



Full wwPDB EM Validation Report ⓘ

Dec 4, 2025 – 12:32 PM EST

PDB ID : 9O19 / pdb_00009o19
EMDB ID : EMD-49999
Title : Pseudomonas aeruginosa ATPase State1
Authors : Stewart, A.G.; Sobti, M.
Deposited on : 2025-04-03
Resolution : 2.00 Å(reported)

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<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.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

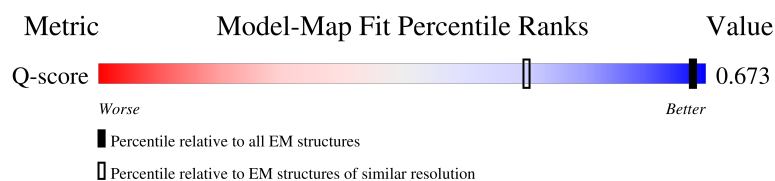
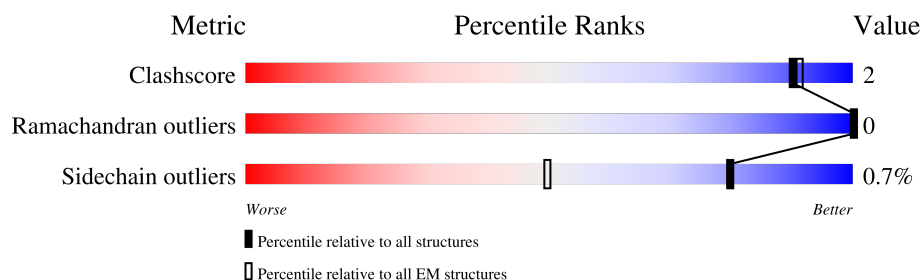
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.00 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	1659 (1.50 - 2.50)

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	A	513	 95% 5%
1	B	513	 95% 5%
1	C	513	 95% 5%
2	D	464	 94% 5%

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Mol	Chain	Length	Quality of chain
2	E	464	<div><div></div><div>90%</div><div>8%</div><div></div><div></div></div>
2	F	464	<div><div></div><div>95%</div><div></div><div></div><div></div></div>
3	G	286	<div><div>12%</div><div></div><div>92%</div><div></div><div></div><div></div><div></div></div>
4	H	141	<div><div>38%</div><div></div><div>82%</div><div></div><div>9%</div><div>9%</div><div></div></div>
5	W	178	<div><div></div><div>96%</div><div></div><div></div><div></div></div>
6	X	156	<div><div>21%</div><div></div><div>58%</div><div></div><div></div><div></div><div>39%</div></div>
6	Y	156	<div><div>7%</div><div></div><div>54%</div><div></div><div>6%</div><div></div><div>40%</div></div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 29299 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	507	Total	C	N	O	S	0	0
			3831	2409	663	746	13		
1	B	512	Total	C	N	O	S	0	0
			3872	2435	671	752	14		
1	C	509	Total	C	N	O	S	0	0
			3846	2420	666	747	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	457	Total	C	N	O	S	0	0
			3473	2194	592	675	12		
2	E	456	Total	C	N	O	S	0	0
			3464	2188	591	673	12		
2	F	456	Total	C	N	O	S	0	0
			3464	2188	591	673	12		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	expression tag	UNP A6VF32
D	2	HIS	-	expression tag	UNP A6VF32
D	3	HIS	-	expression tag	UNP A6VF32
D	4	HIS	-	expression tag	UNP A6VF32
D	5	HIS	-	expression tag	UNP A6VF32
D	6	HIS	-	expression tag	UNP A6VF32
D	7	HIS	-	expression tag	UNP A6VF32
E	1	MET	-	expression tag	UNP A6VF32
E	2	HIS	-	expression tag	UNP A6VF32
E	3	HIS	-	expression tag	UNP A6VF32
E	4	HIS	-	expression tag	UNP A6VF32
E	5	HIS	-	expression tag	UNP A6VF32
E	6	HIS	-	expression tag	UNP A6VF32

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Chain	Residue	Modelled	Actual	Comment	Reference
E	7	HIS	-	expression tag	UNP A6VF32
F	1	MET	-	expression tag	UNP A6VF32
F	2	HIS	-	expression tag	UNP A6VF32
F	3	HIS	-	expression tag	UNP A6VF32
F	4	HIS	-	expression tag	UNP A6VF32
F	5	HIS	-	expression tag	UNP A6VF32
F	6	HIS	-	expression tag	UNP A6VF32
F	7	HIS	-	expression tag	UNP A6VF32

- Molecule 3 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	276	Total	C	N	O	S	0	0
			2132	1339	381	399	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	128	Total	C	N	O	S	0	0
			933	590	159	181	3		

- Molecule 5 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	W	177	Total	C	N	O	S	0	0
			1345	840	237	266	2		

- Molecule 6 is a protein called ATP synthase subunit b.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	95	Total	C	N	O		0	0
			714	431	136	147			
6	Y	93	Total	C	N	O		0	0
			696	420	134	142			

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

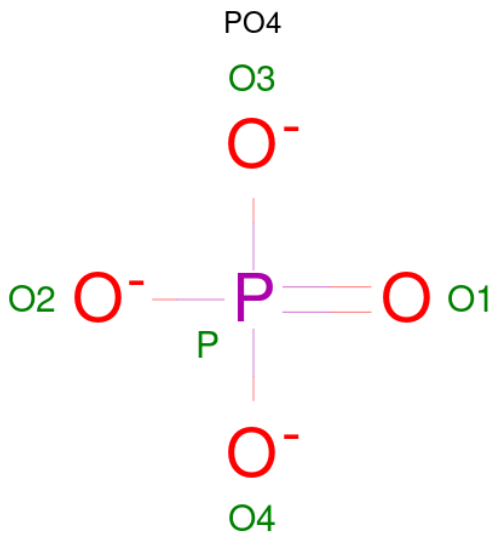
Mol	Chain	Residues	Atoms	AltConf
8	A	1	Total Mg 1 1	0
8	B	1	Total Mg 1 1	0
8	C	1	Total Mg 1 1	0
8	D	1	Total Mg 1 1	0
8	E	1	Total Mg 1 1	0

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 10 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
10	F	1	Total	O	P	0
			5	4	1	

- Molecule 11 is water.

Mol	Chain	Residues	Atoms			AltConf
11	A	161	Total	O		0
			161	161		
11	B	209	Total	O		0
			209	209		
11	C	290	Total	O		0
			290	290		
11	D	129	Total	O		0
			129	129		
11	E	230	Total	O		0
			230	230		
11	F	227	Total	O		0
			227	227		
11	G	54	Total	O		0
			54	54		
11	H	1	Total	O		0
			1	1		
11	W	43	Total	O		0
			43	43		
11	Y	1	Total	O		0
			1	1		

3 Residue-property plots [i](#)

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

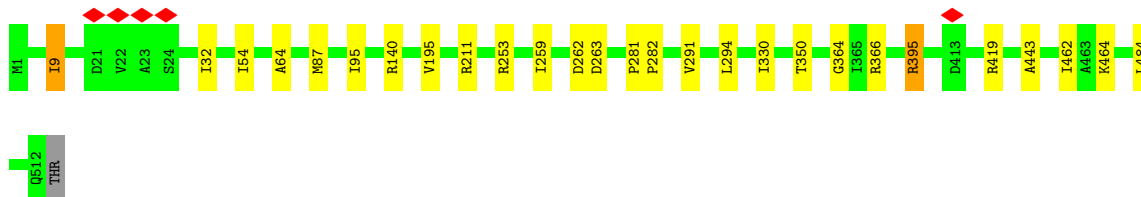
- Molecule 1: ATP synthase subunit alpha

Chain A: 



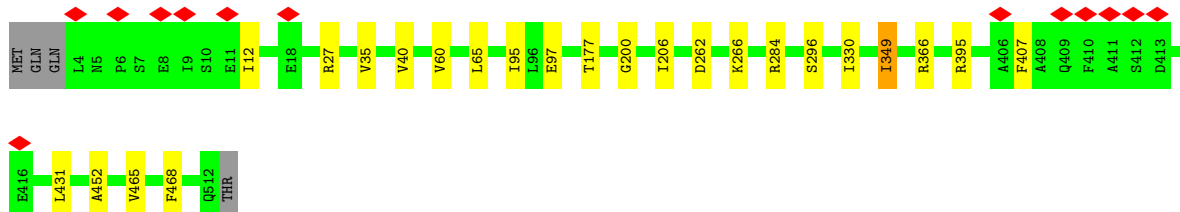
- Molecule 1: ATP synthase subunit alpha

Chain B: 



- Molecule 1: ATP synthase subunit alpha

Chain C: 

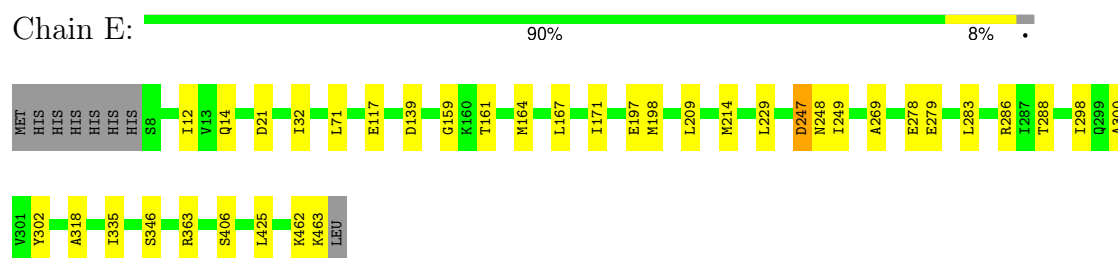


- Molecule 2: ATP synthase subunit beta

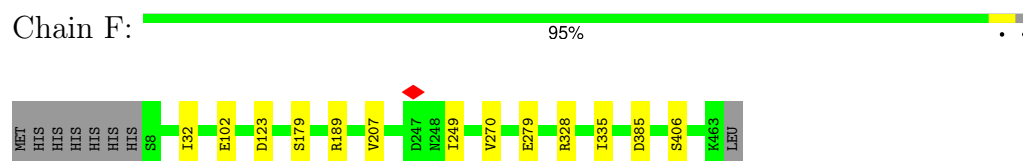
Chain D: 



