



## Full wwPDB EM Validation Report ⓘ

Dec 4, 2025 – 01:15 PM EST

PDB ID : 9O1J / pdb\_00009o1j  
EMDB ID : EMD-70009  
Title : Pseudomonas aeruginosa ATPase State3 F1Fo focused  
Authors : Stewart, A.G.; Sobti, M.  
Deposited on : 2025-04-03  
Resolution : 3.02 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](mailto: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>.

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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

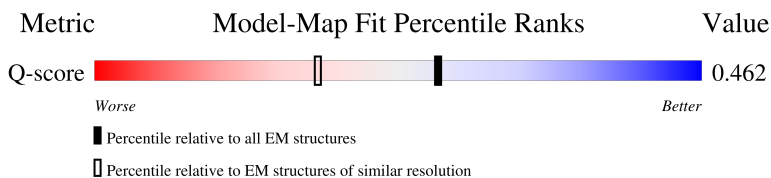
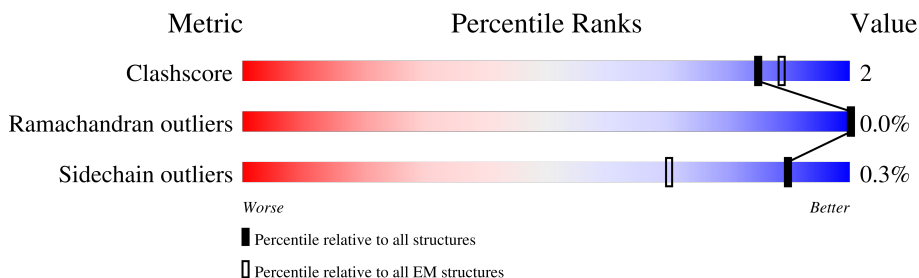
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*



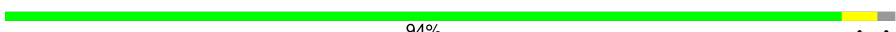

The reported resolution of this entry is 3.02 Å.

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.

















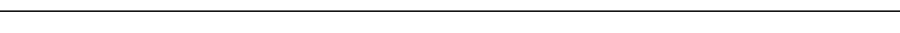
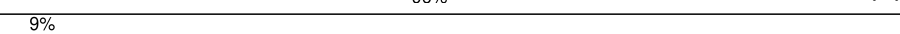
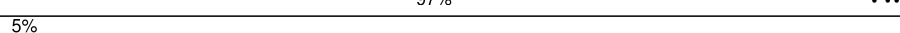
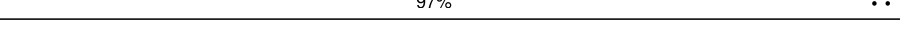
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	13913 ( 2.52 - 3.52 )

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  $\geq 3$ , 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	514	 94% ..
1	B	514	 90% 7% .
1	C	514	 94% ..
2	D	464	 84% 14% ..

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Mol	Chain	Length	Quality of chain
2	E	464	 91% 7% .
2	F	464	 93% 5% .
3	G	286	 87% 7% 6%
4	H	141	 82% 9% 10%
5	I	85	 85% 13% .
5	J	85	 86% 12% .
5	L	85	 91% 7% .
5	M	85	 95% . .
5	N	85	 93% . . .
5	O	85	 93% 5% .
5	P	85	 88% 7% . .
5	Q	85	 86% 12% .
5	R	85	 92% 5% . .
5	S	85	 93% . . .
6	W	178	 96% . .
7	X	156	 9% 97% . . .
7	Y	156	 5% 97% . .
8	a	289	 95% . .

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 36919 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	506	Total	C	N	O	S	0	0
			3823	2405	662	743	13		
1	B	504	Total	C	N	O	S	0	0
			3808	2397	660	738	13		
1	C	506	Total	C	N	O	S	0	0
			3823	2405	662	743	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	456	Total	C	N	O	S	0	0
			3464	2188	591	673	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	269	Total	C	N	O	S	0	0
			2074	1304	367	390	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	127	Total	C	N	O	S	0	0
			929	588	158	180	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	83	Total	C	N	O	S	0	0
			594	397	92	100	5		
5	J	83	Total	C	N	O	S	0	0
			594	397	92	100	5		
5	L	83	Total	C	N	O	S	0	0
			594	397	92	100	5		
5	M	83	Total	C	N	O	S	0	0
			594	397	92	100	5		
5	N	83	Total	C	N	O	S	0	0
			594	397	92	100	5		
5	O	83	Total	C	N	O	S	0	0
			594	397	92	100	5		
5	P	83	Total	C	N	O	S	0	0
			591	394	92	100	5		
5	Q	83	Total	C	N	O	S	0	0
			594	397	92	100	5		
5	R	83	Total	C	N	O	S	0	0
			594	397	92	100	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	83	Total	C	N	O	S	0	0
			594	397	92	100	5		

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

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

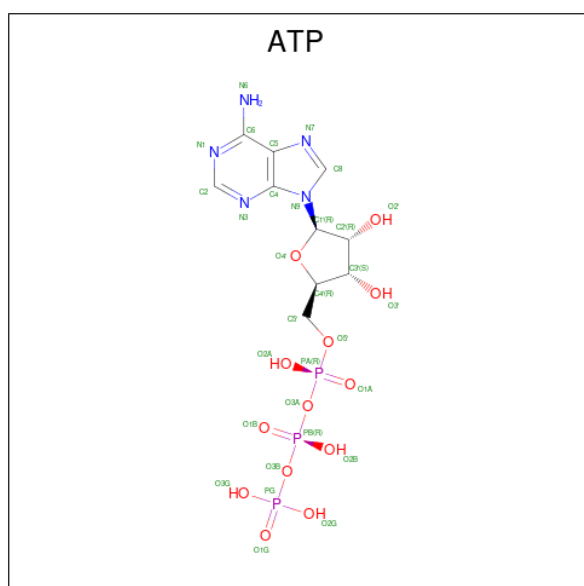
- Molecule 7 is a protein called ATP synthase subunit b.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	X	155	Total	C	N	O	S	0	0
			1183	736	218	226	3		
7	Y	155	Total	C	N	O	S	0	0
			1183	736	218	226	3		

- Molecule 8 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	a	286	Total	C	N	O	S	0	0
			2243	1503	354	377	9		

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).

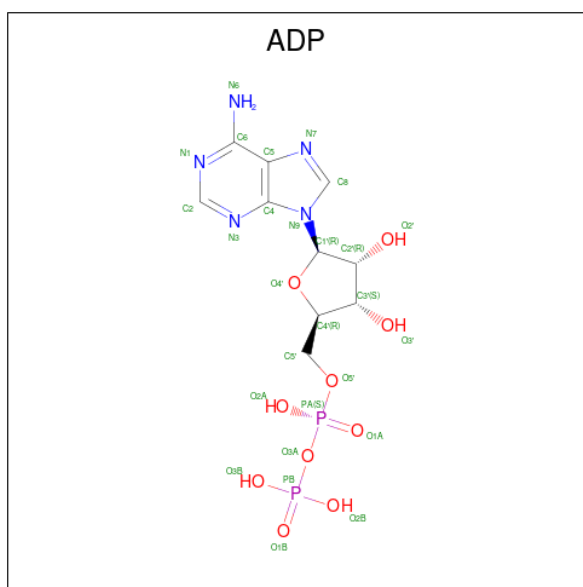


Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
9	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
9	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



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

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



### 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.

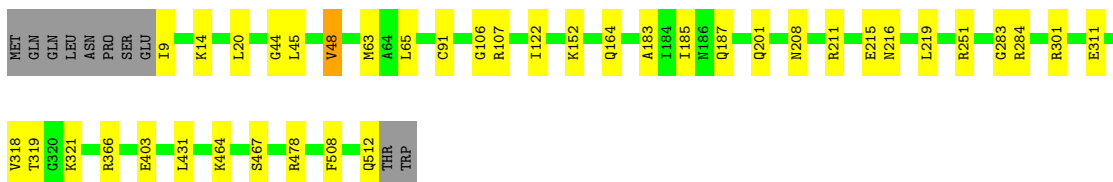
- Molecule 1: ATP synthase subunit alpha

Chain A:  94%



- Molecule 1: ATP synthase subunit alpha

Chain B:  90% 7%




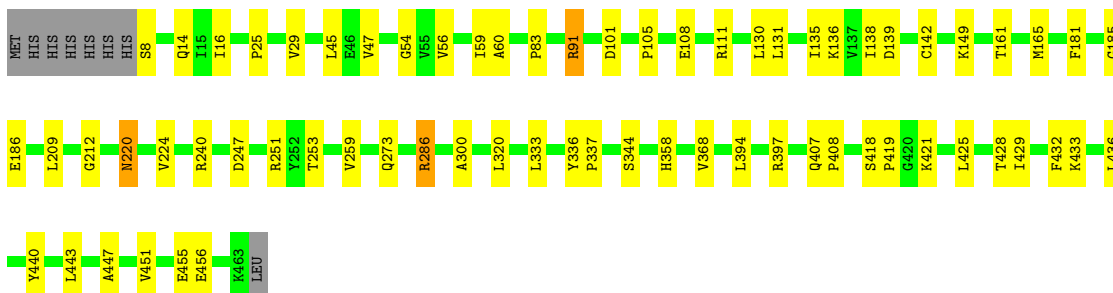
- Molecule 1: ATP synthase subunit alpha

Chain C:  94%

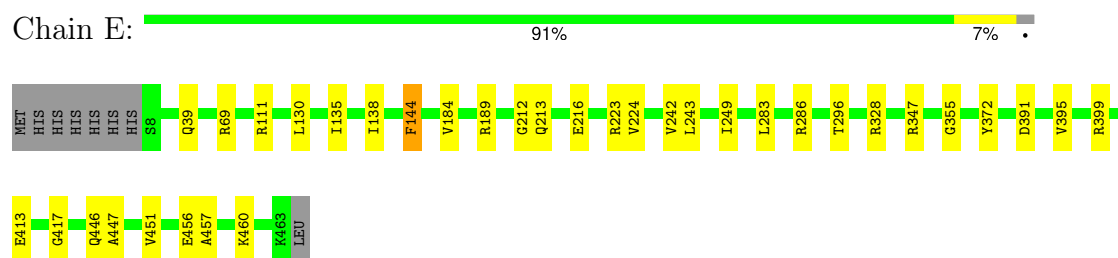


- Molecule 2: ATP synthase subunit beta

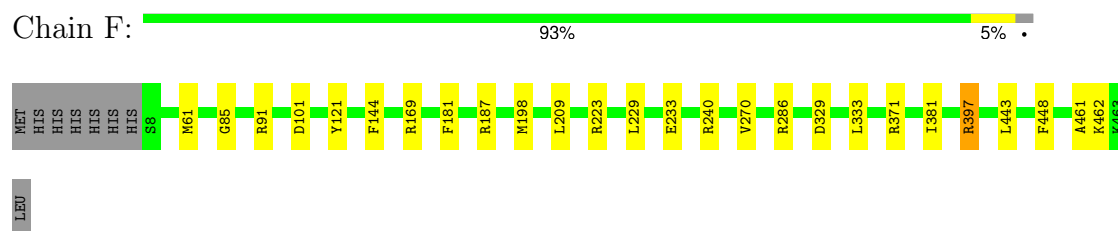
Chain D:  84% 14%



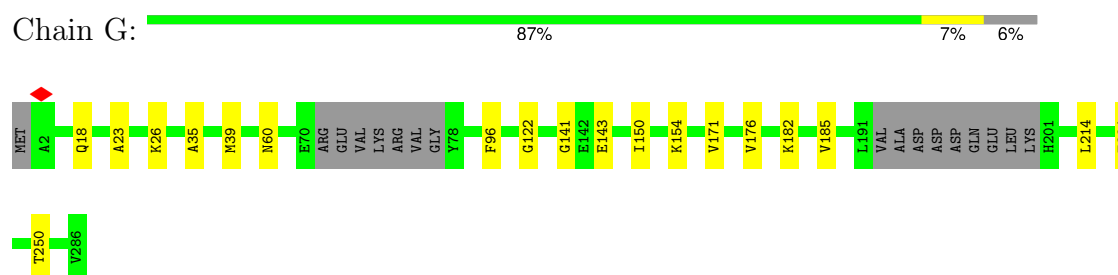
- Molecule 2: ATP synthase subunit beta



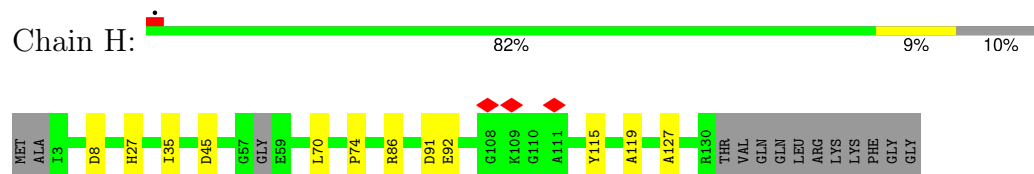
- Molecule 2: ATP synthase subunit beta



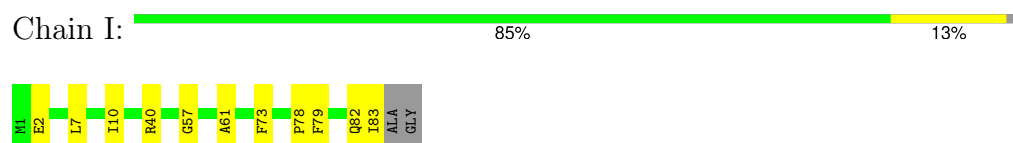
- Molecule 3: ATP synthase gamma chain



- Molecule 4: ATP synthase epsilon chain



- Molecule 5: ATP synthase subunit c



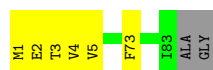
- Molecule 5: ATP synthase subunit c





- Molecule 5: ATP synthase subunit c

Chain L: 91% 7% •



- Molecule 5: ATP synthase subunit c

Chain M: 95% • •



- Molecule 5: ATP synthase subunit c

Chain N: 93% • • •



- Molecule 5: ATP synthase subunit c

Chain O: 93% 5% •



- Molecule 5: ATP synthase subunit c

Chain P: 88% 7% • •



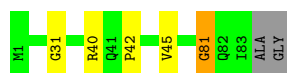
- Molecule 5: ATP synthase subunit c

Chain Q: 86% 12% •



- Molecule 5: ATP synthase subunit c

Chain R: 92% 5% • •



- Molecule 5: ATP synthase subunit c

Chain S:  93%



- Molecule 6: ATP synthase subunit delta

Chain W:  96%



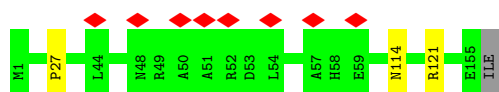
- Molecule 7: ATP synthase subunit b

Chain X:  97%



- Molecule 7: ATP synthase subunit b

Chain Y:  97%



- Molecule 8: ATP synthase subunit a

Chain a:  95%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25274	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	0.285	Depositor
Minimum map value	-0.096	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.037	Depositor
Map size ( $\text{\AA}$ )	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 ( $\text{\AA}$ )	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

