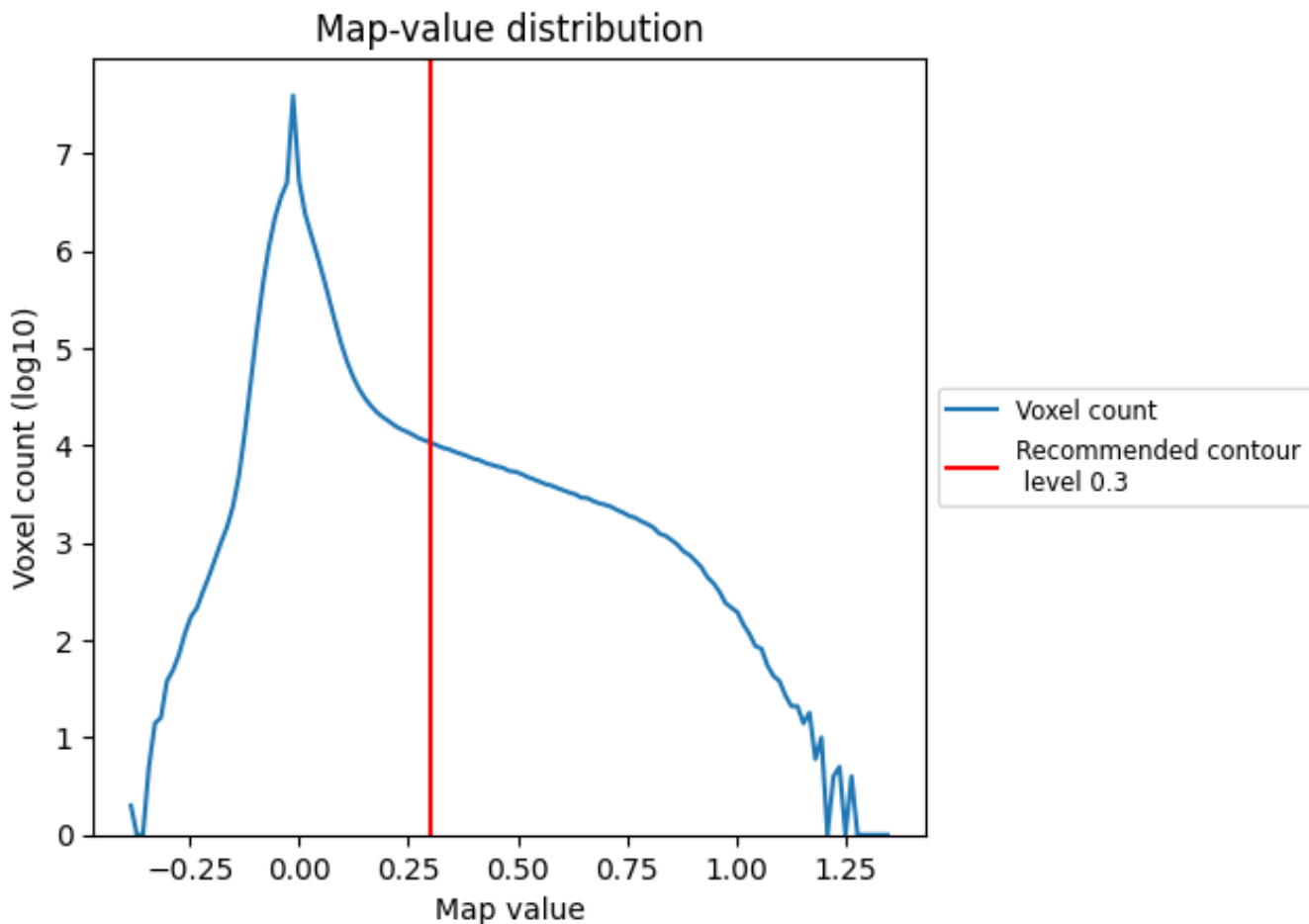
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