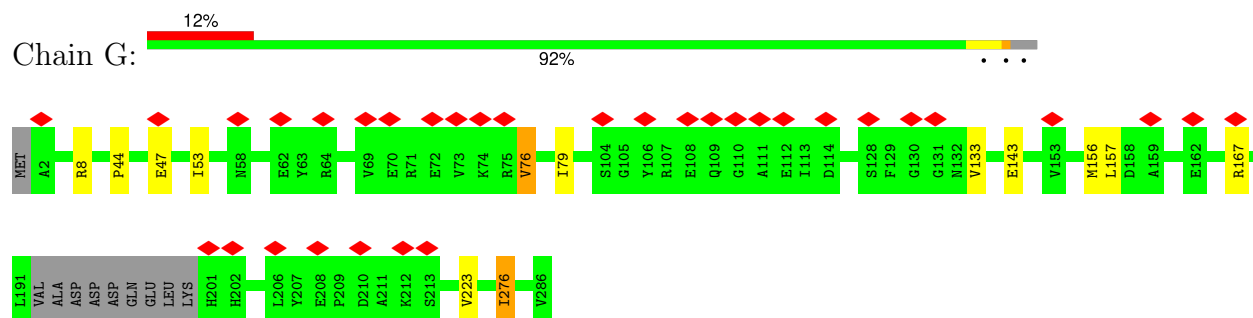
- Molecule 2: ATP synthase subunit beta



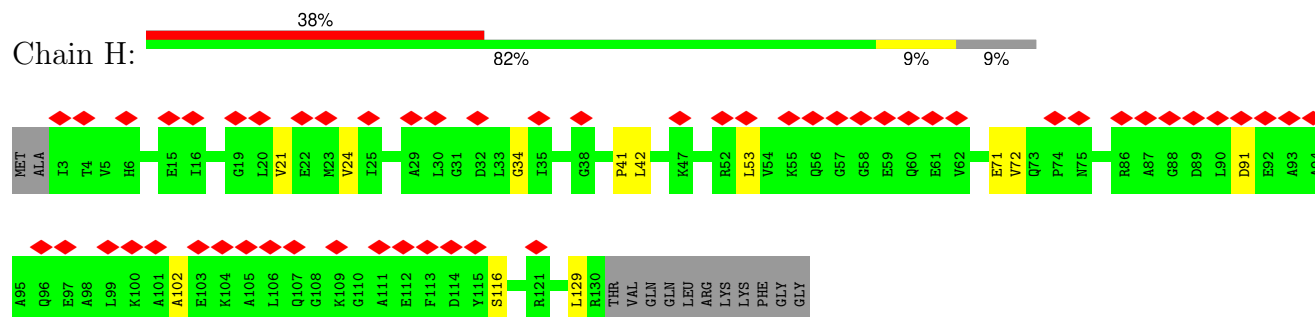
- Molecule 2: ATP synthase subunit beta



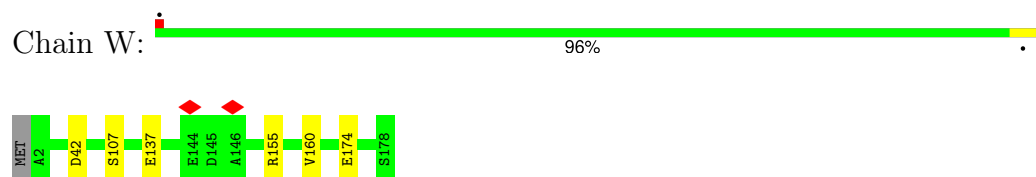
- Molecule 3: ATP synthase gamma chain



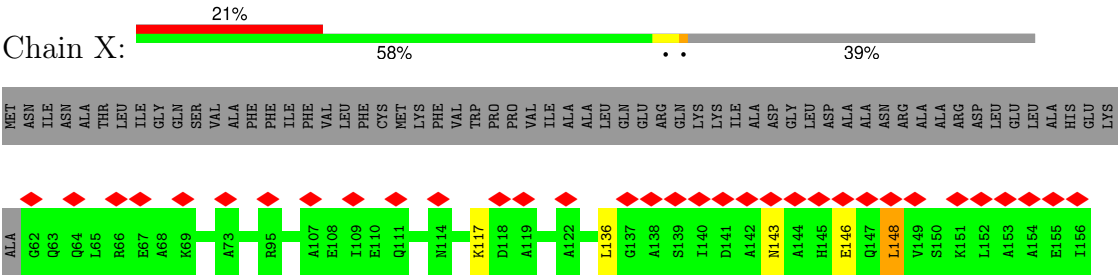
- Molecule 4: ATP synthase epsilon chain



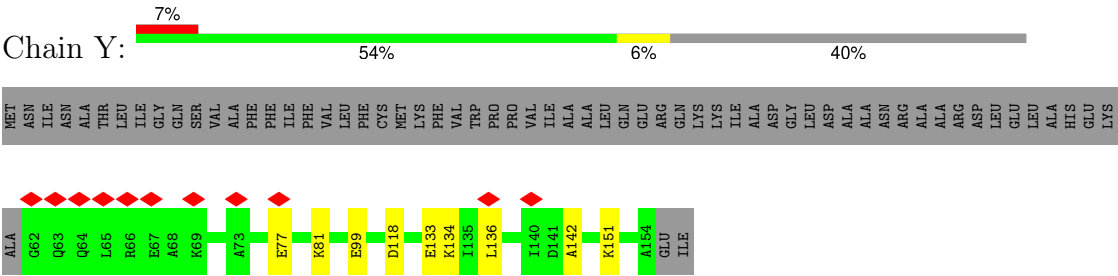
- Molecule 5: ATP synthase subunit delta



- Molecule 6: ATP synthase subunit b



• Molecule 6: ATP synthase subunit b



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	219554	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 ($e^-/\text{\AA}^2$)	65	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.716	Depositor
Minimum map value	-0.243	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.06	Depositor
Map size (\AA)	332.0, 332.0, 332.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ATP, MG, PO4

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	0.50	0/3883	0.90	1/5243 (0.0%)
1	B	0.50	0/3925	0.95	5/5301 (0.1%)
1	C	0.51	0/3899	0.91	6/5267 (0.1%)
2	D	0.54	0/3530	0.98	6/4778 (0.1%)
2	E	0.50	0/3521	0.92	8/4767 (0.2%)
2	F	0.46	0/3521	0.84	4/4767 (0.1%)
3	G	0.51	0/2161	0.85	1/2908 (0.0%)
4	H	0.38	0/946	0.81	1/1282 (0.1%)
5	W	0.47	0/1358	0.96	1/1833 (0.1%)
6	X	0.55	0/714	1.01	6/956 (0.6%)
6	Y	0.62	0/696	1.10	2/933 (0.2%)
All	All	0.50	0/28154	0.92	41/38035 (0.1%)

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	B	0	4
1	C	0	2
2	D	0	1
2	E	0	2
All	All	0	9

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	247	ASP	CA-C-N	-9.75	108.41	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	247	ASP	C-N-CA	-9.75	108.41	123.13
1	C	407	PHE	CA-CB-CG	7.84	121.64	113.80
6	X	146	GLU	CA-CB-CG	7.25	128.60	114.10
2	D	399	ARG	NE-CZ-NH2	6.55	125.10	119.20
6	X	148	LEU	CA-CB-CG	6.32	138.43	116.30
6	X	148	LEU	CA-C-N	-6.20	116.89	122.97
6	X	148	LEU	C-N-CA	-6.20	116.89	122.97
3	G	143	GLU	CA-CB-CG	6.05	126.19	114.10
1	B	95	ILE	CB-CG1-CD1	5.97	126.35	113.80
2	D	451	VAL	N-CA-C	5.79	116.54	111.56
1	B	462	ILE	N-CA-C	5.79	116.44	110.36
2	D	32	ILE	CA-C-N	5.71	130.24	122.19
2	D	32	ILE	C-N-CA	5.71	130.24	122.19
2	E	32	ILE	CA-C-N	5.68	132.16	123.47
2	E	32	ILE	C-N-CA	5.68	132.16	123.47
1	A	301	ARG	NE-CZ-NH2	5.66	124.29	119.20
1	B	395	ARG	NE-CZ-NH2	5.64	124.28	119.20
2	F	189	ARG	NE-CZ-NH2	5.63	124.27	119.20
2	F	32	ILE	CA-C-N	5.60	130.81	122.74
2	F	32	ILE	C-N-CA	5.60	130.81	122.74
2	E	248	ASN	CB-CA-C	5.49	120.46	111.23
6	Y	151	LYS	CA-CB-CG	5.47	125.05	114.10
1	B	350	THR	N-CA-C	5.42	117.08	110.41
2	F	189	ARG	CD-NE-CZ	5.39	131.95	124.40
5	W	174	GLU	CB-CG-CD	5.35	121.70	112.60
1	C	12	ILE	CA-C-N	5.30	127.73	120.46
1	C	12	ILE	C-N-CA	5.30	127.73	120.46
1	C	349	ILE	CA-C-O	-5.28	115.66	120.73
2	D	203	VAL	CA-C-N	5.28	127.88	120.28
2	D	203	VAL	C-N-CA	5.28	127.88	120.28
4	H	91	ASP	CA-CB-CG	5.26	117.86	112.60
2	E	248	ASN	CA-CB-CG	-5.24	107.36	112.60
2	E	269	ALA	CA-C-N	5.22	131.36	121.97
2	E	269	ALA	C-N-CA	5.22	131.36	121.97
6	X	117	LYS	CB-CG-CD	5.21	123.28	111.30
6	Y	99	GLU	CB-CG-CD	5.14	121.33	112.60
1	B	95	ILE	CA-CB-CG1	5.12	119.11	110.40
1	C	95	ILE	CA-C-N	5.09	129.36	121.26
1	C	95	ILE	C-N-CA	5.09	129.36	121.26
6	X	117	LYS	CA-CB-CG	5.08	124.26	114.10

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	140	ARG	Sidechain
1	B	253	ARG	Sidechain
1	B	395	ARG	Sidechain
1	B	419	ARG	Sidechain
1	C	27	ARG	Sidechain
1	C	284	ARG	Sidechain
2	D	328	ARG	Sidechain
2	E	159	GLY	Mainchain
2	E	302	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3831	0	3879	10	0
1	B	3872	0	3924	11	0
1	C	3846	0	3897	15	0
2	D	3473	0	3493	11	0
2	E	3464	0	3482	23	0
2	F	3464	0	3482	7	0
3	G	2132	0	2171	8	0
4	H	933	0	940	5	0
5	W	1345	0	1384	2	0
6	X	714	0	726	2	0
6	Y	696	0	709	5	0
7	A	31	0	12	0	0
7	B	31	0	12	0	0
7	C	31	0	12	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	1	0
8	D	1	0	0	0	0
8	E	1	0	0	0	0
9	D	27	0	12	0	0
9	E	27	0	12	3	0
9	F	27	0	12	0	0
10	F	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	161	0	0	1	0
11	B	209	0	0	3	0
11	C	290	0	0	7	0
11	D	129	0	0	3	0
11	E	230	0	0	8	0
11	F	227	0	0	4	0
11	G	54	0	0	1	0
11	H	1	0	0	0	0
11	W	43	0	0	0	0
11	Y	1	0	0	1	0
All	All	29299	0	28159	91	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 2.

