



## Full wwPDB EM Validation Report ⓘ

Nov 3, 2024 – 05:31 AM EST

PDB ID : 6VOH  
EMDB ID : EMD-21264  
Title : Chloroplast ATP synthase (O1, CF1FO)  
Authors : Yang, J.-H.; Williams, D.; Kandiah, E.; Fromme, P.; Chiu, P.-L.  
Deposited on : 2020-01-30  
Resolution : 4.16 Å (reported)  
Based on initial model : 6FKF

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:

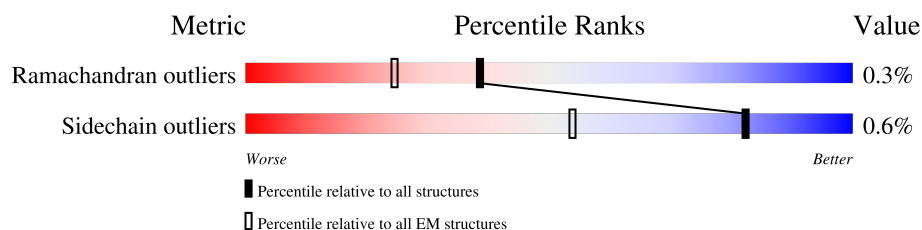
EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.16 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	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	507	
1	B	507	
1	C	507	
2	D	498	
2	E	498	
2	F	498	
3	d	257	
4	g	364	
5	e	134	

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Mol	Chain	Length	Quality of chain
6	J	222	
7	I	184	
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

There are 11 unique types of molecules in this entry. The entry contains 39159 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	501	Total	C	N	O	S	0	0
			3850	2421	665	751	13		
1	C	500	Total	C	N	O	S	0	0
			3843	2417	666	747	13		
1	B	502	Total	C	N	O	S	0	0
			3854	2425	667	749	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	478	Total	C	N	O	S	0	0
			3619	2282	622	699	16		
2	E	481	Total	C	N	O	S	0	0
			3645	2299	626	704	16		
2	F	480	Total	C	N	O	S	0	0
			3636	2294	625	701	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
			1384	876	229	277	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	g	323	Total	C	N	O	S	0	0
			2508	1580	431	484	13		

- 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
			1007	621	189	194	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	136	Total	C	N	O	S	0	0
			1068	675	174	214	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	153	Total	C	N	O	S	0	0
			1237	772	227	233	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	a	223	Total	C	N	O	S	0	0
			1741	1172	268	299	2		

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

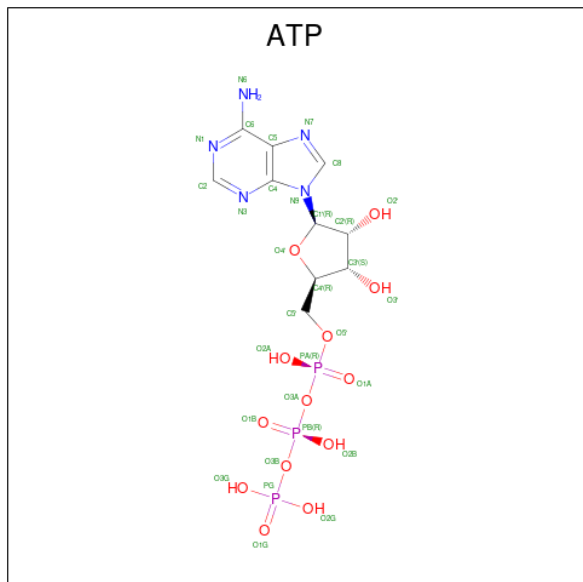
Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
9	Y	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
9	X	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
9	W	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
9	V	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
9	U	79	Total	C	N	O	S	0	0
		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

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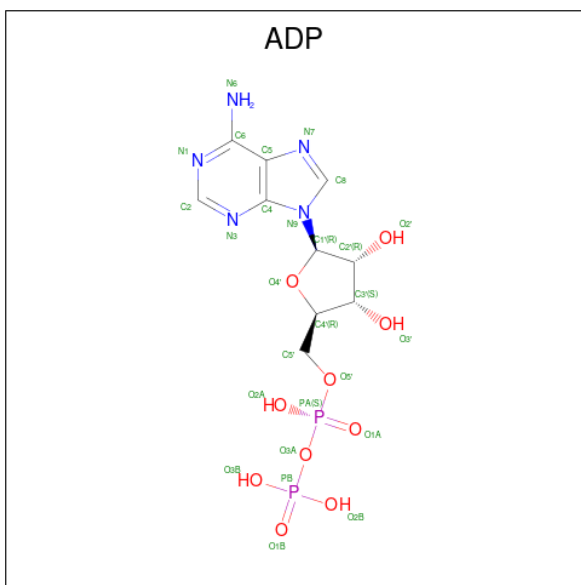
Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
9	M	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
9	N	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
9	O	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
9	P	79	Total	C	N	O	S	0	0
			544	355	90	98	1		

- 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	C	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	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

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



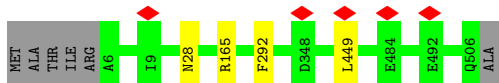
Mol	Chain	Residues	Atoms					AltConf
11	F	1	Total 27	C 10	N 5	O 10	P 2	0

### 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.

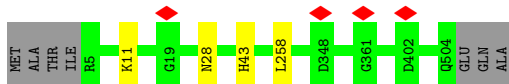
- Molecule 1: ATP synthase subunit alpha, chloroplastic

Chain A:  98%



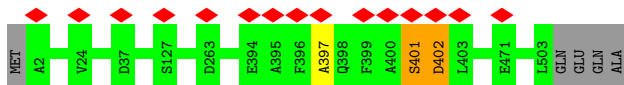
- Molecule 1: ATP synthase subunit alpha, chloroplastic

Chain C:  98%



- Molecule 1: ATP synthase subunit alpha, chloroplastic

Chain B:  98%



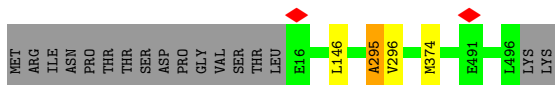
- Molecule 2: ATP synthase subunit beta, chloroplastic

Chain D:  95%



- Molecule 2: ATP synthase subunit beta, chloroplastic

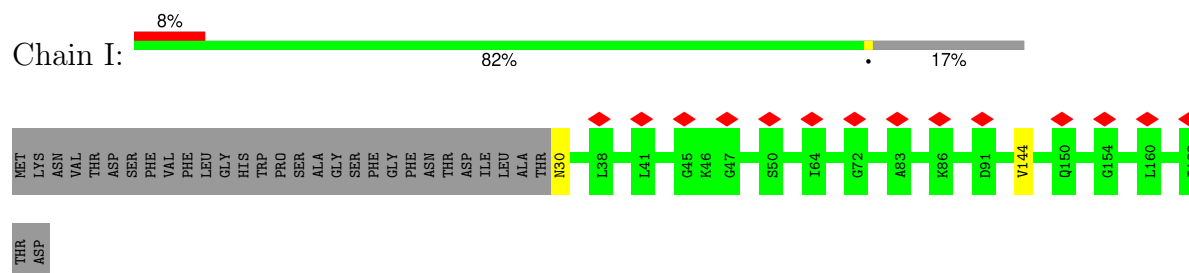
Chain E:  96%



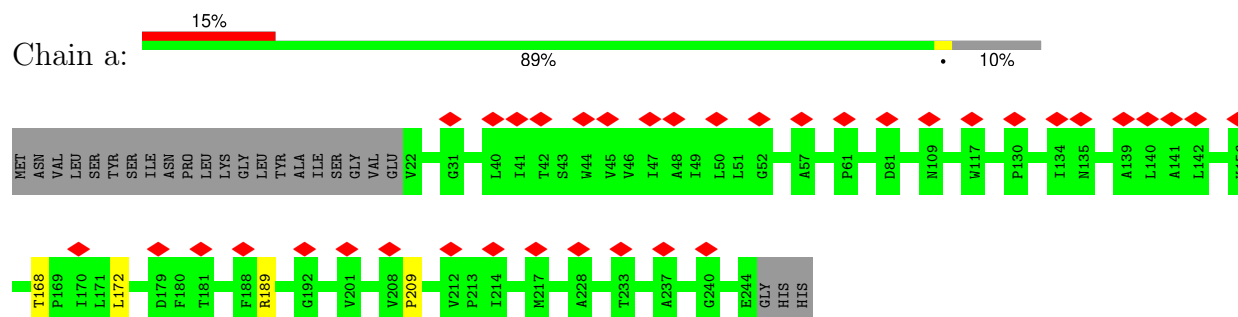




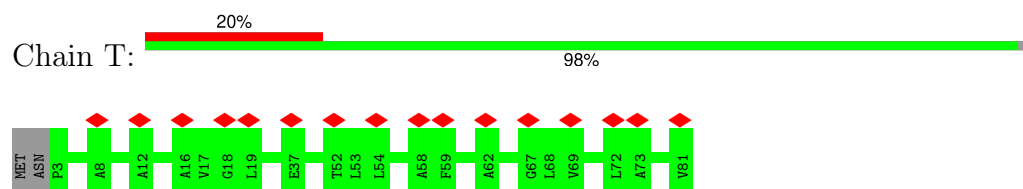
- Molecule 7: ATP synthase subunit b, chloroplastic



