Full wwPDB EM Validation Report ⓘ

Nov 12, 2022 – 09:52 PM EST

PDB ID	:	6VOL
EMDB ID	:	EMD-21268
Title	:	Chloroplast ATP synthase (R2, CF1FO)
Authors	:	Yang, J.-H.; Williams, D.; Kandiah, E.; Fromme, P.; Chiu, P.-L.
Deposited on	:	2020-01-30
Resolution	:	4.06 Å(reported)
Based on initial model	:	6FKH

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

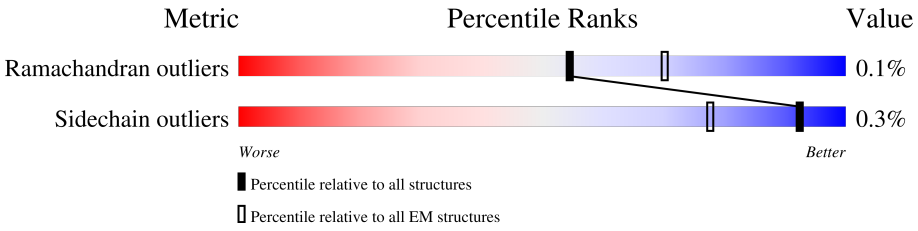
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.06 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.



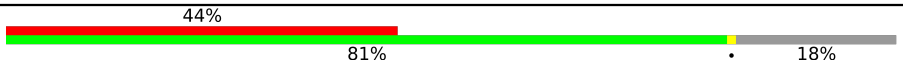
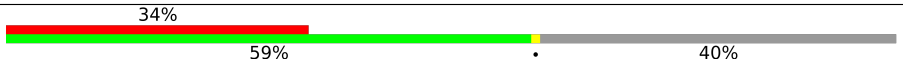
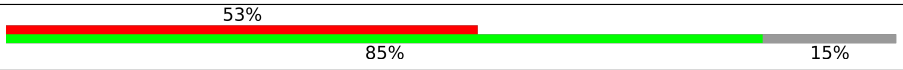
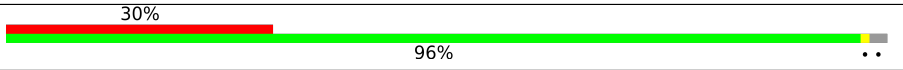
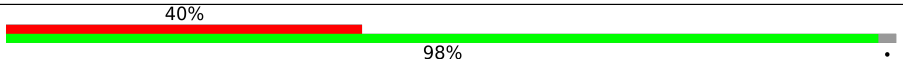
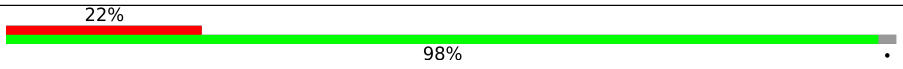
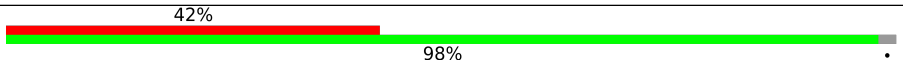
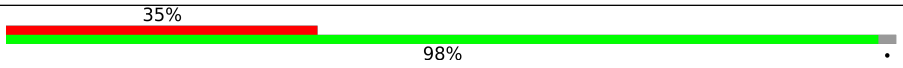
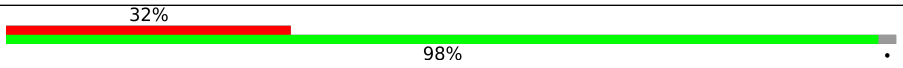
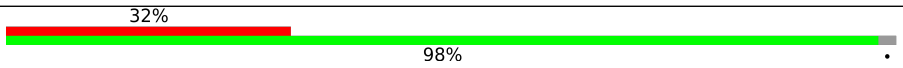
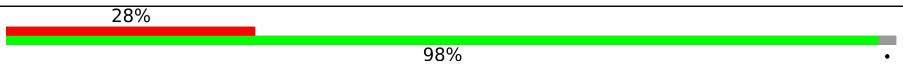
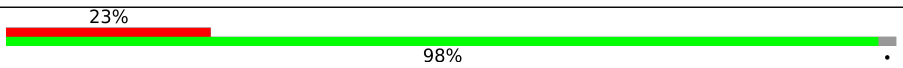
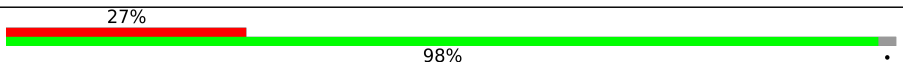
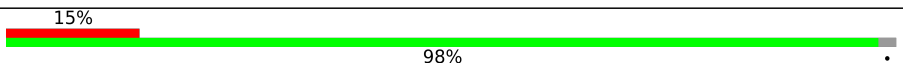
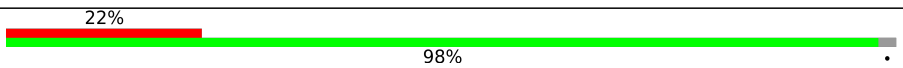
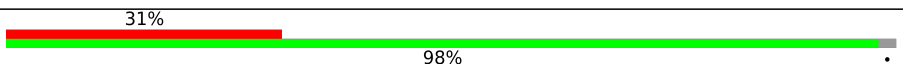
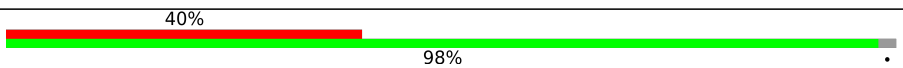
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	507	98%
1	B	507	98%
1	C	507	98%
2	D	498	96%
2	E	498	96%
2	F	498	96%
3	d	257	5% 70% 30%
4	g	364	88% 12%
5	e	134	6% 96%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	I	184	
7	J	222	
8	a	247	
9	M	81	
9	N	81	
9	O	81	
9	P	81	
9	Q	81	
9	R	81	
9	S	81	
9	T	81	
9	U	81	
9	V	81	
9	W	81	
9	X	81	
9	Y	81	
9	Z	81	

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 38991 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, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	497	Total	C	N	O	S	0	0
			3818	2403	659	743	13		
1	B	501	Total	C	N	O	S	0	0
			3851	2423	667	748	13		
1	C	500	Total	C	N	O	S	0	0
			3843	2417	666	747	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	479	Total	C	N	O	S	0	0
			3627	2288	623	700	16		
2	E	480	Total	C	N	O	S	0	0
			3636	2294	625	701	16		
2	F	478	Total	C	N	O	S	0	0
			3619	2282	622	699	16		

- Molecule 3 is a protein called ATP synthase delta chain, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	179	Total	C	N	O	S	0	0
			1383	876	229	277	1		

- Molecule 4 is a protein called ATP synthase gamma chain, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	g	321	Total	C	N	O	S	0	0
			2497	1574	429	482	12		

- Molecule 5 is a protein called ATP synthase epsilon chain, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	131	Total	C	N	O	S	0	0
			1010	622	190	195	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	150	Total	C	N	O	S	0	0
			1213	756	223	229	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	133	Total	C	N	O	S	0	0
			1041	658	170	208	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	a	210	Total	C	N	O	S	0	0
			1629	1096	249	282	2		

- Molecule 9 is a protein called ATP synthase subunit c, chloroplastic.

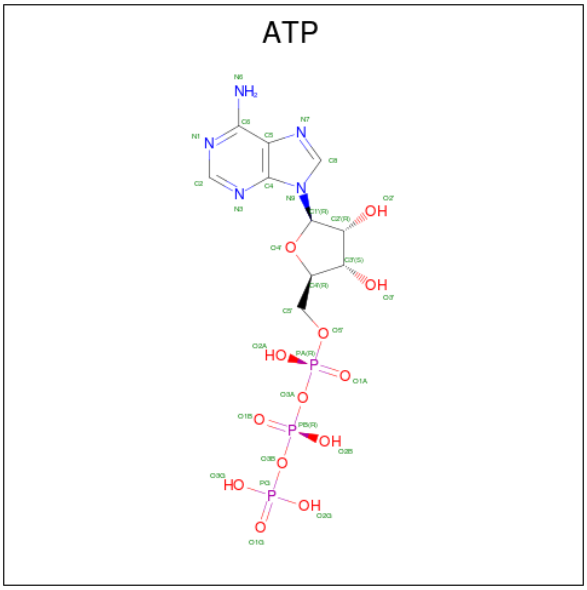
Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
9	N	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
9	O	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
9	P	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
9	Q	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
9	R	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
9	S	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
9	T	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
9	U	79	Total	C	N	O	S	0	0
			544	355	90	98	1		

Continued on next page...

Continued from previous page...

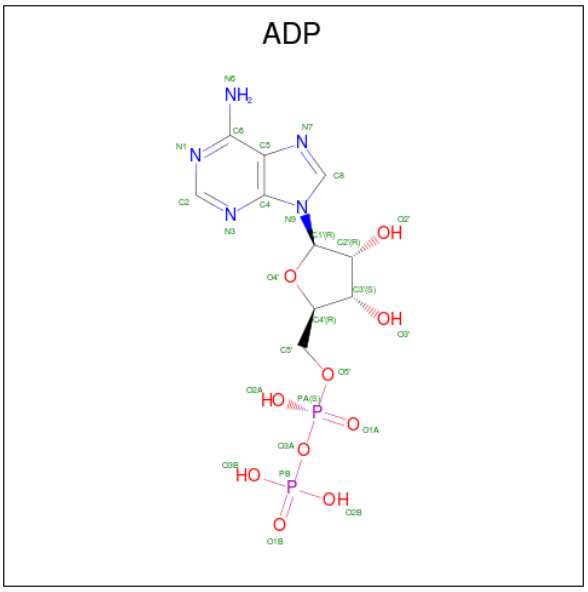
Mol	Chain	Residues	Atoms					AltConf	Trace
9	V	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
9	W	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
9	X	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
9	Y	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
9	Z	79	Total	C	N	O	S	0	0
			544	355	90	98	1		

- Molecule 10 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



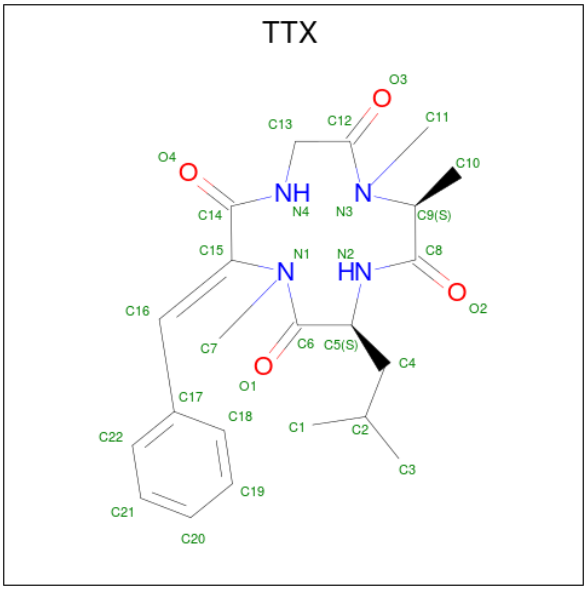
Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
10	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
10	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
10	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 12 is TENTOXIN (three-letter code: TTX) (formula: $C_{22}H_{30}N_4O_4$).