All (91) 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)
2:E:279:GLU:OE2	11:E:601:HOH:O	1.82	0.97
4:H:41:PRO:HA	4:H:72:VAL:O	1.78	0.84
2:D:248:ASN:ND2	11:D:602:HOH:O	2.10	0.83
2:F:123:ASP:OD2	11:F:601:HOH:O	1.96	0.83
1:C:296:SER:HB2	2:E:214:MET:HE3	1.61	0.81
2:D:314:ALA:O	11:D:601:HOH:O	1.99	0.81
2:E:318:ALA:N	11:E:602:HOH:O	2.09	0.80
1:C:349:ILE:HG23	2:E:214:MET:HE1	1.64	0.80
2:E:247:ASP:O	2:E:300:ALA:HB3	1.84	0.77
2:E:164:MET:HE2	2:E:298:ILE:HG22	1.67	0.75
1:C:177:THR:OG1	8:C:602:MG:MG	1.30	0.73
1:C:465:VAL:O	1:C:468:PHE:HB3	1.89	0.72
3:G:8:ARG:CZ	11:G:301:HOH:O	2.39	0.70
2:E:197:GLU:OE2	11:E:603:HOH:O	2.13	0.65
2:E:288:THR:HG23	11:E:792:HOH:O	1.96	0.65
2:F:328:ARG:HG3	11:F:652:HOH:O	2.01	0.61
2:D:254:LEU:O	2:D:257:THR:HB	2.05	0.56
2:E:278:GLU:OE2	11:E:604:HOH:O	2.18	0.56
1:B:211:ARG:NH1	11:B:706:HOH:O	2.40	0.54
9:E:501:ADP:O1B	11:E:605:HOH:O	2.18	0.53
2:F:279:GLU:HG3	11:F:800:HOH:O	2.09	0.52
1:B:291:VAL:O	1:B:294:LEU:HB3	2.10	0.52
1:A:295:HIS:CD2	11:A:773:HOH:O	2.64	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:11:ARG:NH1	11:D:610:HOH:O	2.43	0.51
1:C:60:VAL:HG13	11:C:938:HOH:O	2.10	0.50
1:C:366:ARG:HB2	11:C:717:HOH:O	2.12	0.50
6:X:136:LEU:HD11	6:Y:142:ALA:HB1	1.94	0.49
2:D:143:PRO:HG2	2:D:348:GLN:HB2	1.94	0.49
2:E:198:MET:HE1	2:E:209:LEU:HD21	1.94	0.49
2:E:161:THR:HG21	11:E:618:HOH:O	2.12	0.49
2:E:249:ILE:HD11	2:E:283:LEU:HD21	1.94	0.48
5:W:155:ARG:HG3	5:W:160:VAL:HG22	1.95	0.48
6:Y:133:GLU:HG3	6:Y:136:LEU:HD12	1.96	0.48
1:A:172:ARG:HB3	1:A:332:GLU:OE1	2.13	0.48
1:C:97:GLU:HG2	11:C:768:HOH:O	2.13	0.48
1:B:9:ILE:HG23	11:B:702:HOH:O	2.13	0.48
2:D:11:ARG:NH2	2:D:70:GLY:HA2	2.29	0.48
2:E:14:GLN:HB3	2:E:21:ASP:HB2	1.96	0.47
3:G:157:LEU:HD21	3:G:223:VAL:HG11	1.95	0.47
3:G:44:PRO:HA	3:G:47:GLU:HG2	1.96	0.47
1:A:262:ASP:HA	1:A:330:ILE:HD12	1.97	0.47
2:E:161:THR:HG22	9:E:501:ADP:O1A	2.14	0.47
6:Y:118:ASP:OD2	11:Y:201:HOH:O	2.20	0.47
1:A:334:GLN:HB3	2:D:309:THR:HB	1.97	0.47
1:B:443:ALA:HB1	1:B:484:LEU:HD22	1.96	0.47
1:A:200:GLY:HA3	1:A:266:LYS:HD2	1.96	0.46
1:B:262:ASP:HA	1:B:330:ILE:HD12	1.98	0.46
1:B:464:LYS:NZ	11:B:713:HOH:O	2.48	0.46
1:C:262:ASP:HA	1:C:330:ILE:HD12	1.97	0.46
1:B:195:VAL:O	1:B:259:ILE:HA	2.15	0.45
3:G:76:VAL:HG12	3:G:167:ARG:HB2	1.98	0.45
1:A:263:ASP:OD1	1:A:265:SER:HB2	2.16	0.45
2:D:259:VAL:HG12	2:D:263:LEU:HG	1.99	0.45
2:D:130:LEU:HD11	2:D:143:PRO:HB2	1.98	0.45
1:C:206:ILE:HD11	11:C:776:HOH:O	2.17	0.45
1:C:395:ARG:HB3	11:C:965:HOH:O	2.17	0.44
2:E:167:LEU:O	2:E:171:ILE:HB	2.17	0.44
1:C:395:ARG:CB	11:C:965:HOH:O	2.66	0.43
1:B:54:ILE:HD11	1:B:64:ALA:HB2	2.01	0.43
1:C:200:GLY:HA3	1:C:266:LYS:HD3	2.01	0.42
2:F:179:SER:O	2:F:207:VAL:HA	2.18	0.42
2:F:335:ILE:HG23	2:F:406:SER:HB2	2.01	0.42
1:B:32:ILE:HD12	1:B:87:MET:HB2	2.01	0.42
2:E:117:GLU:OE1	11:E:606:HOH:O	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Y:81:LYS:HB2	6:Y:81:LYS:HE3	1.89	0.42
6:X:143:ASN:HD21	6:Y:134:LYS:HG2	1.84	0.42
2:E:161:THR:HG22	9:E:501:ADP:PA	2.59	0.42
2:E:462:LYS:C	2:E:463:LYS:HG2	2.43	0.42
1:A:138:ILE:HG21	2:F:102:GLU:HG2	2.02	0.42
1:C:177:THR:HB	11:C:739:HOH:O	2.19	0.42
3:G:133:VAL:HG13	4:H:102:ALA:HB1	2.02	0.42
4:H:21:VAL:HG11	4:H:53:LEU:HD23	2.01	0.42
1:A:95:ILE:C	1:A:95:ILE:HD12	2.45	0.41
2:E:335:ILE:HG23	2:E:406:SER:HB3	2.02	0.41
1:A:284:ARG:HA	3:G:276:ILE:HD11	2.02	0.41
4:H:24:VAL:O	4:H:34:GLY:HA2	2.21	0.41
1:A:347:ILE:HG12	1:A:353:GLN:HG2	2.02	0.41
1:B:364:GLY:HA2	2:E:363:ARG:HH11	1.84	0.41
4:H:42:LEU:O	4:H:71:GLU:HA	2.20	0.41
2:E:229:LEU:HD21	2:E:286:ARG:HB2	2.02	0.41
2:F:249:ILE:HG23	11:F:644:HOH:O	2.20	0.41
2:E:12:ILE:HD12	2:E:71:LEU:HB2	2.03	0.41
3:G:79:ILE:HD11	3:G:156:MET:HG2	2.03	0.41
1:B:281:PRO:HA	1:B:282:PRO:HD3	2.01	0.40
5:W:107:SER:HA	5:W:137:GLU:O	2.21	0.40
2:D:88:THR:HB	2:D:93:MET:HE1	2.04	0.40
2:D:372:TYR:HD1	2:D:395:VAL:HG22	1.86	0.40
3:G:53:ILE:HD13	3:G:53:ILE:HA	1.96	0.40
1:C:35:VAL:HG22	1:C:40:VAL:HG22	2.04	0.40
1:C:431:LEU:HD22	1:C:452:ALA:HB2	2.03	0.40
2:E:139:ASP:HB3	2:E:425:LEU:HD13	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	A	505/513 (98%)	499 (99%)	6 (1%)	0	100	100
1	B	510/513 (99%)	499 (98%)	11 (2%)	0	100	100
1	C	507/513 (99%)	496 (98%)	11 (2%)	0	100	100
2	D	455/464 (98%)	448 (98%)	7 (2%)	0	100	100
2	E	454/464 (98%)	442 (97%)	12 (3%)	0	100	100
2	F	454/464 (98%)	445 (98%)	9 (2%)	0	100	100
3	G	272/286 (95%)	270 (99%)	2 (1%)	0	100	100
4	H	126/141 (89%)	124 (98%)	2 (2%)	0	100	100
5	W	175/178 (98%)	175 (100%)	0	0	100	100
6	X	93/156 (60%)	93 (100%)	0	0	100	100
6	Y	91/156 (58%)	90 (99%)	1 (1%)	0	100	100
All	All	3642/3848 (95%)	3581 (98%)	61 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	399/405 (98%)	396 (99%)	3 (1%)	79	84
1	B	404/405 (100%)	401 (99%)	3 (1%)	81	86
1	C	401/405 (99%)	400 (100%)	1 (0%)	92	94
2	D	369/376 (98%)	367 (100%)	2 (0%)	86	90
2	E	368/376 (98%)	367 (100%)	1 (0%)	91	94
2	F	368/376 (98%)	366 (100%)	2 (0%)	86	90
3	G	226/235 (96%)	224 (99%)	2 (1%)	75	81
4	H	91/101 (90%)	89 (98%)	2 (2%)	47	51
5	W	141/142 (99%)	140 (99%)	1 (1%)	81	86
6	X	69/117 (59%)	68 (99%)	1 (1%)	62	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	Y	67/117 (57%)	66 (98%)	1 (2%)	60	66
All	All	2903/3055 (95%)	2884 (99%)	19 (1%)	80	86

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ILE
1	A	394	ILE
1	A	461	GLU
1	B	9	ILE
1	B	263	ASP
1	B	366	ARG
1	C	65	LEU
2	D	270	VAL
2	D	378	ILE
2	E	346	SER
2	F	270	VAL
2	F	385	ASP
3	G	76	VAL
3	G	276	ILE
4	H	116	SER
4	H	129	LEU
5	W	42	ASP
6	X	148	LEU
6	Y	77	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	145	GLN
1	A	295	HIS
1	A	480	HIS
1	B	145	GLN
1	B	334	GLN
1	C	66	ASN
1	C	203	GLN
2	D	128	ASN
2	D	196	HIS
2	D	348	GLN
2	D	370	GLN

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Mol	Chain	Res	Type
2	E	14	GLN
2	E	124	GLN
2	E	175	HIS
2	E	192	ASN
2	E	220	ASN
2	F	72	ASN
2	F	284	GLN
2	F	299	GLN
2	F	442	HIS
3	G	60	ASN
3	G	147	ASN
3	G	187	GLN
3	G	261	GLN
3	G	274	GLN
4	H	6	HIS
4	H	128	GLN
5	W	40	GLN
5	W	71	ASN
6	X	147	GLN
6	Y	63	GLN
6	Y	145	HIS

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 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 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	ATP	C	601	8	28,33,33	1.03	2 (7%)	34,52,52	0.70	1 (2%)
7	ATP	A	601	8	28,33,33	0.79	1 (3%)	34,52,52	0.69	1 (2%)
10	PO4	F	502	-	4,4,4	0.83	0	6,6,6	0.49	0
9	ADP	F	501	-	24,29,29	0.99	2 (8%)	29,45,45	1.14	2 (6%)
9	ADP	D	501	8	24,29,29	0.80	0	29,45,45	0.77	1 (3%)
7	ATP	B	601	8	28,33,33	0.82	1 (3%)	34,52,52	0.71	1 (2%)
9	ADP	E	501	8	24,29,29	0.83	0	29,45,45	0.75	1 (3%)

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	ATP	C	601	8	-	2/18/38/38	0/3/3/3
7	ATP	A	601	8	-	3/18/38/38	0/3/3/3
9	ADP	F	501	-	-	1/12/32/32	0/3/3/3
9	ADP	D	501	8	-	3/12/32/32	0/3/3/3
7	ATP	B	601	8	-	3/18/38/38	0/3/3/3
9	ADP	E	501	8	-	2/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	601	ATP	PB-O3B	-3.01	1.56	1.59
7	C	601	ATP	PA-O3A	-2.97	1.56	1.59
7	B	601	ATP	PB-O3B	-2.59	1.56	1.59
9	F	501	ADP	PA-O3A	2.34	1.62	1.59
7	A	601	ATP	PB-O3B	-2.04	1.57	1.59
9	F	501	ADP	O4'-C1'	2.01	1.43	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	501	ADP	N3-C2-N1	-4.09	123.13	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	501	ADP	C5-C6-N6	2.42	123.99	120.31
9	F	501	ADP	C4-C5-N7	-2.35	106.85	109.34
9	D	501	ADP	C5-C6-N6	2.35	123.89	120.31
7	B	601	ATP	C5-C6-N6	2.22	123.69	120.31
7	A	601	ATP	C5-C6-N6	2.19	123.65	120.31
7	C	601	ATP	C5-C6-N6	2.17	123.62	120.31

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	601	ATP	PB-O3B-PG-O2G
7	C	601	ATP	PB-O3B-PG-O2G
9	D	501	ADP	PA-O3A-PB-O3B
9	F	501	ADP	C5'-O5'-PA-O1A
7	A	601	ATP	O4'-C4'-C5'-O5'
7	A	601	ATP	C3'-C4'-C5'-O5'
9	D	501	ADP	PA-O3A-PB-O2B
9	E	501	ADP	PA-O3A-PB-O2B
9	E	501	ADP	PA-O3A-PB-O3B
7	B	601	ATP	PB-O3B-PG-O1G
7	C	601	ATP	PB-O3B-PG-O1G
9	D	501	ADP	PA-O3A-PB-O1B
7	B	601	ATP	PB-O3B-PG-O3G
7	A	601	ATP	PB-O3A-PA-O2A

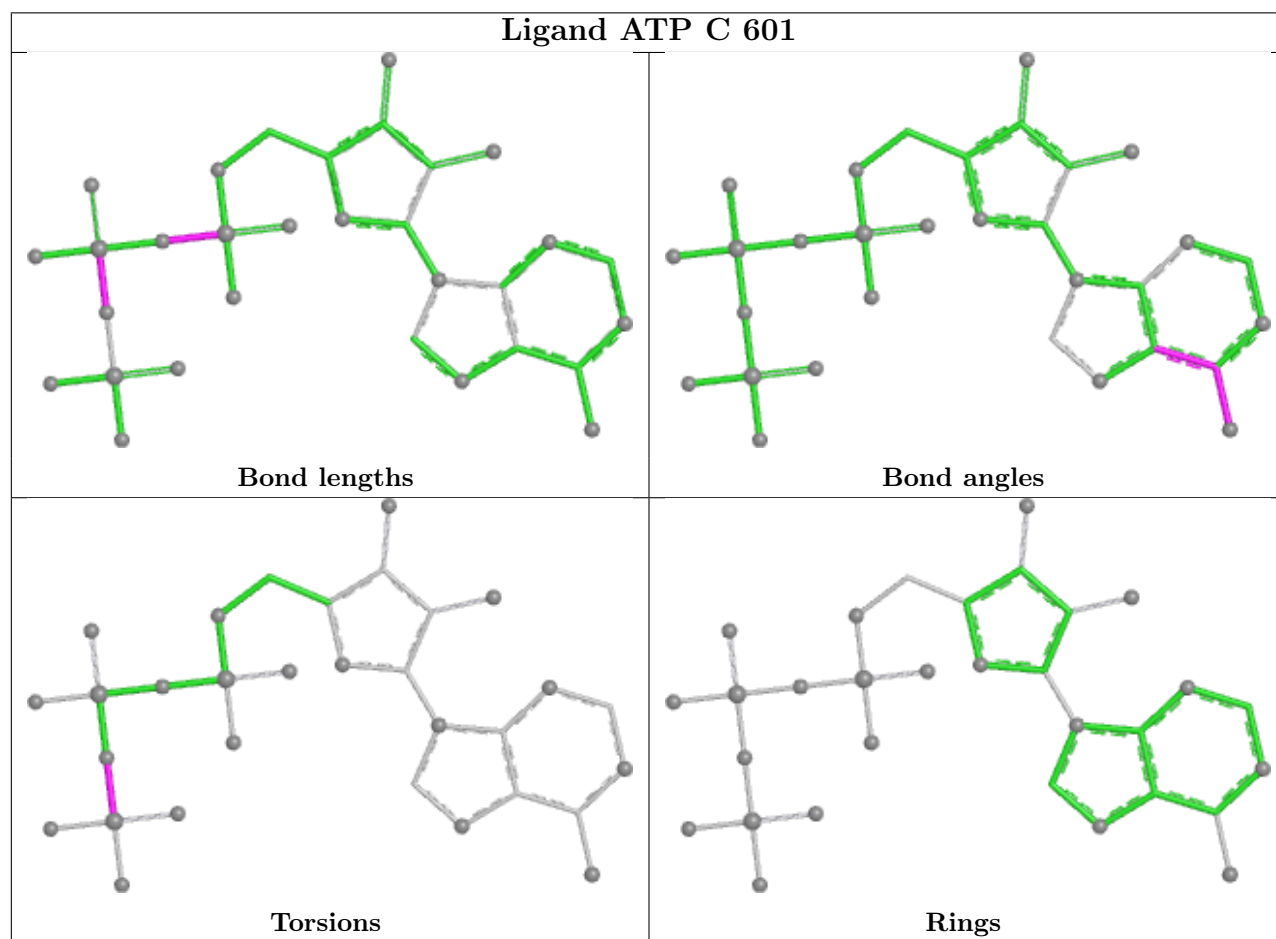
There are no ring outliers.