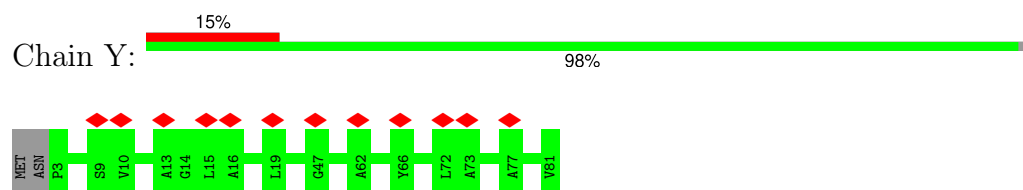
- Molecule 8: ATP synthase subunit a, chloroplastic



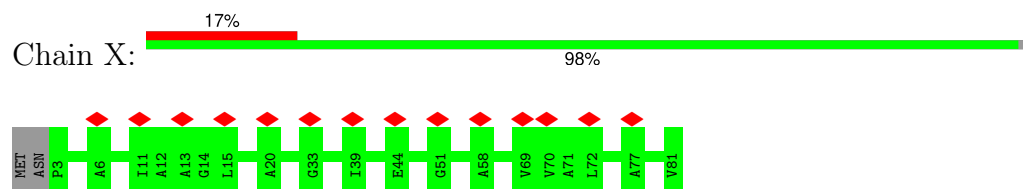
- Molecule 9: ATP synthase subunit c, chloroplastic



- Molecule 9: ATP synthase subunit c, chloroplastic

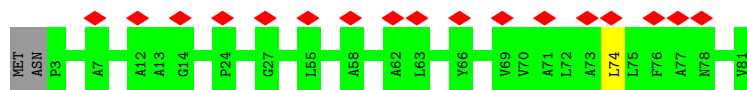


- Molecule 9: ATP synthase subunit c, chloroplastic

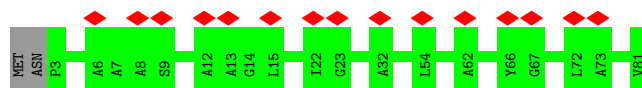


- Molecule 9: ATP synthase subunit c, chloroplastic

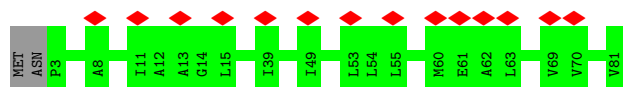




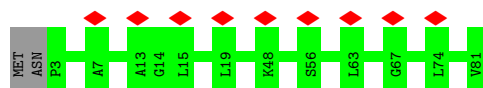
- Molecule 9: ATP synthase subunit c, chloroplastic



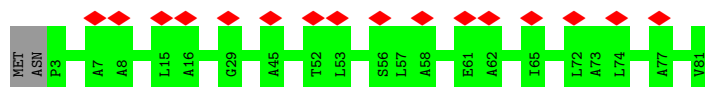
- Molecule 9: ATP synthase subunit c, chloroplastic



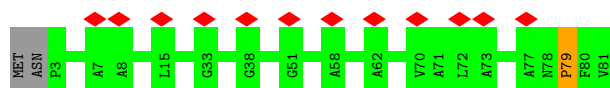
- Molecule 9: ATP synthase subunit c, chloroplastic



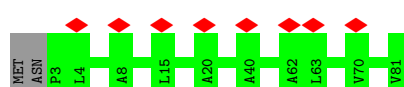
- Molecule 9: ATP synthase subunit c, chloroplastic



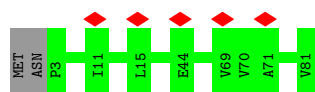
- Molecule 9: ATP synthase subunit c, chloroplastic



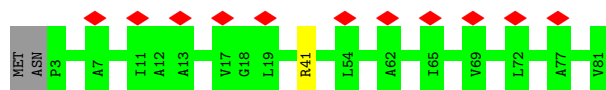
- Molecule 9: ATP synthase subunit c, chloroplastic



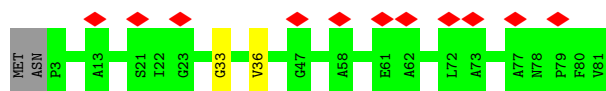
- Molecule 9: ATP synthase subunit c, chloroplastic



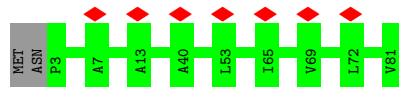
- Molecule 9: ATP synthase subunit c, chloroplastic



- Molecule 9: ATP synthase subunit c, chloroplastic



- Molecule 9: ATP synthase subunit c, chloroplastic



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	304879	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	43.5	Depositor
Minimum defocus (nm)	-1500	Depositor
Maximum defocus (nm)	-4000	Depositor
Magnification	48077	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.109	Depositor
Minimum map value	-0.068	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	374.4, 374.4, 374.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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

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	0.31	0/3899	0.50	0/5275
1	B	0.32	0/3903	0.53	0/5281
1	C	0.32	0/3892	0.51	0/5265
2	D	0.32	0/3676	0.51	0/4983
2	E	0.31	0/3702	0.50	0/5017
2	F	0.31	0/3693	0.51	0/5005
3	d	0.27	0/1400	0.46	0/1898
4	g	0.29	0/2537	0.53	0/3427
5	e	0.26	0/1016	0.60	0/1377
6	J	0.28	0/1077	0.60	2/1443 (0.1%)
7	I	0.26	0/1247	0.45	0/1670
8	a	0.28	0/1792	0.56	1/2454 (0.0%)
9	M	0.30	0/551	0.53	0/750
9	N	0.29	0/551	0.56	0/750
9	O	0.28	0/551	0.56	0/750
9	P	0.28	0/551	0.46	0/750
9	Q	0.27	0/551	0.53	0/750
9	R	0.30	0/551	0.53	0/750
9	S	0.27	0/551	0.49	0/750
9	T	0.29	0/551	0.52	0/750
9	U	0.27	0/551	0.49	0/750
9	V	0.28	0/551	0.51	0/750
9	W	0.29	0/551	0.55	1/750 (0.1%)
9	X	0.31	0/551	0.53	0/750
9	Y	0.31	0/551	0.48	0/750
9	Z	0.30	0/551	0.49	0/750
All	All	0.30	0/39548	0.52	4/53595 (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	A	0	1
1	B	0	1
2	D	0	2
2	E	0	1
2	F	0	1
6	J	0	1
8	a	0	1
9	R	0	1
All	All	0	9

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	219	LEU	CA-CB-CG	7.81	133.27	115.30
6	J	90	LEU	CA-CB-CG	6.97	131.34	115.30
8	a	172	LEU	CA-CB-CG	5.42	127.76	115.30
9	W	74	LEU	CA-CB-CG	5.41	127.75	115.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	449	LEU	Peptide
1	B	401	SER	Peptide
2	D	295	ALA	Peptide
2	D	405	ILE	Peptide
2	E	295	ALA	Peptide
2	F	295	ALA	Peptide
6	J	86	PHE	Peptide
9	R	79	PRO	Peptide
8	a	168	THR	Peptide

## 5.2 Too-close contacts

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

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	499/507 (98%)	461 (92%)	38 (8%)	0	100	100
1	B	500/507 (99%)	445 (89%)	52 (10%)	3 (1%)	22	59
1	C	498/507 (98%)	462 (93%)	36 (7%)	0	100	100
2	D	476/498 (96%)	423 (89%)	50 (10%)	3 (1%)	22	59
2	E	479/498 (96%)	441 (92%)	36 (8%)	2 (0%)	30	67
2	F	478/498 (96%)	441 (92%)	35 (7%)	2 (0%)	30	67
3	d	177/257 (69%)	160 (90%)	17 (10%)	0	100	100
4	g	321/364 (88%)	285 (89%)	34 (11%)	2 (1%)	22	59
5	e	129/134 (96%)	115 (89%)	14 (11%)	0	100	100
6	J	134/222 (60%)	131 (98%)	3 (2%)	0	100	100
7	I	151/184 (82%)	147 (97%)	4 (3%)	0	100	100
8	a	221/247 (90%)	195 (88%)	25 (11%)	1 (0%)	25	62
9	M	77/81 (95%)	72 (94%)	5 (6%)	0	100	100
9	N	77/81 (95%)	72 (94%)	5 (6%)	0	100	100
9	O	77/81 (95%)	70 (91%)	6 (8%)	1 (1%)	10	43
9	P	77/81 (95%)	77 (100%)	0	0	100	100
9	Q	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
9	R	77/81 (95%)	71 (92%)	5 (6%)	1 (1%)	10	43
9	S	77/81 (95%)	73 (95%)	4 (5%)	0	100	100
9	T	77/81 (95%)	73 (95%)	4 (5%)	0	100	100
9	U	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
9	V	77/81 (95%)	75 (97%)	2 (3%)	0	100	100
9	W	77/81 (95%)	73 (95%)	4 (5%)	0	100	100
9	X	77/81 (95%)	73 (95%)	4 (5%)	0	100	100
9	Y	77/81 (95%)	74 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	Z	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
All	All	5141/5557 (92%)	4731 (92%)	395 (8%)	15 (0%)	38	72

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	296	VAL
2	F	296	VAL
1	B	402	ASP
2	D	407	ILE
4	g	130	CYS
1	B	397	ALA
1	B	401	SER
2	E	295	ALA
2	F	295	ALA
2	D	406	ALA
2	D	296	VAL
9	R	79	PRO
4	g	242	ILE
8	a	209	PRO
9	O	33	GLY