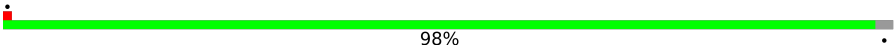
Mol	Chain	Residues	Atoms				AltConf
12	F	1	Total	C	N	O	0
			30	22	4	4	

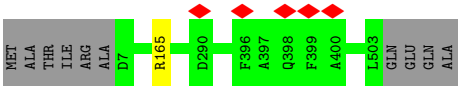
3 Residue-property plots (i)

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, chloroplastic

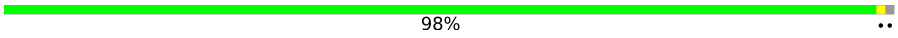
Chain A:

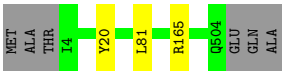




• Molecule 1: ATP synthase subunit alpha, chloroplastic

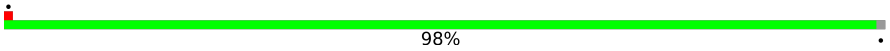
Chain B:

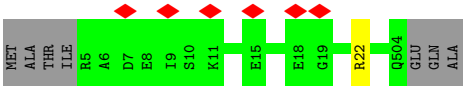




• Molecule 1: ATP synthase subunit alpha, chloroplastic

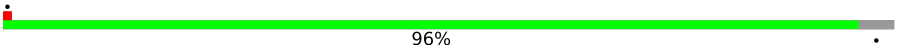
Chain C:

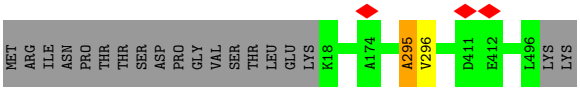




• Molecule 2: ATP synthase subunit beta, chloroplastic

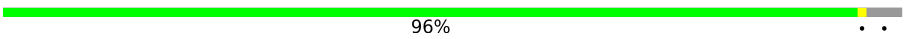
Chain D:

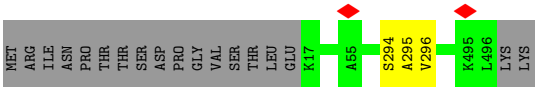




• Molecule 2: ATP synthase subunit beta, chloroplastic

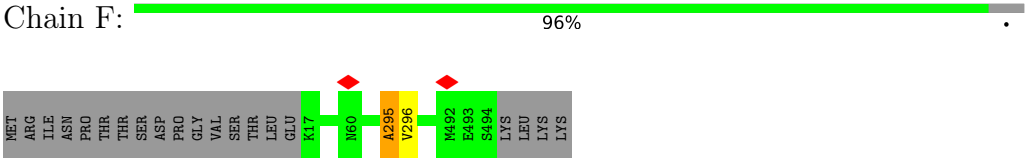
Chain E:





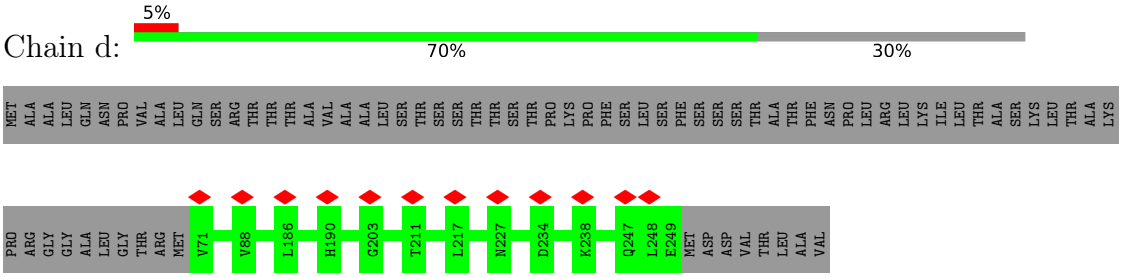
• Molecule 2: ATP synthase subunit beta, chloroplastic

Chain F:



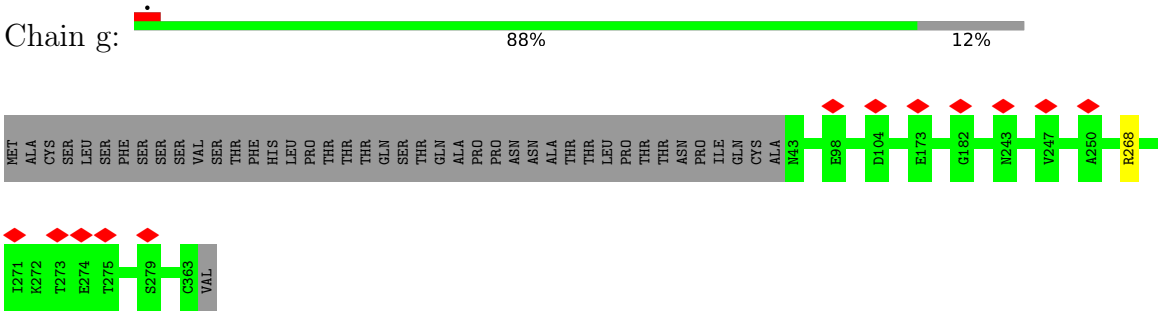
• Molecule 3: ATP synthase delta chain, chloroplastic

Chain d:



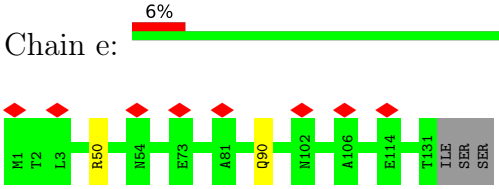
• Molecule 4: ATP synthase gamma chain, chloroplastic

Chain g:



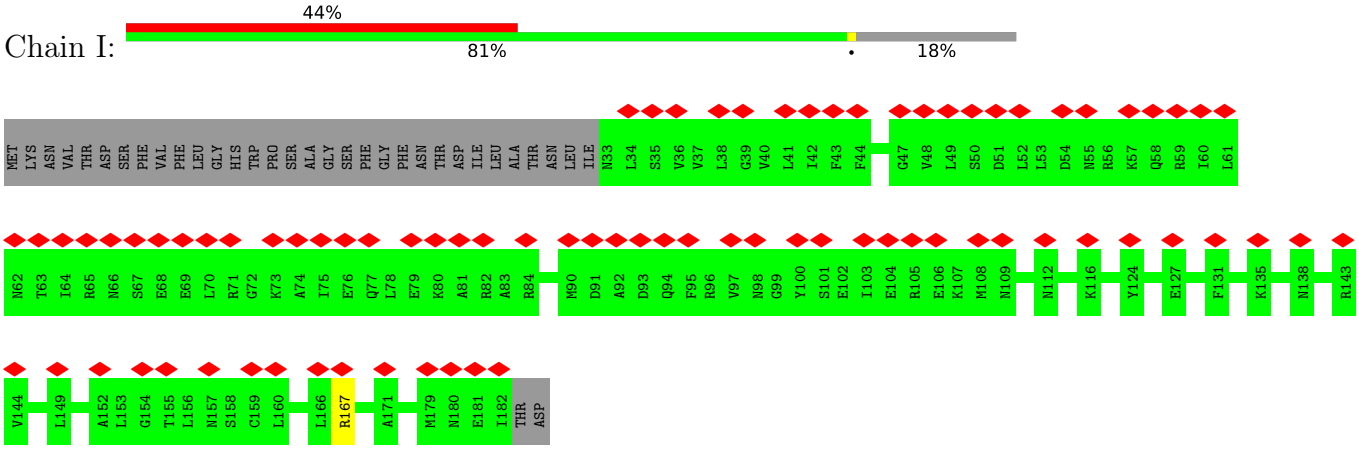
• Molecule 5: ATP synthase epsilon chain, chloroplastic

Chain e:



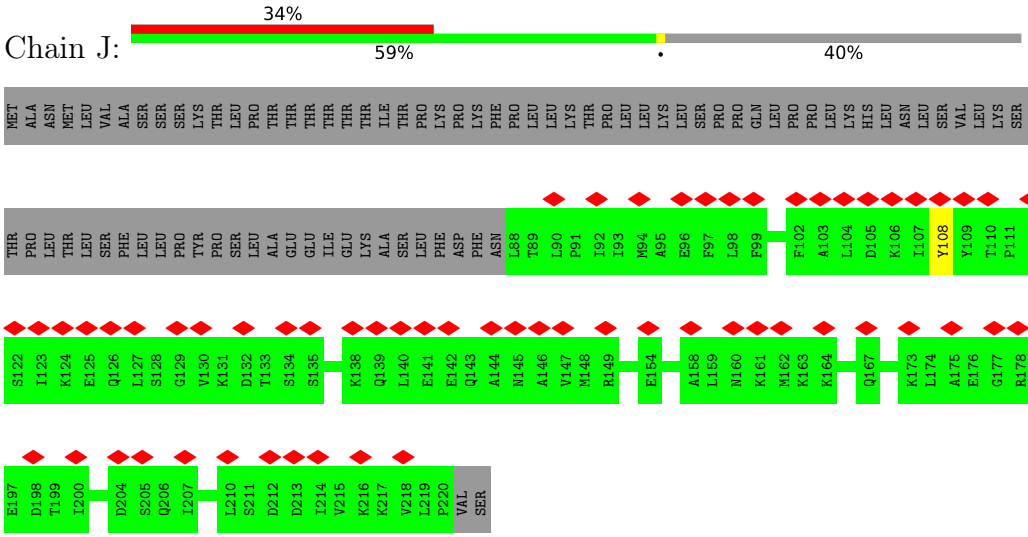
• Molecule 6: ATP synthase subunit b, chloroplastic

Chain I:



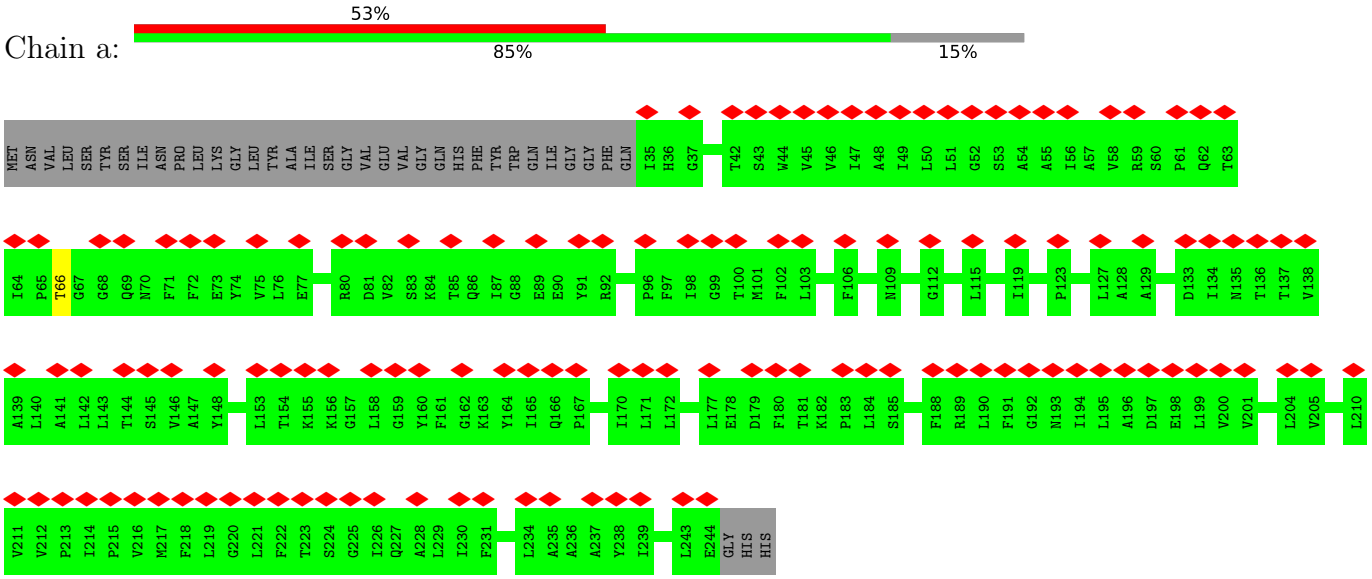
• Molecule 7: ATP synthase subunit b', chloroplastic

Chain J:



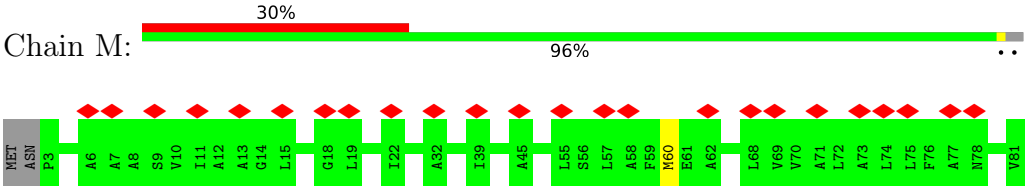
• Molecule 8: ATP synthase subunit a, chloroplastic

Chain a:



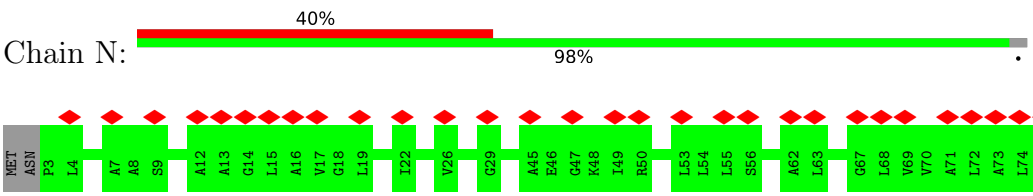
• Molecule 9: ATP synthase subunit c, chloroplastic