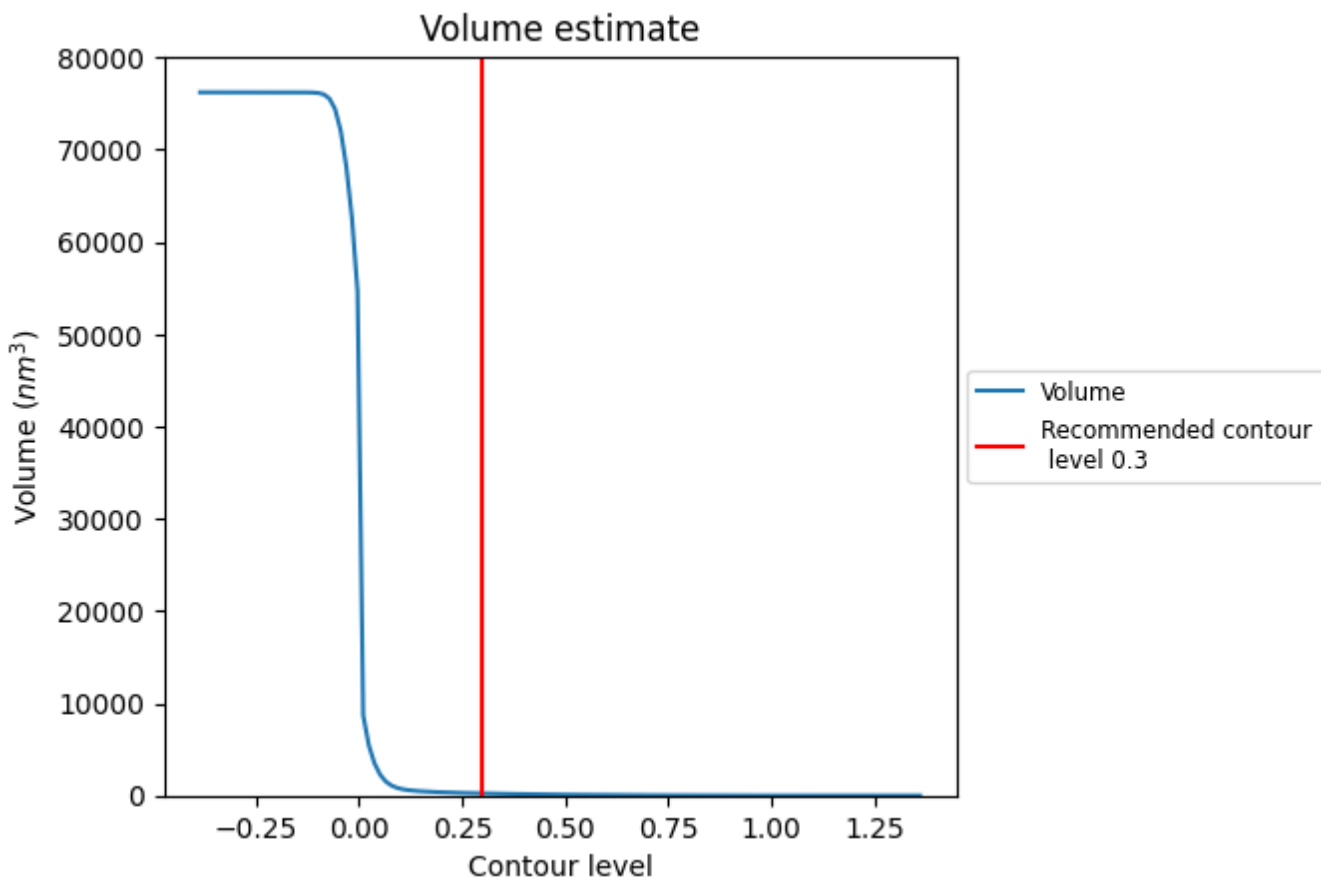
This section contains the results of statistical analysis of the map.

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.