### 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	410/414 (99%)	407 (99%)	3 (1%)	81	87
1	B	410/414 (99%)	409 (100%)	1 (0%)	92	94
1	C	409/414 (99%)	405 (99%)	4 (1%)	73	81
2	D	389/408 (95%)	387 (100%)	2 (0%)	86	90
2	E	392/408 (96%)	390 (100%)	2 (0%)	86	90
2	F	391/408 (96%)	391 (100%)	0	100	100
3	d	156/220 (71%)	154 (99%)	2 (1%)	65	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	g	277/315 (88%)	273 (99%)	4 (1%)	62	75
5	e	108/112 (96%)	108 (100%)	0	100	100
6	J	118/197 (60%)	118 (100%)	0	100	100
7	I	135/161 (84%)	133 (98%)	2 (2%)	60	74
8	a	187/207 (90%)	186 (100%)	1 (0%)	86	90
9	M	51/53 (96%)	51 (100%)	0	100	100
9	N	51/53 (96%)	50 (98%)	1 (2%)	50	68
9	O	51/53 (96%)	50 (98%)	1 (2%)	50	68
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
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	4096/4420 (93%)	4073 (99%)	23 (1%)	82	88

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	165	ARG
1	A	292	PHE
1	C	11	LYS
1	C	28	ASN
1	C	43	HIS
1	C	258	LEU
1	B	402	ASP
2	D	52	ARG
2	D	442	THR
2	E	146	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	E	374	MET
3	d	190	HIS
3	d	235	MET
4	g	231	LEU
4	g	246	CYS
4	g	270	MET
4	g	301	ASN
7	I	30	ASN
7	I	144	VAL
8	a	189	ARG
9	N	41	ARG
9	O	36	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	GLN
1	C	164	GLN
2	D	210	ASN
2	D	472	GLN
2	F	210	ASN
2	F	264	ASN
7	I	150	GLN
8	a	193	ASN
8	a	227	GLN
9	T	28	GLN
9	Y	78	ASN
9	W	28	GLN
9	U	28	GLN
9	Z	78	ASN
9	R	34	GLN
9	R	78	ASN
9	Q	34	GLN
9	M	42	GLN
9	P	28	GLN
9	P	42	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
10	ATP	C	601	-	28,33,33	0.85	0	34,52,52	1.15	2 (5%)
10	ATP	D	601	-	28,33,33	0.89	0	34,52,52	1.20	2 (5%)
10	ATP	A	601	-	28,33,33	0.90	0	34,52,52	1.17	2 (5%)
11	ADP	F	601	-	24,29,29	0.79	0	29,45,45	1.25	4 (13%)
10	ATP	B	601	-	28,33,33	0.88	0	34,52,52	1.19	2 (5%)

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	C	601	-	-	4/18/38/38	0/3/3/3
10	ATP	D	601	-	-	5/18/38/38	0/3/3/3
10	ATP	A	601	-	-	0/18/38/38	0/3/3/3
11	ADP	F	601	-	-	2/12/32/32	0/3/3/3
10	ATP	B	601	-	-	3/18/38/38	0/3/3/3

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	601	ATP	N3-C2-N1	-3.66	123.71	128.67
10	A	601	ATP	N3-C2-N1	-3.65	123.71	128.67
11	F	601	ADP	N3-C2-N1	-3.51	123.92	128.67
10	B	601	ATP	N3-C2-N1	-3.45	124.00	128.67
10	D	601	ATP	N3-C2-N1	-3.43	124.02	128.67
10	D	601	ATP	C4-C5-N7	-2.95	106.22	109.34
10	A	601	ATP	C4-C5-N7	-2.67	106.52	109.34
10	B	601	ATP	C4-C5-N7	-2.49	106.70	109.34
11	F	601	ADP	C4-C5-N7	-2.35	106.86	109.34
10	C	601	ATP	C4-C5-N7	-2.20	107.02	109.34
11	F	601	ADP	O3A-PA-O1A	-2.06	104.51	110.70
11	F	601	ADP	O2A-PA-O1A	2.01	121.81	112.44

There are no chirality outliers.

All (14) torsion outliers are listed below:

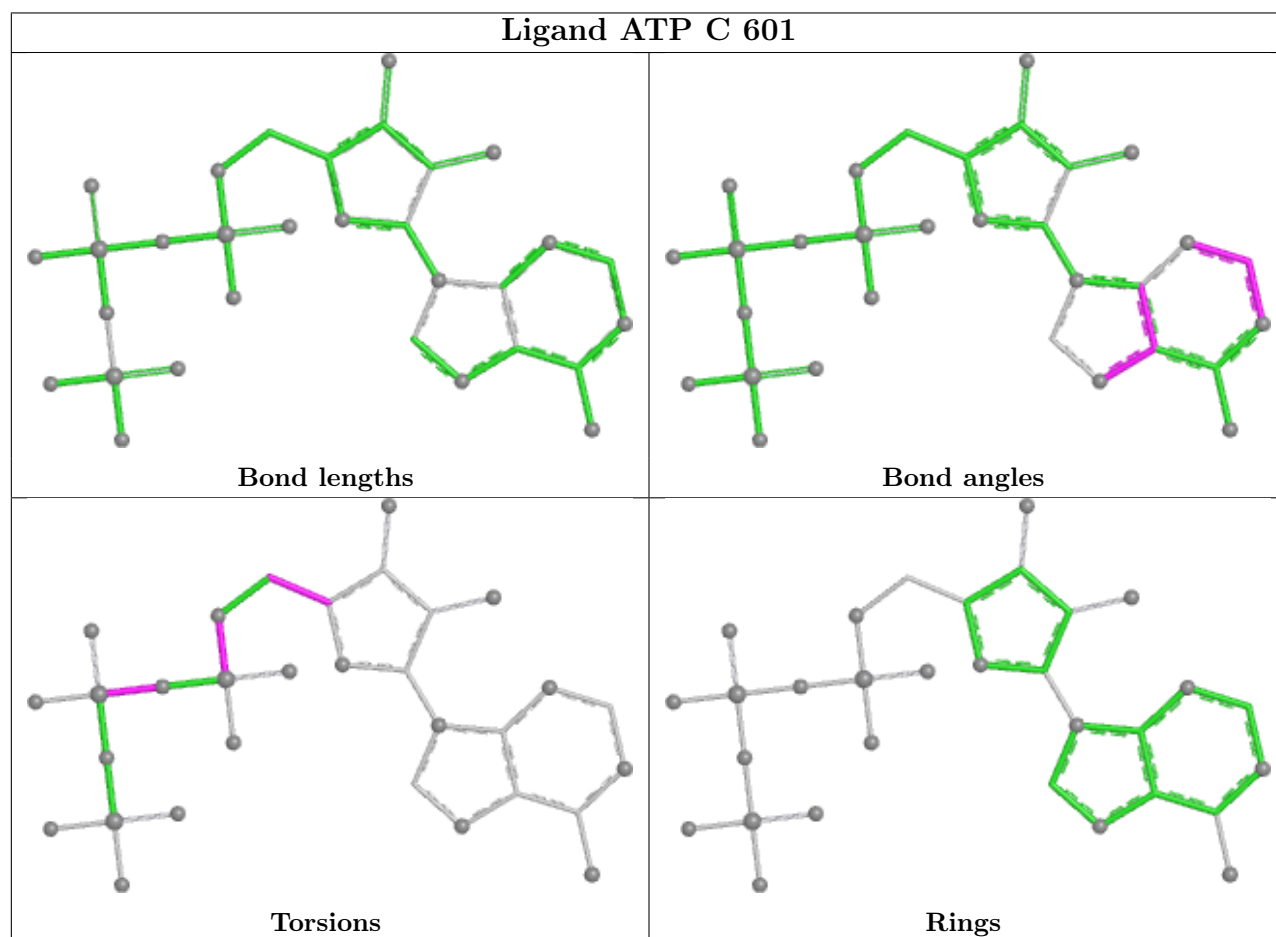
Mol	Chain	Res	Type	Atoms
10	C	601	ATP	C5'-O5'-PA-O2A
10	B	601	ATP	C5'-O5'-PA-O3A
10	D	601	ATP	C5'-O5'-PA-O1A
10	D	601	ATP	C5'-O5'-PA-O2A
10	D	601	ATP	C5'-O5'-PA-O3A
10	D	601	ATP	O4'-C4'-C5'-O5'
10	D	601	ATP	C3'-C4'-C5'-O5'
11	F	601	ADP	O4'-C4'-C5'-O5'
11	F	601	ADP	C4'-C5'-O5'-PA
10	C	601	ATP	C5'-O5'-PA-O3A
10	B	601	ATP	C5'-O5'-PA-O1A
10	B	601	ATP	C4'-C5'-O5'-PA
10	C	601	ATP	C3'-C4'-C5'-O5'
10	C	601	ATP	PA-O3A-PB-O1B