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	0.76	0/3875	1.31	7/5233 (0.1%)
1	B	0.79	1/3860 (0.0%)	1.34	9/5213 (0.2%)
1	C	0.80	0/3875	1.34	10/5233 (0.2%)
2	D	0.86	0/3521	1.27	5/4767 (0.1%)
2	E	0.81	0/3521	1.34	13/4767 (0.3%)
2	F	0.78	0/3521	1.35	11/4767 (0.2%)
3	G	0.80	0/2102	1.37	2/2829 (0.1%)
4	H	0.81	0/941	1.45	4/1274 (0.3%)
5	I	0.66	0/603	1.25	2/816 (0.2%)
5	J	0.68	0/603	1.31	4/816 (0.5%)
5	L	0.67	0/603	1.23	1/816 (0.1%)
5	M	0.68	0/603	1.28	1/816 (0.1%)
5	N	0.69	0/603	1.31	2/816 (0.2%)
5	O	0.68	0/603	1.33	2/816 (0.2%)
5	P	0.75	1/600 (0.2%)	1.28	2/812 (0.2%)
5	Q	0.71	0/603	1.25	0/816
5	R	0.74	0/603	1.60	4/816 (0.5%)
5	S	0.67	0/603	1.29	1/816 (0.1%)
6	W	0.77	0/1358	1.43	4/1833 (0.2%)
7	X	0.79	0/1193	1.77	6/1605 (0.4%)
7	Y	0.78	0/1193	1.40	3/1605 (0.2%)
8	a	0.81	0/2306	1.43	5/3141 (0.2%)
All	All	0.78	2/37293 (0.0%)	1.36	98/50423 (0.2%)

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	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1
2	E	0	3
2	F	0	3
5	N	0	1
5	P	0	1
5	Q	0	1
5	R	0	1
7	X	0	1
8	a	0	1
All	All	0	15

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	82	GLN	C-O	-6.46	1.14	1.23
1	B	284	ARG	CZ-NH2	-6.28	1.25	1.33

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	X	60	LYS	O-C-N	-41.92	61.23	122.43
8	a	284	ALA	O-C-N	-25.34	90.67	122.34
5	R	81	GLY	O-C-N	-25.18	90.56	122.29
8	a	284	ALA	CA-C-N	9.12	136.21	121.99
8	a	284	ALA	C-N-CA	9.12	136.21	121.99
5	R	81	GLY	CA-C-N	8.26	135.29	122.49
5	R	81	GLY	C-N-CA	8.26	135.29	122.49
7	X	60	LYS	CA-C-O	-8.03	108.84	119.11
2	F	144	PHE	CA-CB-CG	7.53	121.33	113.80
5	N	75	PHE	CA-CB-CG	-7.00	106.80	113.80
2	F	91	ARG	NE-CZ-NH2	6.90	125.41	119.20
5	P	82	GLN	O-C-N	-6.88	110.30	122.21
7	X	60	LYS	CA-C-N	6.79	132.04	120.71
7	X	60	LYS	C-N-CA	6.79	132.04	120.71
2	D	91	ARG	NE-CZ-NH2	6.69	125.22	119.20
1	C	284	ARG	NE-CZ-NH2	6.68	125.21	119.20
7	Y	121	ARG	NE-CZ-NH2	6.64	125.17	119.20
8	a	200	ILE	N-CA-CB	6.58	114.65	110.50
1	C	16	ARG	NE-CZ-NH2	6.41	124.97	119.20
2	D	111	ARG	NE-CZ-NH2	6.40	124.96	119.20
1	B	283	GLY	CA-C-N	6.31	129.60	120.38
1	B	283	GLY	C-N-CA	6.31	129.60	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	39	GLN	N-CA-C	6.31	117.82	111.07
1	B	251	ARG	NE-CZ-NH2	6.18	124.76	119.20
1	A	495	ASP	CA-CB-CG	6.16	118.76	112.60
1	C	511	THR	N-CA-C	6.06	117.68	111.14
1	B	284	ARG	N-CA-C	5.99	119.42	111.75
1	C	377	ARG	NE-CZ-NH2	5.99	124.59	119.20
2	F	101	ASP	CA-CB-CG	5.99	118.59	112.60
6	W	124	ASP	CA-C-N	5.89	128.98	120.38
6	W	124	ASP	C-N-CA	5.89	128.98	120.38
2	E	189	ARG	NE-CZ-NH2	5.88	124.49	119.20
2	D	286	ARG	NE-CZ-NH2	5.86	124.47	119.20
4	H	74	PRO	CA-C-N	5.85	130.48	120.71
4	H	74	PRO	C-N-CA	5.85	130.48	120.71
3	G	60	ASN	CA-C-N	5.79	125.65	119.28
3	G	60	ASN	C-N-CA	5.79	125.65	119.28
5	J	41	GLN	OE1-CD-NE2	-5.75	116.85	122.60
1	A	201	GLN	OE1-CD-NE2	-5.72	116.88	122.60
8	a	188	PHE	CA-CB-CG	5.72	119.52	113.80
2	F	397	ARG	NE-CZ-NH2	5.72	124.35	119.20
2	F	286	ARG	NE-CZ-NH2	5.69	124.32	119.20
1	A	410	PHE	CA-C-N	5.67	128.44	120.28
1	A	410	PHE	C-N-CA	5.67	128.44	120.28
6	W	115	ALA	N-CA-C	5.67	117.26	111.14
1	C	278	LEU	N-CA-C	-5.66	105.96	112.92
2	D	240	ARG	NE-CZ-NH2	5.63	124.27	119.20
2	F	240	ARG	NE-CZ-NH2	5.62	124.26	119.20
2	E	399	ARG	NE-CZ-NH2	5.62	124.25	119.20
5	L	73	PHE	CA-CB-CG	5.60	119.40	113.80
1	C	226	ALA	N-CA-C	5.58	117.50	108.41
1	B	164	GLN	OE1-CD-NE2	-5.53	117.07	122.60
2	E	144	PHE	CA-CB-CG	5.50	119.31	113.80
4	H	8	ASP	CA-CB-CG	5.50	118.10	112.60
5	I	40	ARG	NE-CZ-NH2	5.45	124.10	119.20
1	B	44	GLY	N-CA-C	5.37	121.89	114.92
5	N	73	PHE	CA-CB-CG	5.33	119.12	113.80
4	H	27	HIS	CB-CG-CD2	-5.32	124.28	131.20
5	I	73	PHE	CA-CB-CG	5.32	119.12	113.80
2	E	184	VAL	CA-C-N	5.30	128.11	120.11
2	E	184	VAL	C-N-CA	5.30	128.11	120.11
6	W	137	GLU	CB-CA-C	5.30	118.71	109.65
2	F	85	GLY	CA-C-N	5.29	127.63	120.38
2	F	85	GLY	C-N-CA	5.29	127.63	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	213	GLN	N-CA-C	5.29	117.65	110.35
2	E	355	GLY	CA-C-O	-5.27	118.02	122.29
5	J	73	PHE	CA-CB-CG	5.23	119.03	113.80
1	C	367	PRO	N-CA-C	-5.22	101.71	112.47
5	O	1	MET	CA-C-N	5.21	127.25	120.28
5	O	1	MET	C-N-CA	5.21	127.25	120.28
2	E	223	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	C	341	PHE	N-CA-C	5.18	116.61	111.07
2	E	347	ARG	NE-CZ-NH2	5.18	123.86	119.20
5	J	39	ALA	CA-C-N	5.17	127.16	120.44
5	J	39	ALA	C-N-CA	5.17	127.16	120.44
1	A	229	ALA	N-CA-C	5.16	117.65	111.71
5	S	40	ARG	NE-CZ-NH2	5.16	123.84	119.20
2	E	69	ARG	NE-CZ-NH2	5.16	123.84	119.20
1	C	70	ASP	N-CA-CB	-5.15	102.96	110.53
7	Y	114	ASN	CA-CB-CG	5.14	117.74	112.60
2	F	187	ARG	NE-CZ-NH2	5.12	123.81	119.20
2	E	216	GLU	N-CA-C	5.12	117.71	110.24
5	R	40	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	A	278	LEU	N-CA-C	-5.11	107.05	113.28
2	D	101	ASP	CA-CB-CG	5.11	117.71	112.60
7	Y	27	PRO	N-CA-C	5.10	116.92	110.70
5	M	73	PHE	CA-CB-CG	5.09	118.89	113.80
1	B	48	VAL	CG1-CB-CG2	-5.08	99.62	110.80
7	X	140	ILE	N-CA-CB	-5.08	106.28	112.33
7	X	49	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	A	172	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	B	201	GLN	OE1-CD-NE2	-5.05	117.55	122.60
2	F	169	ARG	NE-CZ-NH2	5.03	123.73	119.20
1	B	301	ARG	NE-CZ-NH2	5.03	123.72	119.20
2	F	223	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	C	512	GLN	OE1-CD-NE2	-5.01	117.59	122.60
5	P	73	PHE	CA-CB-CG	5.01	118.81	113.80
2	E	213	GLN	OE1-CD-NE2	-5.00	117.60	122.60