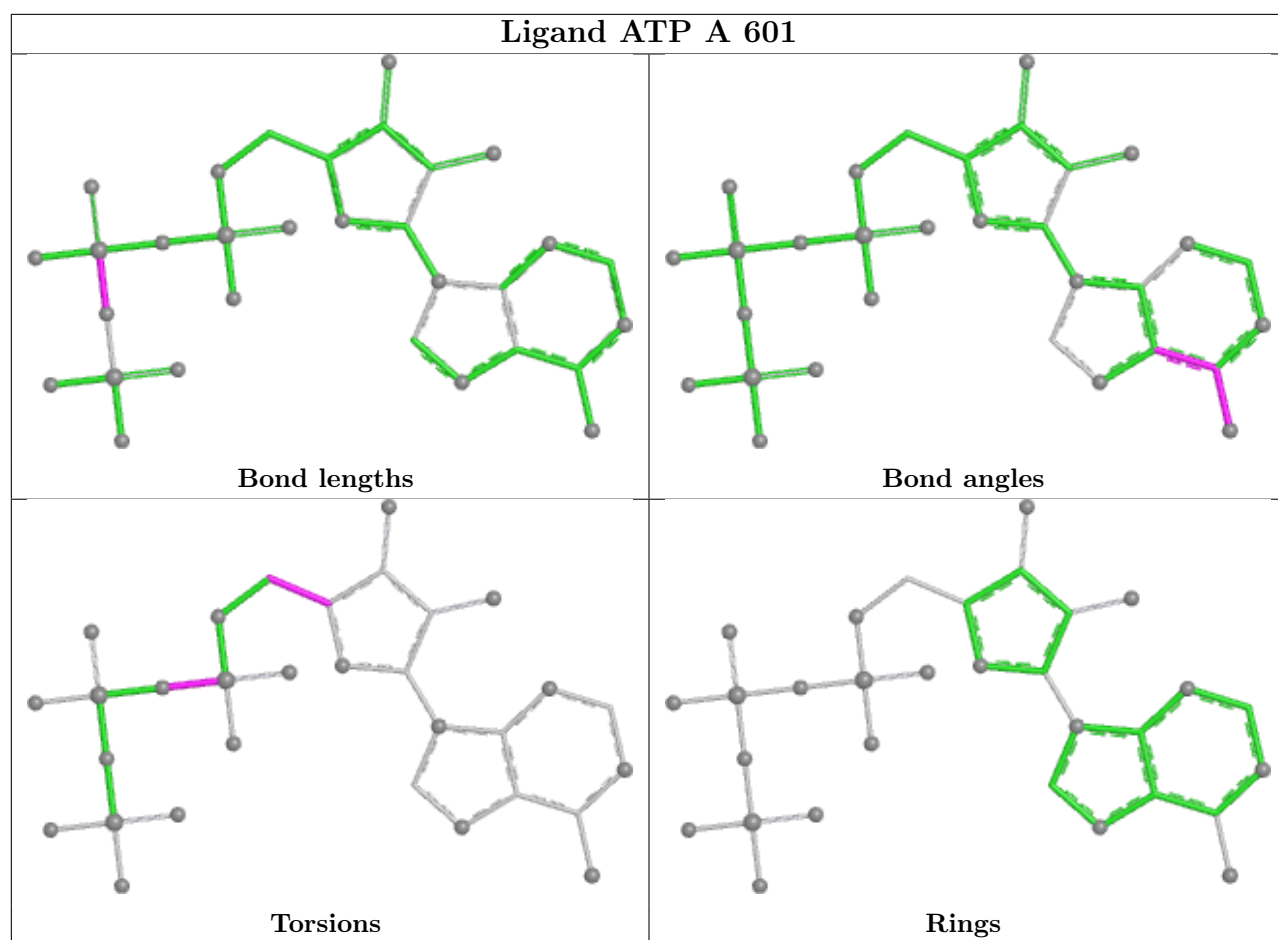
1 monomer is involved in 3 short contacts:

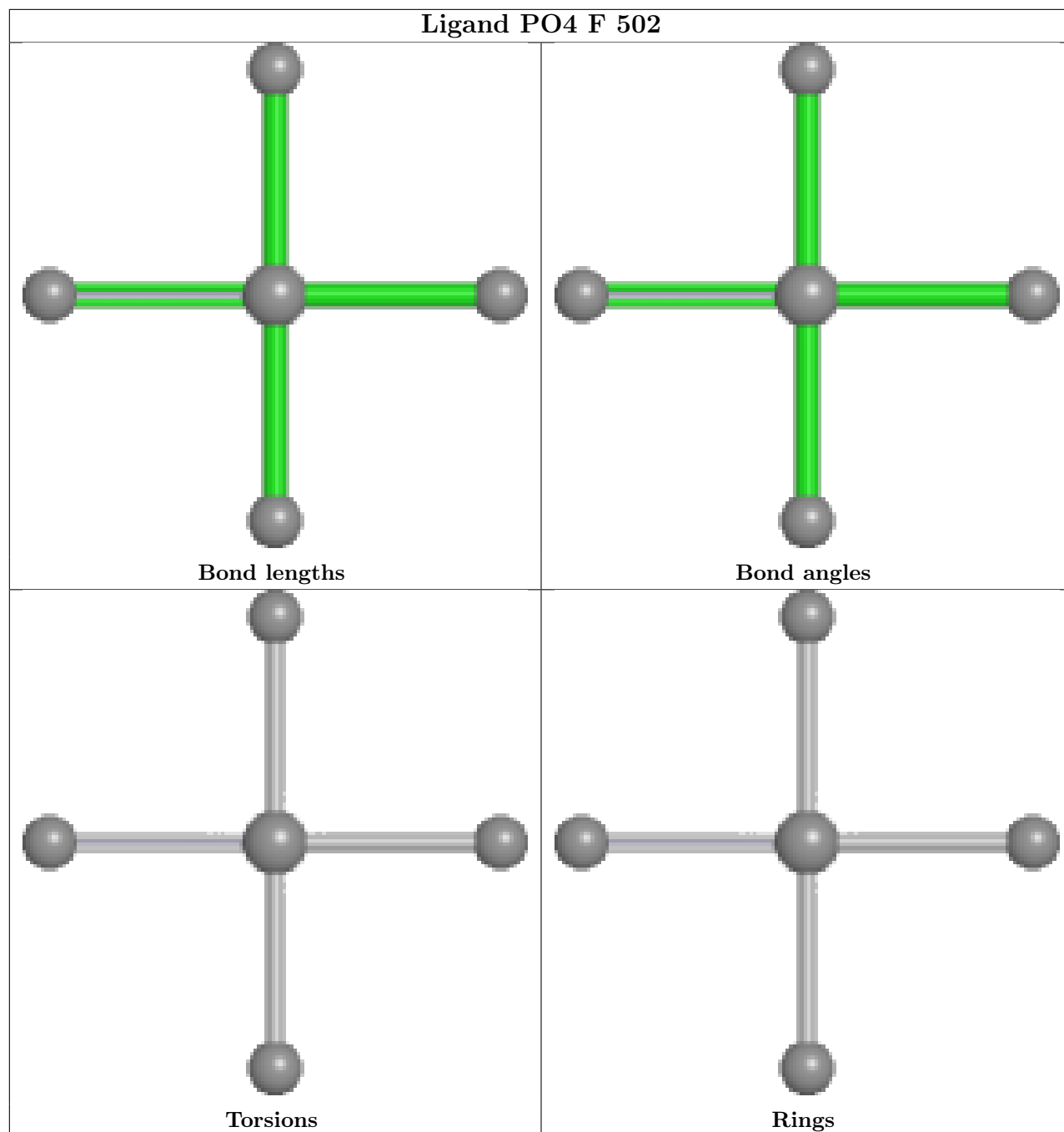
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	E	501	ADP	3	0

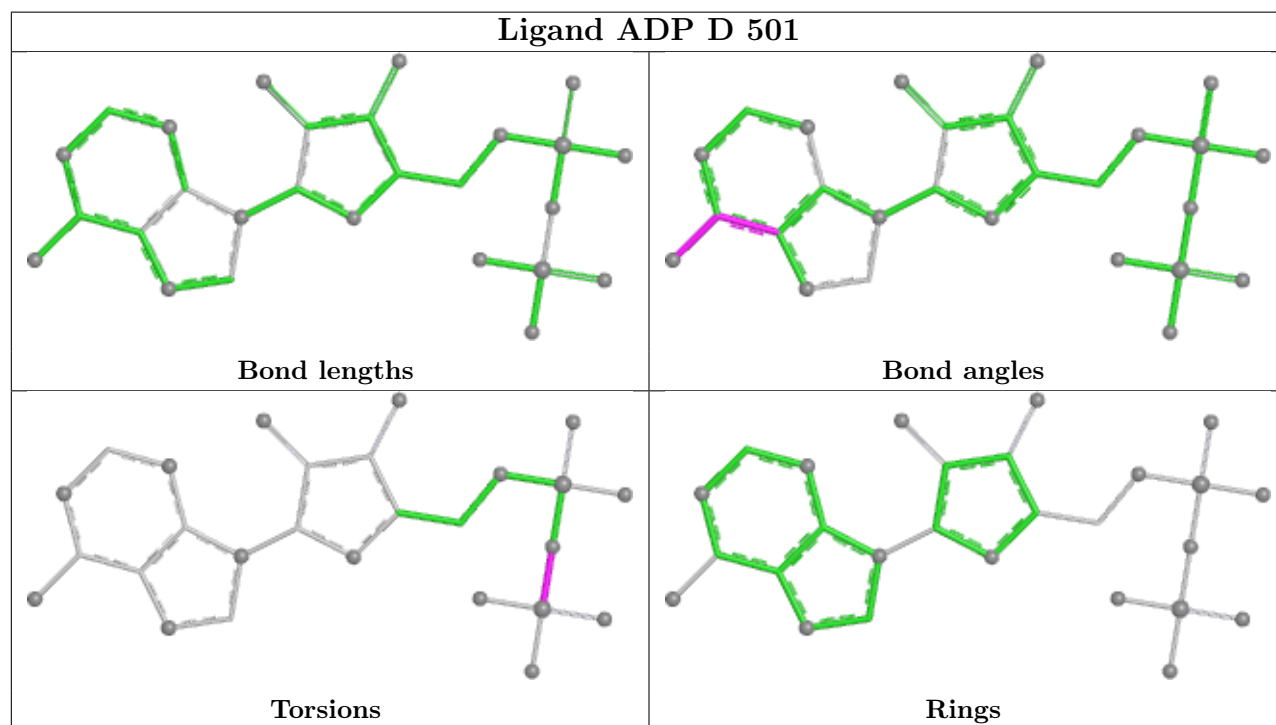
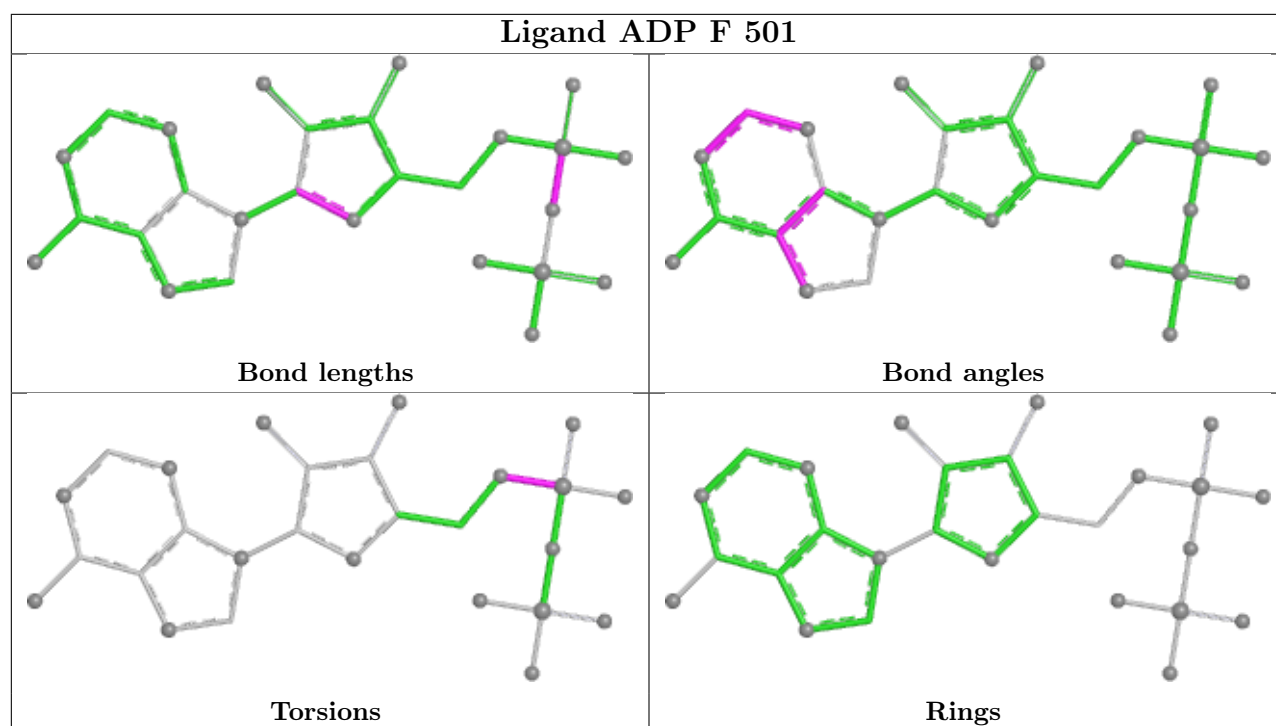
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