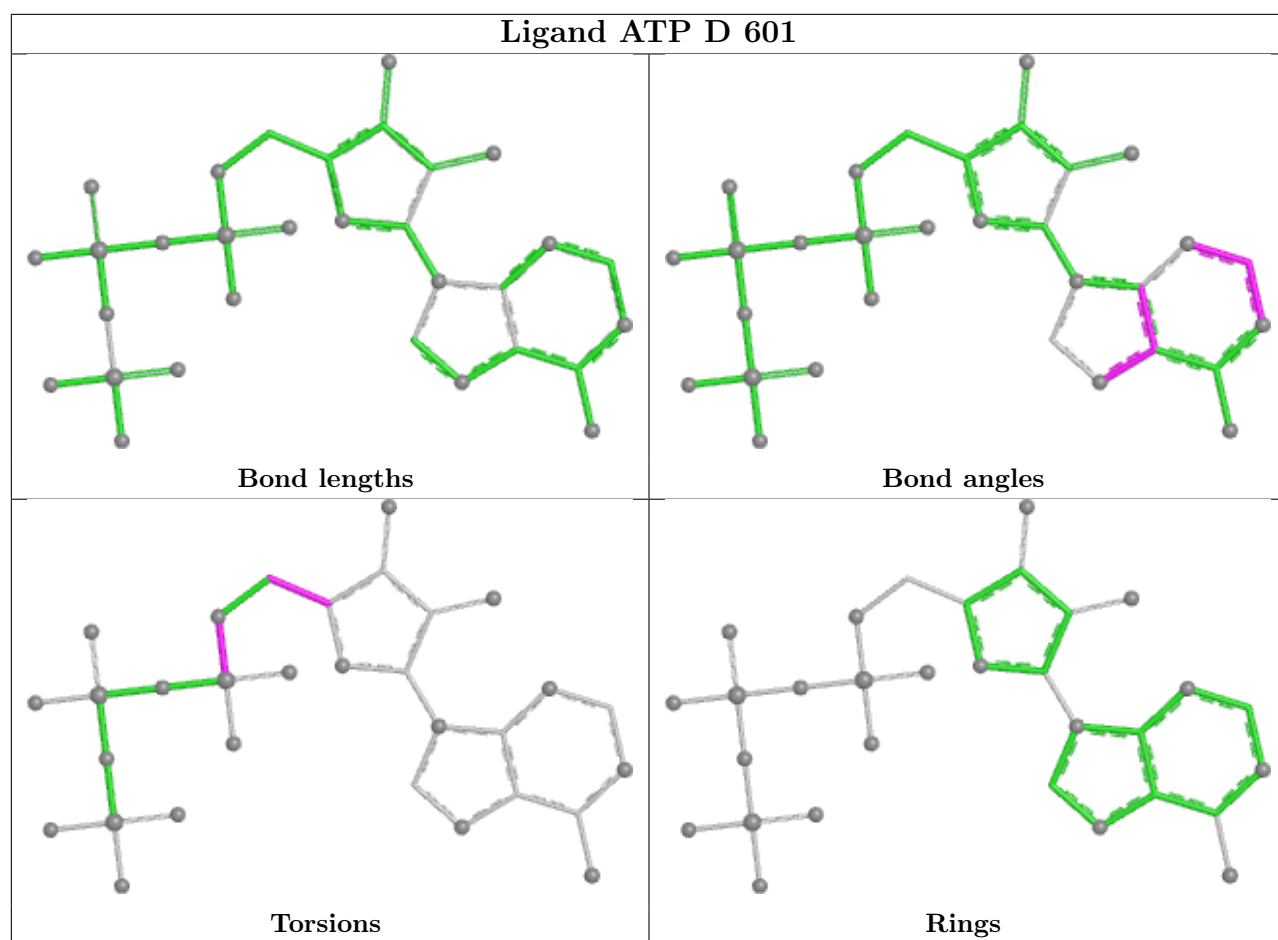
There are no ring outliers.

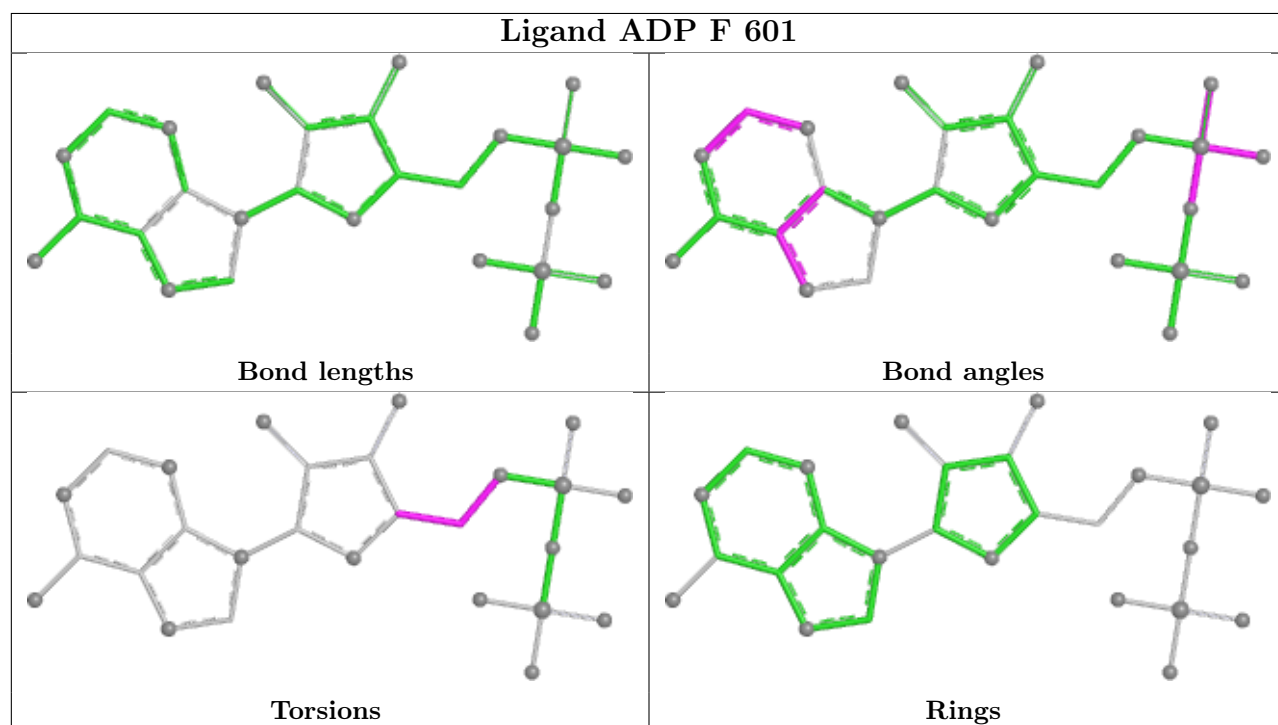
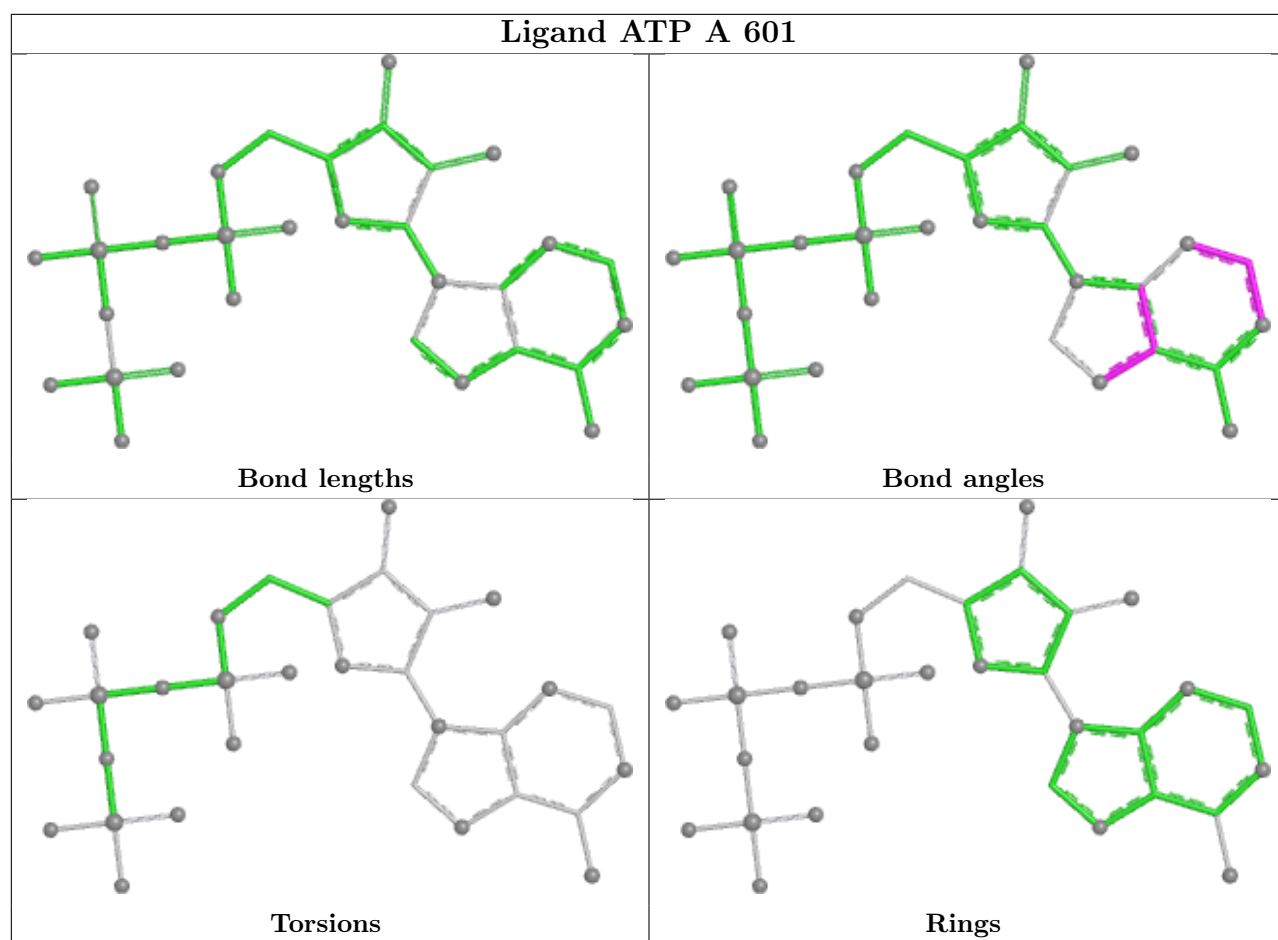
No monomer is involved in short contacts.