Chain M:



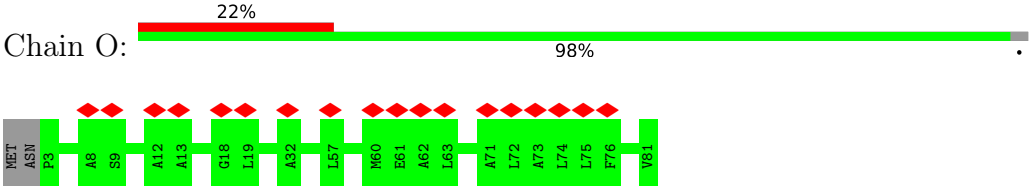
• Molecule 9: ATP synthase subunit c, chloroplastic

Chain N:



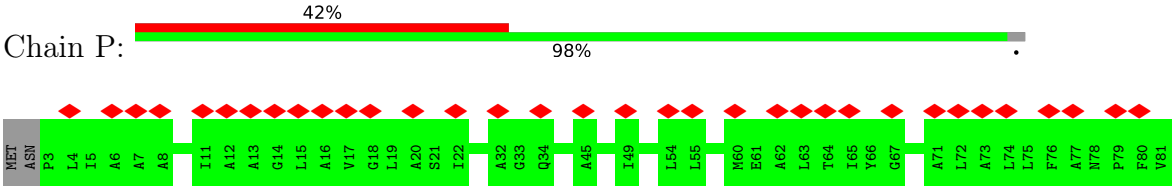
• Molecule 9: ATP synthase subunit c, chloroplastic

Chain O:



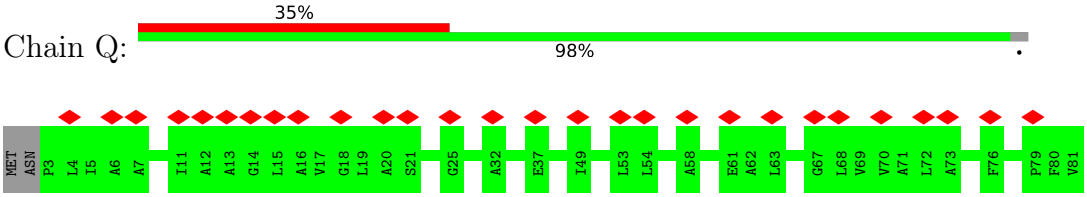
• Molecule 9: ATP synthase subunit c, chloroplastic

Chain P:



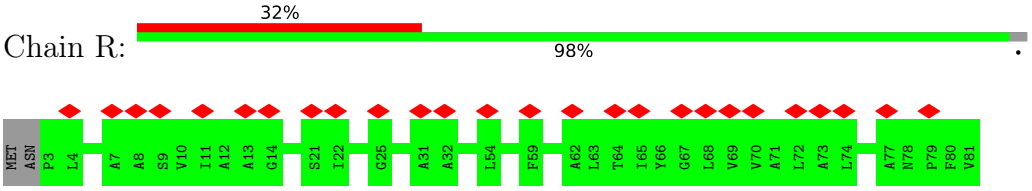
• Molecule 9: ATP synthase subunit c, chloroplastic

Chain Q:



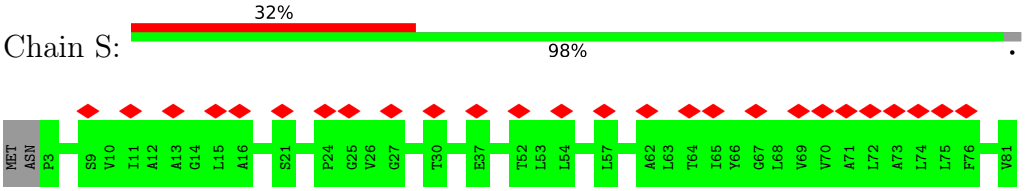
• Molecule 9: ATP synthase subunit c, chloroplastic

Chain R:



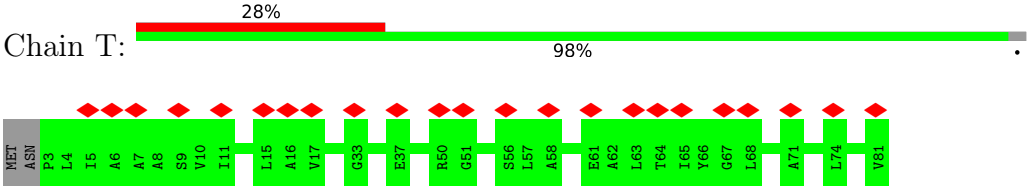
• Molecule 9: ATP synthase subunit c, chloroplastic

Chain S:



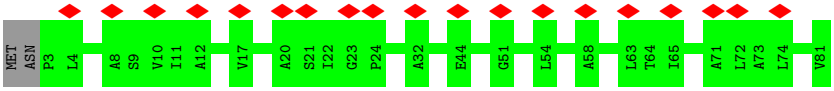
• Molecule 9: ATP synthase subunit c, chloroplastic

Chain T:

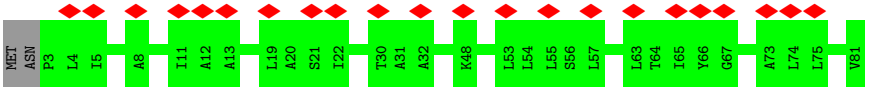


• Molecule 9: ATP synthase subunit c, chloroplastic

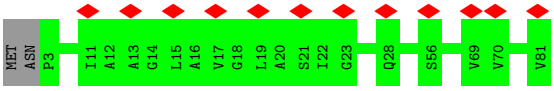
Chain U:



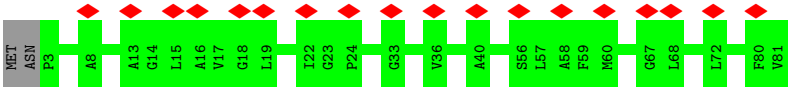
• Molecule 9: ATP synthase subunit c, chloroplastic



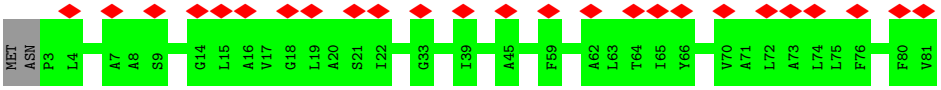
• Molecule 9: ATP synthase subunit c, chloroplastic



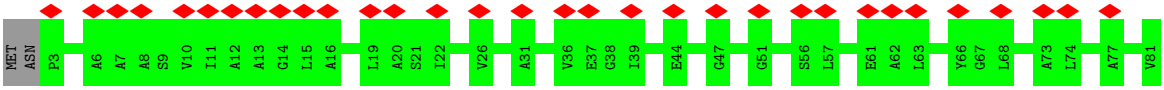
• Molecule 9: ATP synthase subunit c, chloroplastic



• Molecule 9: ATP synthase subunit c, chloroplastic



• Molecule 9: ATP synthase subunit c, chloroplastic



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	29667	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	43.5	Depositor
Minimum defocus (nm)	-1500	Depositor
Maximum defocus (nm)	-2800	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.074	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	442.25998, 442.25998, 442.25998	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.053, 1.053, 1.053	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.32	0/3867	0.48	0/5232
1	B	0.31	0/3900	0.51	1/5276 (0.0%)
1	C	0.32	0/3892	0.48	0/5265
2	D	0.31	0/3684	0.48	0/4994
2	E	0.31	0/3693	0.48	0/5005
2	F	0.33	0/3676	0.48	0/4983
3	d	0.27	0/1399	0.46	0/1898
4	g	0.29	0/2526	0.48	0/3412
5	e	0.28	0/1019	0.56	0/1381
6	I	0.28	0/1223	0.49	0/1637
7	J	0.31	0/1049	0.53	0/1405
8	a	0.28	0/1674	0.49	0/2294
9	M	0.29	0/551	0.51	0/750
9	N	0.30	0/551	0.50	0/750
9	O	0.28	0/551	0.47	0/750
9	P	0.29	0/551	0.48	0/750
9	Q	0.30	0/551	0.46	0/750
9	R	0.30	0/551	0.47	0/750
9	S	0.29	0/551	0.48	0/750
9	T	0.29	0/551	0.46	0/750
9	U	0.28	0/551	0.45	0/750
9	V	0.29	0/551	0.50	0/750
9	W	0.31	0/551	0.48	0/750
9	X	0.28	0/551	0.45	0/750
9	Y	0.29	0/551	0.47	0/750
9	Z	0.29	0/551	0.48	0/750
All	All	0.30	0/39316	0.49	1/53282 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	D	0	1
2	F	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	81	LEU	CA-CB-CG	5.21	127.28	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	20	TYR	Peptide
2	D	295	ALA	Peptide
2	F	295	ALA	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	495/507 (98%)	470 (95%)	25 (5%)	0	100	100
1	B	499/507 (98%)	468 (94%)	31 (6%)	0	100	100
1	C	498/507 (98%)	477 (96%)	21 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	477/498 (96%)	443 (93%)	32 (7%)	2 (0%)	34	71
2	E	478/498 (96%)	451 (94%)	24 (5%)	3 (1%)	25	63
2	F	476/498 (96%)	439 (92%)	35 (7%)	2 (0%)	34	71
3	d	177/257 (69%)	167 (94%)	10 (6%)	0	100	100
4	g	319/364 (88%)	300 (94%)	19 (6%)	0	100	100
5	e	129/134 (96%)	113 (88%)	16 (12%)	0	100	100
6	I	148/184 (80%)	148 (100%)	0	0	100	100
7	J	131/222 (59%)	129 (98%)	2 (2%)	0	100	100
8	a	208/247 (84%)	192 (92%)	16 (8%)	0	100	100
9	M	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
9	N	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
9	O	77/81 (95%)	75 (97%)	2 (3%)	0	100	100
9	P	77/81 (95%)	75 (97%)	2 (3%)	0	100	100
9	Q	77/81 (95%)	75 (97%)	2 (3%)	0	100	100
9	R	77/81 (95%)	76 (99%)	1 (1%)	0	100	100
9	S	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
9	T	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
9	U	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
9	V	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
9	W	77/81 (95%)	76 (99%)	1 (1%)	0	100	100
9	X	77/81 (95%)	76 (99%)	1 (1%)	0	100	100
9	Y	77/81 (95%)	73 (95%)	4 (5%)	0	100	100
9	Z	77/81 (95%)	73 (95%)	4 (5%)	0	100	100
All	All	5113/5557 (92%)	4840 (95%)	266 (5%)	7 (0%)	54	84

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	296	VAL
2	E	296	VAL
2	D	295	ALA
2	E	295	ALA
2	F	295	ALA
2	E	294	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	296	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	407/414 (98%)	406 (100%)	1 (0%)	93 96
1	B	410/414 (99%)	409 (100%)	1 (0%)	93 96
1	C	409/414 (99%)	408 (100%)	1 (0%)	93 96
2	D	390/408 (96%)	390 (100%)	0	100 100
2	E	391/408 (96%)	391 (100%)	0	100 100
2	F	389/408 (95%)	389 (100%)	0	100 100
3	d	156/220 (71%)	156 (100%)	0	100 100
4	g	276/315 (88%)	275 (100%)	1 (0%)	91 94
5	e	109/112 (97%)	107 (98%)	2 (2%)	59 77
6	I	132/161 (82%)	131 (99%)	1 (1%)	81 89
7	J	115/197 (58%)	113 (98%)	2 (2%)	60 78
8	a	177/207 (86%)	176 (99%)	1 (1%)	86 92
9	M	51/53 (96%)	50 (98%)	1 (2%)	55 73
9	N	51/53 (96%)	51 (100%)	0	100 100
9	O	51/53 (96%)	51 (100%)	0	100 100
9	P	51/53 (96%)	51 (100%)	0	100 100
9	Q	51/53 (96%)	51 (100%)	0	100 100
9	R	51/53 (96%)	51 (100%)	0	100 100
9	S	51/53 (96%)	51 (100%)	0	100 100
9	T	51/53 (96%)	51 (100%)	0	100 100
9	U	51/53 (96%)	51 (100%)	0	100 100
9	V	51/53 (96%)	51 (100%)	0	100 100
9	W	51/53 (96%)	51 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	X	51/53 (96%)	51 (100%)	0	100 100
9	Y	51/53 (96%)	51 (100%)	0	100 100
9	Z	51/53 (96%)	51 (100%)	0	100 100
All	All	4075/4420 (92%)	4064 (100%)	11 (0%)	92 95