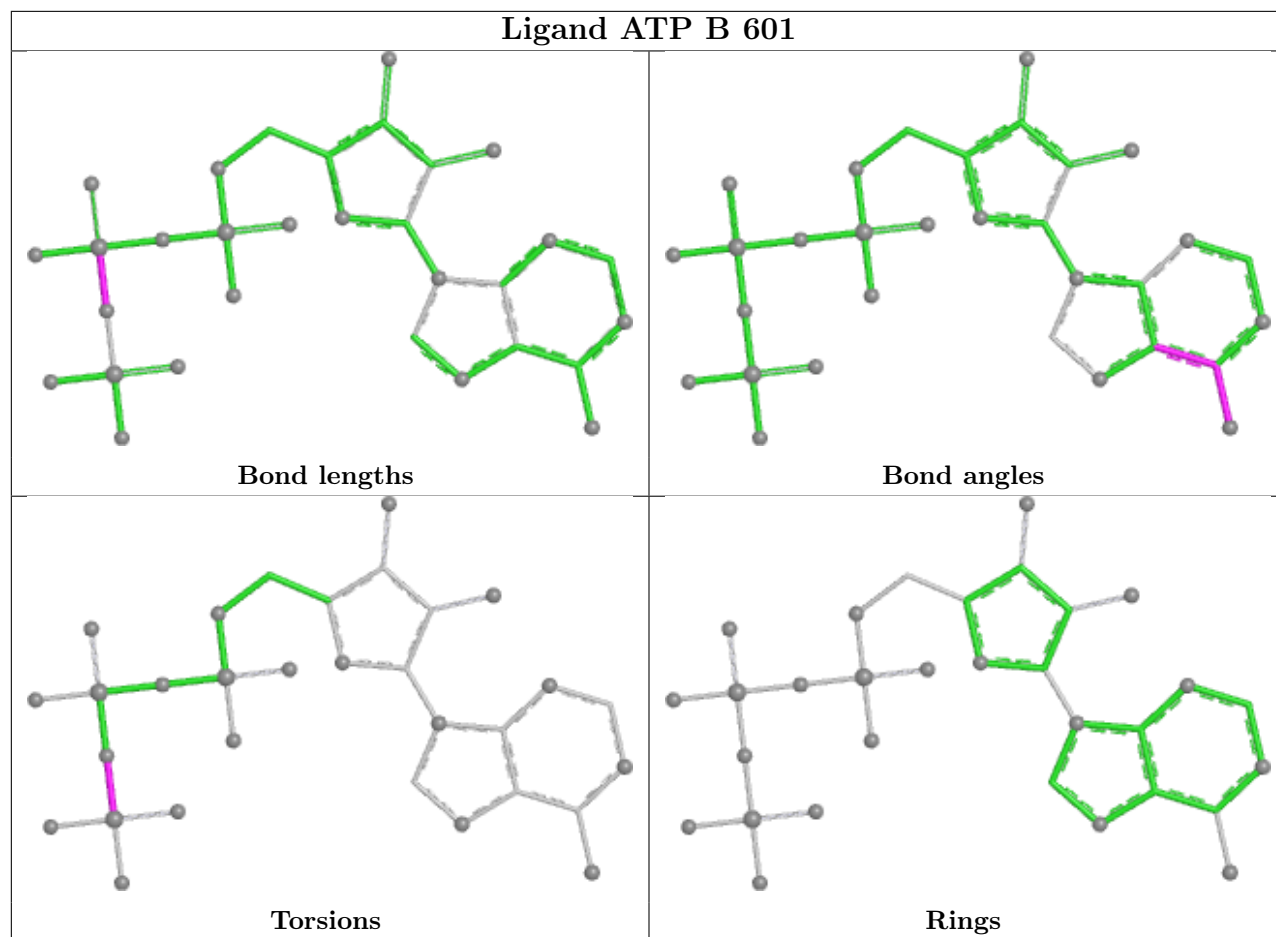




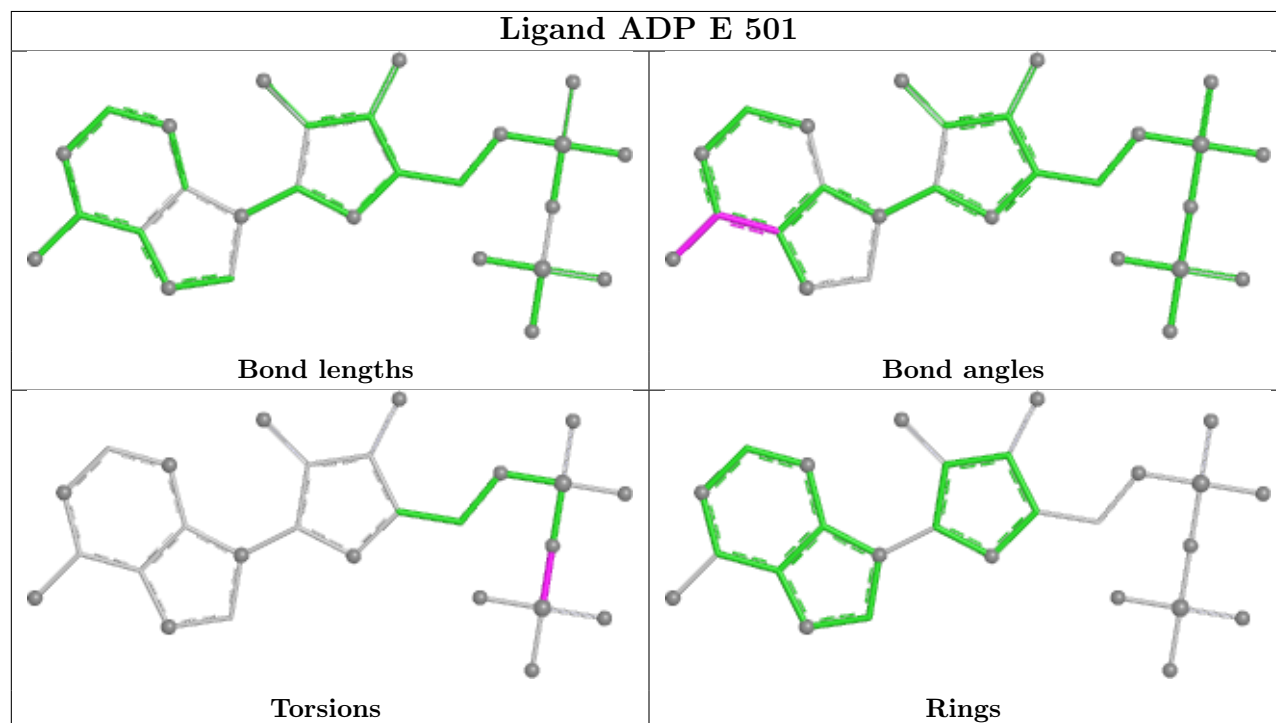




Ligand ATP B 601



Ligand ADP E 501



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

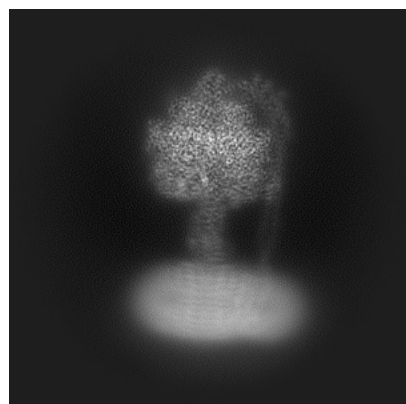
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49999. These allow visual inspection of the internal detail of the map and identification of artifacts.

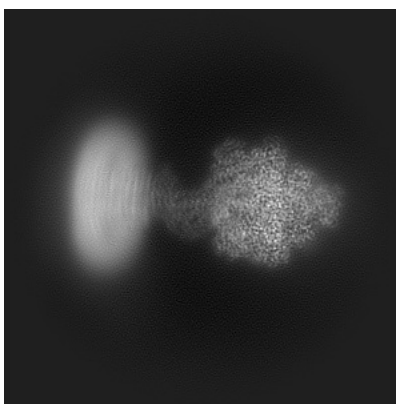
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

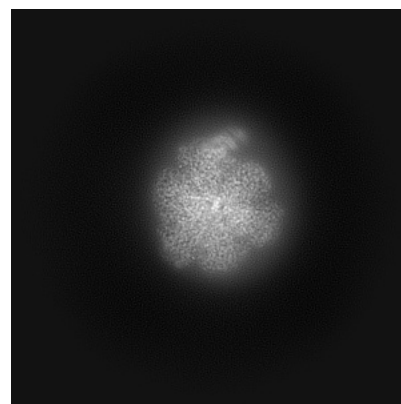
6.1.1 Primary map



X

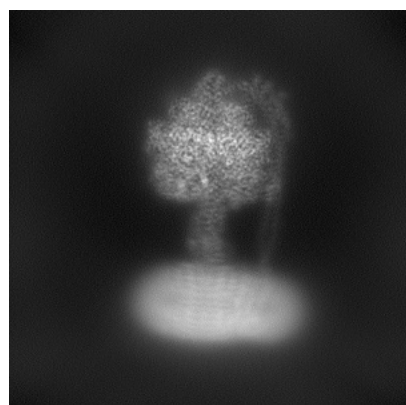


Y

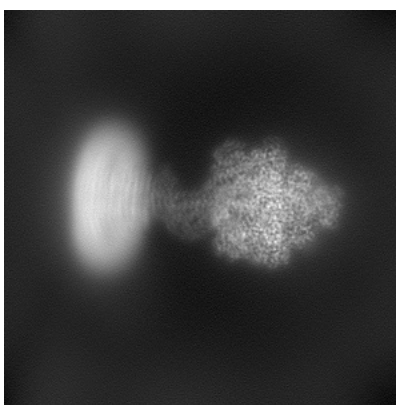


Z

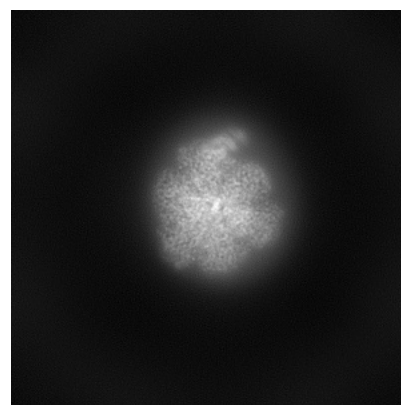
6.1.2 Raw map



X



Y

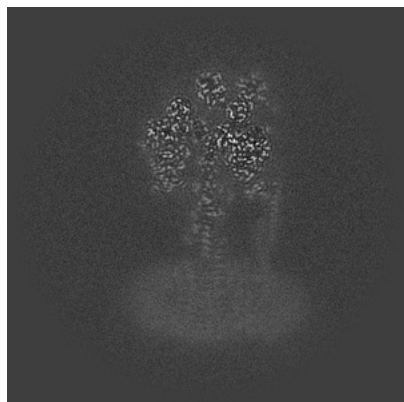


Z

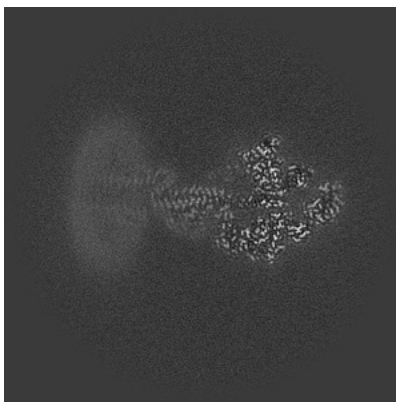
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