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 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

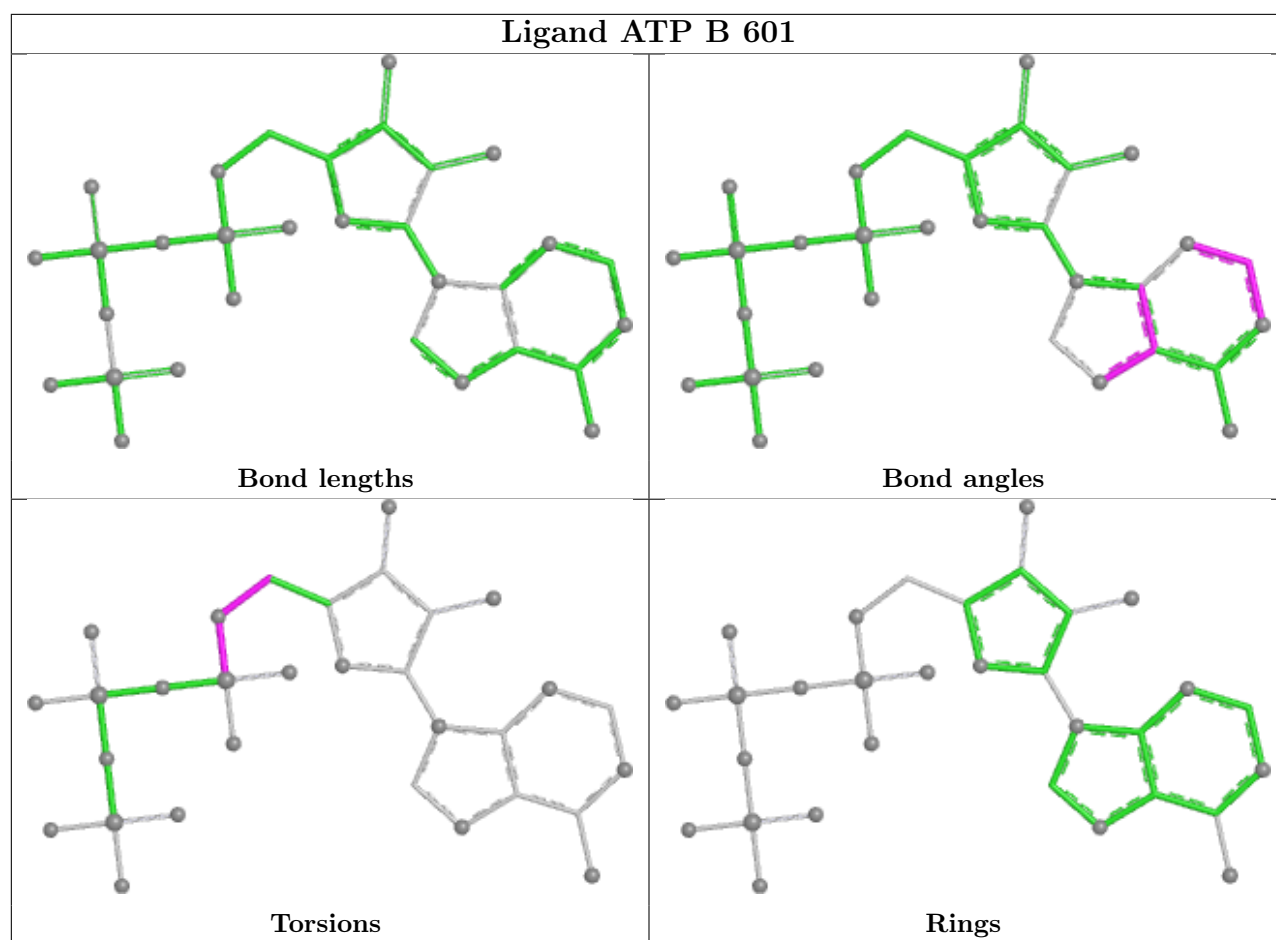
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

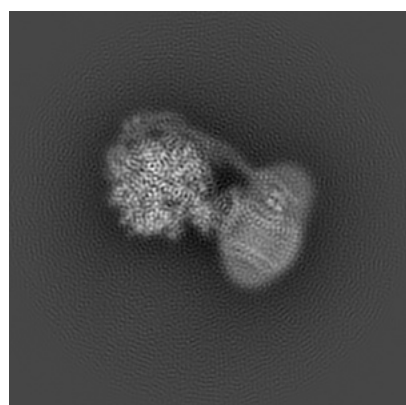
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21264. These allow visual inspection of the internal detail of the map and identification of artifacts.

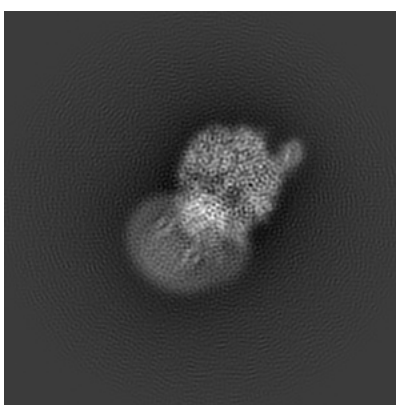
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

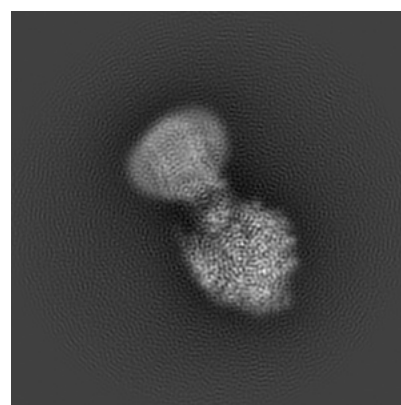
#### 6.1.1 Primary map



X



Y

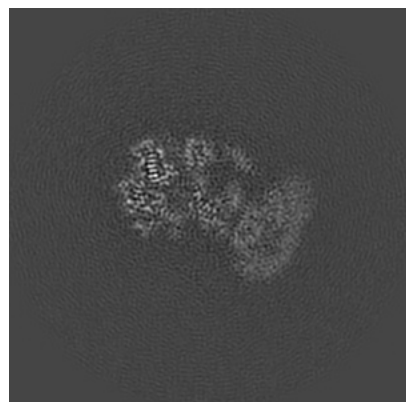


Z

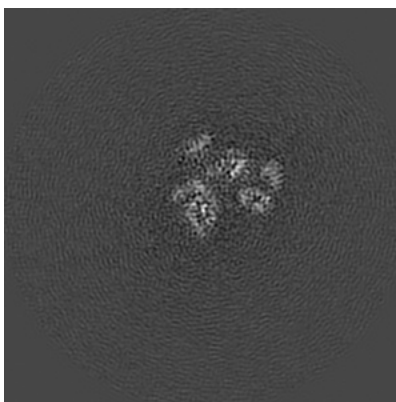
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

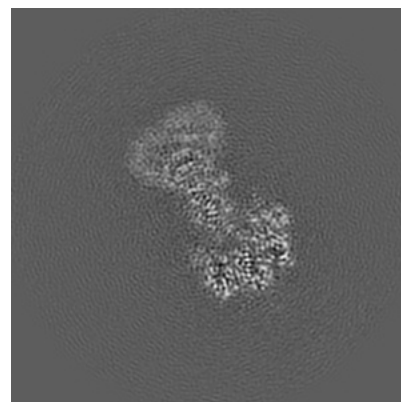
#### 6.2.1 Primary map



X Index: 180



Y Index: 180

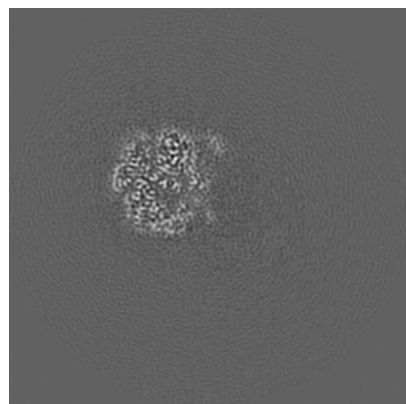


Z Index: 180

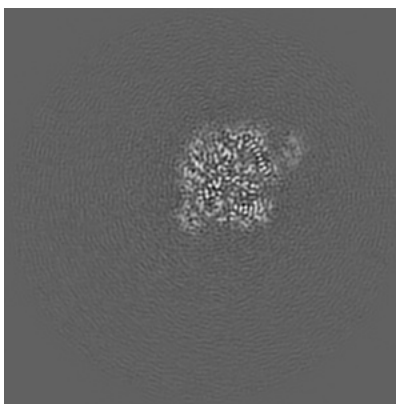
The images above show central slices of the map in three orthogonal directions.