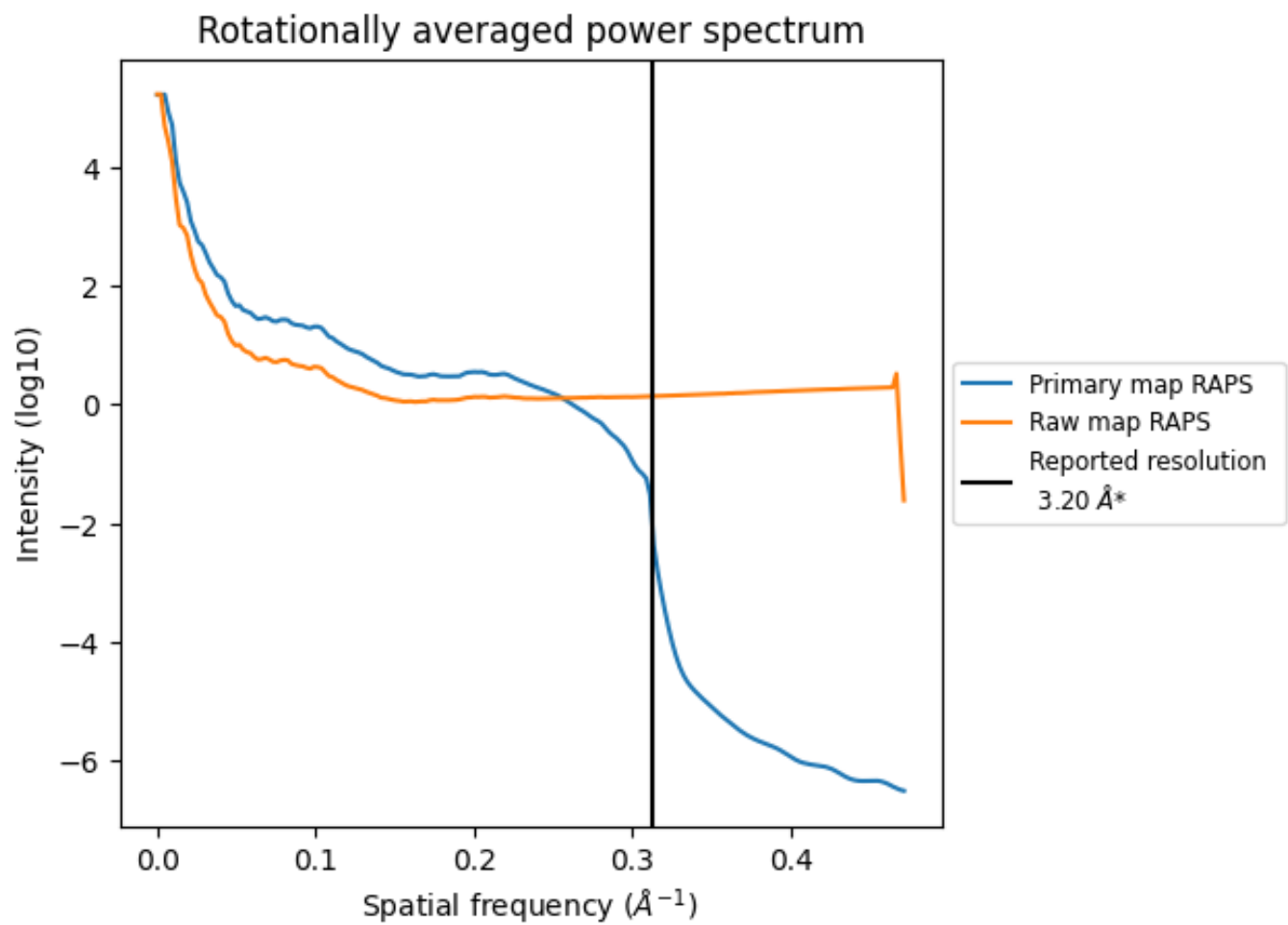
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 232 nm³; this corresponds to an approximate mass of 209 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