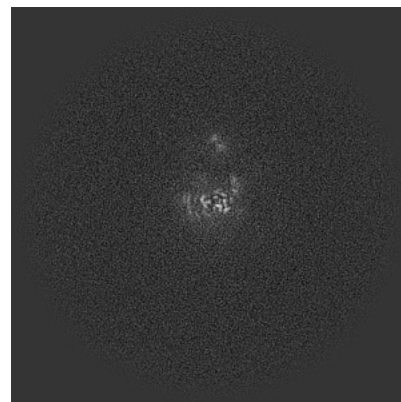
6.2.1 Primary map



X Index: 200

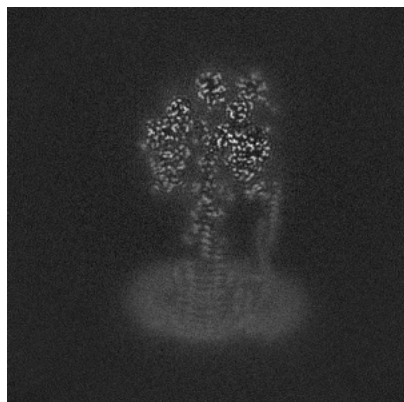


Y Index: 200

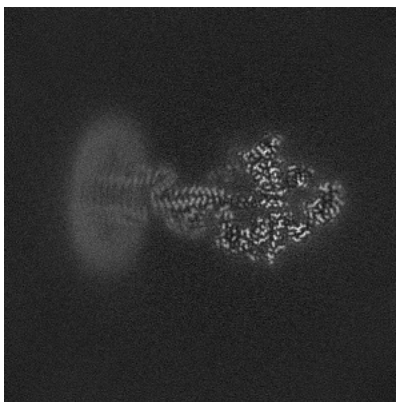


Z Index: 200

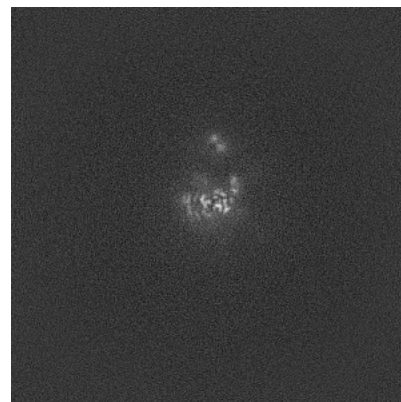
6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

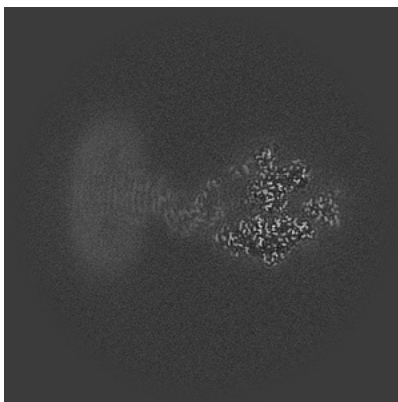
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

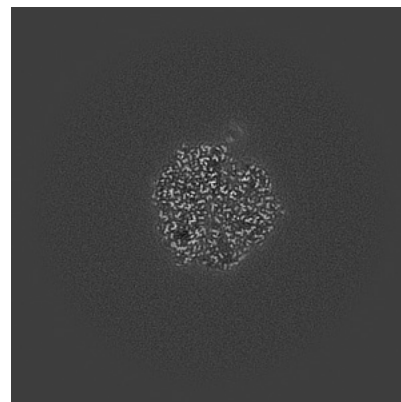
6.3.1 Primary map



X Index: 204

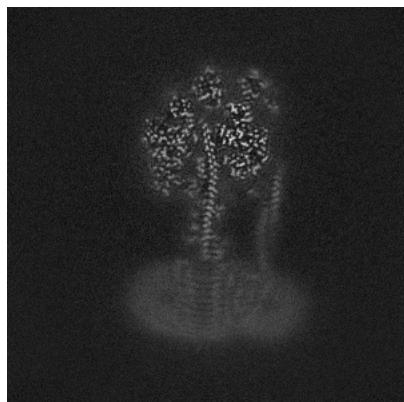


Y Index: 211

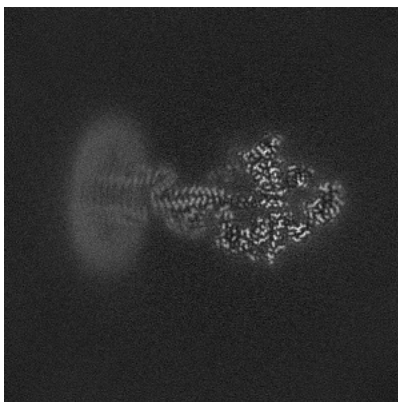


Z Index: 270

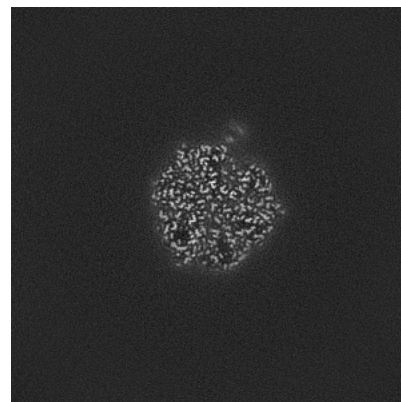
6.3.2 Raw map



X Index: 204



Y Index: 200



Z Index: 270

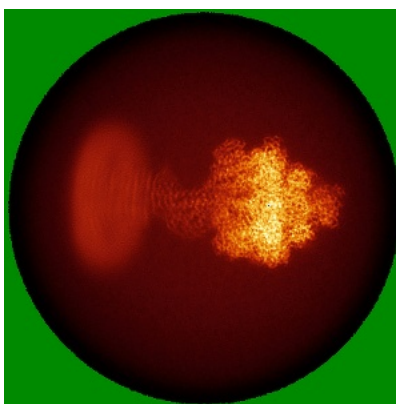
The images above show the largest variance slices of the map in three orthogonal directions.

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

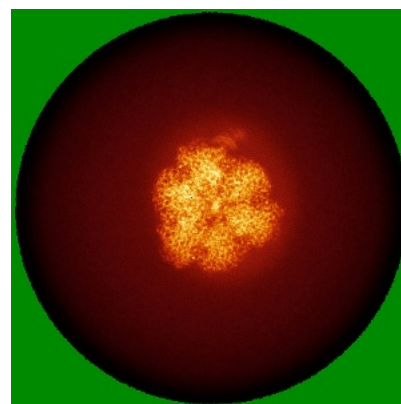
6.4.1 Primary map



X

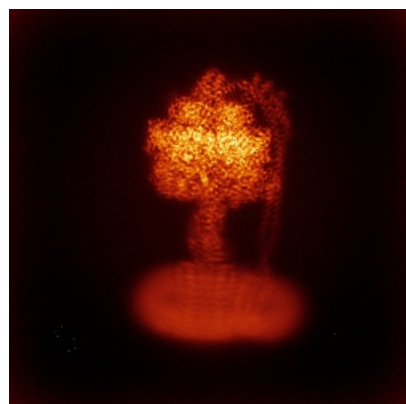


Y

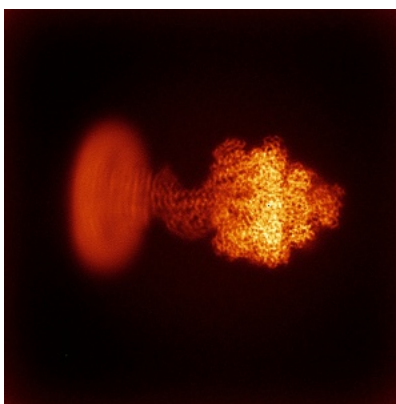


Z

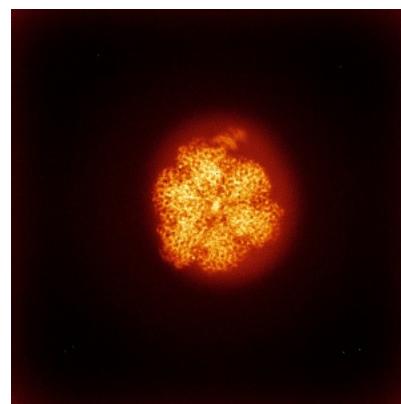
6.4.2 Raw map



X



Y

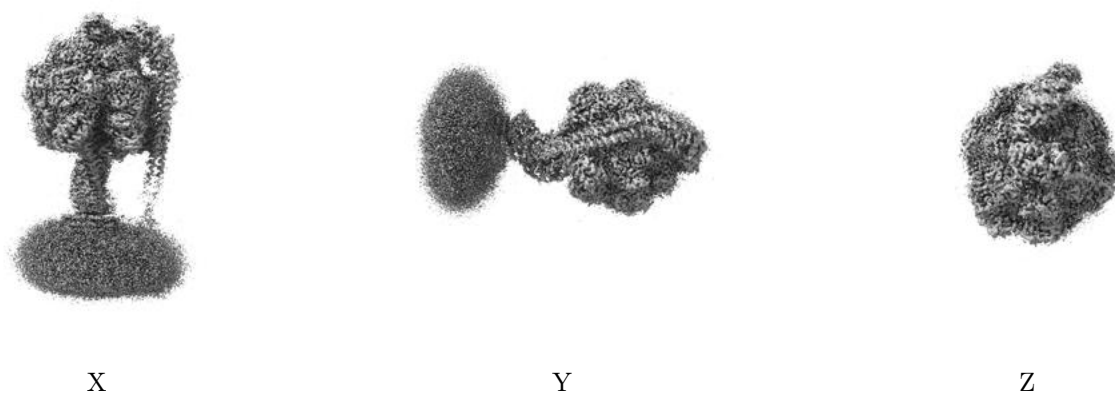


Z

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.

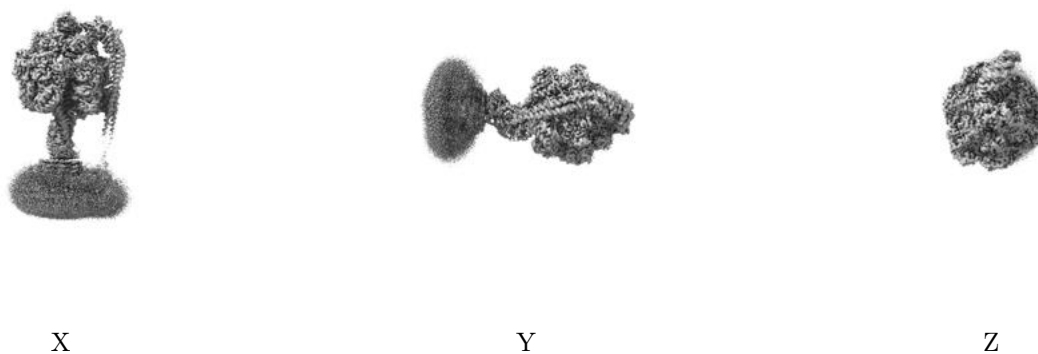
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. 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.