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

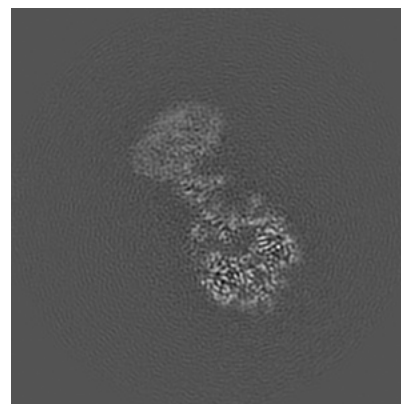
### 6.3.1 Primary map



X Index: 204



Y Index: 127

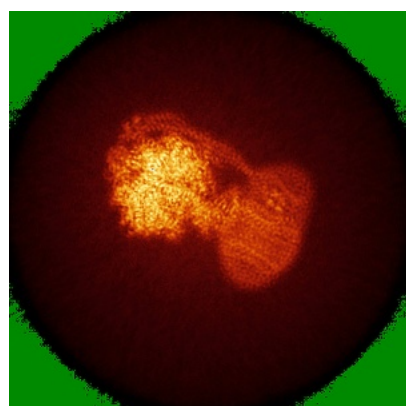


Z Index: 190

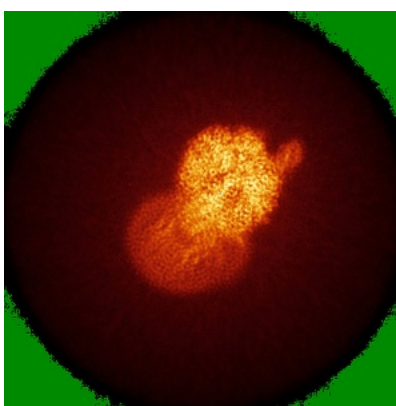
The images above show the largest variance slices of the map in three orthogonal directions.

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

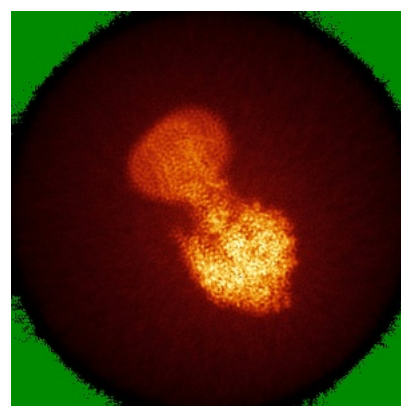
### 6.4.1 Primary map



X



Y



Z

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 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

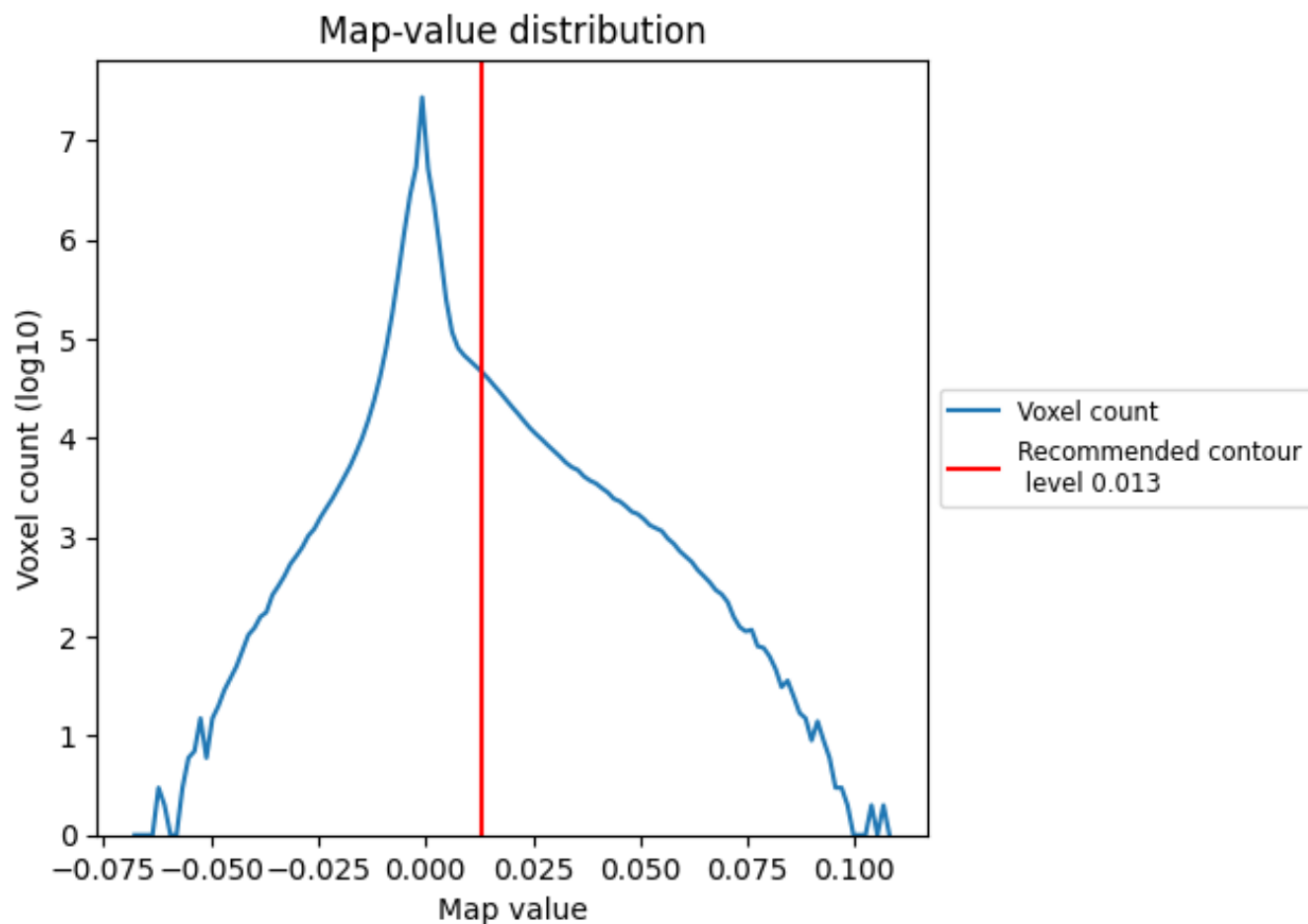
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

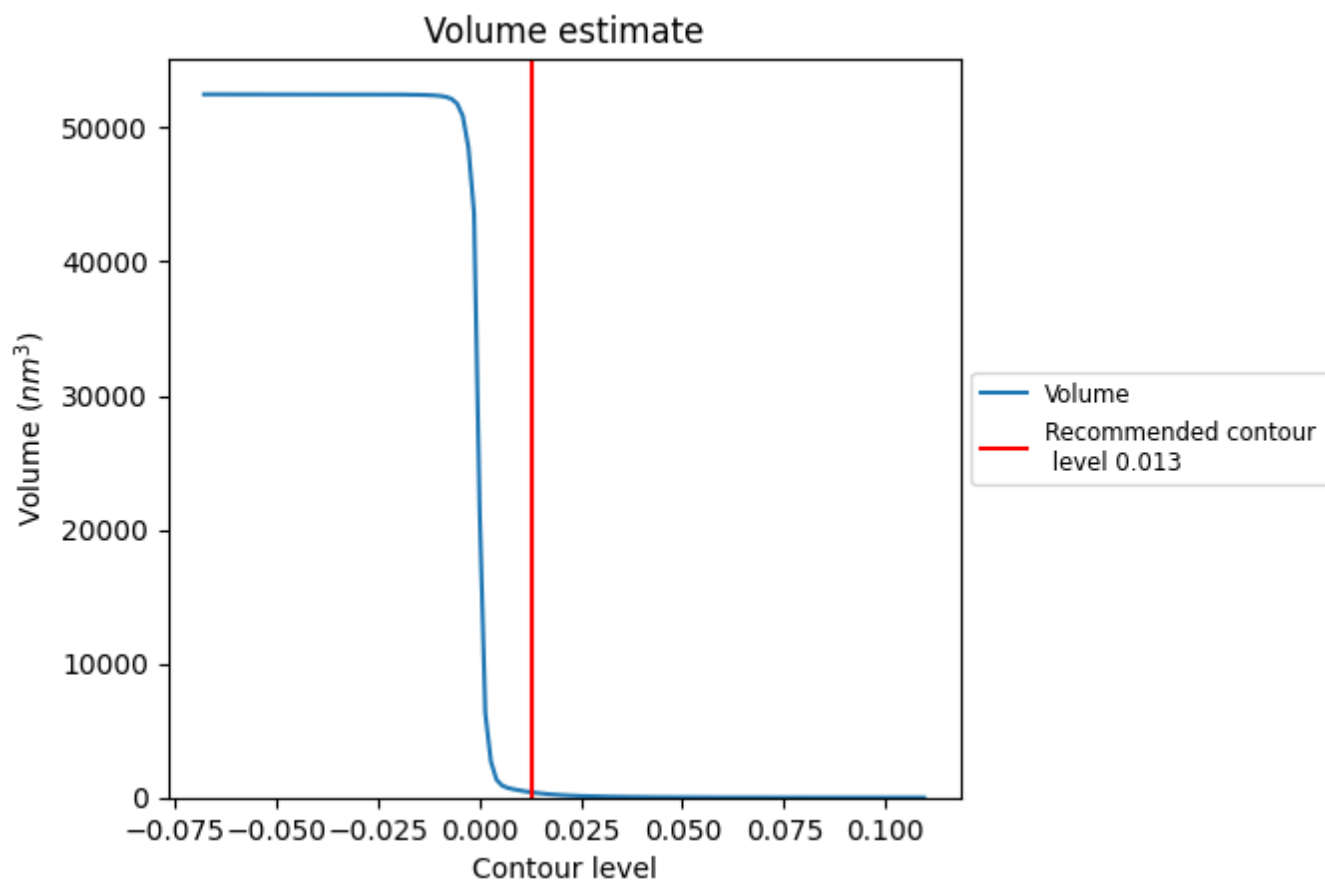
This section contains the results of statistical analysis of the map.