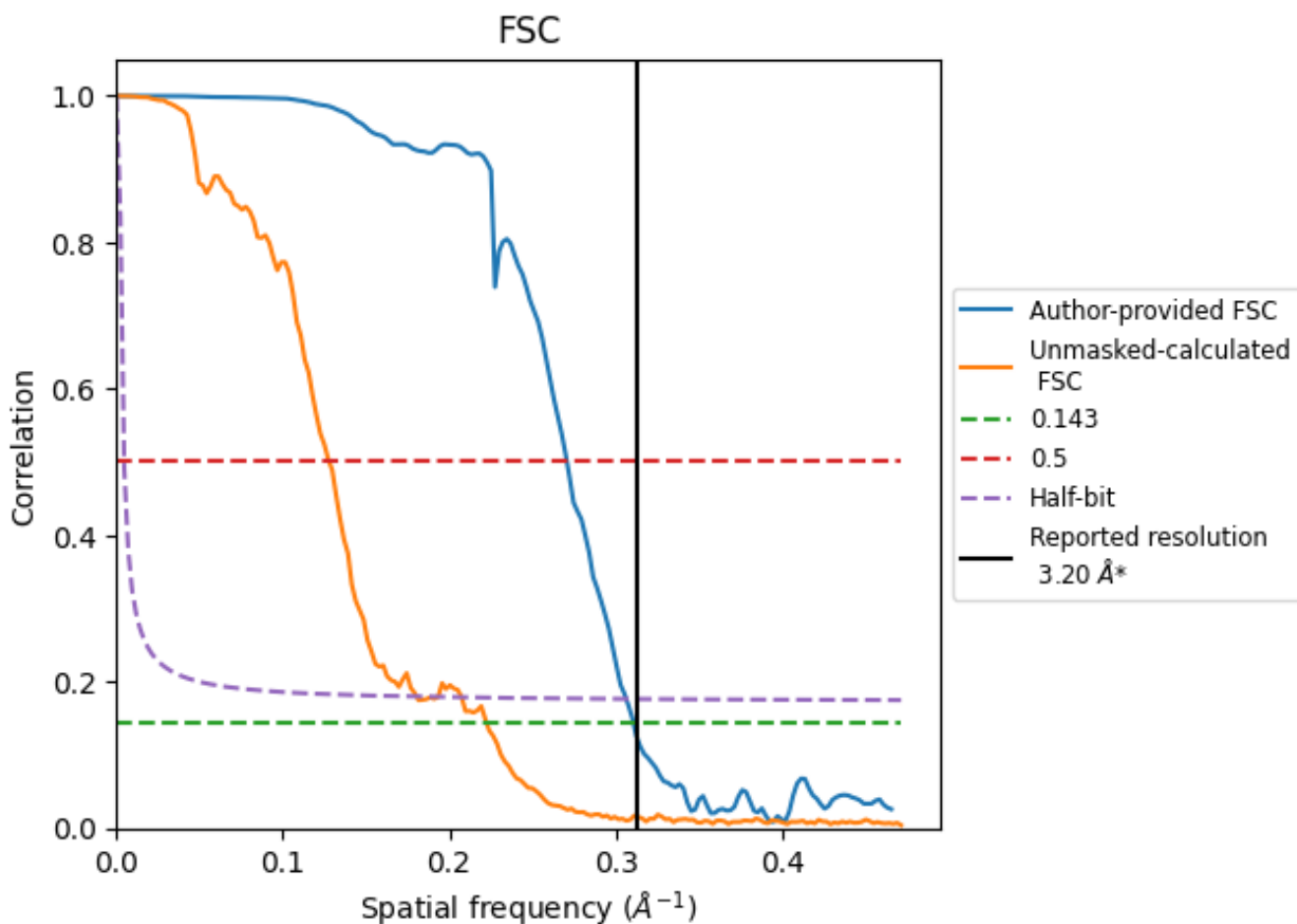


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312\AA^{-1}

8.2 Resolution estimates [i](#)

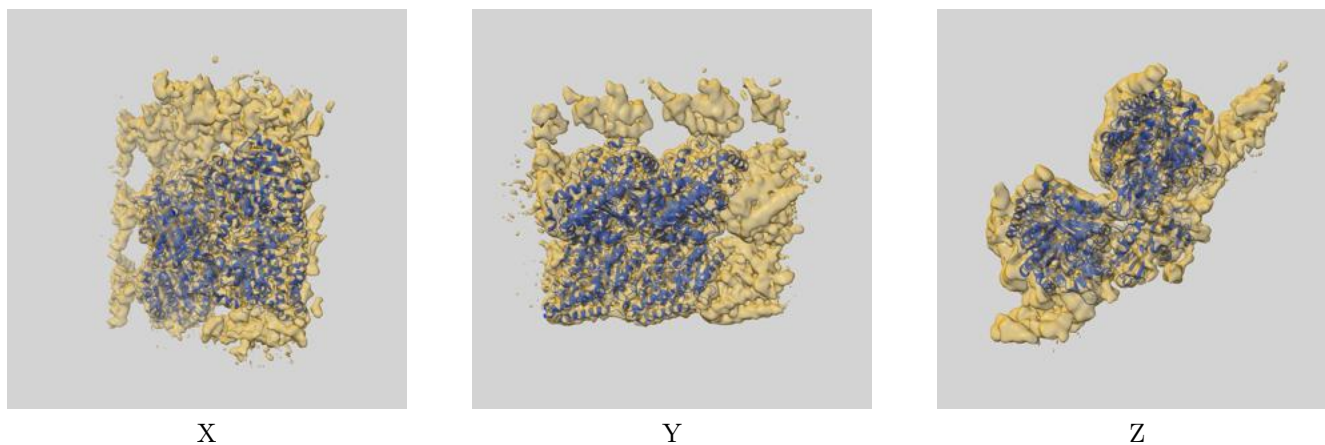
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.22	3.69	3.26
Unmasked-calculated*	4.49	7.82	5.54