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	251	ARG	Sidechain
1	C	475	TYR	Sidechain
2	D	286	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	E	111	ARG	Sidechain
2	E	286	ARG	Sidechain
2	E	328	ARG	Sidechain
2	F	121	TYR	Sidechain
2	F	371	ARG	Sidechain
2	F	397	ARG	Sidechain
5	N	75	PHE	Sidechain
5	P	82	GLN	Mainchain
5	Q	40	ARG	Sidechain
5	R	81	GLY	Mainchain
7	X	60	LYS	Mainchain
8	a	284	ALA	Mainchain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3823	0	3872	8	0
1	B	3808	0	3862	20	0
1	C	3823	0	3872	8	0
2	D	3464	0	3482	42	0
2	E	3464	0	3482	13	0
2	F	3464	0	3482	9	0
3	G	2074	0	2104	14	0
4	H	929	0	936	8	0
5	I	594	0	641	12	0
5	J	594	0	641	14	0
5	L	594	0	641	5	0
5	M	594	0	641	1	0
5	N	594	0	641	3	0
5	O	594	0	641	3	0
5	P	591	0	632	7	0
5	Q	594	0	641	17	0
5	R	594	0	641	3	0
5	S	594	0	641	3	0
6	W	1345	0	1384	2	0
7	X	1183	0	1210	1	0
7	Y	1183	0	1210	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	a	2243	0	2290	7	0
9	A	31	0	12	0	0
9	B	31	0	12	1	0
9	C	31	0	12	1	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	C	1	0	0	0	0
10	D	1	0	0	0	0
10	E	1	0	0	0	0
11	D	27	0	12	1	0
11	E	27	0	12	0	0
11	F	27	0	12	0	0
All	All	36919	0	37659	158	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 (158) 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:63:MET:HE3	1:B:65:LEU:HD21	1.69	0.74
5:J:16:ILE:HD13	5:Q:69:ILE:HD12	1.74	0.70
1:C:45:LEU:HD22	1:C:91:CYS:SG	2.32	0.69
6:W:72:ALA:HB3	6:W:73:PRO:HD3	1.75	0.69
5:J:63:THR:HG21	5:Q:62:VAL:HG21	1.76	0.67
2:D:447:ALA:O	2:D:451:VAL:HG11	1.96	0.66
3:G:18:GLN:HG2	3:G:250:THR:HG23	1.78	0.66
1:B:403:GLU:HB2	2:D:333:LEU:HD22	1.80	0.64
5:L:1:MET:HA	5:L:1:MET:HE2	1.79	0.63
5:L:3:THR:HB	5:Q:2:GLU:HB3	1.81	0.63
2:D:139:ASP:HB3	2:D:425:LEU:HD13	1.81	0.62
2:D:247:ASP:O	2:D:300:ALA:HB3	1.99	0.62
1:B:403:GLU:HB2	2:D:333:LEU:CD2	2.30	0.61
4:H:35:ILE:HD11	4:H:70:LEU:HD21	1.83	0.61
2:D:185:GLY:HA3	2:D:251:ARG:HG3	1.84	0.60
1:B:106:GLY:HA2	1:B:219:LEU:O	2.01	0.59
1:B:464:LYS:HG2	1:B:467:SER:HB2	1.83	0.59
5:I:61:ALA:HB1	8:a:209:VAL:HG12	1.84	0.59
4:H:115:TYR:CE2	4:H:119:ALA:HB2	2.38	0.59
2:D:83:PRO:HB3	2:D:108:GLU:OE1	2.01	0.59
2:D:455:GLU:H	2:D:455:GLU:CD	2.10	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:2:GLU:HG3	5:P:4:VAL:HG23	1.83	0.59
2:D:142:CYS:SG	2:D:344:SER:HB3	2.44	0.58
1:B:311:GLU:HG2	1:B:319:THR:HA	1.84	0.58
5:P:42:PRO:HG3	5:S:44:MET:SD	2.43	0.57
2:D:440:TYR:HB3	2:D:443:LEU:HD12	1.86	0.57
1:C:407:PHE:CE1	4:H:127:ALA:O	2.58	0.56
8:a:65:LEU:O	8:a:69:LYS:HG2	2.06	0.56
5:I:61:ALA:HB1	8:a:209:VAL:CG1	2.36	0.56
2:F:61:MET:HA	2:F:61:MET:HE2	1.88	0.55
5:J:12:VAL:HG11	5:Q:73:PHE:HZ	1.71	0.55
5:J:75:PHE:CE1	5:Q:72:PHE:CZ	2.94	0.55
1:C:436:GLN:HB2	9:C:600:ATP:C6	2.41	0.55
2:E:130:LEU:HD12	2:E:144:PHE:O	2.07	0.54
5:J:63:THR:CG2	5:Q:62:VAL:HG21	2.36	0.54
2:D:220:ASN:O	2:D:224:VAL:HG23	2.07	0.54
2:E:447:ALA:O	2:E:451:VAL:HG11	2.08	0.54
5:I:82:GLN:O	5:I:83:ILE:C	2.51	0.54
2:D:429:ILE:HG22	2:D:433:LYS:HE2	1.90	0.54
1:C:407:PHE:CD1	4:H:127:ALA:O	2.61	0.53
5:I:82:GLN:OE1	5:M:5:VAL:HG13	2.09	0.53
2:D:368:VAL:HG13	2:D:394:LEU:HD11	1.91	0.53
2:D:186:GLU:HG3	2:D:247:ASP:OD2	2.09	0.53
5:J:75:PHE:CZ	5:Q:72:PHE:CE2	2.97	0.53
2:D:212:GLY:HA3	2:D:224:VAL:HG21	1.89	0.53
3:G:150:ILE:HG22	4:H:91:ASP:OD1	2.09	0.52
5:L:1:MET:HB3	5:L:4:VAL:HB	1.91	0.52
2:F:198:MET:HE1	2:F:209:LEU:HD21	1.91	0.51
5:P:1:MET:SD	5:P:80:VAL:HG13	2.51	0.51
2:F:381:ILE:HD11	3:G:26:LYS:HA	1.91	0.51
2:D:358:HIS:CE1	2:D:425:LEU:HD11	2.45	0.51
2:E:451:VAL:O	2:E:456:GLU:HB2	2.11	0.51
1:C:95:ILE:O	1:C:97:GLU:HG3	2.10	0.51
2:D:358:HIS:HE1	2:D:425:LEU:HD11	1.76	0.51
2:E:243:LEU:HD23	2:E:296:THR:HB	1.91	0.51
2:D:451:VAL:O	2:D:456:GLU:HB2	2.11	0.50
2:D:418:SER:HB2	2:D:419:PRO:HD2	1.94	0.50
5:O:44:MET:HE3	5:R:42:PRO:HG2	1.94	0.50
5:J:13:ALA:HA	5:Q:15:LEU:CD2	2.42	0.49
6:W:71:ASN:O	6:W:72:ALA:C	2.55	0.49
5:J:16:ILE:HD13	5:Q:69:ILE:CD1	2.41	0.49
5:P:39:ALA:O	5:S:41:GLN:NE2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:10:ILE:HD11	5:N:10:ILE:HB	1.95	0.49
1:A:426:GLN:HB3	1:A:462:ILE:HD13	1.95	0.49
2:D:59:ILE:HD13	2:D:259:VAL:HG11	1.94	0.49
5:I:79:PHE:HA	5:I:82:GLN:NE2	2.28	0.49
2:D:161:THR:O	2:D:165:MET:HG2	2.13	0.48
3:G:141:GLY:C	3:G:143:GLU:N	2.71	0.48
8:a:51:TRP:NE1	8:a:146:ALA:HA	2.28	0.48
1:B:403:GLU:CB	2:D:333:LEU:HD22	2.42	0.48
1:B:211:ARG:O	1:B:215:GLU:HG3	2.13	0.48
2:D:181:PHE:HB3	2:D:209:LEU:HD23	1.95	0.48
1:A:314:THR:HG21	1:A:318:VAL:HB	1.96	0.48
1:A:407:PHE:CE1	3:G:23:ALA:HA	2.48	0.47
1:B:366:ARG:HB3	9:B:600:ATP:C6	2.48	0.47
2:E:413:GLU:O	2:E:417:GLY:N	2.47	0.47
2:E:249:ILE:HD11	2:E:283:LEU:HD23	1.95	0.47
2:D:14:GLN:HE21	2:D:16:ILE:HD11	1.79	0.47
2:D:47:VAL:HG13	2:D:56:VAL:HB	1.95	0.47
2:D:29:VAL:HG22	2:D:54:GLY:HA2	1.96	0.47
2:D:45:LEU:HD23	2:D:60:ALA:HA	1.97	0.47
1:B:152:LYS:HE2	1:B:431:LEU:O	2.14	0.47
3:G:214:LEU:CD2	4:H:45:ASP:HB2	2.45	0.46
3:G:96:PHE:CZ	3:G:122:GLY:HA2	2.50	0.46
5:I:79:PHE:HA	5:I:82:GLN:CD	2.41	0.46
2:E:372:TYR:CE1	2:E:395:VAL:HG13	2.50	0.46
1:A:251:ARG:NH2	1:A:301:ARG:O	2.50	0.45
5:P:77:ASN:ND2	5:P:80:VAL:HG23	2.32	0.45
1:B:9:ILE:O	1:B:14:LYS:HG2	2.17	0.45
5:J:16:ILE:HG21	5:Q:66:GLY:HA2	1.99	0.45
1:B:478:ARG:O	1:B:478:ARG:HG2	2.17	0.45
1:C:95:ILE:O	1:C:96:LEU:C	2.60	0.45
2:D:336:TYR:HA	2:D:337:PRO:C	2.42	0.44
2:D:8:SER:HB3	2:D:25:PRO:HG2	1.99	0.44
8:a:51:TRP:CH2	8:a:129:LEU:HD13	2.52	0.44
3:G:35:ALA:O	3:G:39:MET:HG3	2.17	0.44
3:G:96:PHE:HZ	3:G:122:GLY:HA2	1.82	0.44
2:D:408:PRO:HG2	2:D:421:LYS:HG2	1.99	0.44
2:F:461:ALA:O	2:F:462:LYS:C	2.61	0.44
5:I:7:LEU:HD23	5:N:7:LEU:HD13	1.99	0.44
5:L:1:MET:HB2	5:L:5:VAL:HG23	2.00	0.44
5:Q:23:THR:CG2	5:Q:63:THR:HG21	2.48	0.44
7:X:26:TRP:CH2	8:a:105:ALA:HB1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:149:LYS:CD	2:D:320:LEU:HD23	2.48	0.44
5:Q:23:THR:HG23	5:Q:63:THR:HG21	1.98	0.43
1:A:407:PHE:HB3	1:A:414:LEU:HD21	2.00	0.43
5:I:10:ILE:CD1	5:N:10:ILE:HB	2.48	0.43
5:O:55:VAL:HG11	5:R:31:GLY:HA3	2.00	0.43
1:B:9:ILE:O	1:B:14:LYS:HE2	2.18	0.43
2:D:149:LYS:HD2	2:D:320:LEU:HD23	2.00	0.43
2:D:428:THR:O	2:D:432:PHE:HD2	2.01	0.43
2:E:212:GLY:HA3	2:E:224:VAL:HG21	2.01	0.43
5:J:75:PHE:HE1	5:Q:72:PHE:CZ	2.37	0.43
5:P:42:PRO:CG	5:S:44:MET:SD	3.07	0.43
1:B:107:ARG:NH2	1:B:122:ILE:HG12	2.34	0.43
2:D:149:LYS:HG2	2:D:320:LEU:HD23	2.01	0.43
2:E:249:ILE:HD11	2:E:283:LEU:CD2	2.49	0.43
2:E:446:GLN:O	2:E:460:LYS:HE2	2.18	0.43
5:J:16:ILE:CD1	5:Q:69:ILE:CD1	2.96	0.43
2:D:253:THR:HG23	2:D:273:GLN:HE22	1.83	0.42
5:I:78:PRO:O	5:I:82:GLN:HG3	2.19	0.42
1:B:183:ALA:O	1:B:187:GLN:HG2	2.19	0.42
2:D:91:ARG:NH1	2:D:105:PRO:O	2.52	0.42
2:E:451:VAL:HG21	2:E:457:ALA:HB2	2.01	0.42
5:I:2:GLU:H	5:I:2:GLU:CD	2.27	0.42
2:D:130:LEU:HD23	2:D:131:LEU:N	2.34	0.42
2:D:397:ARG:NH2	2:D:436:LEU:O	2.52	0.42
1:A:53:MET:HE2	1:A:53:MET:HB3	1.79	0.42
5:O:51:LYS:HE3	5:R:45:VAL:CG2	2.49	0.42
1:B:318:VAL:HG13	1:B:321:LYS:HD2	2.01	0.42
2:E:391:ASP:O	2:E:395:VAL:HG23	2.20	0.42
2:F:443:LEU:HB2	2:F:448:PHE:CZ	2.55	0.42
1:C:53:MET:HE3	1:C:96:LEU:HD12	2.01	0.42
2:D:135:ILE:HD12	2:D:138:ILE:HD12	2.02	0.42
2:F:229:LEU:O	2:F:233:GLU:HG3	2.19	0.42
2:F:329:ASP:O	2:F:333:LEU:HD13	2.18	0.42
5:P:4:VAL:HG11	5:P:80:VAL:HA	2.01	0.42
3:G:224:GLU:OE1	4:H:86:ARG:NH1	2.49	0.42
5:J:20:ALA:HB1	5:Q:63:THR:HG22	2.01	0.42
3:G:154:LYS:NZ	4:H:92:GLU:OE1	2.28	0.41
1:B:508:PHE:O	1:B:512:GLN:HG2	2.21	0.41
1:B:185:ILE:HD13	1:B:216:ASN:HD22	1.85	0.41
2:D:429:ILE:O	2:D:433:LYS:HG3	2.20	0.41
2:F:181:PHE:HB3	2:F:209:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:LEU:HD22	1:B:91:CYS:SG	2.61	0.41
1:C:357:GLU:OE2	1:C:359:ALA:HB3	2.20	0.41
2:D:336:TYR:HB3	11:D:501:ADP:N6	2.36	0.41
2:E:135:ILE:HD12	2:E:138:ILE:HD12	2.02	0.41
5:I:57:GLY:O	8:a:210:THR:HG22	2.20	0.41
1:A:461:GLU:C	1:A:463:ALA:N	2.78	0.41
1:B:208:ASN:OD1	1:B:211:ARG:NH1	2.53	0.41
5:J:71:LEU:HD21	5:Q:69:ILE:HD11	2.03	0.41
2:F:381:ILE:HD11	3:G:26:LYS:CA	2.51	0.40
1:A:63:MET:HE3	1:A:65:LEU:HD21	2.02	0.40
2:D:136:LYS:HE2	2:D:407:GLN:HB2	2.04	0.40
3:G:176:VAL:HG21	3:G:182:LYS:HB2	2.02	0.40
5:J:13:ALA:HA	5:Q:15:LEU:HD21	2.02	0.40
3:G:171:VAL:HG22	3:G:185:VAL:HG22	2.03	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	504/514 (98%)	488 (97%)	16 (3%)	0	100	100
1	B	502/514 (98%)	479 (95%)	23 (5%)	0	100	100
1	C	504/514 (98%)	488 (97%)	15 (3%)	1 (0%)	44	76
2	D	454/464 (98%)	434 (96%)	20 (4%)	0	100	100
2	E	454/464 (98%)	442 (97%)	12 (3%)	0	100	100
2	F	454/464 (98%)	442 (97%)	11 (2%)	1 (0%)	44	76
3	G	263/286 (92%)	260 (99%)	3 (1%)	0	100	100
4	H	123/141 (87%)	117 (95%)	6 (5%)	0	100	100
5	I	81/85 (95%)	81 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	J	81/85 (95%)	81 (100%)	0	0	100	100
5	L	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
5	M	81/85 (95%)	81 (100%)	0	0	100	100
5	N	81/85 (95%)	77 (95%)	4 (5%)	0	100	100
5	O	81/85 (95%)	80 (99%)	1 (1%)	0	100	100
5	P	81/85 (95%)	80 (99%)	1 (1%)	0	100	100
5	Q	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
5	R	81/85 (95%)	80 (99%)	1 (1%)	0	100	100
5	S	81/85 (95%)	81 (100%)	0	0	100	100
6	W	175/178 (98%)	169 (97%)	6 (3%)	0	100	100
7	X	153/156 (98%)	153 (100%)	0	0	100	100
7	Y	153/156 (98%)	151 (99%)	2 (1%)	0	100	100
8	a	284/289 (98%)	277 (98%)	7 (2%)	0	100	100
All	All	4833/4990 (97%)	4698 (97%)	133 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	22	VAL
2	F	270	VAL

### 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	398/406 (98%)	395 (99%)	3 (1%)	79	90
1	B	396/406 (98%)	394 (100%)	2 (0%)	86	94
1	C	398/406 (98%)	396 (100%)	2 (0%)	86	94
2	D	368/376 (98%)	367 (100%)	1 (0%)	91	96
2	E	368/376 (98%)	367 (100%)	1 (0%)	91	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	368/376 (98%)	368 (100%)	0	100	100
3	G	220/235 (94%)	220 (100%)	0	100	100
4	H	91/101 (90%)	91 (100%)	0	100	100
5	I	59/59 (100%)	59 (100%)	0	100	100
5	J	59/59 (100%)	59 (100%)	0	100	100
5	L	59/59 (100%)	59 (100%)	0	100	100
5	M	59/59 (100%)	59 (100%)	0	100	100
5	N	59/59 (100%)	59 (100%)	0	100	100
5	O	59/59 (100%)	59 (100%)	0	100	100
5	P	58/59 (98%)	57 (98%)	1 (2%)	56	80
5	Q	59/59 (100%)	59 (100%)	0	100	100
5	R	59/59 (100%)	59 (100%)	0	100	100
5	S	59/59 (100%)	57 (97%)	2 (3%)	32	65
6	W	141/142 (99%)	140 (99%)	1 (1%)	81	91
7	X	116/117 (99%)	116 (100%)	0	100	100
7	Y	116/117 (99%)	116 (100%)	0	100	100
8	a	238/239 (100%)	238 (100%)	0	100	100
All	All	3807/3887 (98%)	3794 (100%)	13 (0%)	90	96