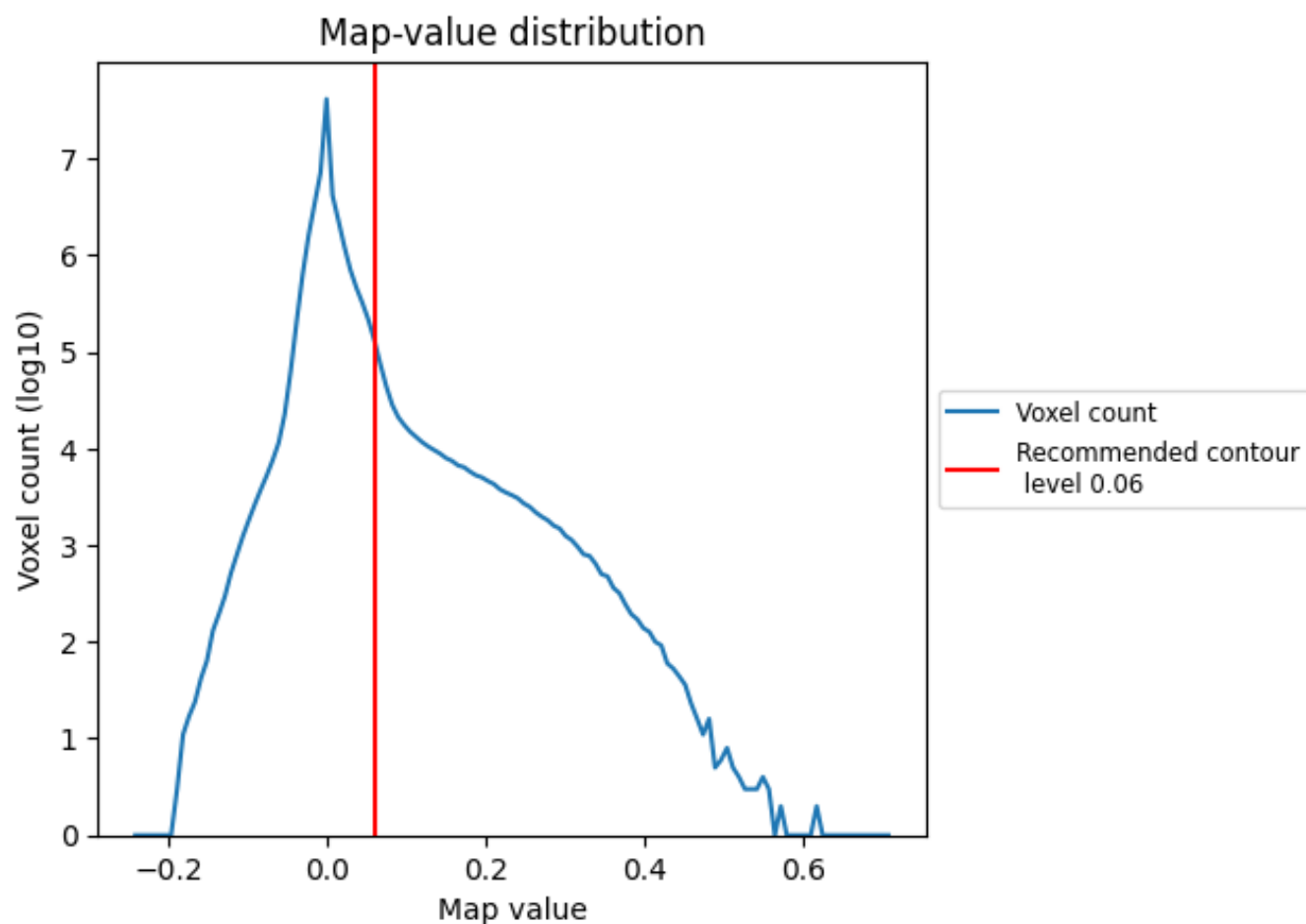
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

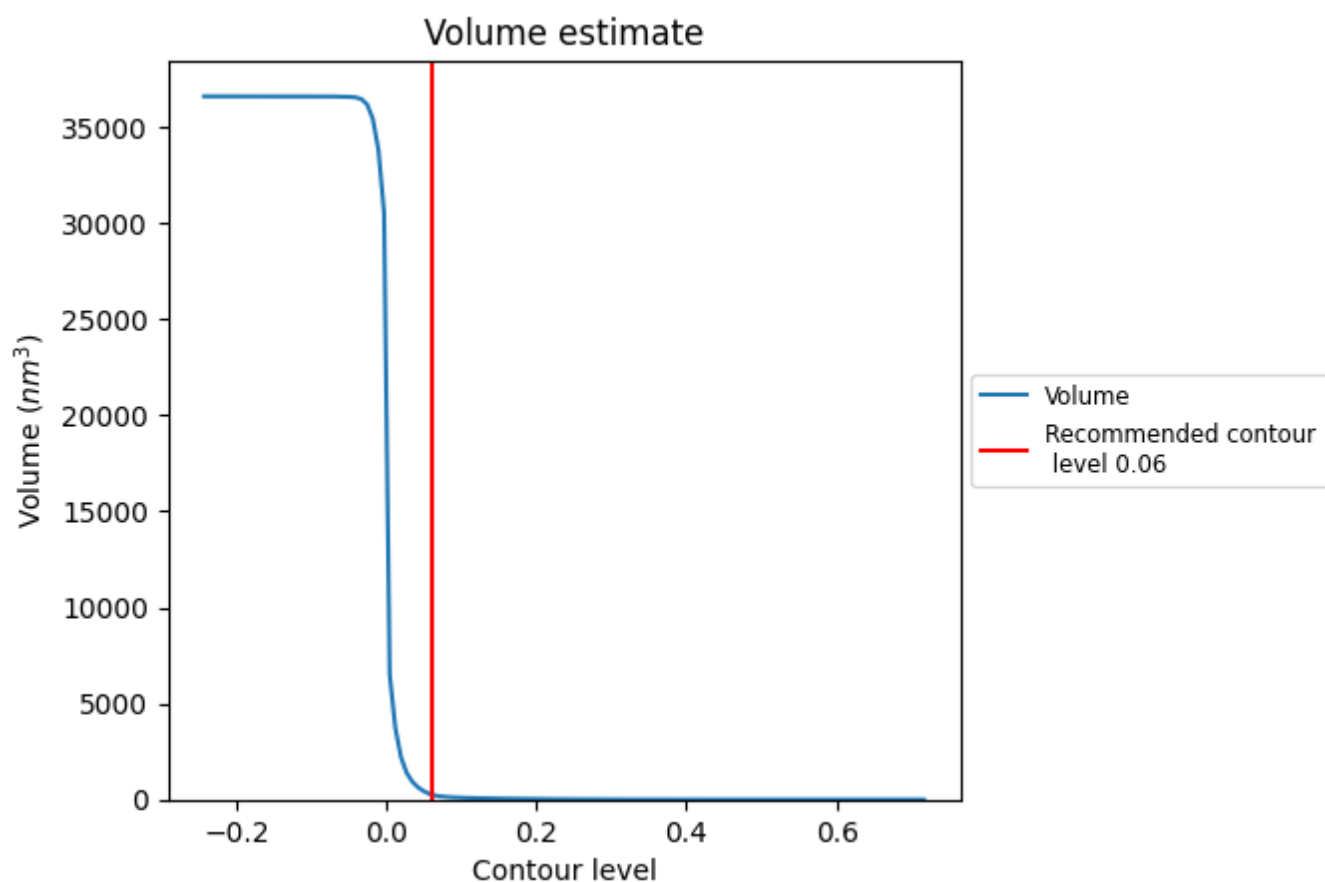
This section contains the results of statistical analysis of the map.

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.

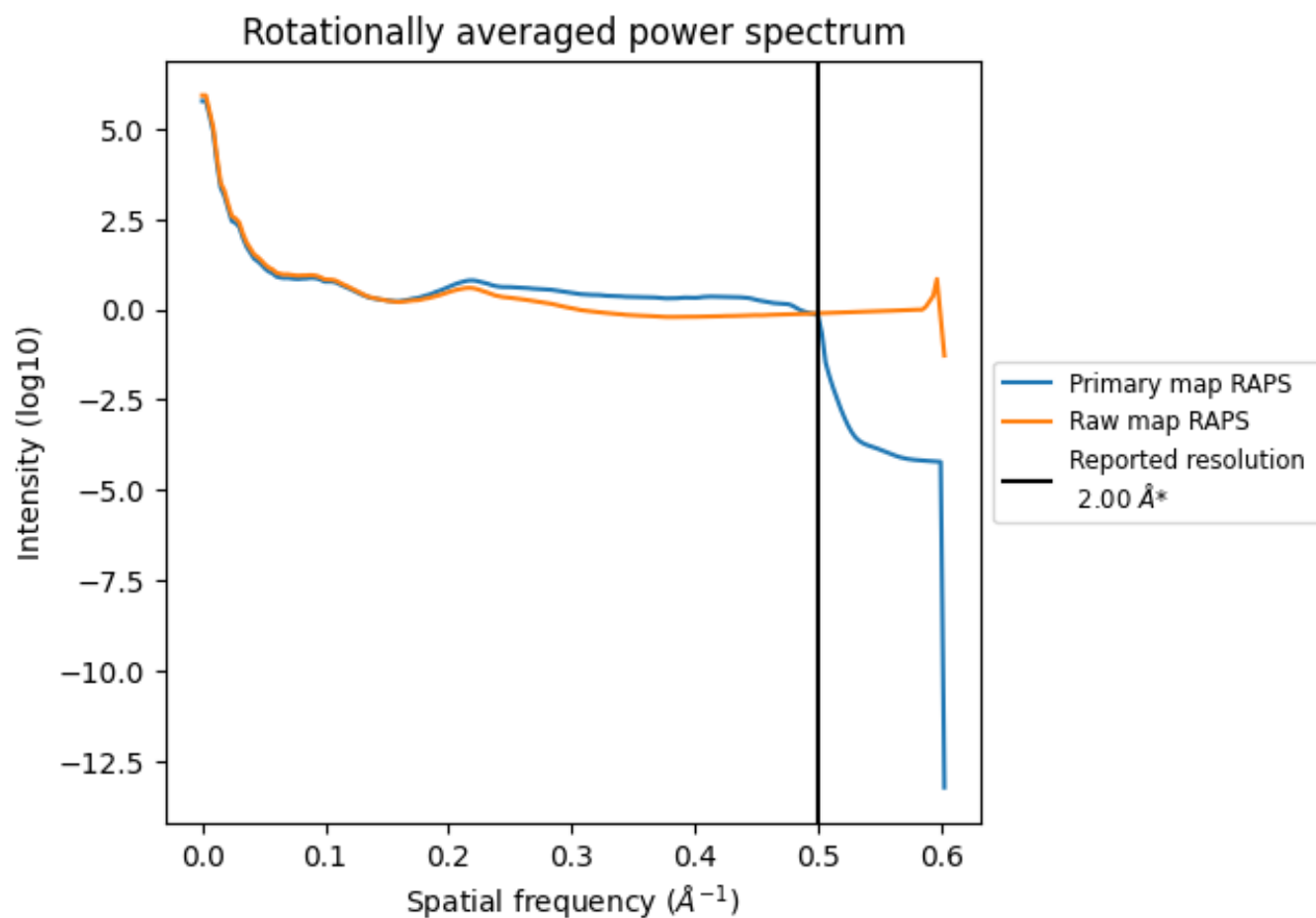
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 270 nm³; this corresponds to an approximate mass of 244 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 ⓘ