*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 4.49 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

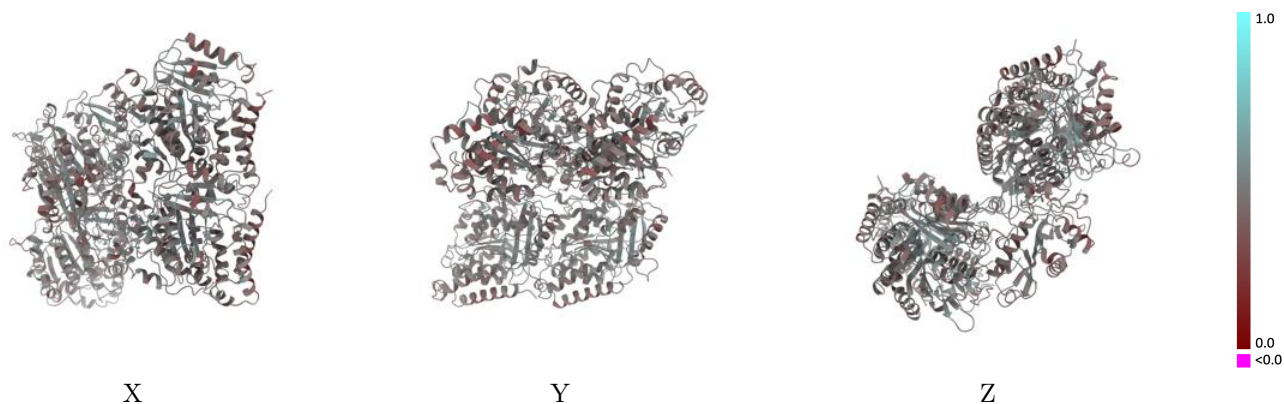
This section contains information regarding the fit between EMDB map EMD-39100 and PDB model 8YAJ. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



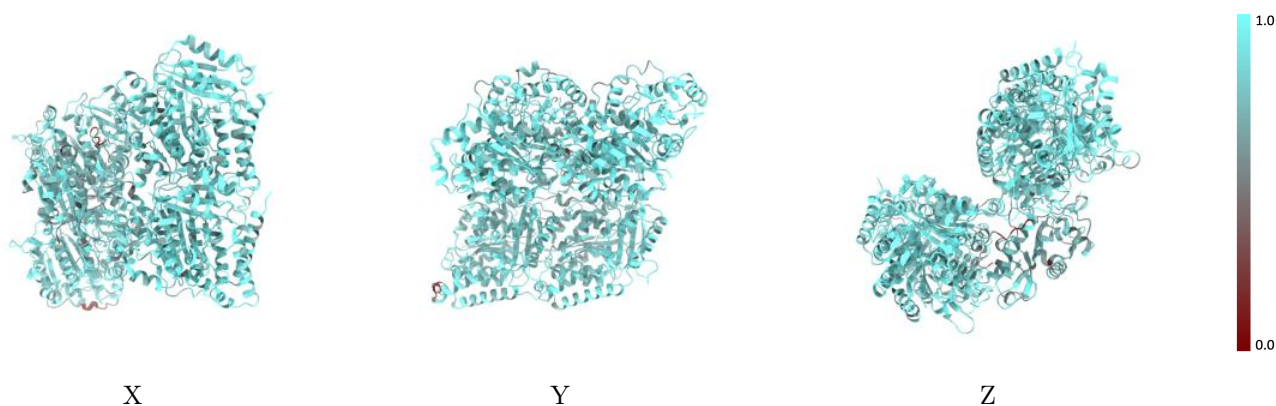
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