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	ARG
1	A	495	ASP
1	A	511	THR
1	B	20	LEU
1	B	48	VAL
1	C	22	VAL
1	C	237	TYR
2	D	220	ASN
2	E	242	VAL
5	P	4	VAL
5	S	23	THR
5	S	44	MET
6	W	169	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	GLN
1	A	203	GLN
1	A	221	ASN
1	A	273	GLN
1	A	383	GLN
1	B	145	GLN
1	B	203	GLN
1	B	424	HIS
1	C	66	ASN
1	C	273	GLN
1	C	362	ASN
2	D	14	GLN
2	D	124	GLN
2	D	175	HIS
2	D	192	ASN
2	D	356	GLN
2	D	370	GLN
2	D	437	ASN
2	E	14	GLN
2	E	48	GLN
2	E	192	ASN
2	E	319	HIS
2	F	192	ASN
3	G	36	GLN
3	G	201	HIS
5	N	41	GLN
5	N	82	GLN
5	O	41	GLN
7	X	84	ASN
7	X	104	GLN
7	X	145	HIS
7	Y	58	HIS
7	Y	85	GLN
8	a	13	HIS
8	a	31	HIS
8	a	45	HIS
8	a	255	ASN
8	a	269	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	ATP	C	600	10	28,33,33	1.32	3 (10%)	34,52,52	1.33	4 (11%)
11	ADP	D	501	10	24,29,29	0.77	0	29,45,45	0.85	2 (6%)
11	ADP	E	501	10	24,29,29	1.27	2 (8%)	29,45,45	1.60	6 (20%)
11	ADP	F	501	-	24,29,29	1.25	1 (4%)	29,45,45	1.40	4 (13%)
9	ATP	A	600	10	28,33,33	1.45	4 (14%)	34,52,52	1.41	6 (17%)
9	ATP	B	600	10	28,33,33	1.39	4 (14%)	34,52,52	1.32	4 (11%)

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	ATP	C	600	10	-	0/18/38/38	0/3/3/3
11	ADP	D	501	10	-	6/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	ADP	E	501	10	-	4/12/32/32	0/3/3/3
11	ADP	F	501	-	-	0/12/32/32	0/3/3/3
9	ATP	A	600	10	-	0/18/38/38	0/3/3/3
9	ATP	B	600	10	-	3/18/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	501	ADP	O4'-C1'	3.61	1.45	1.40
11	E	501	ADP	PA-O3A	-3.59	1.55	1.59
9	A	600	ATP	PA-O3A	-3.36	1.55	1.59
9	C	600	ATP	PB-O3B	-3.08	1.56	1.59
9	A	600	ATP	PB-O3A	-3.08	1.56	1.59
9	A	600	ATP	PB-O3B	-2.89	1.56	1.59
9	B	600	ATP	PB-O3B	-2.87	1.56	1.59
9	B	600	ATP	O4'-C1'	2.86	1.44	1.40
9	B	600	ATP	PB-O3A	-2.77	1.56	1.59
9	C	600	ATP	PB-O3A	-2.62	1.56	1.59
9	B	600	ATP	PA-O3A	-2.51	1.56	1.59
9	A	600	ATP	O4'-C1'	2.46	1.44	1.40
9	C	600	ATP	PA-O3A	-2.22	1.57	1.59
11	E	501	ADP	O4'-C1'	2.18	1.43	1.40

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	600	ATP	C4-C5-N7	4.60	114.20	109.34
11	F	501	ADP	C4-C5-N7	4.38	113.97	109.34
11	E	501	ADP	C4-C5-N7	4.28	113.86	109.34
9	B	600	ATP	C4-C5-N7	4.18	113.75	109.34
9	C	600	ATP	C4-C5-N7	4.06	113.62	109.34
9	B	600	ATP	O2A-PA-O3A	3.10	115.65	107.27
11	F	501	ADP	O3B-PB-O3A	2.80	114.04	104.64
9	A	600	ATP	O2B-PB-O3B	2.80	114.85	107.27
11	E	501	ADP	O3B-PB-O3A	2.73	113.79	104.64
9	C	600	ATP	O2B-PB-O3A	2.70	114.57	107.27
9	C	600	ATP	O2B-PB-O3B	2.65	114.44	107.27
11	F	501	ADP	O2B-PB-O1B	-2.65	100.53	110.83
11	E	501	ADP	C4'-O4'-C1'	-2.51	107.63	109.92
11	E	501	ADP	O4'-C1'-N9	2.49	112.05	108.75
11	E	501	ADP	O3B-PB-O2B	-2.37	98.91	107.80
11	D	501	ADP	C5-C6-N6	2.30	123.82	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	501	ADP	O2B-PB-O1B	2.29	119.74	110.83
9	B	600	ATP	O2B-PB-O3B	2.28	113.44	107.27
9	A	600	ATP	O2B-PB-O3A	2.20	113.22	107.27
9	A	600	ATP	O4'-C1'-N9	2.17	111.62	108.75
9	B	600	ATP	C5-C6-N6	2.15	123.59	120.31
9	C	600	ATP	O2G-PG-O3B	2.10	111.67	104.64
11	F	501	ADP	N6-C6-N1	-2.07	113.90	118.33
11	E	501	ADP	N6-C6-N1	-2.01	114.03	118.33
9	A	600	ATP	O2A-PA-O3A	2.01	112.71	107.27
9	A	600	ATP	N6-C6-N1	-2.01	114.04	118.33

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	D	501	ADP	PA-O3A-PB-O2B
11	D	501	ADP	C5'-O5'-PA-O3A
11	E	501	ADP	C5'-O5'-PA-O1A
11	E	501	ADP	C5'-O5'-PA-O3A
11	E	501	ADP	C4'-C5'-O5'-PA
11	D	501	ADP	PA-O3A-PB-O3B
11	D	501	ADP	C5'-O5'-PA-O1A
9	B	600	ATP	O4'-C4'-C5'-O5'
9	B	600	ATP	PB-O3A-PA-O2A
11	D	501	ADP	C3'-C4'-C5'-O5'
9	B	600	ATP	PB-O3A-PA-O1A
11	D	501	ADP	C4'-C5'-O5'-PA
11	E	501	ADP	PB-O3A-PA-O2A

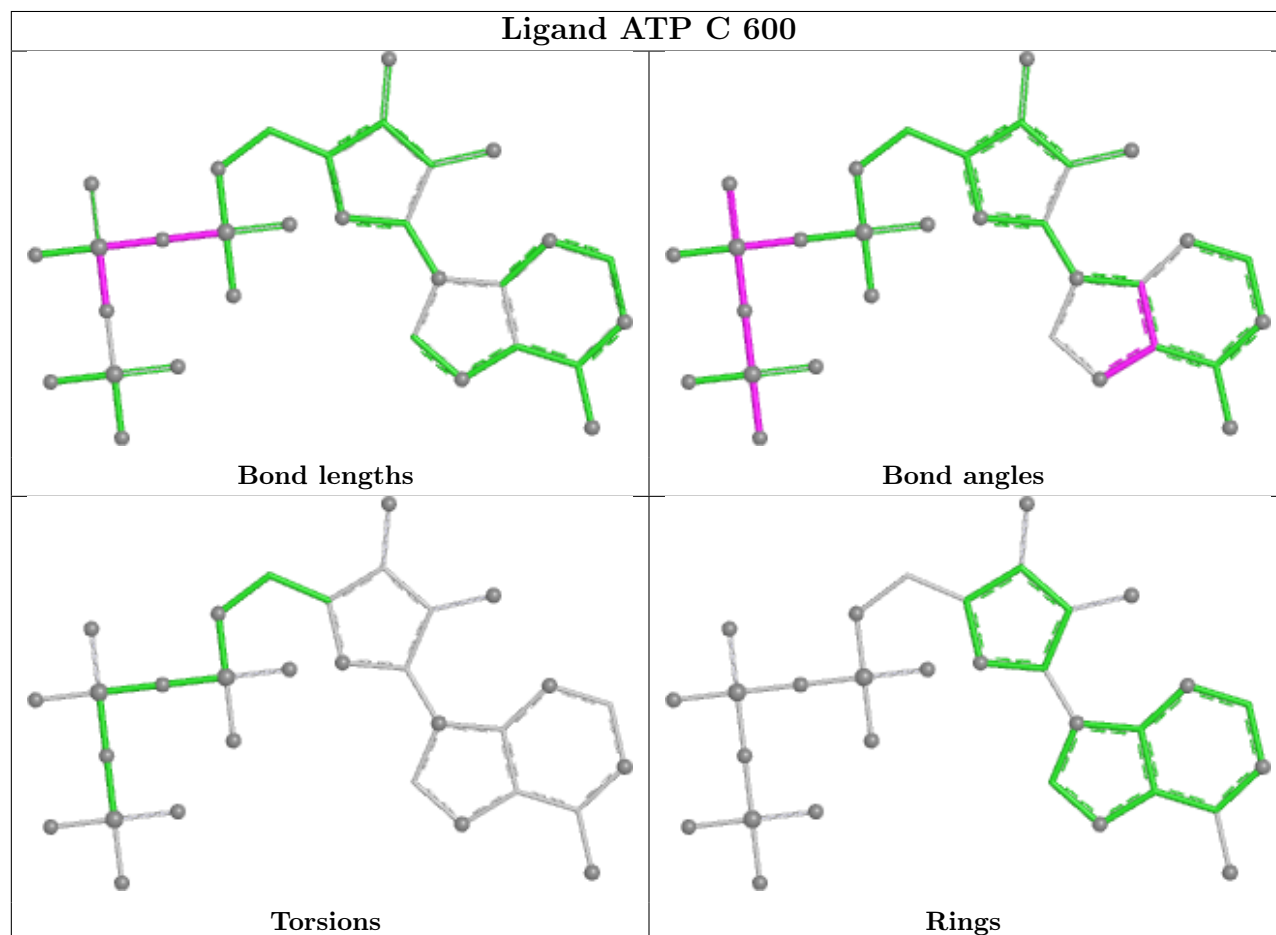
There are no ring outliers.

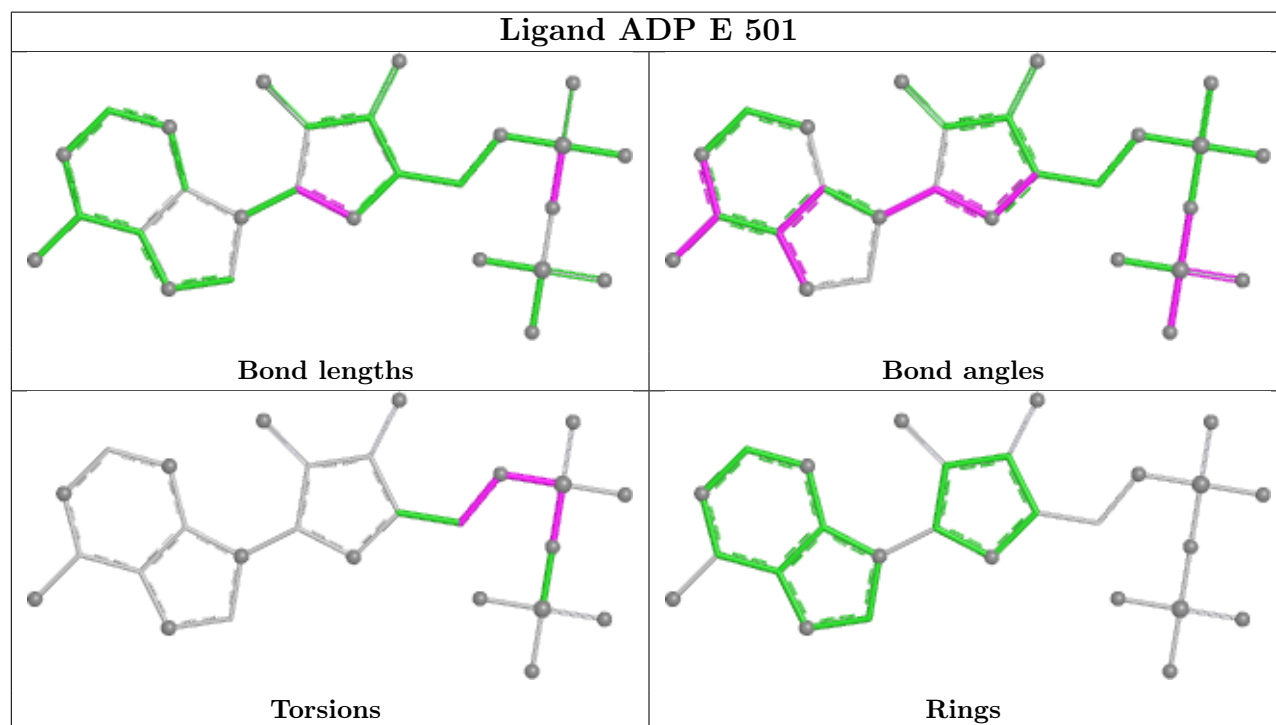
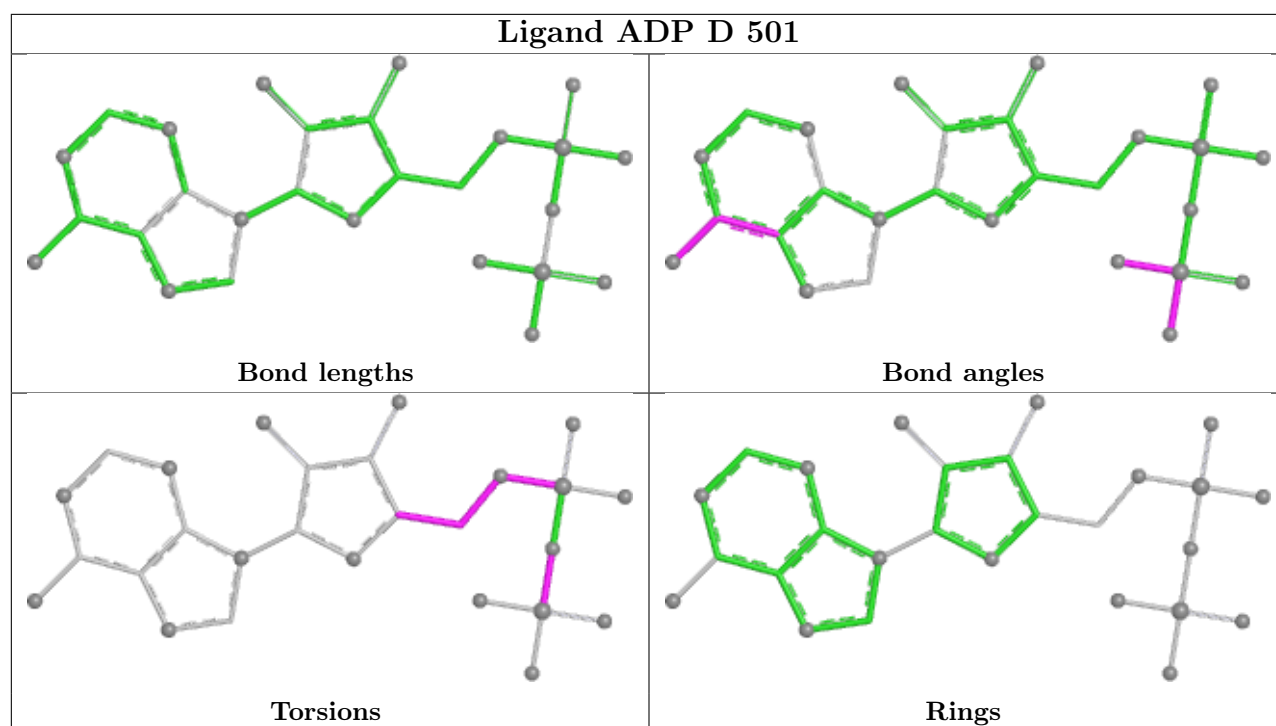
3 monomers are involved in 3 short contacts:

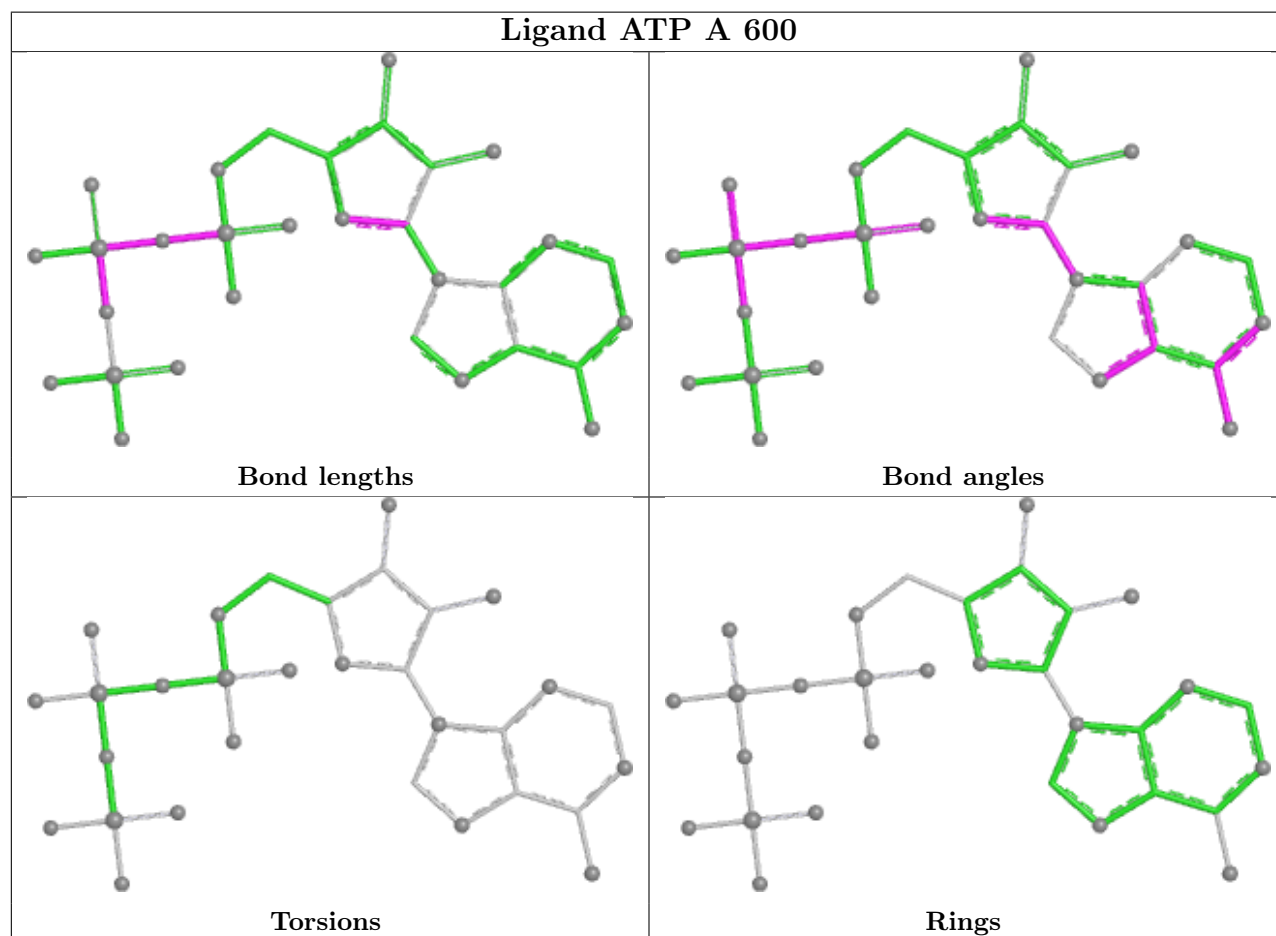
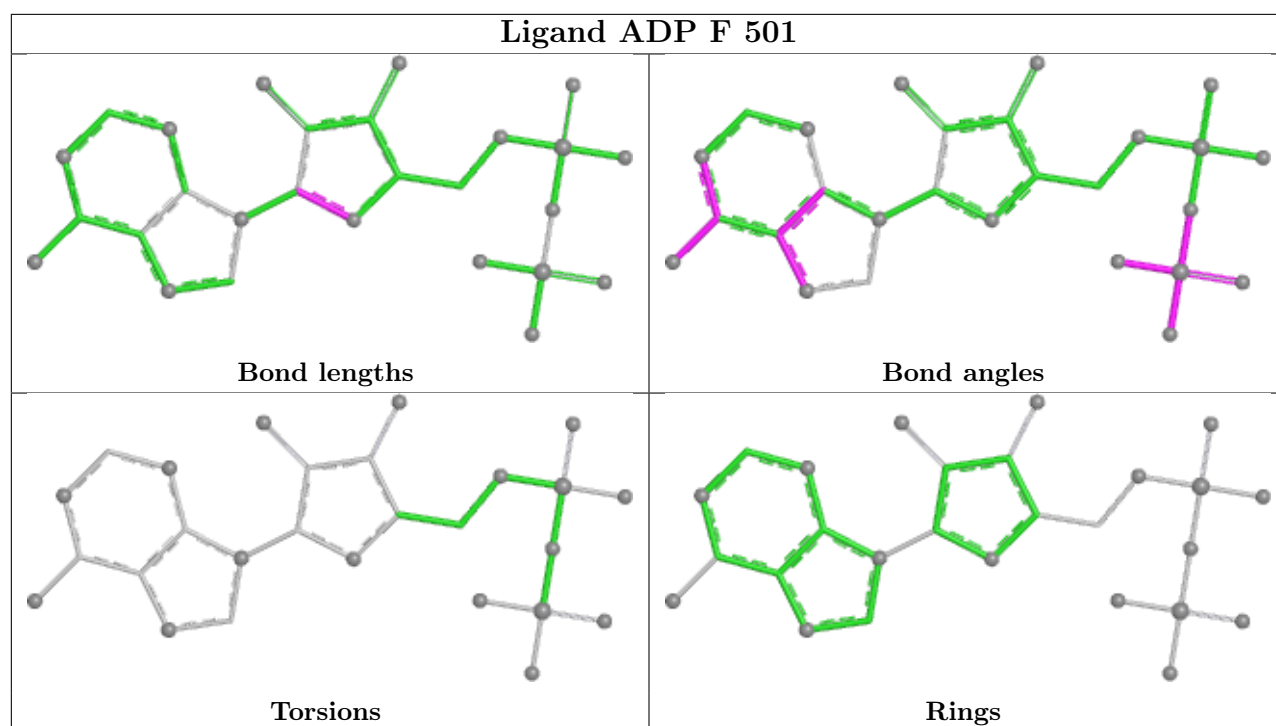
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	600	ATP	1	0
11	D	501	ADP	1	0
9	B	600	ATP	1	0

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.

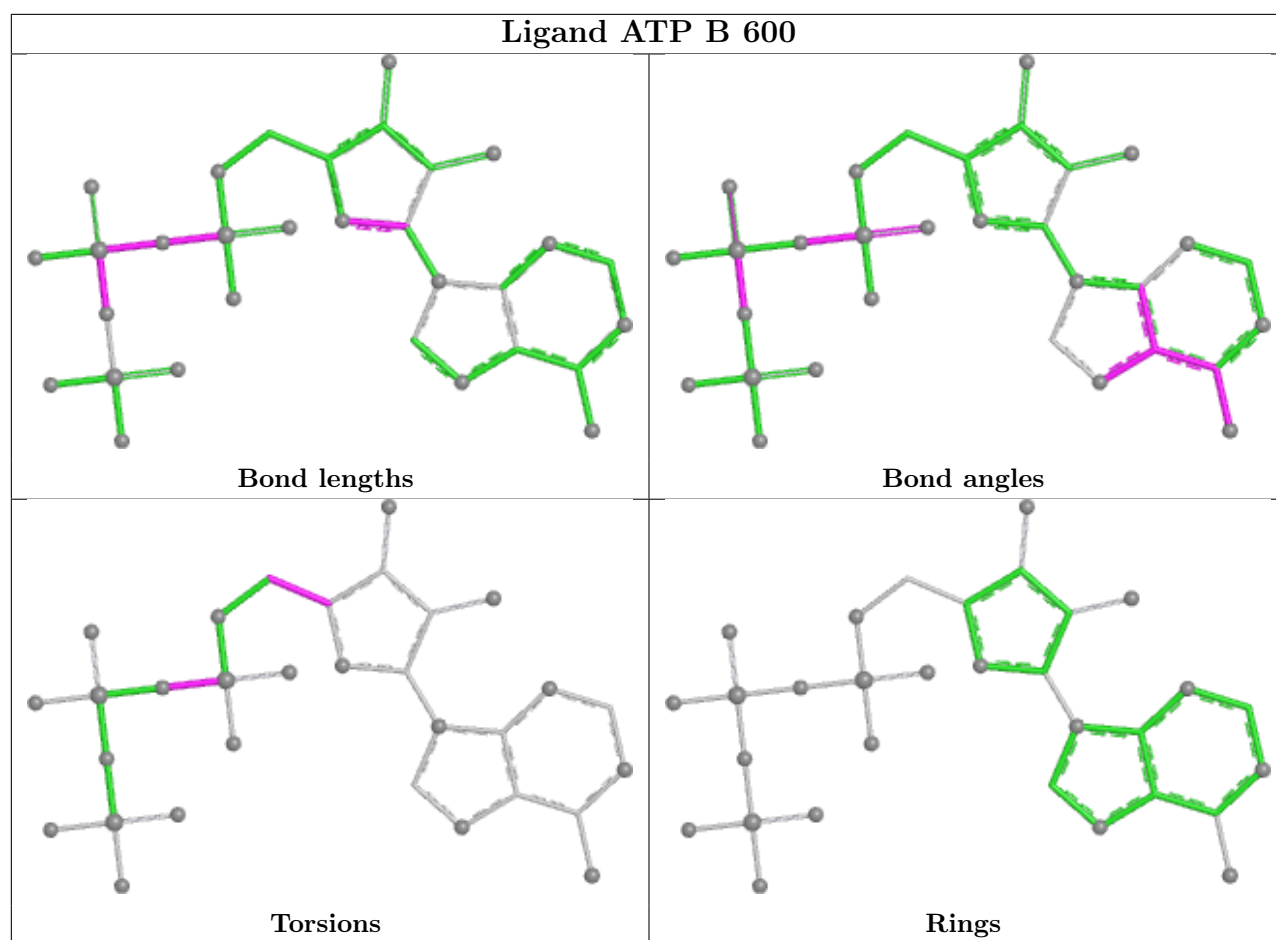
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

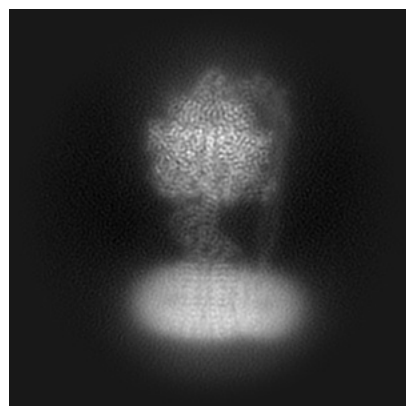
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70009. These allow visual inspection of the internal detail of the map and identification of artifacts.