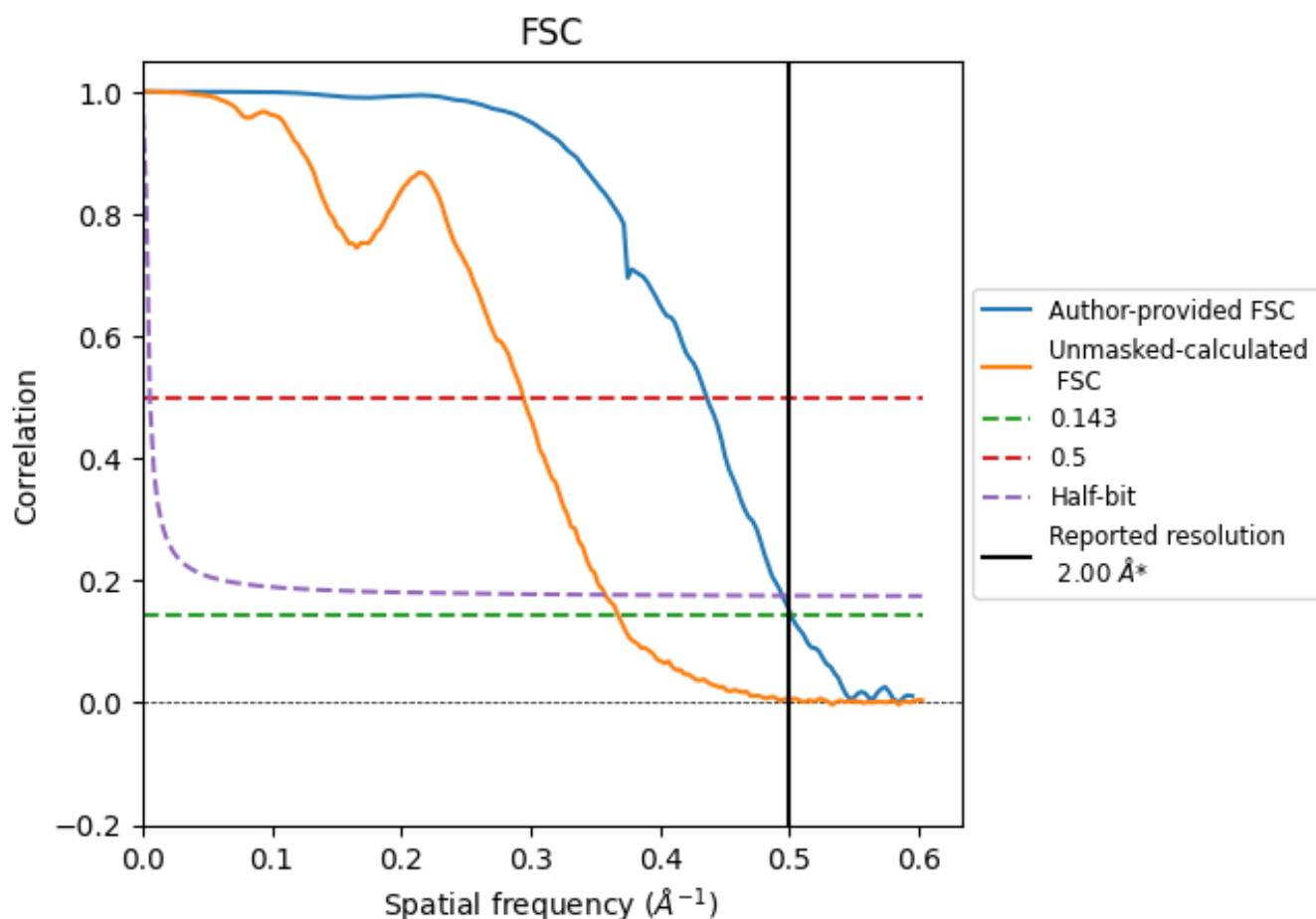


*Reported resolution corresponds to spatial frequency of 0.500 Å⁻¹

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 0.500 \AA^{-1}

8.2 Resolution estimates [i](#)

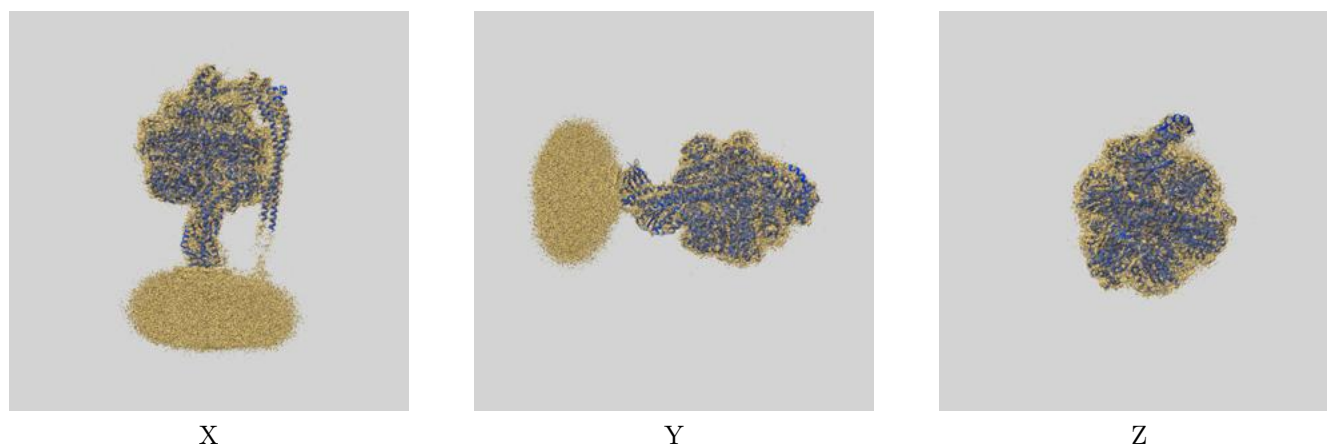
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.00	-	-
Author-provided FSC curve	2.00	2.29	2.02
Unmasked-calculated*	2.72	3.40	2.80

*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 2.72 differs from the reported value 2.0 by more than 10 %

9 Map-model fit [i](#)

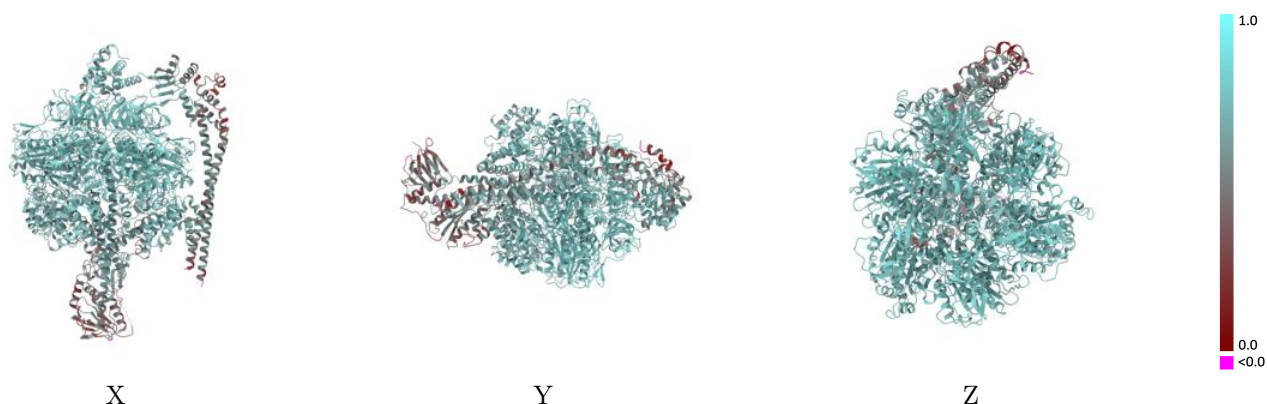
This section contains information regarding the fit between EMDB map EMD-49999 and PDB model 9O19. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



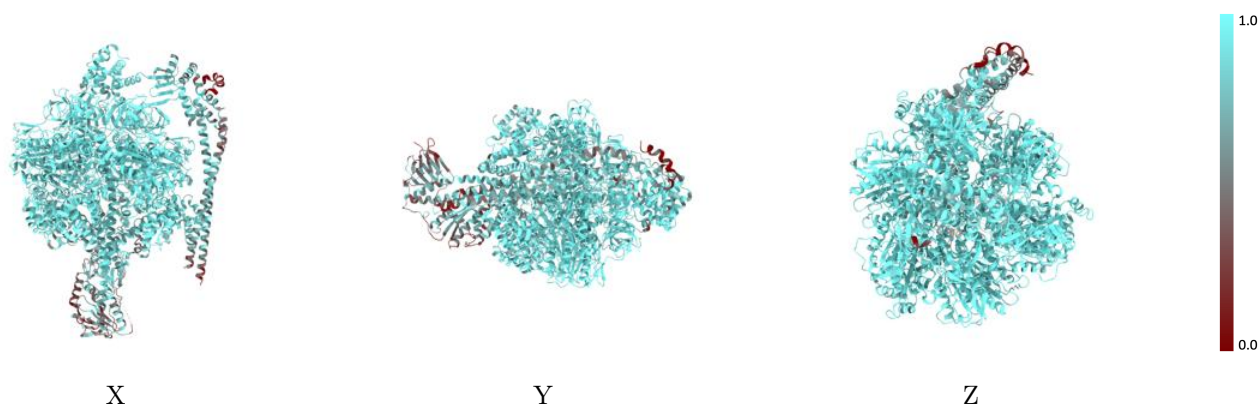
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



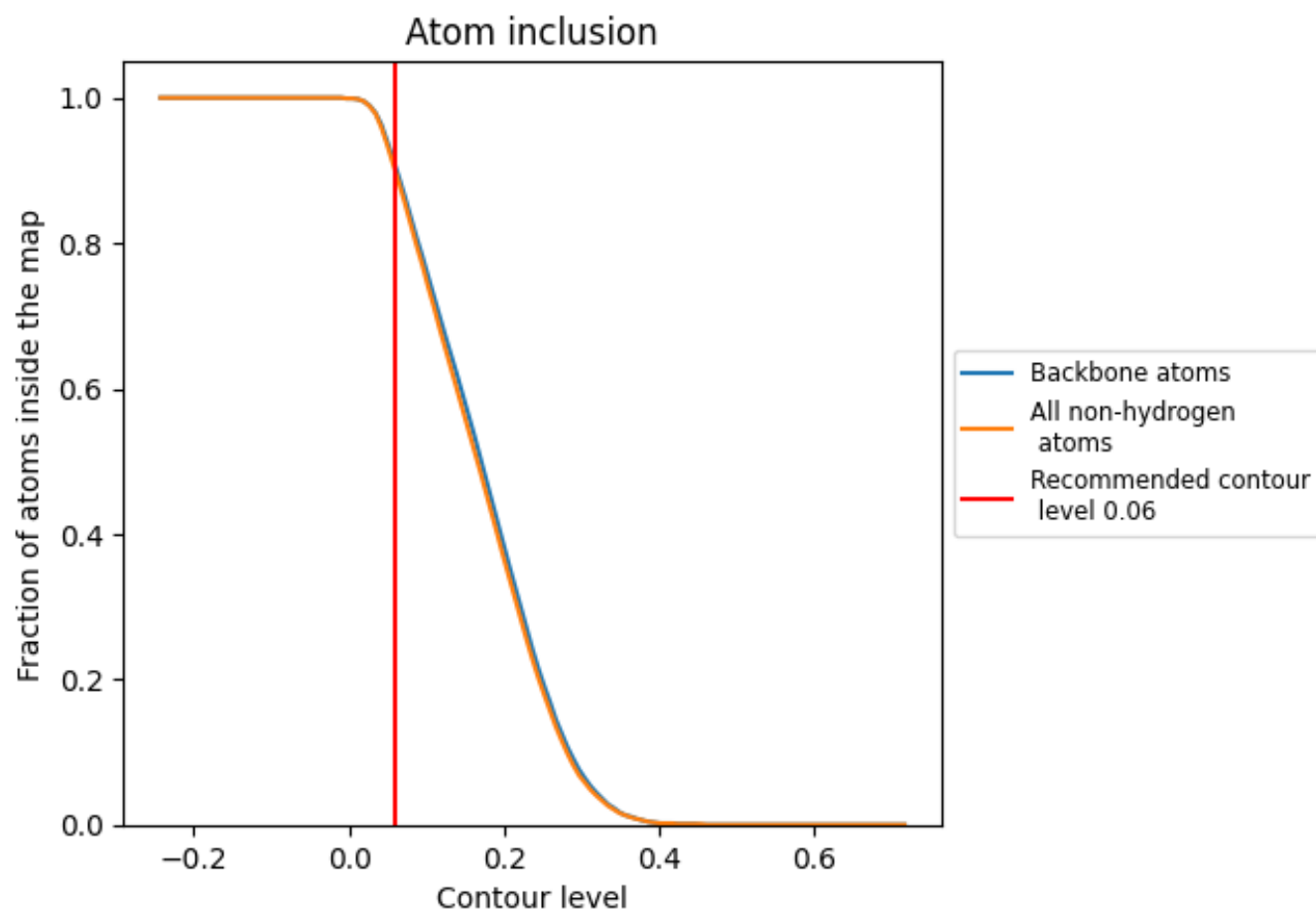
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 90% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8990	<div></div> 0.6730
A	<div></div> 0.9520	<div></div> 0.7130
B	<div></div> 0.9520	<div></div> 0.7080
C	<div></div> 0.9360	<div></div> 0.6990
D	<div></div> 0.9530	<div></div> 0.7080
E	<div></div> 0.9720	<div></div> 0.7340
F	<div></div> 0.9580	<div></div> 0.7170
G	<div></div> 0.7470	<div></div> 0.5330
H	<div></div> 0.4410	<div></div> 0.3790
W	<div></div> 0.9110	<div></div> 0.6580
X	<div></div> 0.5070	<div></div> 0.4040
Y	<div></div> 0.6800	<div></div> 0.5150

1.0

0.0

<0.0