### 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.

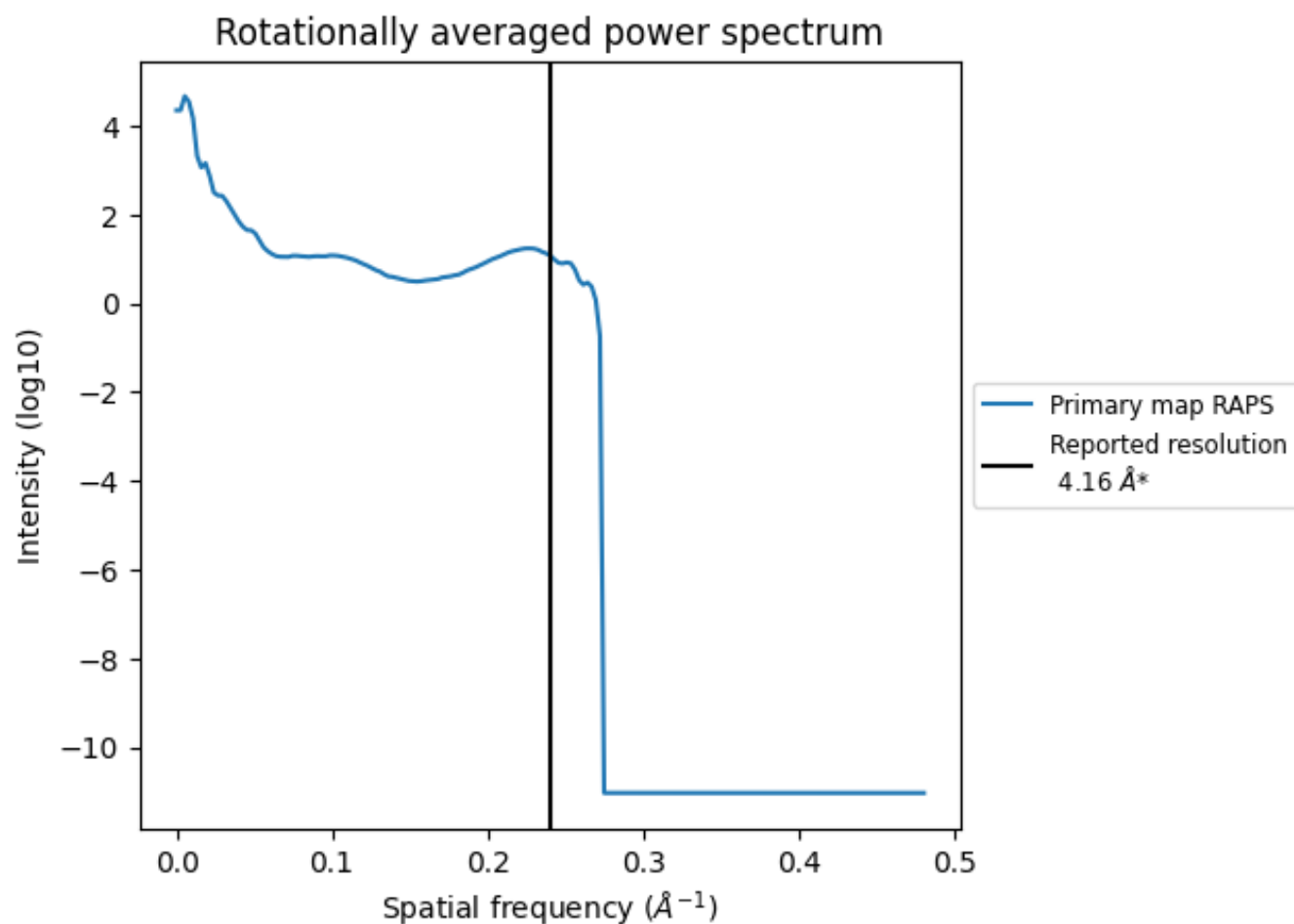
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 388  $\text{nm}^3$ ; this corresponds to an approximate mass of 350 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 ⓘ

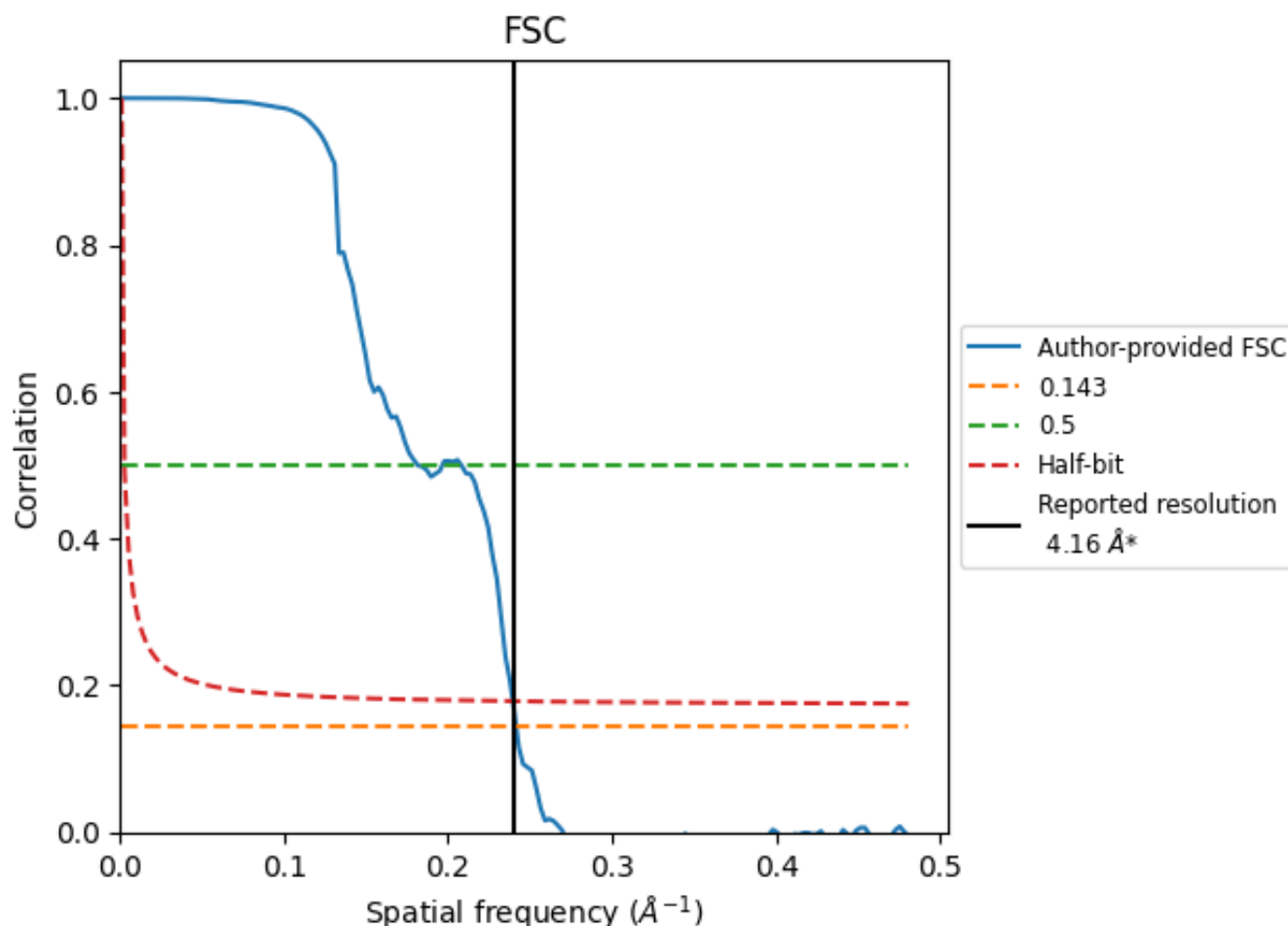


\*Reported resolution corresponds to spatial frequency of 0.240 Å<sup>-1</sup>

## 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 0.240 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

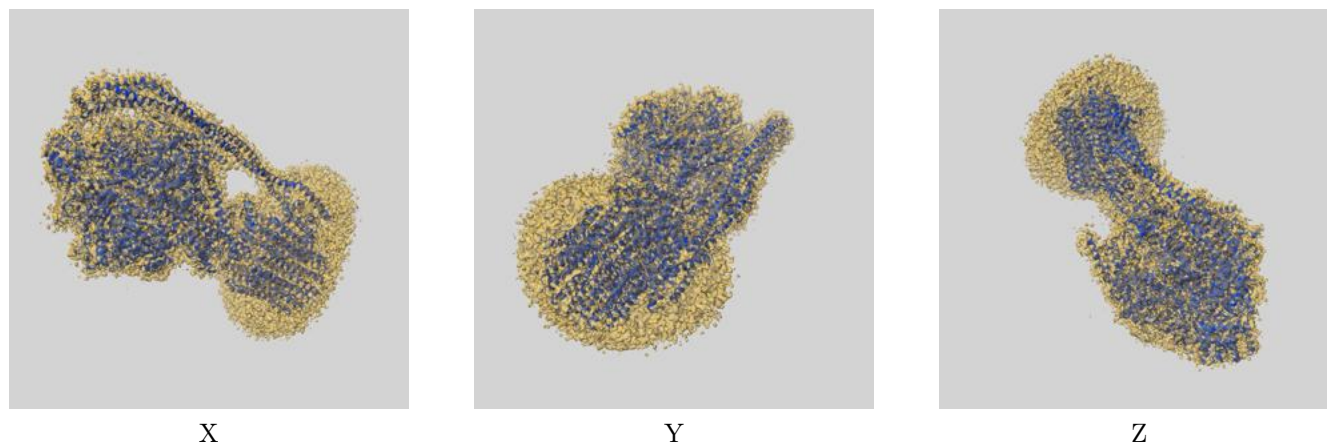
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.16	-	-
Author-provided FSC curve	4.14	5.51	4.18
Unmasked-calculated*	-	-	-