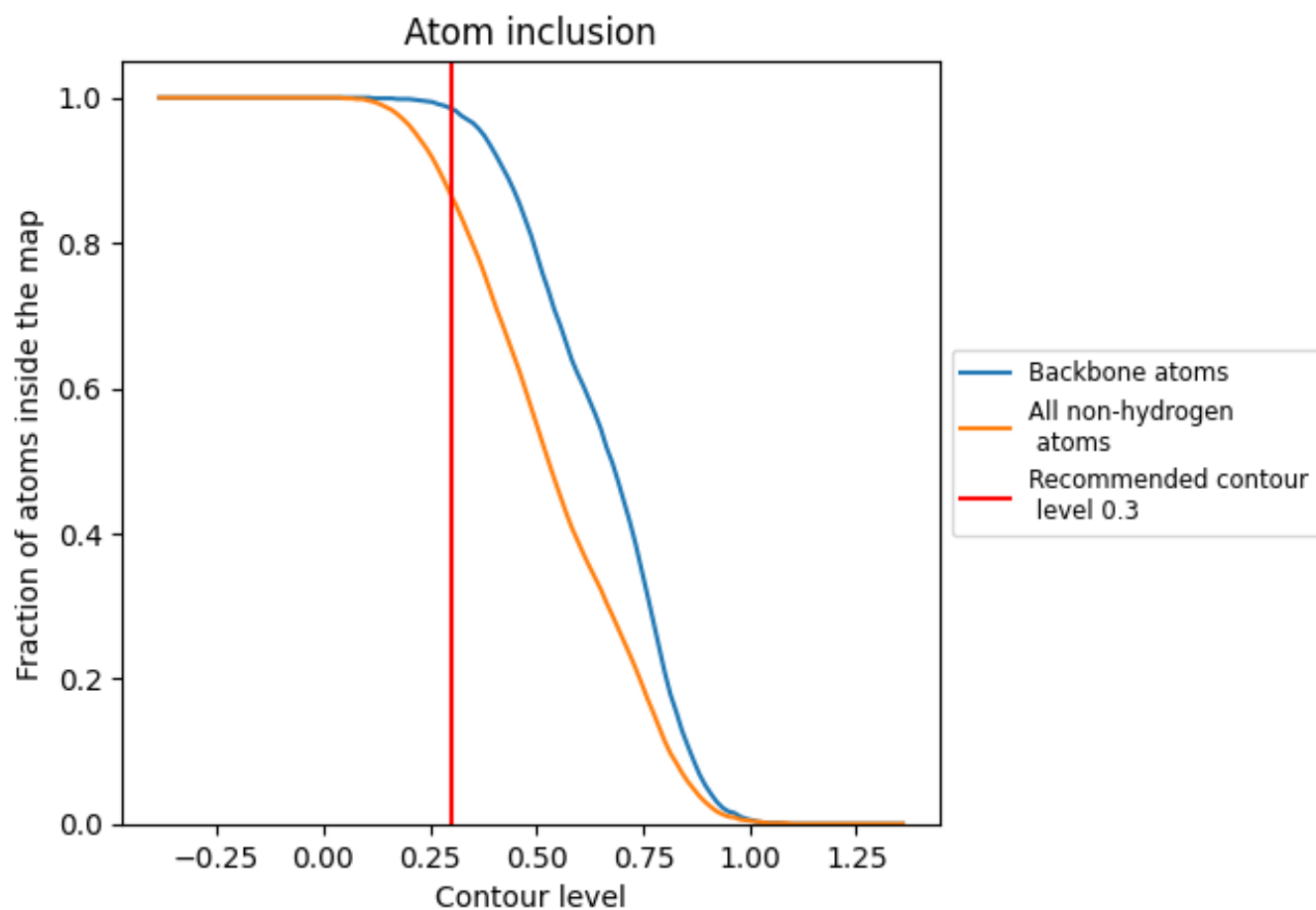
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).















9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 86% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8650	 0.4530
B	 0.8800	 0.4520
C	 0.7730	 0.4420
D	 0.8880	 0.4510
E	 0.8700	 0.4520
F	 0.8840	 0.4610
I	 0.6680	 0.4470