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	165	ARG
1	B	165	ARG
1	C	22	ARG
4	g	268	ARG
5	e	50	ARG
5	e	90	GLN
6	I	167	ARG
7	J	108	TYR
7	J	119	ARG
8	a	66	THR
9	M	60	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	256	HIS
1	A	351	ASN
1	A	389	GLN
1	A	425	GLN
1	A	468	ASN
1	A	497	GLN
1	B	34	GLN
1	B	208	GLN
1	B	212	ASN
1	B	256	HIS
1	B	423	GLN
1	C	70	ASN
1	C	201	GLN
1	C	214	GLN
1	C	295	HIS
1	C	389	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	409	ASN
1	C	425	GLN
2	D	45	ASN
2	D	264	ASN
2	E	25	GLN
2	E	72	ASN
2	E	120	ASN
2	E	188	ASN
2	E	226	ASN
2	E	238	GLN
2	E	240	ASN
2	E	325	GLN
2	F	25	GLN
2	F	112	ASN
2	F	223	ASN
2	F	238	GLN
2	F	479	ASN
3	d	170	ASN
3	d	206	ASN
3	d	240	GLN
4	g	95	ASN
4	g	134	ASN
5	e	4	ASN
5	e	27	ASN
5	e	54	ASN
6	I	55	ASN
6	I	109	ASN
6	I	120	GLN
6	I	150	GLN
6	I	161	ASN
6	I	162	ASN
6	I	172	ASN
6	I	180	ASN
7	J	186	GLN
7	J	195	GLN
8	a	86	GLN
8	a	175	ASN
9	P	34	GLN
9	S	28	GLN
9	S	34	GLN
9	U	34	GLN
9	X	42	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	Z	28	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 monosaccharides in this entry.

5.6 Ligand geometry

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	ATP	A	601	-	26,33,33	0.91	1 (3%)	31,52,52	1.57	6 (19%)
10	ATP	C	601	-	26,33,33	0.91	1 (3%)	31,52,52	1.69	5 (16%)
10	ATP	B	601	-	26,33,33	0.91	1 (3%)	31,52,52	1.70	5 (16%)
10	ATP	F	502	-	26,33,33	0.90	1 (3%)	31,52,52	1.52	5 (16%)
11	ADP	E	601	-	24,29,29	0.91	1 (4%)	29,45,45	1.53	4 (13%)
12	TTX	F	501	-	31,31,31	0.97	1 (3%)	40,43,43	1.30	2 (5%)
11	ADP	D	601	-	24,29,29	0.96	1 (4%)	29,45,45	1.54	4 (13%)

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
10	ATP	A	601	-	-	2/18/38/38	0/3/3/3
10	ATP	C	601	-	-	2/18/38/38	0/3/3/3
10	ATP	B	601	-	-	2/18/38/38	0/3/3/3
10	ATP	F	502	-	-	7/18/38/38	0/3/3/3
11	ADP	E	601	-	-	5/12/32/32	0/3/3/3
12	TTX	F	501	-	-	20/45/45/45	0/1/2/2
11	ADP	D	601	-	-	5/12/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	501	TTX	C6-N1	4.03	1.42	1.35
10	A	601	ATP	C5-C4	2.35	1.47	1.40
11	D	601	ADP	C5-C4	2.33	1.47	1.40
10	F	502	ATP	C5-C4	2.29	1.47	1.40
10	C	601	ATP	C5-C4	2.27	1.46	1.40
10	B	601	ATP	C5-C4	2.23	1.46	1.40
11	E	601	ADP	C5-C4	2.16	1.46	1.40

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	F	501	TTX	C7-N1-C6	-5.20	111.40	118.81
10	B	601	ATP	PA-O3A-PB	-4.54	117.26	132.83
10	C	601	ATP	PB-O3B-PG	-4.30	118.07	132.83
10	C	601	ATP	PA-O3A-PB	-4.27	118.19	132.83
12	F	501	TTX	C6-N1-C15	-4.24	111.83	123.52
10	B	601	ATP	PB-O3B-PG	-3.97	119.20	132.83
10	A	601	ATP	PB-O3B-PG	-3.83	119.67	132.83
11	D	601	ADP	PA-O3A-PB	-3.82	119.71	132.83
11	E	601	ADP	PA-O3A-PB	-3.68	120.20	132.83
10	A	601	ATP	PA-O3A-PB	-3.58	120.53	132.83
11	D	601	ADP	C3'-C2'-C1'	3.46	106.18	100.98
10	F	502	ATP	PA-O3A-PB	-3.43	121.07	132.83
10	C	601	ATP	N3-C2-N1	-3.41	123.35	128.68
11	E	601	ADP	N3-C2-N1	-3.39	123.38	128.68
10	F	502	ATP	PB-O3B-PG	-3.37	121.25	132.83
10	B	601	ATP	C3'-C2'-C1'	3.35	106.02	100.98
11	E	601	ADP	C3'-C2'-C1'	3.33	105.99	100.98
10	A	601	ATP	N3-C2-N1	-3.23	123.63	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	F	502	ATP	N3-C2-N1	-3.13	123.79	128.68
10	B	601	ATP	N3-C2-N1	-3.10	123.84	128.68
10	F	502	ATP	C3'-C2'-C1'	2.95	105.41	100.98
11	D	601	ADP	N3-C2-N1	-2.87	124.20	128.68
10	B	601	ATP	C4-C5-N7	-2.82	106.46	109.40
11	E	601	ADP	C4-C5-N7	-2.72	106.56	109.40
10	C	601	ATP	C4-C5-N7	-2.71	106.58	109.40
10	C	601	ATP	C3'-C2'-C1'	2.64	104.95	100.98
10	F	502	ATP	C4-C5-N7	-2.63	106.65	109.40
10	A	601	ATP	C4-C5-N7	-2.50	106.80	109.40
11	D	601	ADP	C4-C5-N7	-2.36	106.94	109.40
10	A	601	ATP	C3'-C2'-C1'	2.28	104.41	100.98
10	A	601	ATP	C2'-C3'-C4'	2.01	106.55	102.64

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	601	ATP	C5'-O5'-PA-O3A
10	F	502	ATP	C5'-O5'-PA-O3A
11	D	601	ADP	C5'-O5'-PA-O3A
11	D	601	ADP	O4'-C4'-C5'-O5'
11	D	601	ADP	C3'-C4'-C5'-O5'
11	E	601	ADP	C5'-O5'-PA-O1A
11	E	601	ADP	O4'-C4'-C5'-O5'
12	F	501	TTX	C16-C15-N1-C7
12	F	501	TTX	O1-C6-N1-C7
12	F	501	TTX	C5-C6-N1-C7
12	F	501	TTX	C10-C9-N3-C12
12	F	501	TTX	O3-C12-N3-C9
12	F	501	TTX	C13-C12-N3-C9
12	F	501	TTX	O3-C12-N3-C11
12	F	501	TTX	C13-C12-N3-C11
12	F	501	TTX	C15-C14-N4-C13
12	F	501	TTX	O4-C14-N4-C13
11	E	601	ADP	C3'-C4'-C5'-O5'
12	F	501	TTX	C3-C2-C4-C5
10	F	502	ATP	O4'-C4'-C5'-O5'
10	F	502	ATP	C3'-C4'-C5'-O5'
12	F	501	TTX	C1-C2-C4-C5
12	F	501	TTX	C10-C9-N3-C11
12	F	501	TTX	N2-C8-C9-N3

Continued on next page...

Continued from previous page...

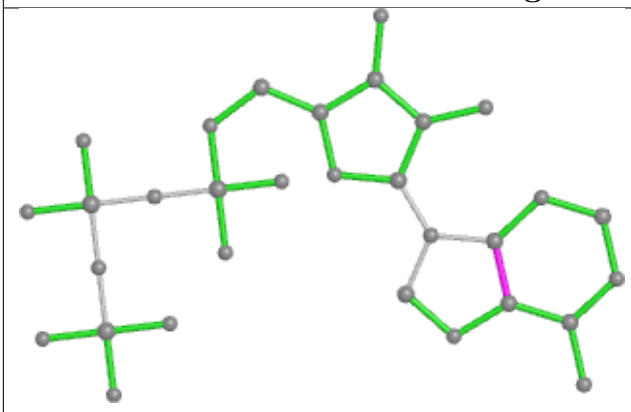
Mol	Chain	Res	Type	Atoms
10	B	601	ATP	PA-O3A-PB-O1B
10	F	502	ATP	PB-O3A-PA-O1A
12	F	501	TTX	O2-C8-C9-N3
11	E	601	ADP	C5'-O5'-PA-O3A
10	C	601	ATP	C5'-O5'-PA-O1A
10	F	502	ATP	C5'-O5'-PA-O1A
10	F	502	ATP	C5'-O5'-PA-O2A
11	D	601	ADP	C5'-O5'-PA-O1A
11	E	601	ADP	C5'-O5'-PA-O2A
12	F	501	TTX	O2-C8-C9-C10
12	F	501	TTX	C14-C15-N1-C7
12	F	501	TTX	N2-C8-C9-C10
10	A	601	ATP	PA-O3A-PB-O1B
10	A	601	ATP	PA-O3A-PB-O2B
10	B	601	ATP	PA-O3A-PB-O2B
12	F	501	TTX	O3-C12-C13-N4
12	F	501	TTX	N3-C12-C13-N4
10	F	502	ATP	PB-O3A-PA-O2A
11	D	601	ADP	PB-O3A-PA-O2A

There are no ring outliers.

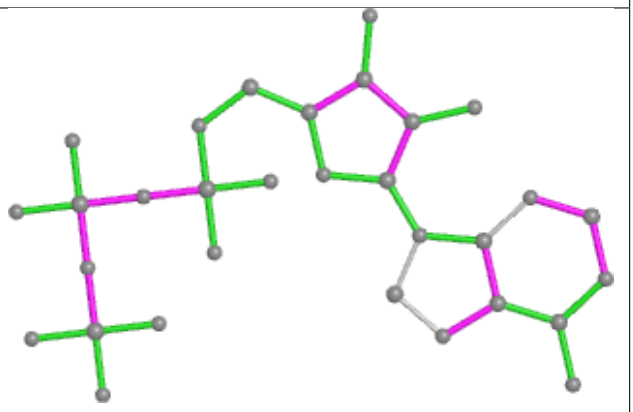
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