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

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

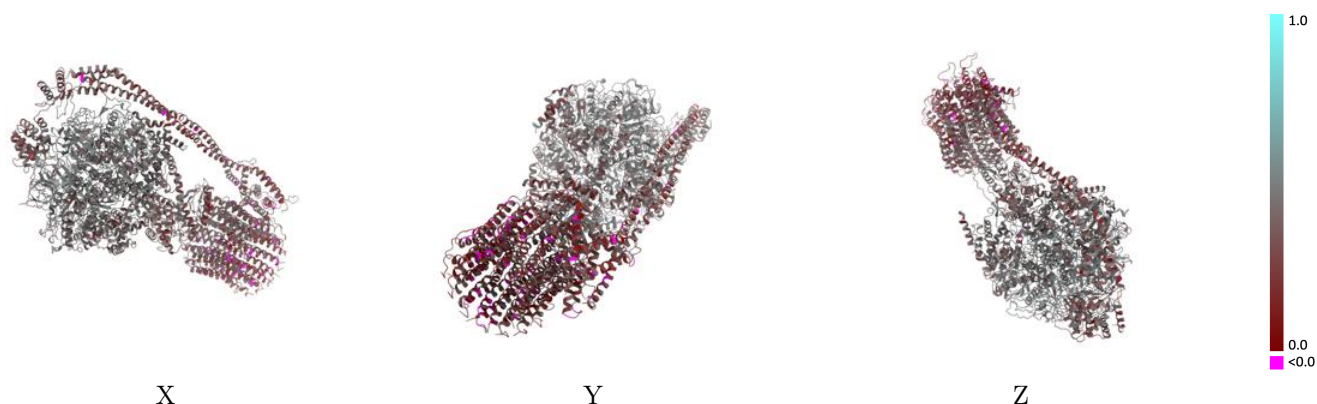
This section contains information regarding the fit between EMDB map EMD-21264 and PDB model 6VOH. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

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



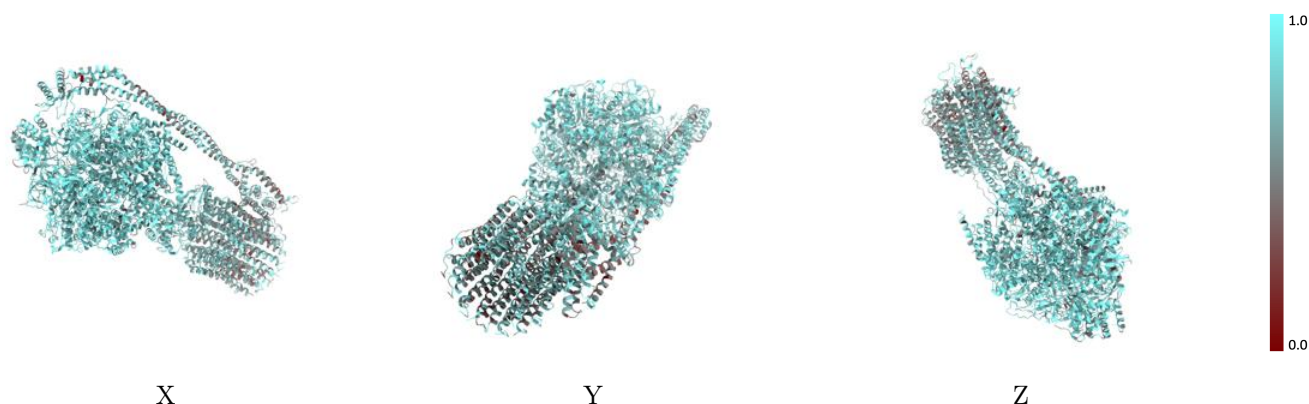
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



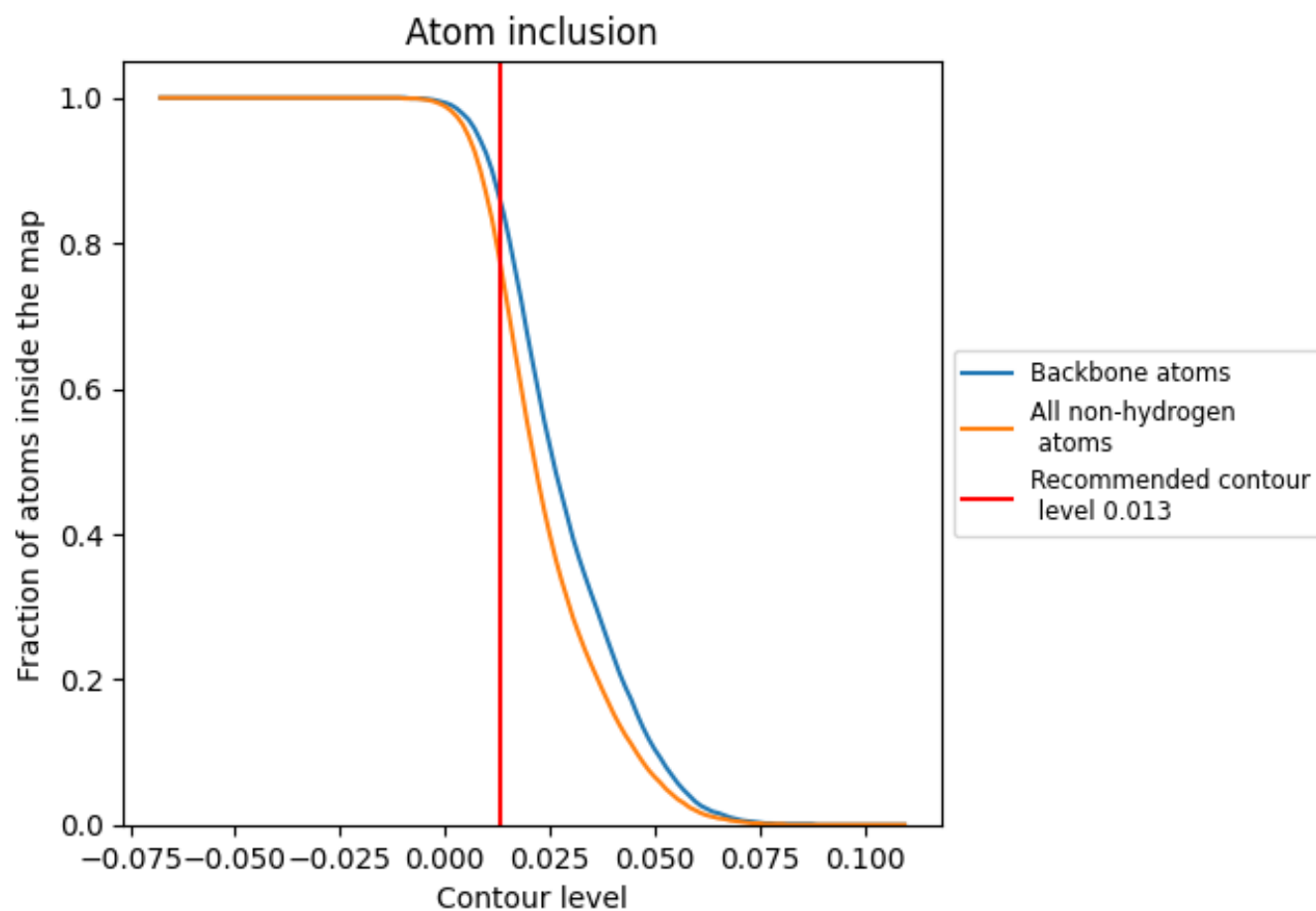
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.013).























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 78% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7780	 0.3900
A	 0.8370	 0.4440
B	 0.8210	 0.4320
C	 0.8470	 0.4540
D	 0.8410	 0.4490
E	 0.8530	 0.4580
F	 0.8470	 0.4560
I	 0.7070	 0.3250
J	 0.6160	 0.2750
M	 0.6960	 0.2960
N	 0.6660	 0.3110
O	 0.6570	 0.2830
P	 0.6850	 0.2910
Q	 0.6720	 0.2700
R	 0.6440	 0.2320
S	 0.6470	 0.2440
T	 0.6460	 0.2340
U	 0.6420	 0.2570
V	 0.6360	 0.2510
W	 0.6180	 0.2060
X	 0.6510	 0.2720
Y	 0.6600	 0.2780
Z	 0.6850	 0.2970
a	 0.6490	 0.2790
d	 0.7950	 0.3860
e	 0.7570	 0.3630
g	 0.7720	 0.4030