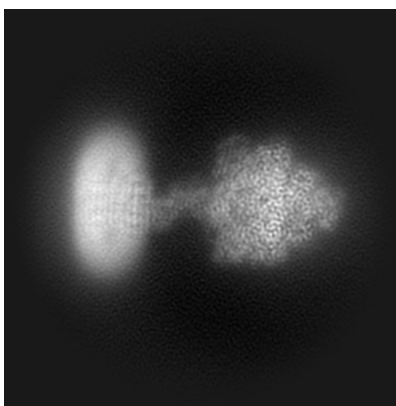
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

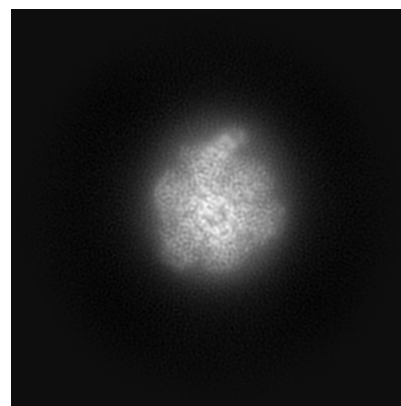
#### 6.1.1 Primary map



X

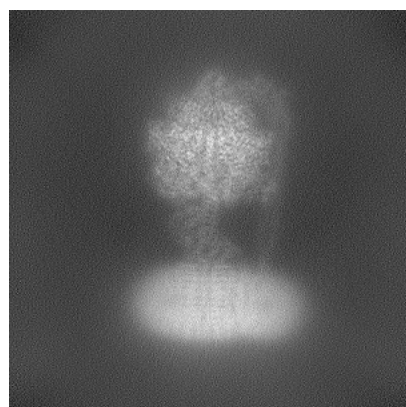


Y

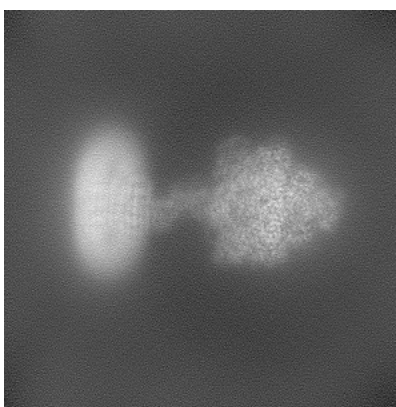


Z

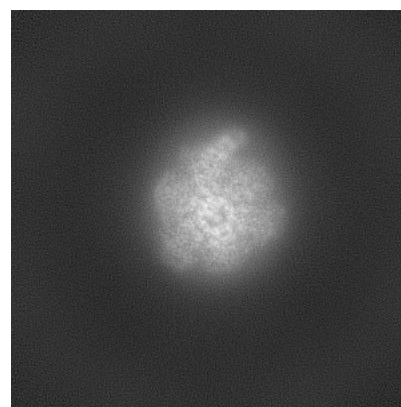
#### 6.1.2 Raw map



X



Y

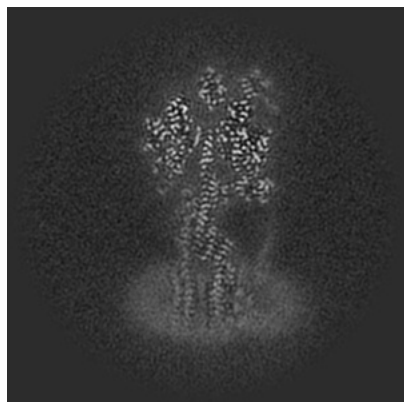


Z

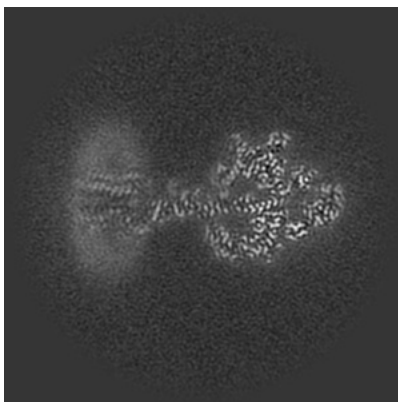
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

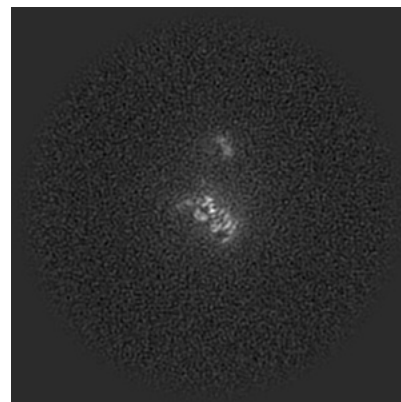
### 6.2.1 Primary map



X Index: 200

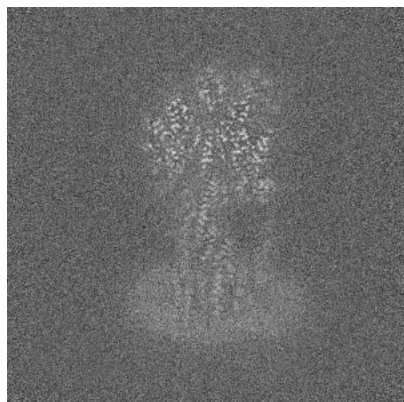


Y Index: 200

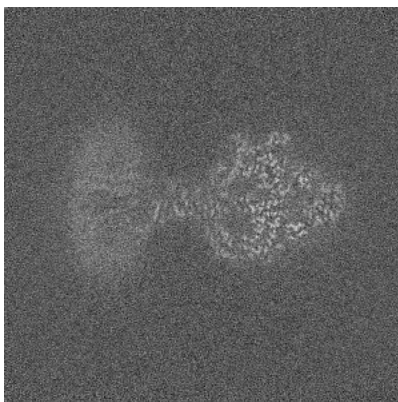


Z Index: 200

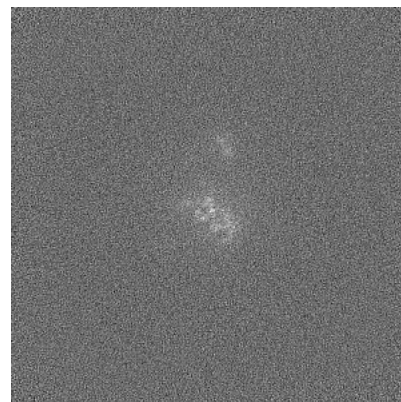
### 6.2.2 Raw map



X Index: 200



Y Index: 200

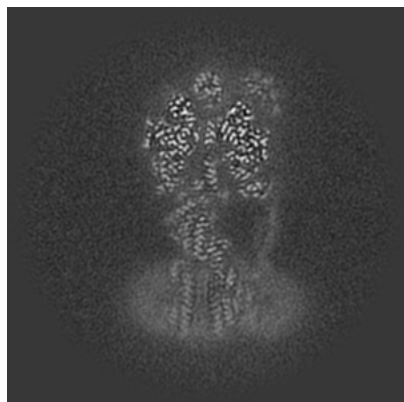


Z Index: 200

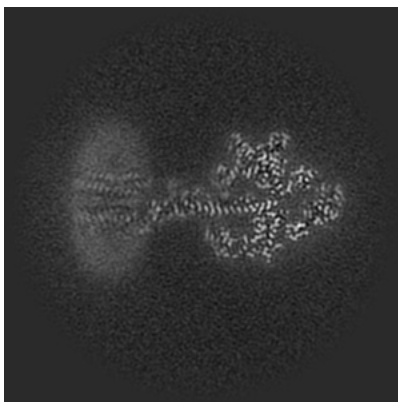
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

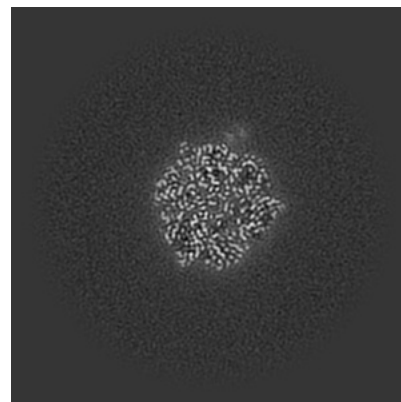
### 6.3.1 Primary map



X Index: 205

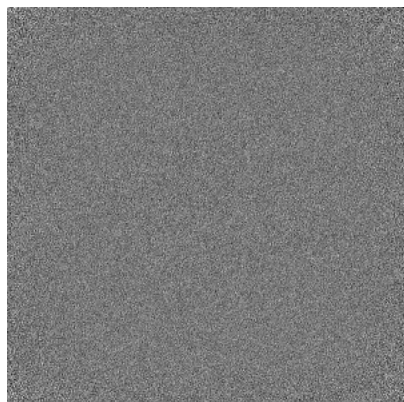


Y Index: 199

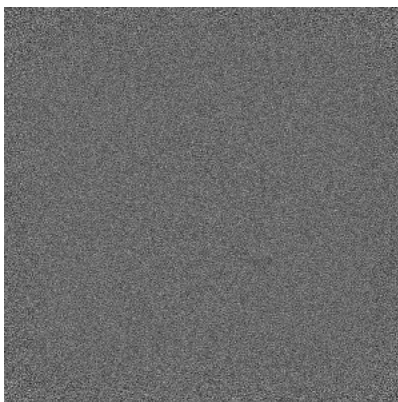


Z Index: 268

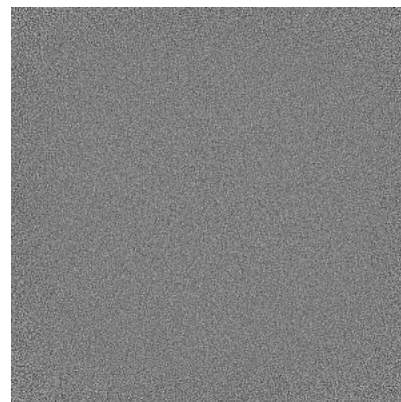
### 6.3.2 Raw map



X Index: 0



Y Index: 0



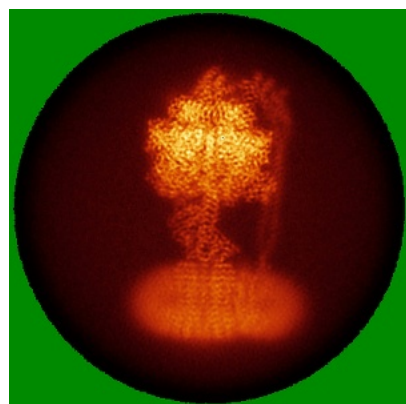
Z Index: 0

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

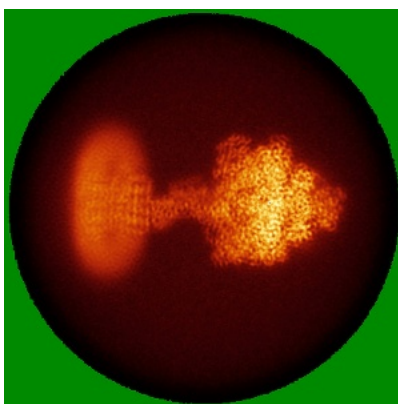


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

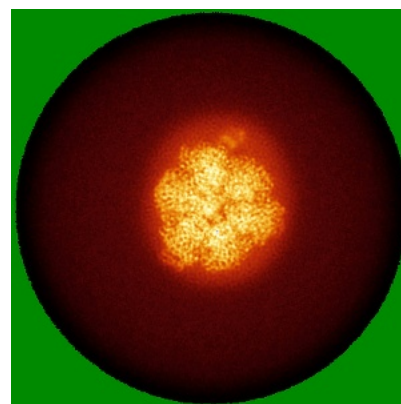
### 6.4.1 Primary map



X

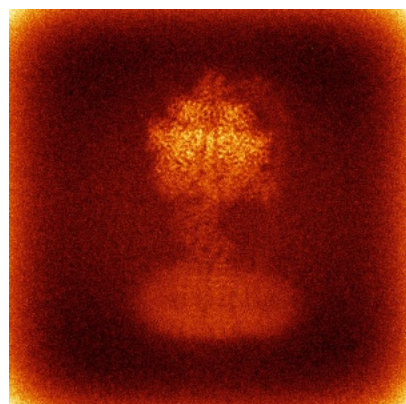


Y

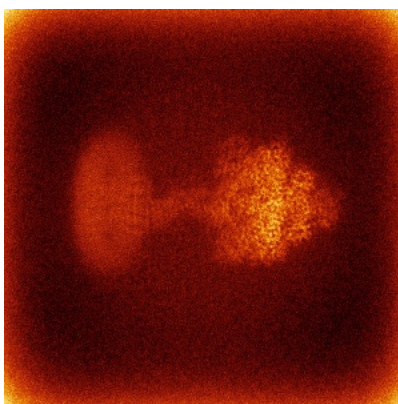


Z

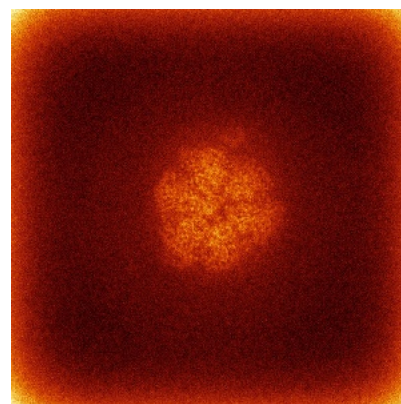
### 6.4.2 Raw map



X



Y

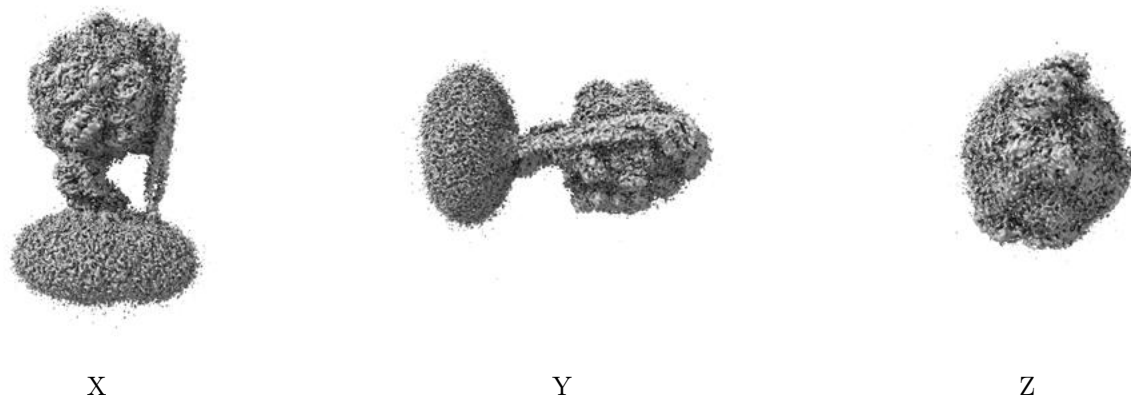


Z

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.