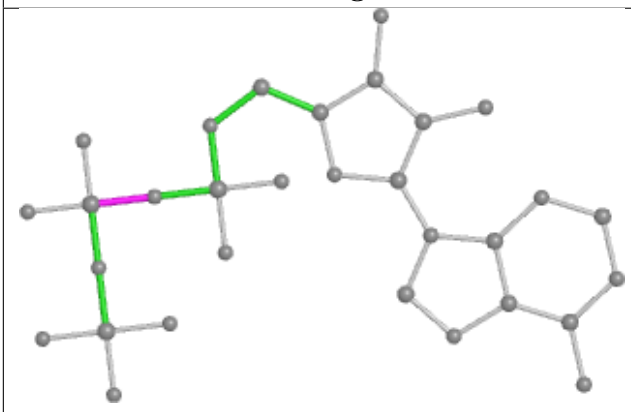
Ligand ATP A 601



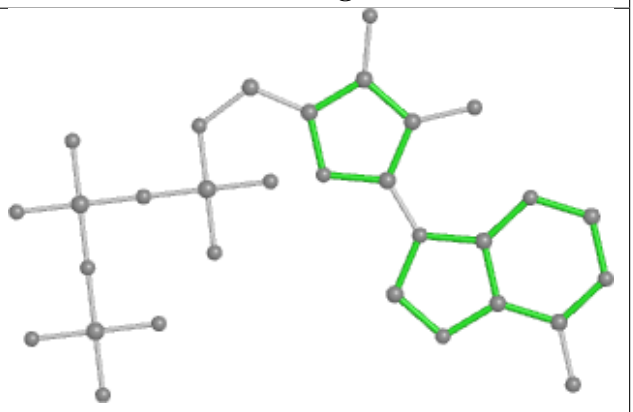
Bond lengths



Bond angles

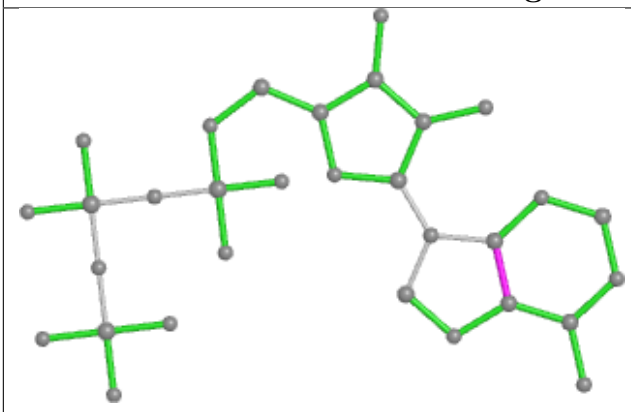


Torsions

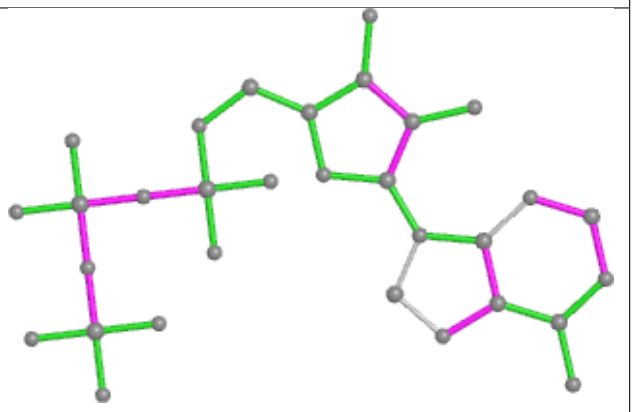


Rings

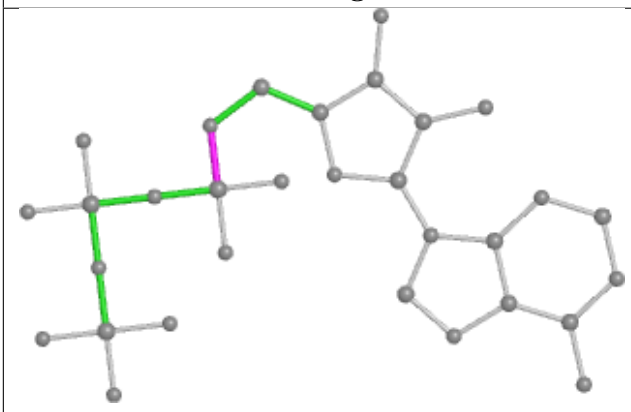
Ligand ATP C 601



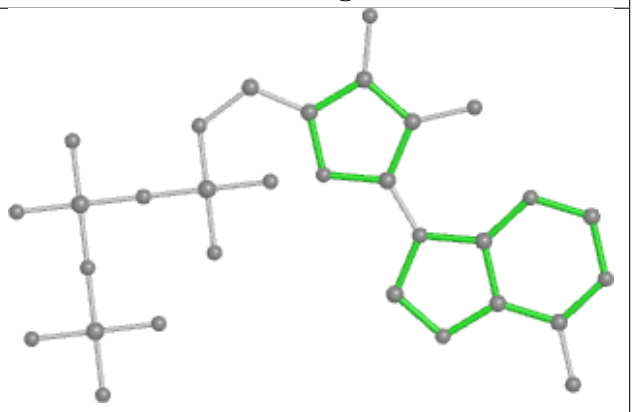
Bond lengths



Bond angles

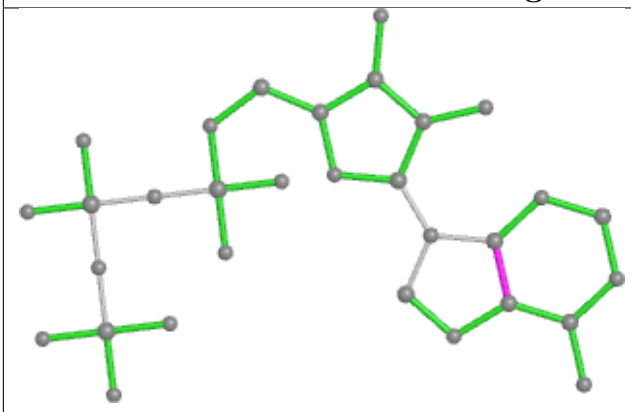


Torsions

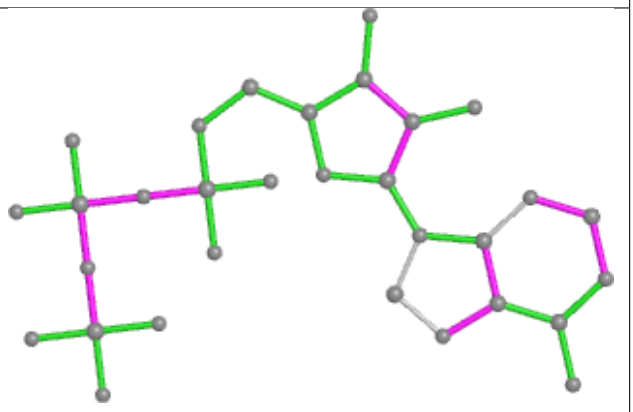


Rings

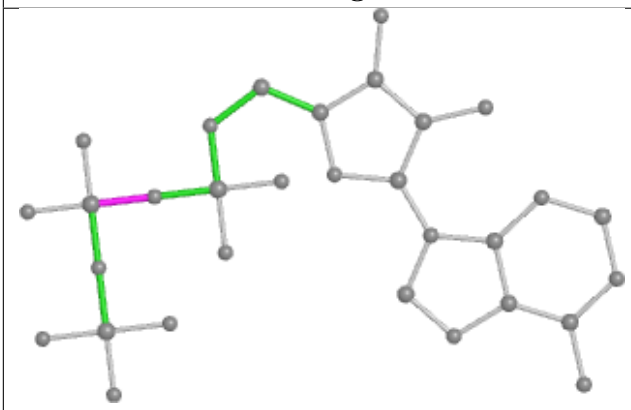
Ligand ATP B 601



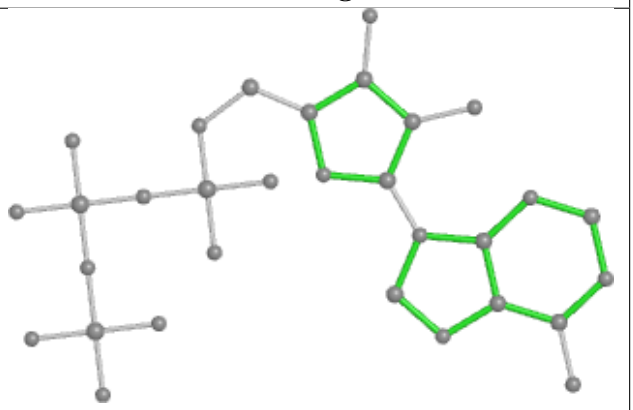
Bond lengths



Bond angles

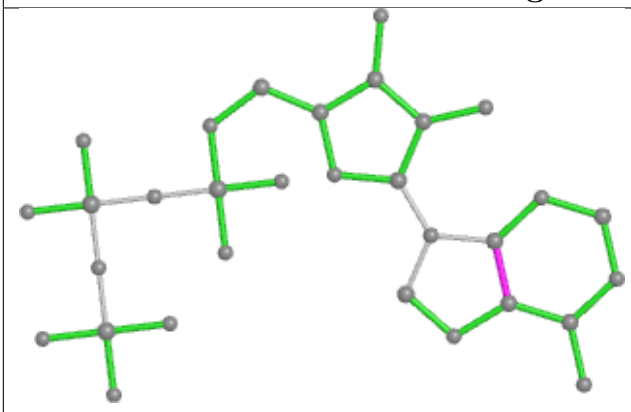


Torsions

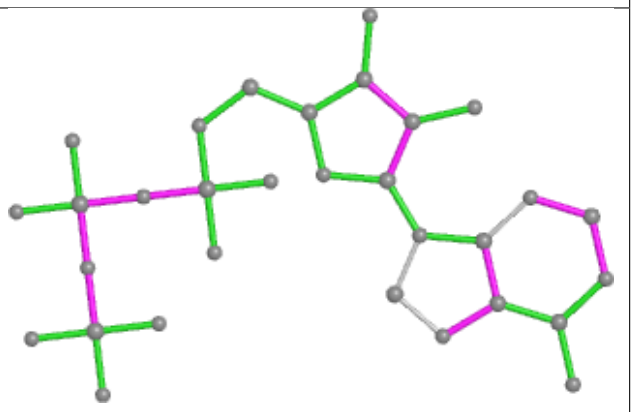


Rings

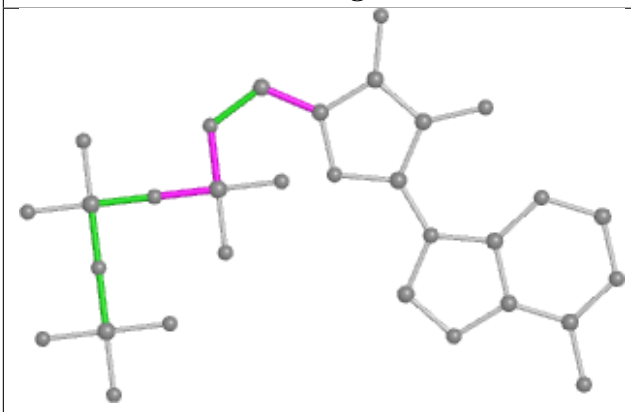
Ligand ATP F 502



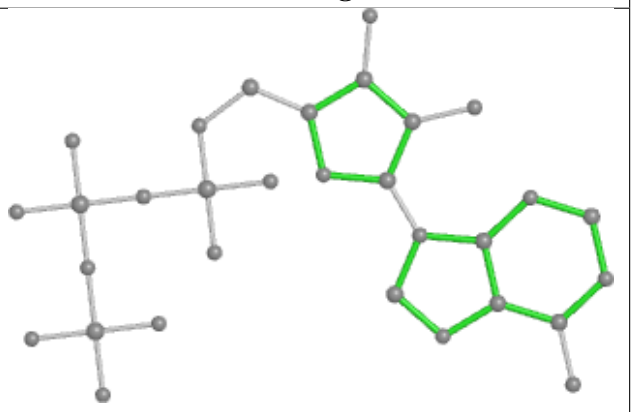
Bond lengths



Bond angles

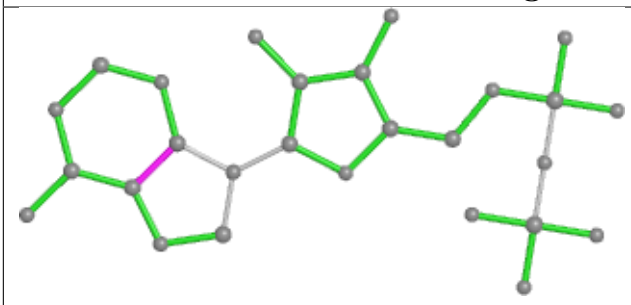


Torsions

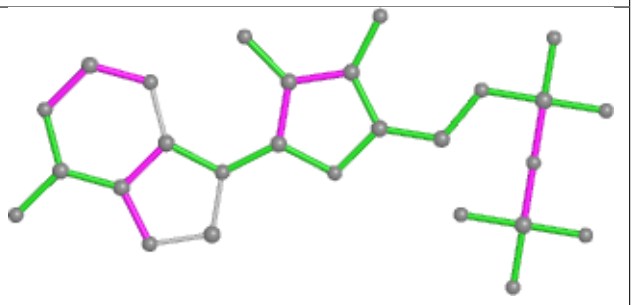


Rings

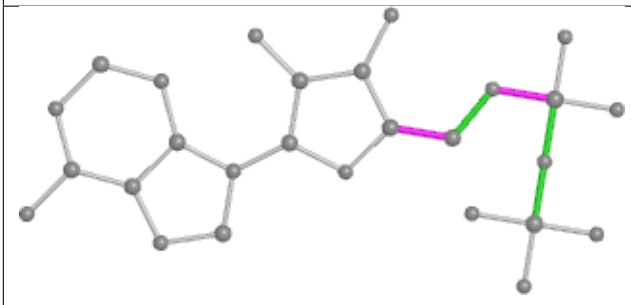
Ligand ADP E 601



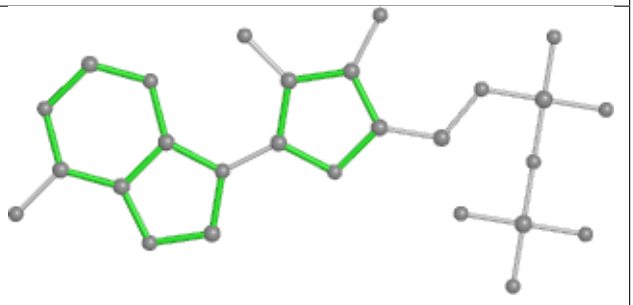
Bond lengths



Bond angles

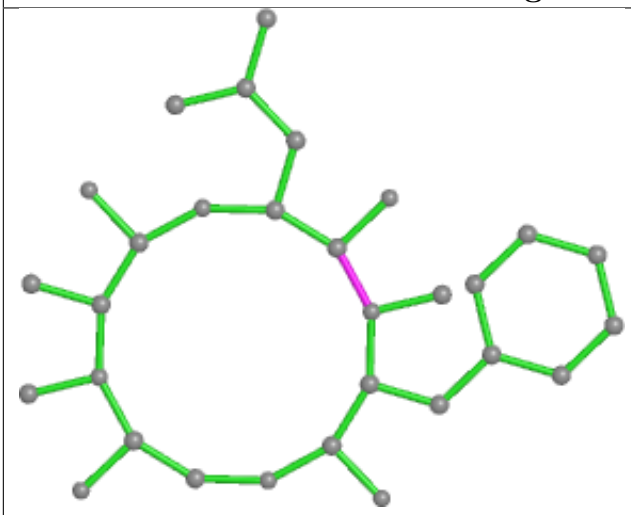


Torsions

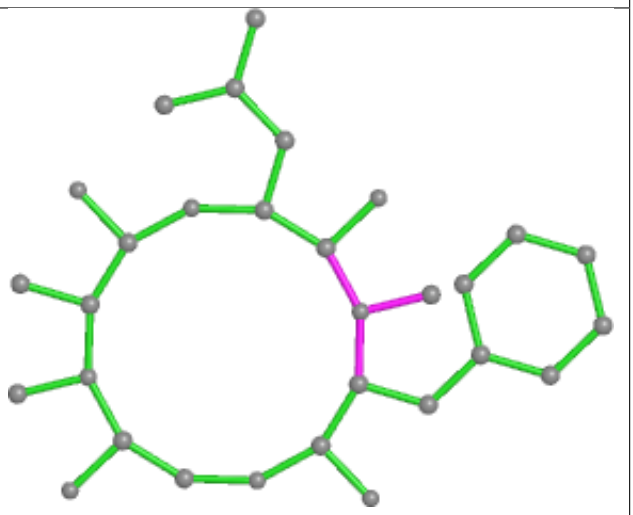


Rings

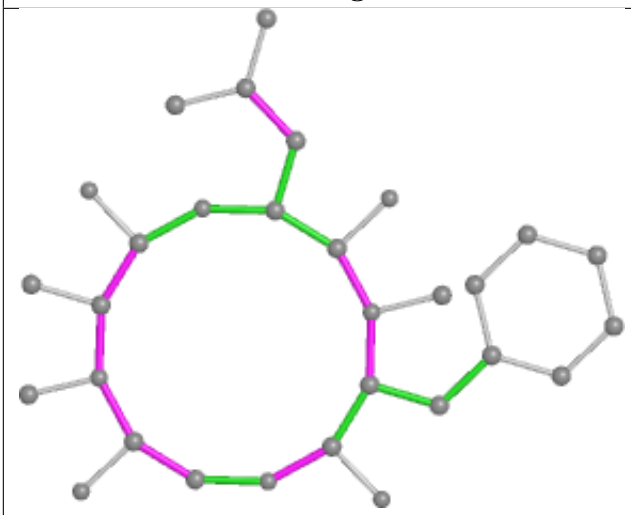
Ligand TTX F 501



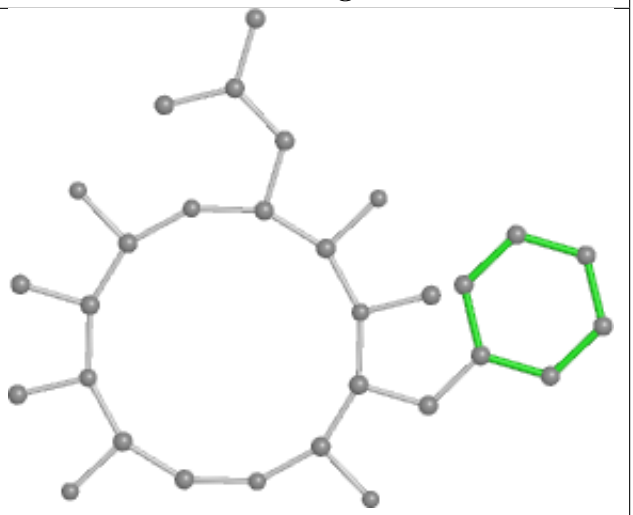
Bond lengths



Bond angles

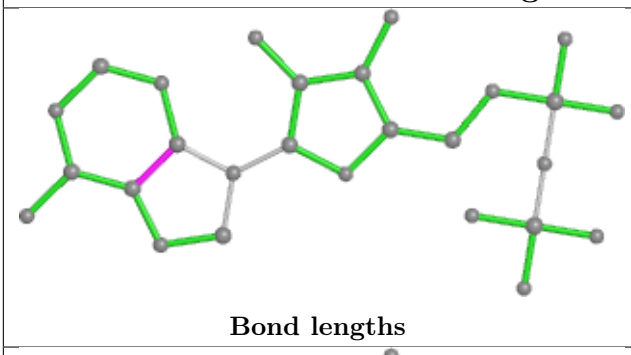


Torsions

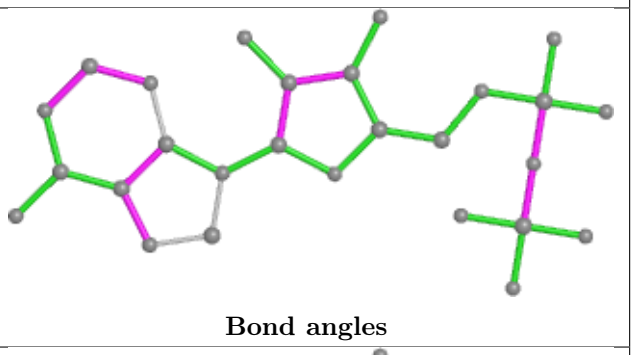


Rings

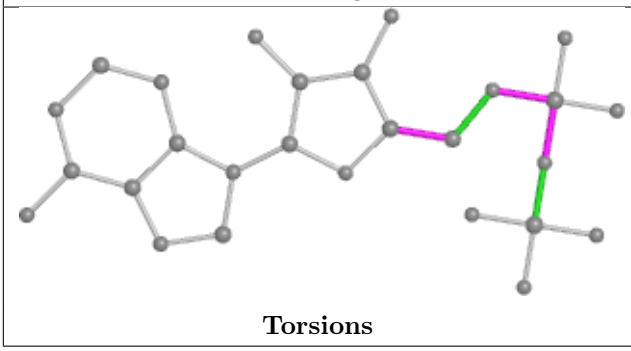
Ligand ADP D 601



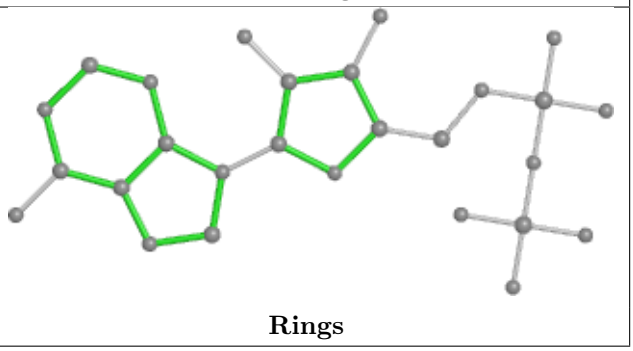
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

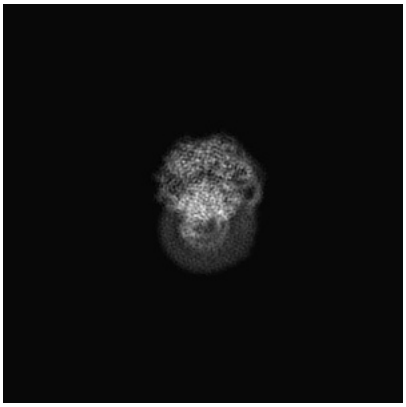
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21268. These allow visual inspection of the internal detail of the map and identification of artifacts.

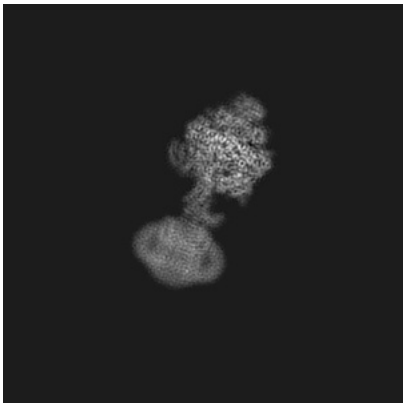
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

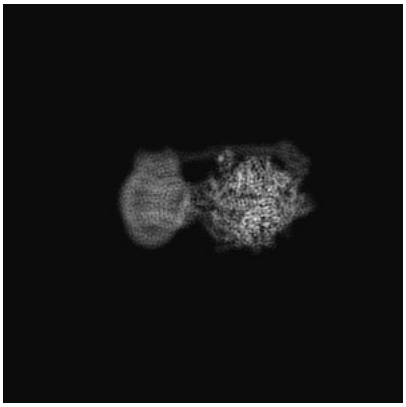
6.1.1 Primary map



X



Y

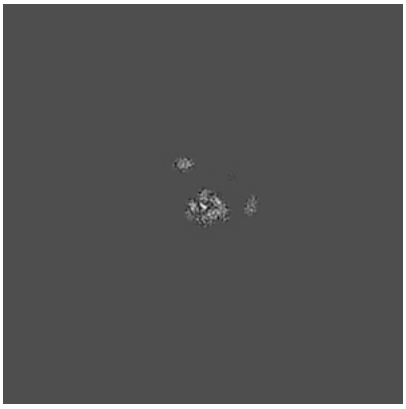


Z

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

6.2 Central slices

6.2.1 Primary map



X Index: 210

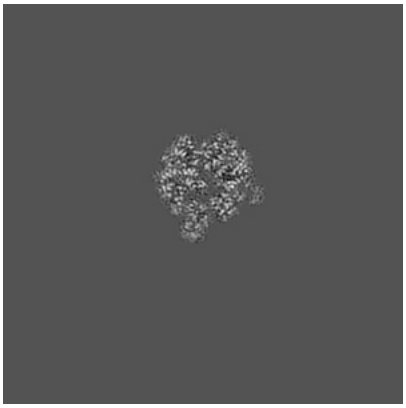
Y Index: 210

Z Index: 210

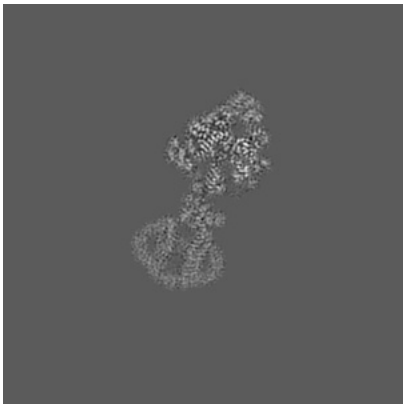
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 259



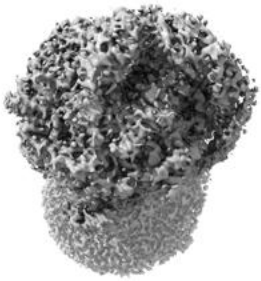
Y Index: 204

Z Index: 214

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

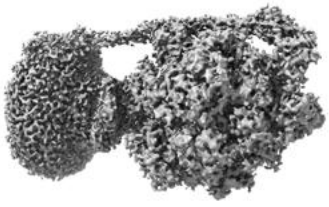
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.011. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