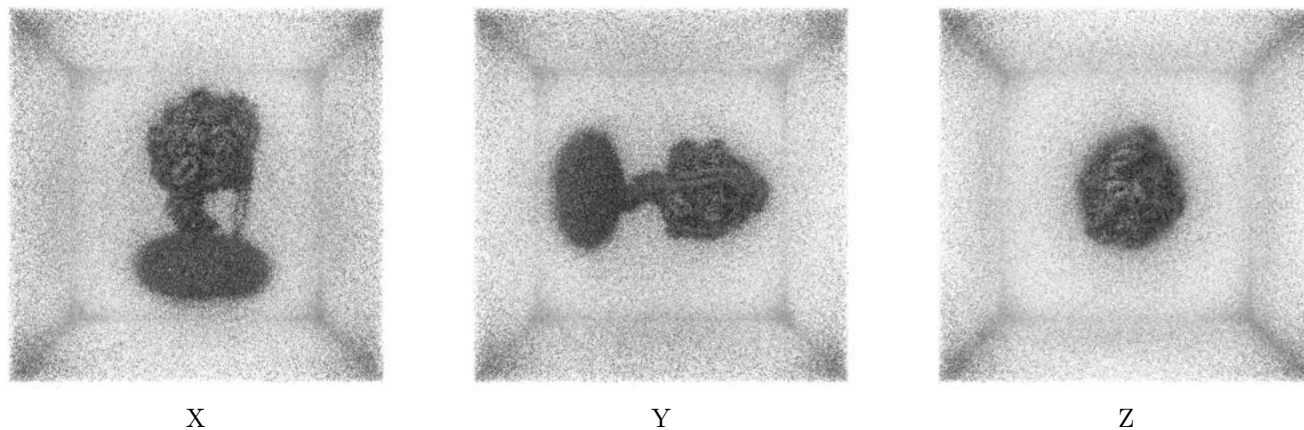
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.037. 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.

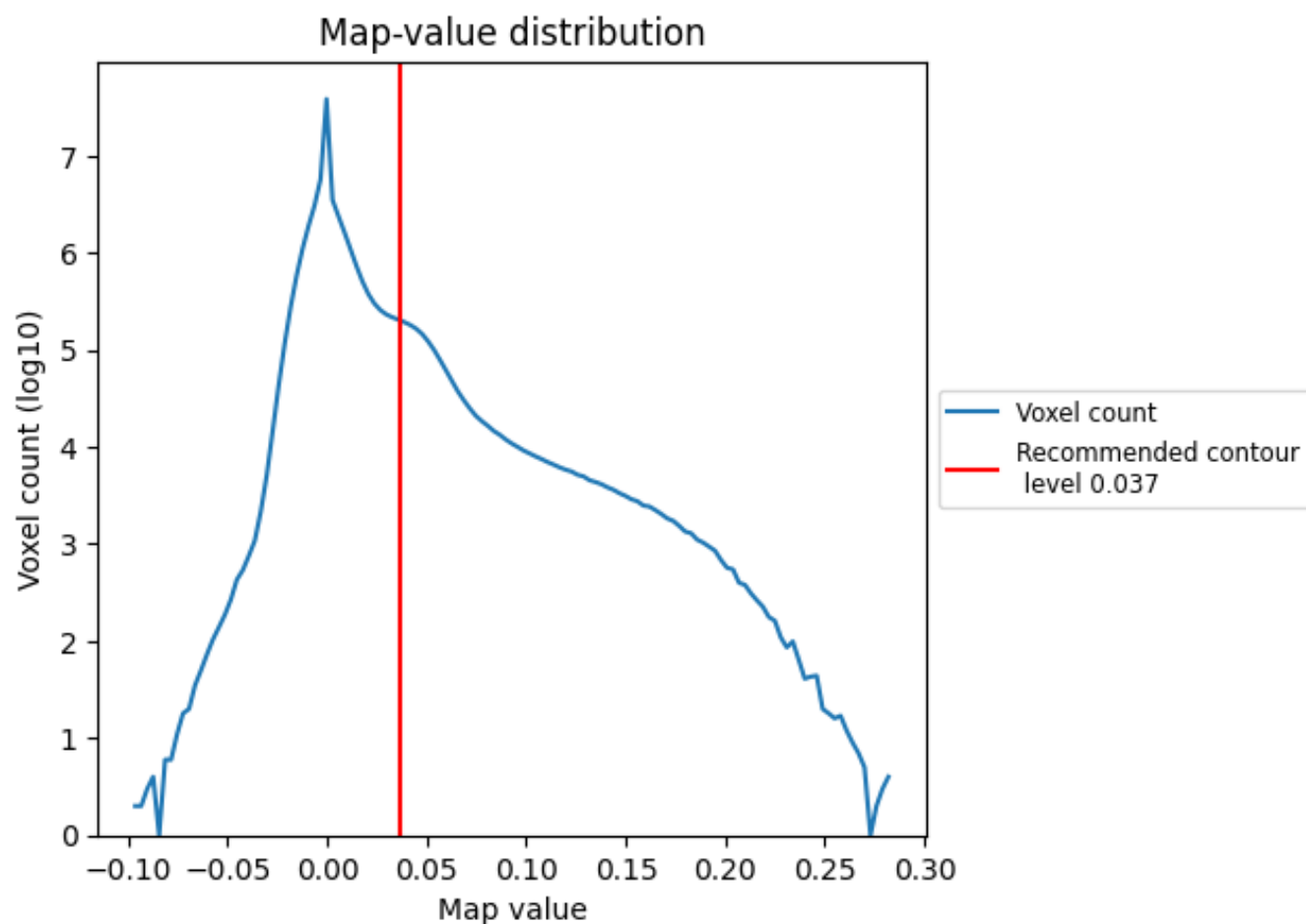
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

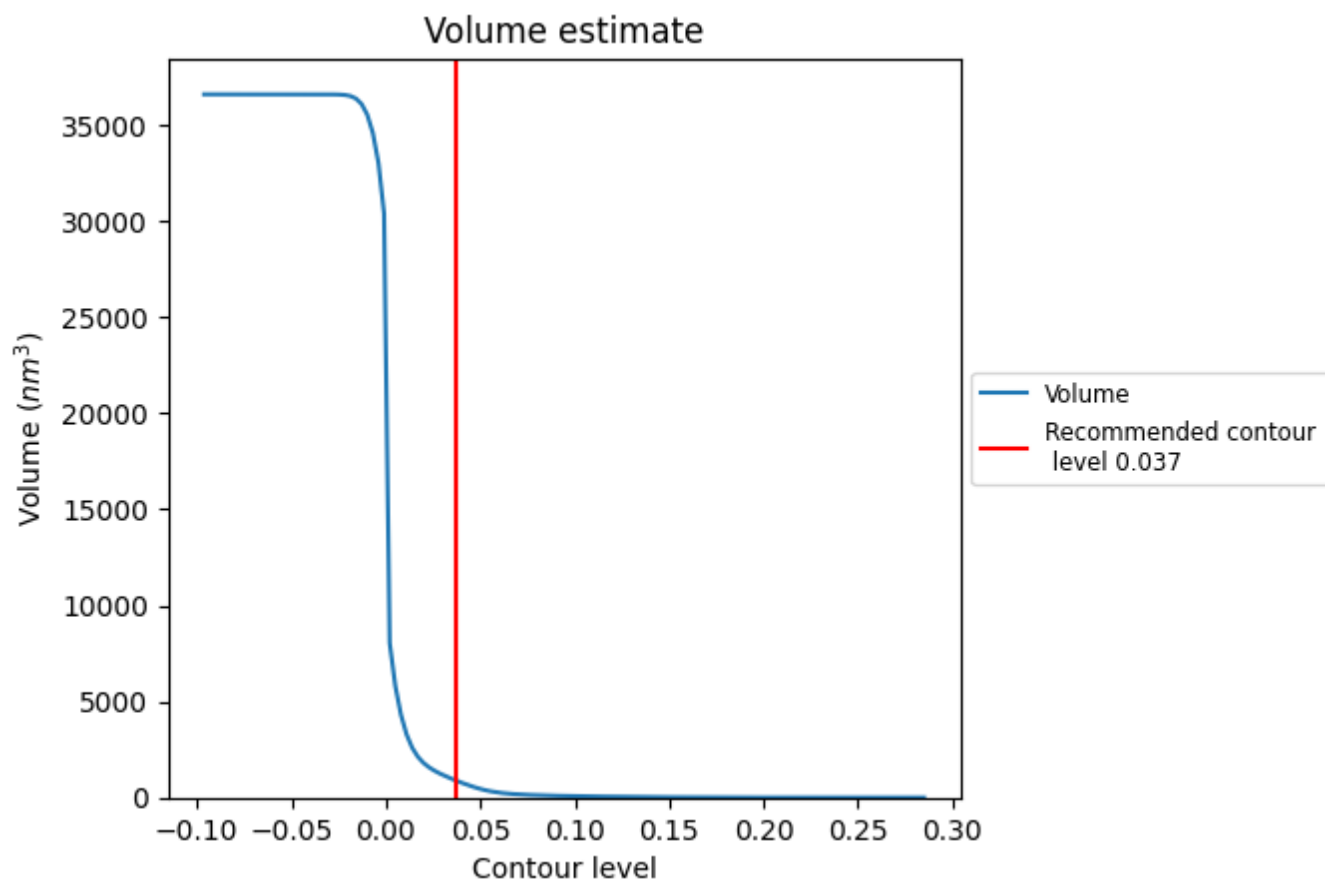
This section contains the results of statistical analysis of the map.

### 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](#)

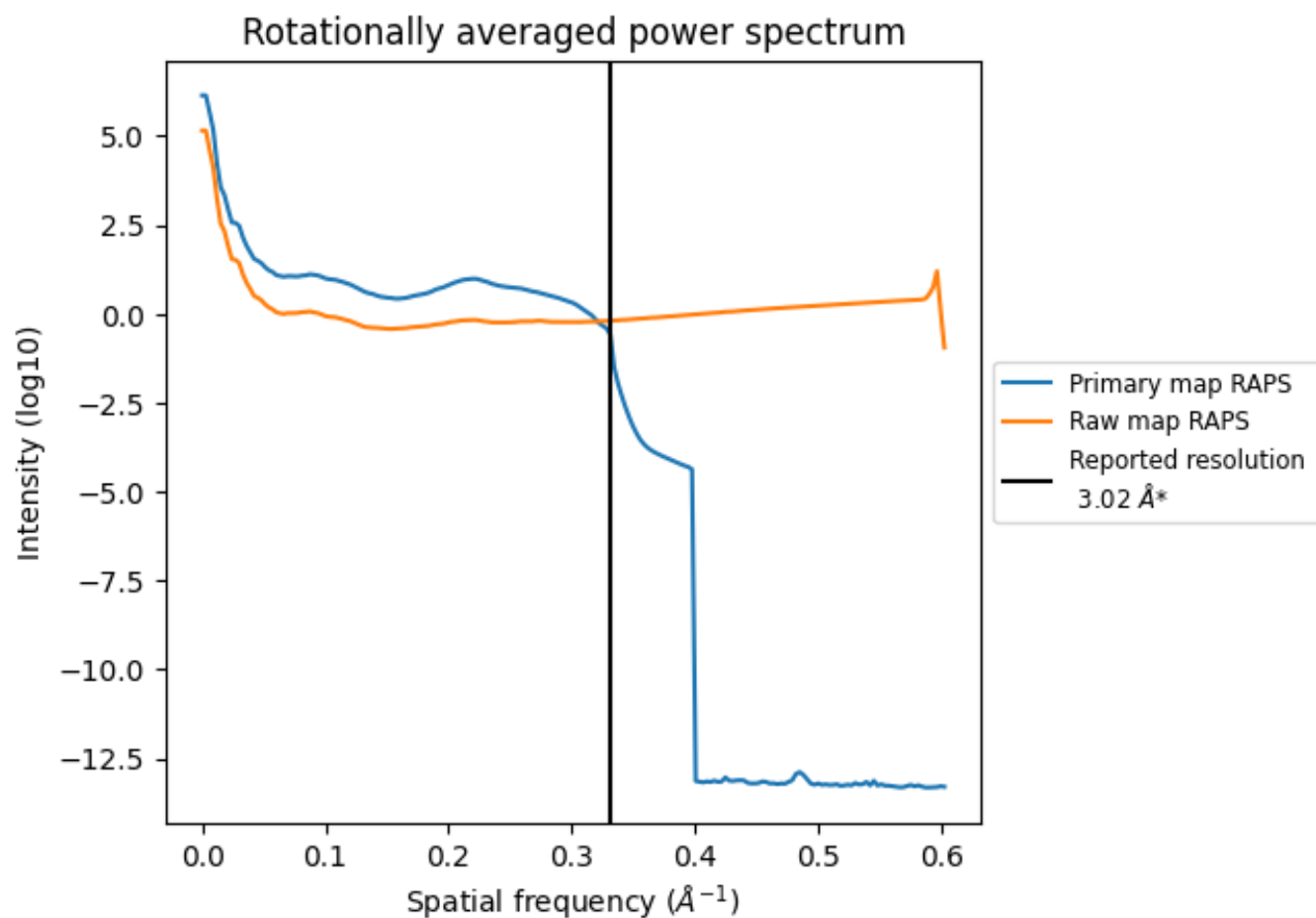


The volume at the recommended contour level is 891 nm<sup>3</sup>; this corresponds to an approximate mass of 805 kDa.