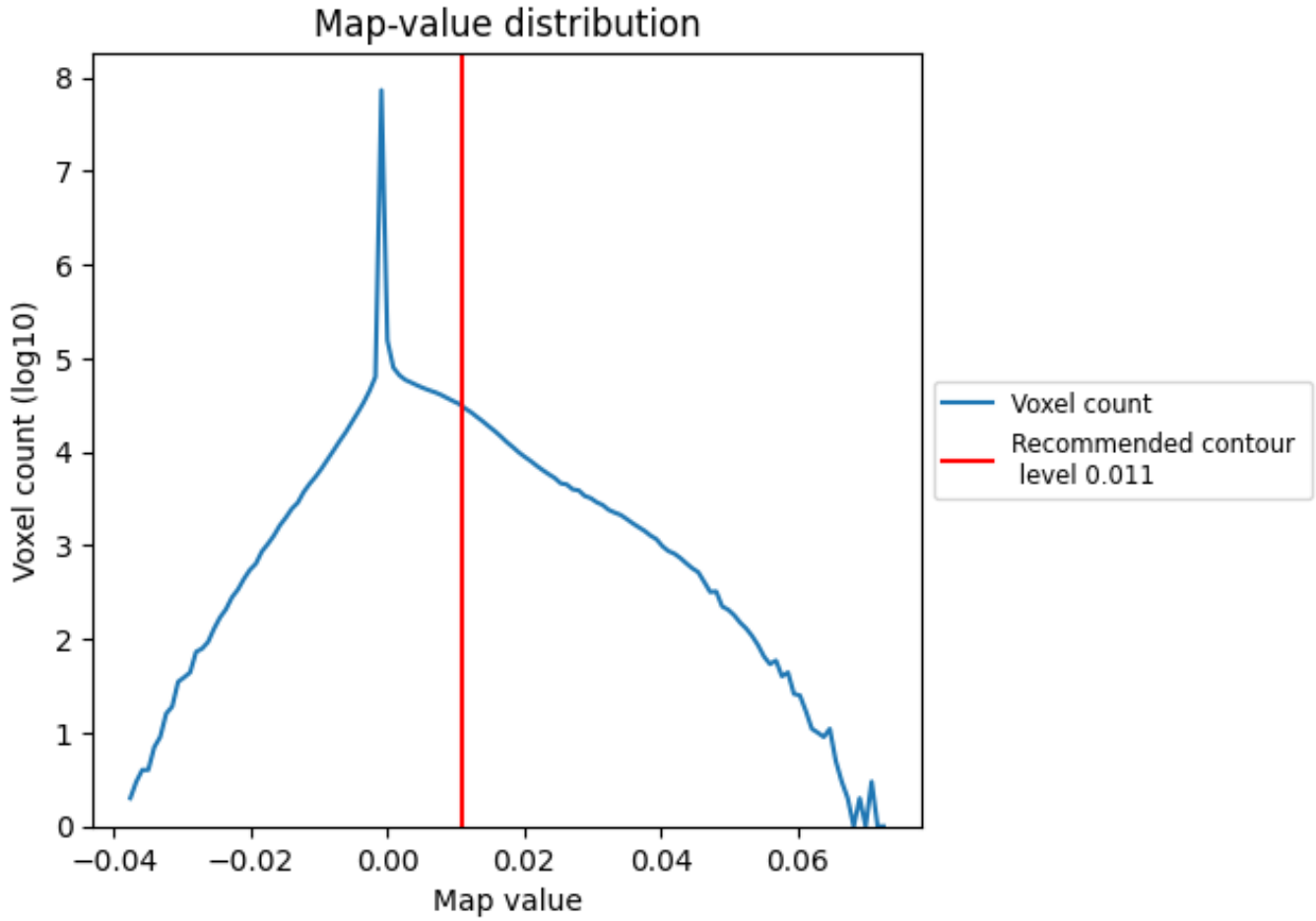
6.5 Mask visualisation (i)

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

7 Map analysis

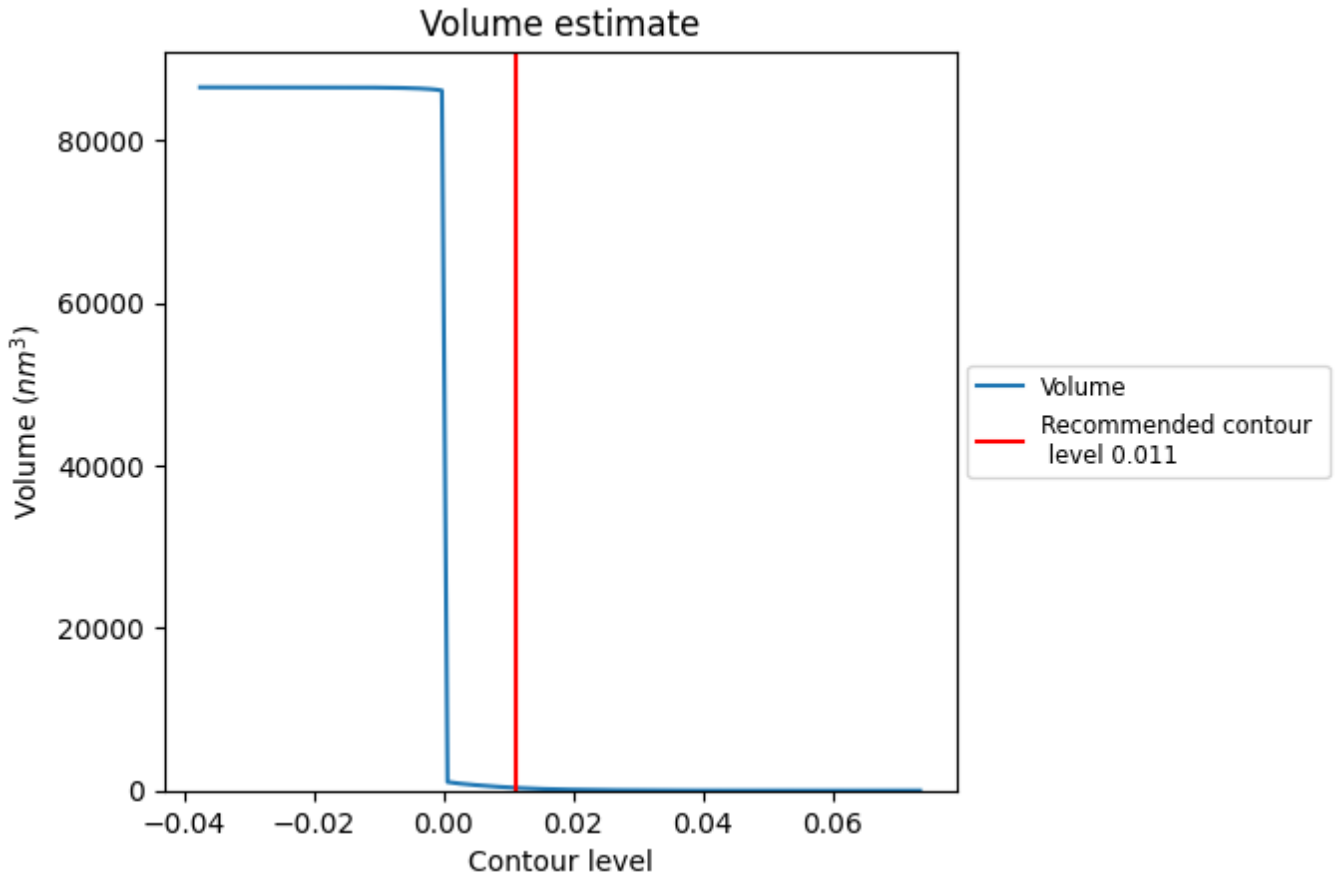
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

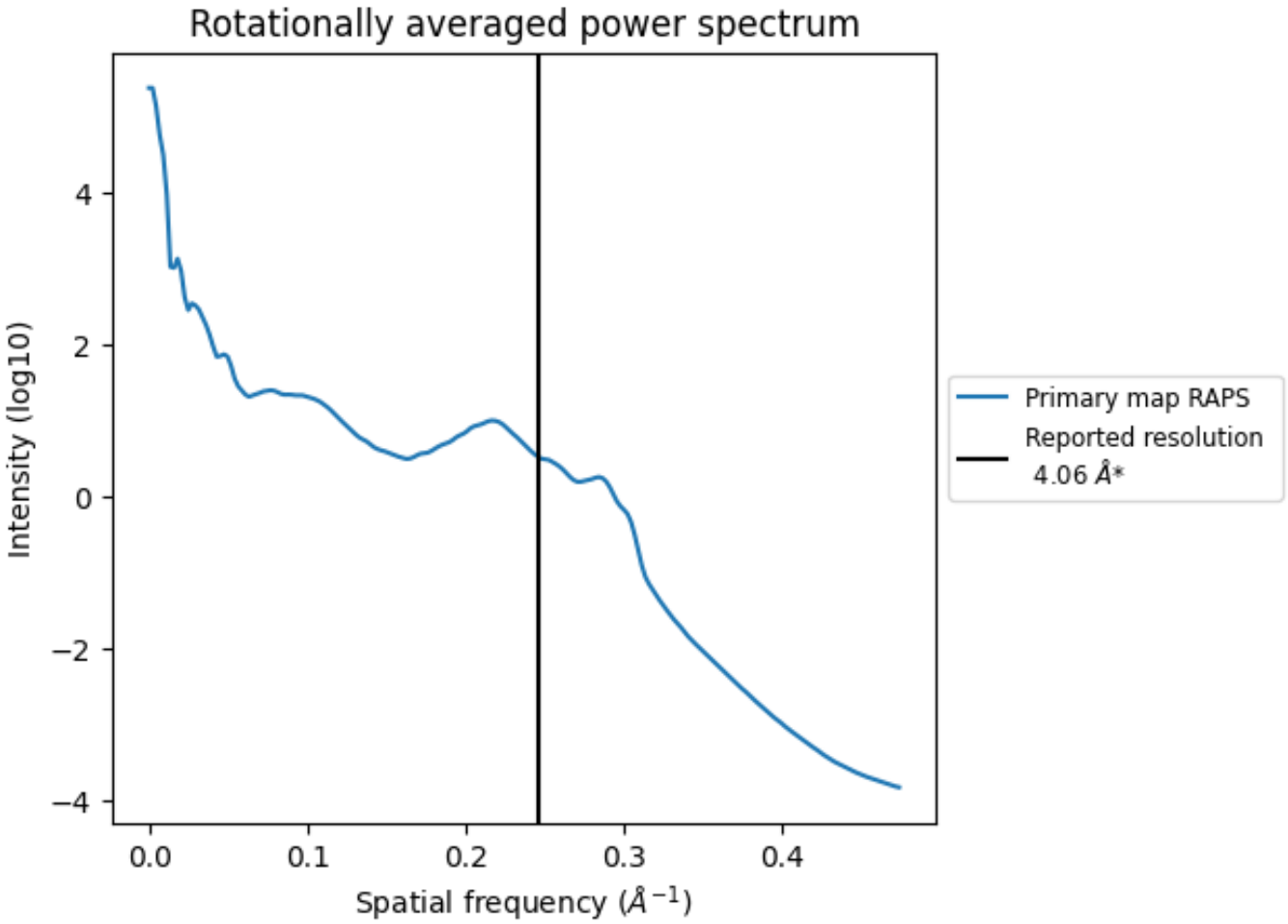
7.2 Volume estimate



The volume at the recommended contour level is 340 nm^3; this corresponds to an approximate mass of 307 kDa.