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 ⓘ

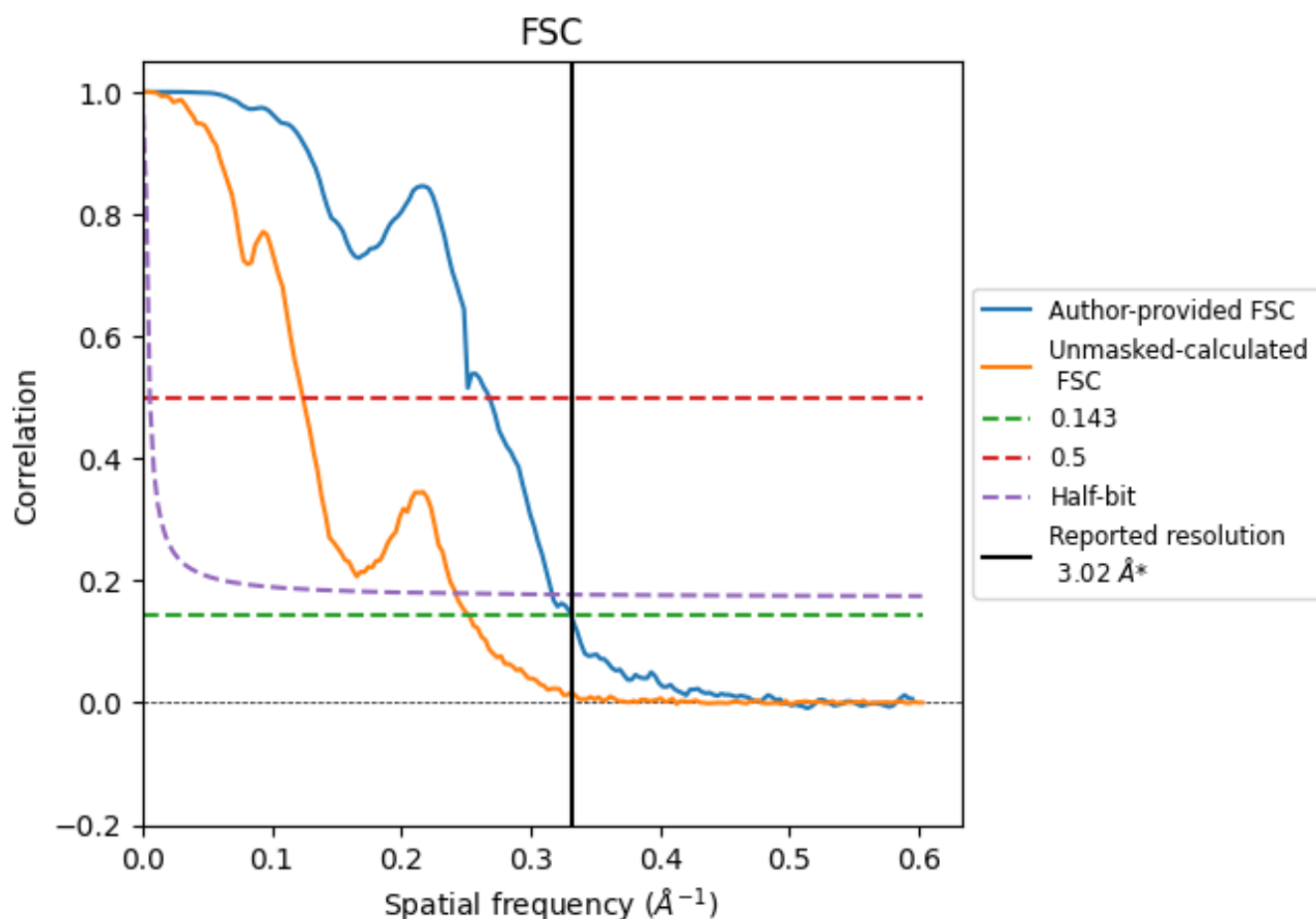


\*Reported resolution corresponds to spatial frequency of 0.331 Å<sup>-1</sup>

## 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 0.331  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

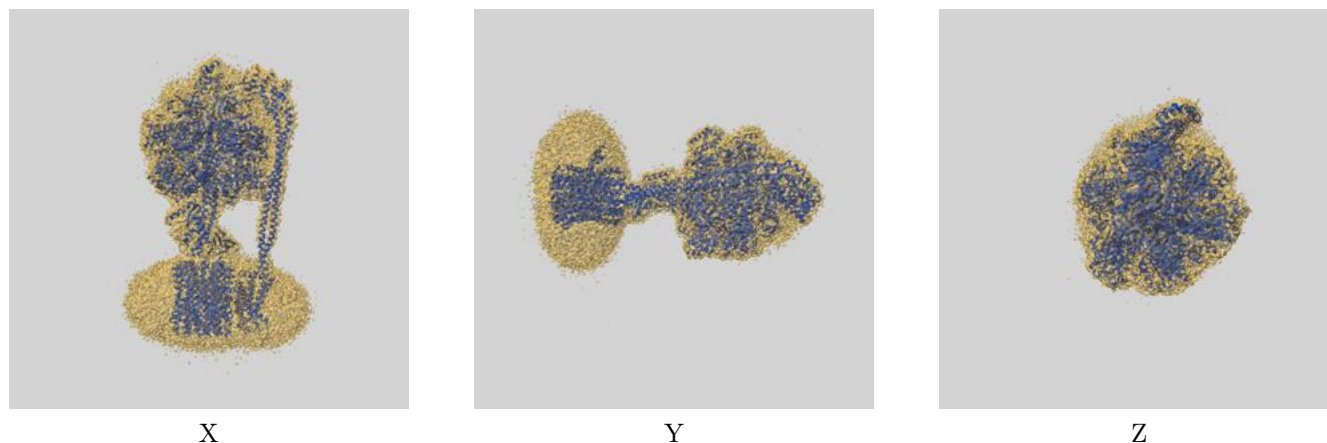
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	3.02	3.73	3.16
Unmasked-calculated*	3.97	8.06	4.13

\*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 3.97 differs from the reported value 3.02 by more than 10 %

## 9 Map-model fit [i](#)

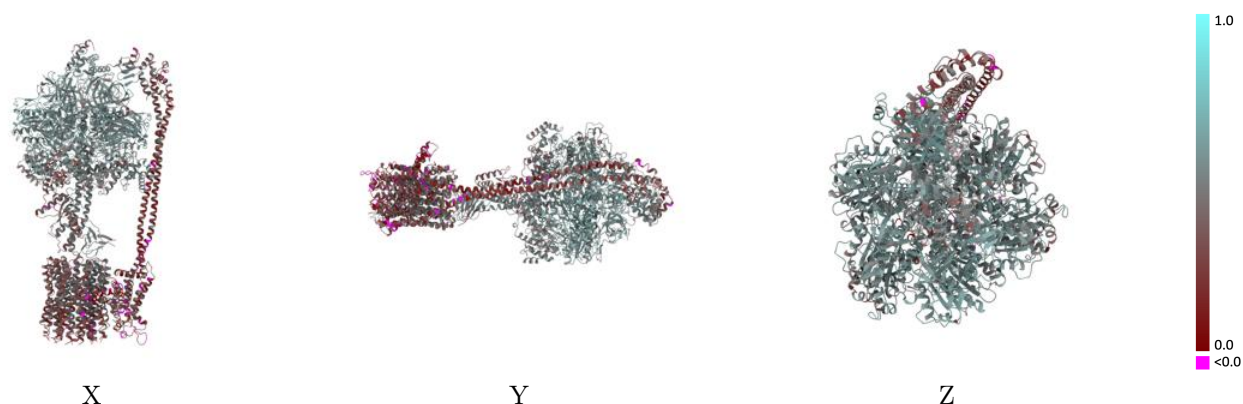
This section contains information regarding the fit between EMDB map EMD-70009 and PDB model 9O1J. Per-residue inclusion information can be found in section [3](#) on page [9](#).

### 9.1 Map-model overlay [i](#)



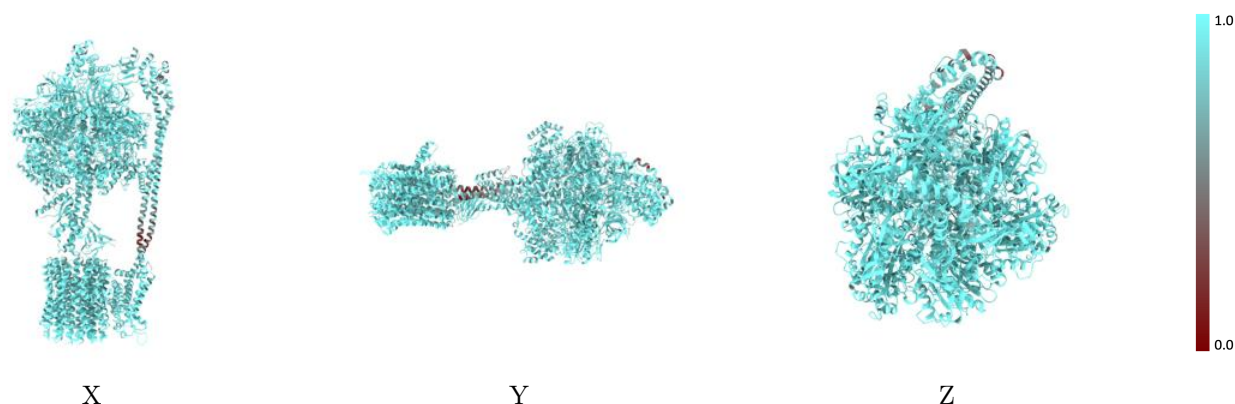
The images above show the 3D surface view of the map at the recommended contour level 0.037 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



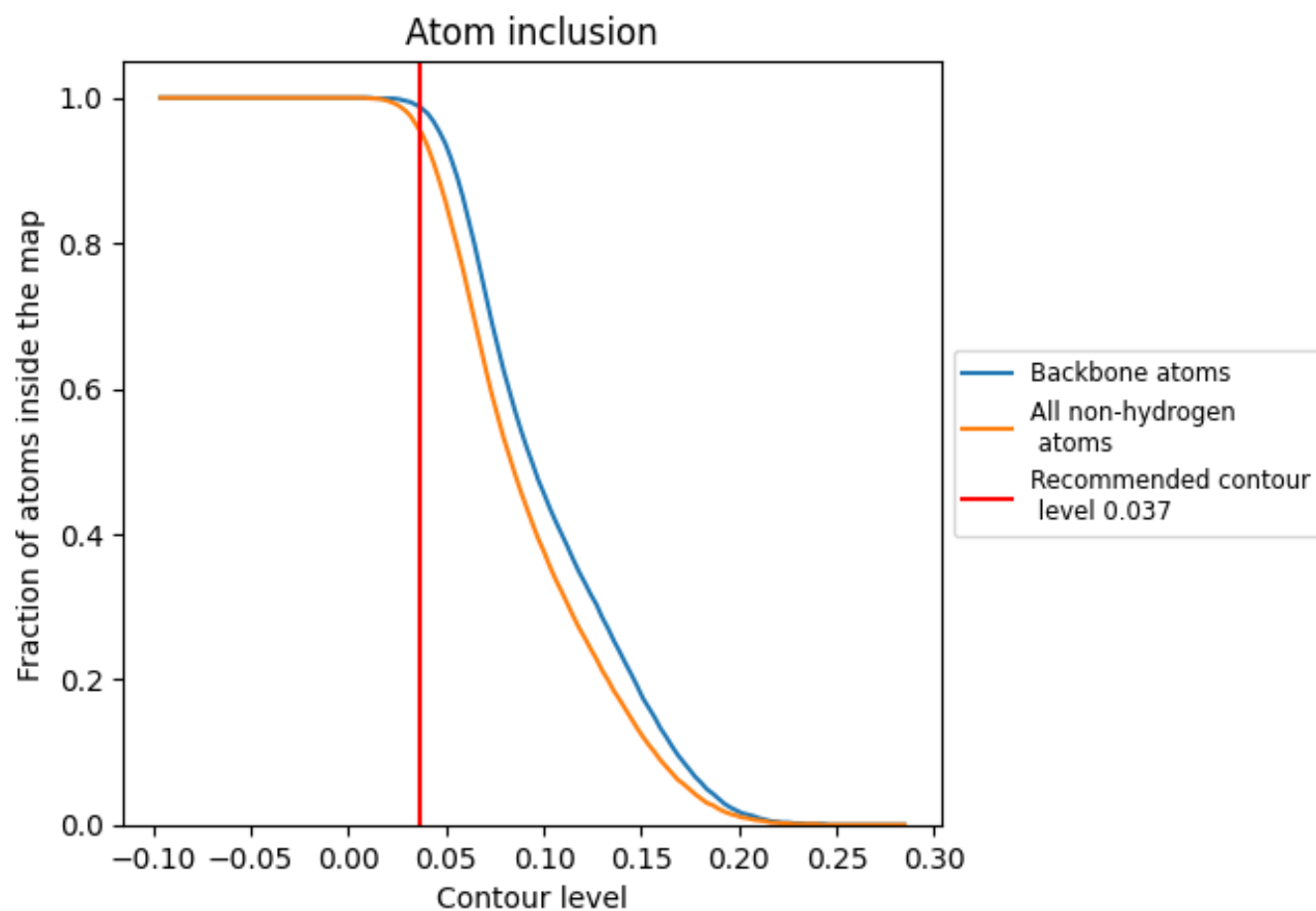
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.037).















































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 99% of all backbone atoms, 95% 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 (0.037) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9530	 0.4620
A	 0.9750	 0.5590
B	 0.9710	 0.5290
C	 0.9660	 0.5140
D	 0.9640	 0.5160
E	 0.9830	 0.5580
F	 0.9780	 0.5420
G	 0.9510	 0.4640
H	 0.8820	 0.4130
I	 0.9540	 0.3660
J	 0.9630	 0.3860
L	 0.9730	 0.3670
M	 0.9480	 0.3360
N	 0.9750	 0.4310
O	 0.9560	 0.2990
P	 0.9610	 0.3580
Q	 0.9700	 0.3840
R	 0.9660	 0.3240
S	 0.9580	 0.3310
W	 0.9470	 0.4760
X	 0.7810	 0.2610
Y	 0.8170	 0.2770
a	 0.9400	 0.2240