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

7.3 Rotationally averaged power spectrum (i)

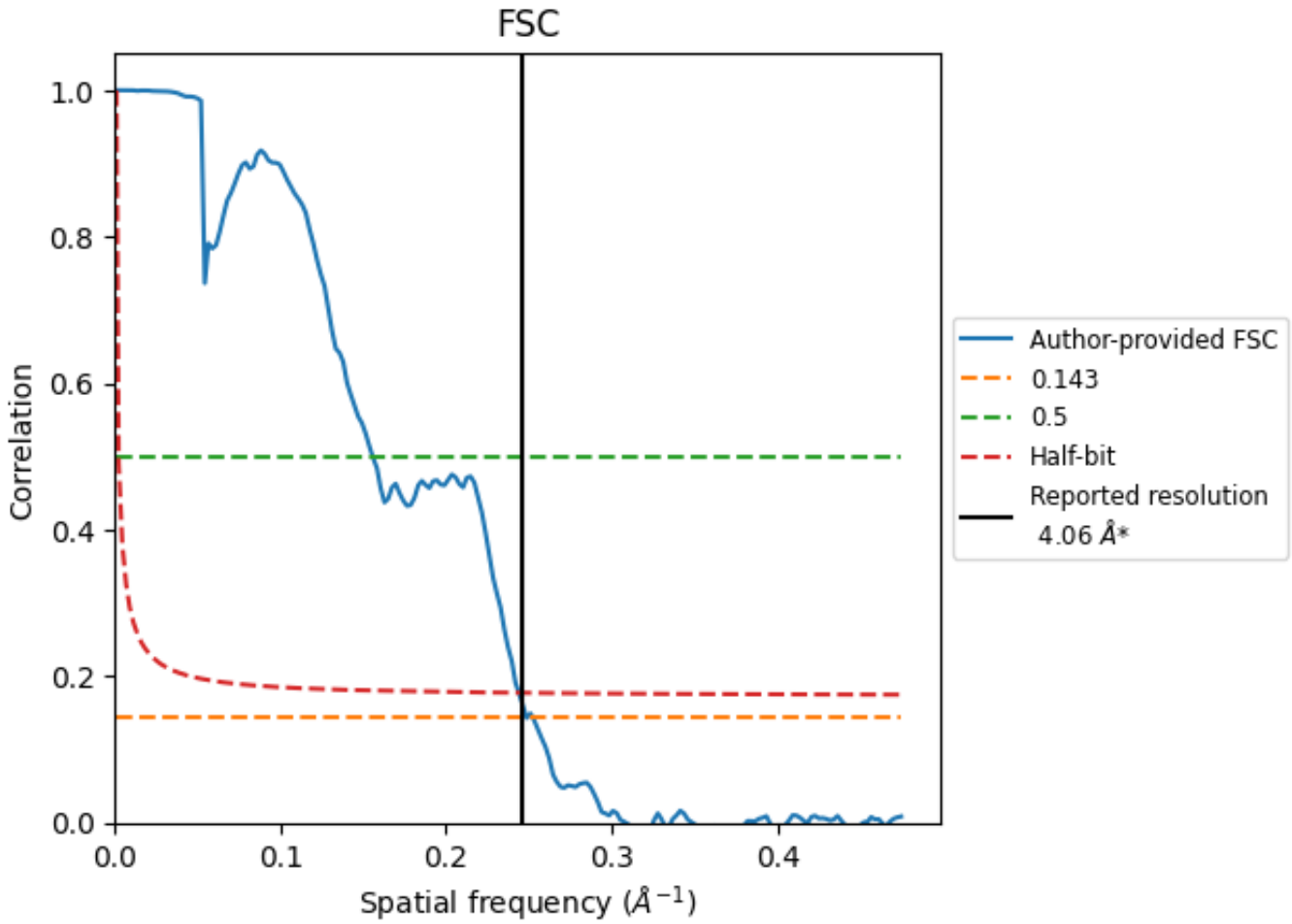


*Reported resolution corresponds to spatial frequency of 0.246 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.246 Å^{-1}

8.2 Resolution estimates (i)

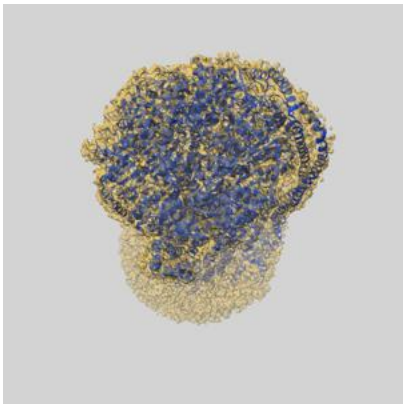
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.06	-	-
Author-provided FSC curve	4.02	6.43	4.10
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

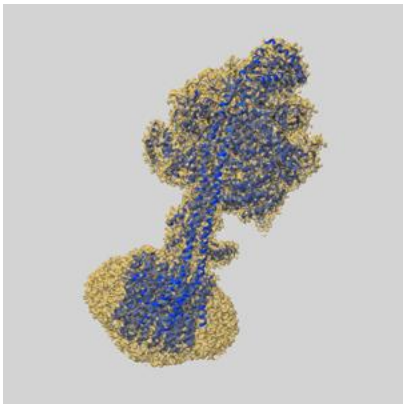
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21268 and PDB model 6VOL. Per-residue inclusion information can be found in section 3 on page 8.

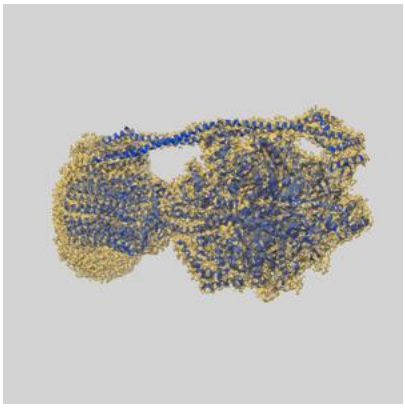
9.1 Map-model overlay



X



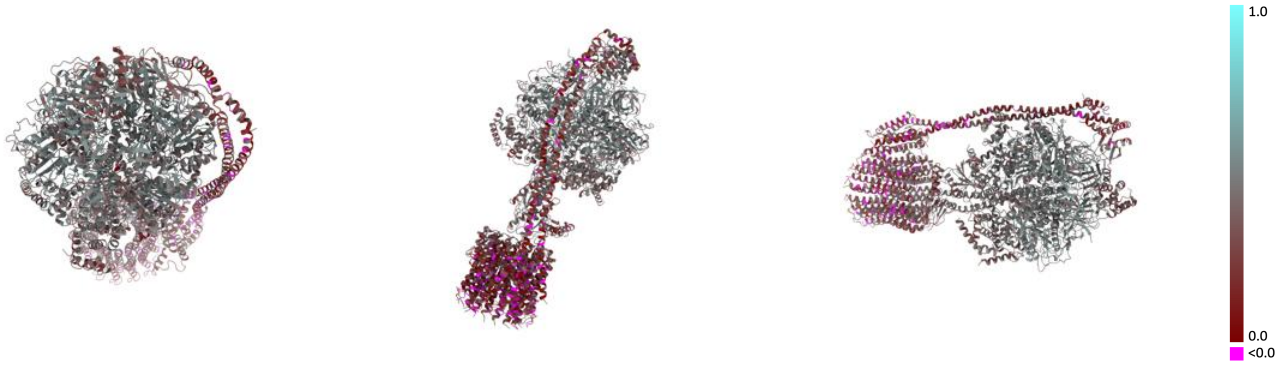
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.011 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.

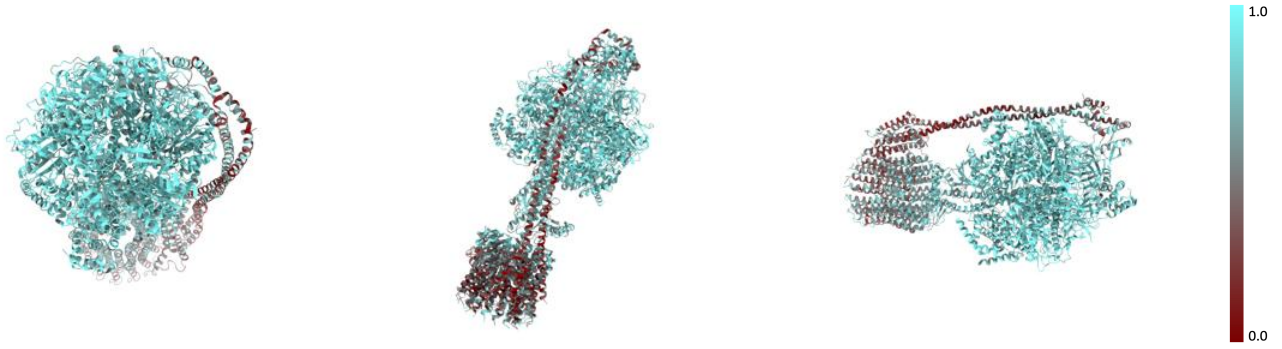
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

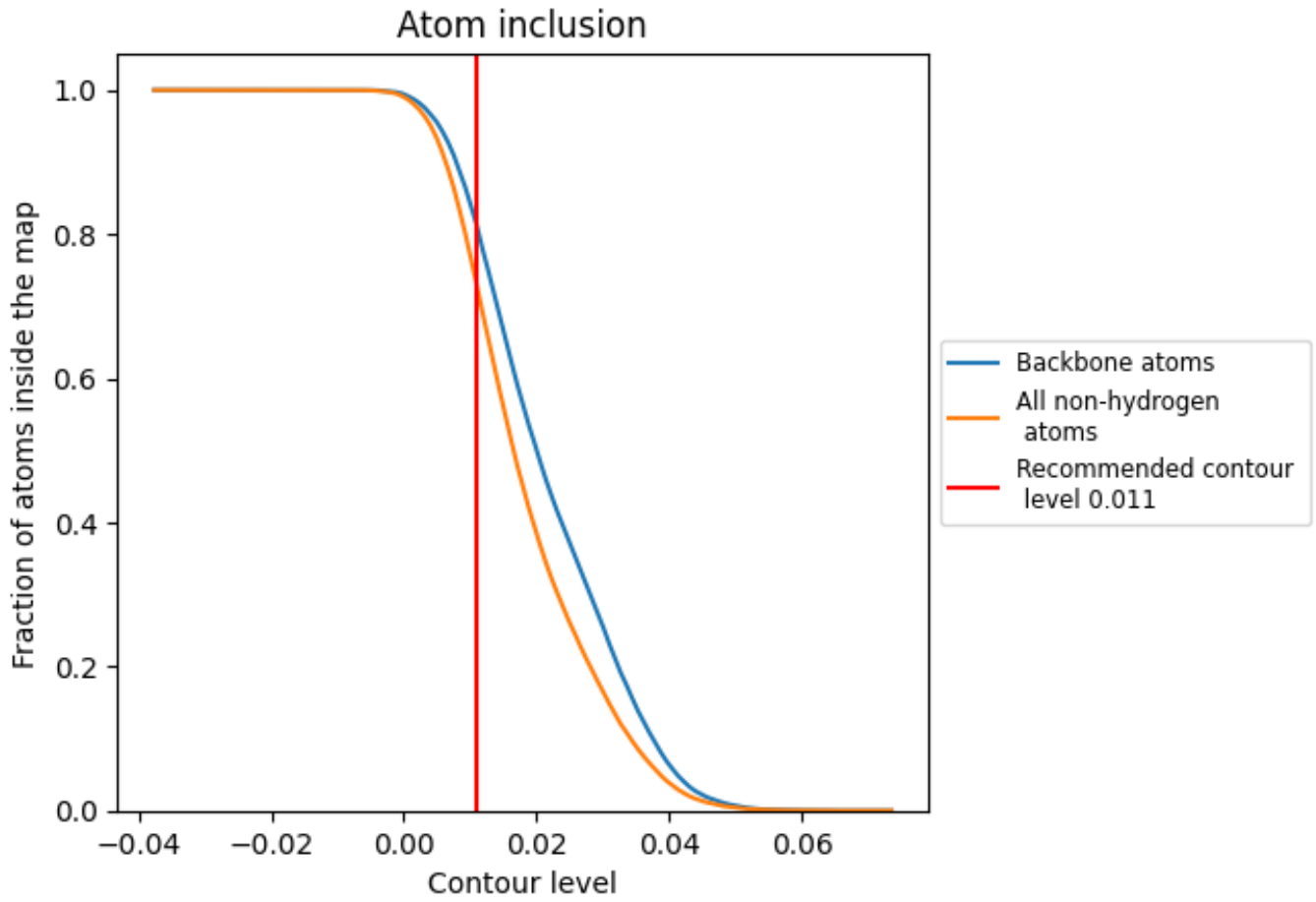
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.011).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 73% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7297	0.3800
A	0.8382	0.4510
B	0.8517	0.4600
C	0.8434	0.4700
D	0.8645	0.4700
E	0.8479	0.4720
F	0.8597	0.4710
I	0.4091	0.2110
J	0.3676	0.2010
M	0.5473	0.2240
N	0.5065	0.2080
O	0.5807	0.1950
P	0.4991	0.2010
Q	0.5009	0.1980
R	0.5455	0.2270
S	0.5399	0.2240
T	0.5881	0.2280
U	0.5788	0.2350
V	0.5492	0.2240
W	0.5993	0.2340
X	0.5900	0.2320
Y	0.5455	0.2030
Z	0.4861	0.2180
a	0.3503	0.1930
d	0.7293	0.3730
e	0.7110	0.3290
g	0.7616	0.4020