wwPDB EM Validation Summary Report (i)

Apr 20, 2024 – 02:53 PM EDT

PDB ID	:	8F39
EMDB ID	:	EMD-28835
Title	:	Yeast ATP synthase in conformation-2, at pH 6
Authors	:	Sharma, S.; Patel, H.; Luo, M.; Mueller, D.M.; Liao, M.
Deposited on	:	2022-11-09
Resolution	:	3.50 Å(reported)

This is a wwPDB EM Validation Summary 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 (i) 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 (1)) were used in the production of this report:

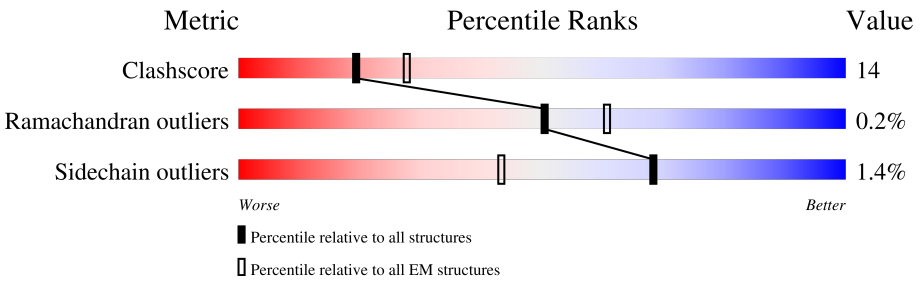
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
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	G	261	8% 67% 32% •
2	Z	155	51% 69% 29% •
3	7	171	82% 71% 26% •
4	6	89	54% 64% 34% •
5	U	85	79% 71% 29%
6	K	75	52% 80% 20%
6	L	75	41% 76% 23% •
6	M	75	27% 75% 24% •

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Mol	Chain	Length	Quality of chain
6	N	75	44% 80% 19%
6	O	75	44% 65% 33%
6	P	75	64% 63% 37%
6	Q	75	61% 56% 43%
6	R	75	65% 73% 24%
6	S	75	60% 76% 23%
6	T	75	55% 79% 20%
7	8	41	63% 68% 29%
8	X	224	68% 66% 33%
9	J	37	54% 81% 19%
10	Y	166	61% 38%
11	A	507	67% 32%
11	B	507	67% 32%
11	C	507	72% 27%
12	D	473	68% 31%
12	E	473	67% 32%
12	F	473	70% 29%
13	H	132	17% 69% 30%
14	I	59	32% 85% 15%

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 38767 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 gamma, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	G	261	2032	1276	353	393	10	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	VAL	deletion	UNP P38077
G	?	-	GLU	deletion	UNP P38077
G	?	-	ALA	deletion	UNP P38077
G	?	-	THR	deletion	UNP P38077
G	?	-	GLU	deletion	UNP P38077
G	?	-	THR	deletion	UNP P38077
G	?	-	GLY	deletion	UNP P38077
G	?	-	ALA	deletion	UNP P38077
G	?	-	PRO	deletion	UNP P38077

- Molecule 2 is a protein called ATP synthase subunit 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	Z	155	1232	778	211	242	1	0	0

- Molecule 3 is a protein called ATP synthase subunit d, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	7	171	1363	856	236	268	3	0	0

- Molecule 4 is a protein called ATP synthase subunit H, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	6	89	710	441	114	155	0	0

- Molecule 5 is a protein called ATP synthase subunit f, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	U	85	639	420	109	109	1	0	0

- Molecule 6 is a protein called ATP synthase subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	S	74	533	357	82	90	4	0	0
6	T	74	533	357	82	90	4	0	0
6	K	75	537	359	83	91	4	0	0
6	L	74	533	357	82	90	4	0	0
6	M	74	533	357	82	90	4	0	0
6	N	74	533	357	82	90	4	0	0
6	O	74	533	357	82	90	4	0	0
6	P	75	537	359	83	91	4	0	0
6	Q	74	533	357	82	90	4	0	0
6	R	74	533	357	82	90	4	0	0

- Molecule 7 is a protein called ATP synthase protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	8	41	356	250	51	52	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	X	224	1772	1210	265	287	10	0	0

- Molecule 9 is a protein called ATP synthase subunit J, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	37	292	197	45	48	2	0	0

- Molecule 10 is a protein called ATP synthase subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	Y	166	1254	799	217	237	1	0	0

- Molecule 11 is a protein called ATP synthase subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	A	507	3858	2435	679	741	3	0	0
11	B	506	3846	2426	678	739	3	0	0
11	C	505	3844	2426	676	739	3	0	0

- Molecule 12 is a protein called ATP synthase subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	D	473	3572	2262	608	696	6	0	0
12	E	473	3572	2262	608	696	6	0	0
12	F	472	3566	2259	607	694	6	0	0

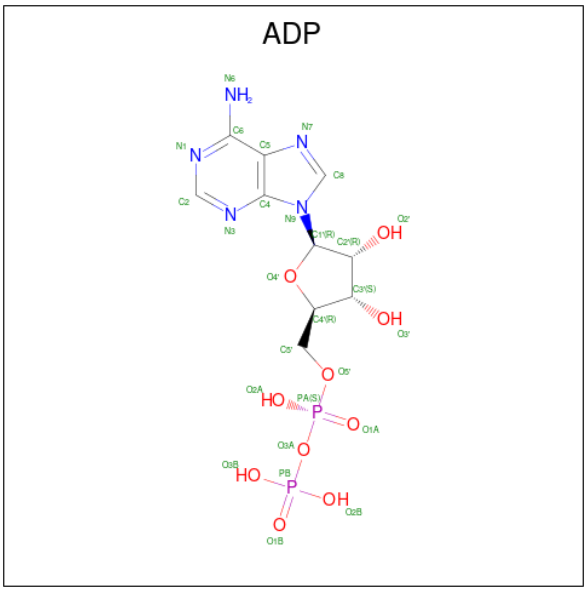
- Molecule 13 is a protein called ATP synthase subunit delta, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	H	132	990	624	165	199	2	0	0

- Molecule 14 is a protein called ATP synthase subunit epsilon, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	I	59	392	243	71	78	0	0

- Molecule 15 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

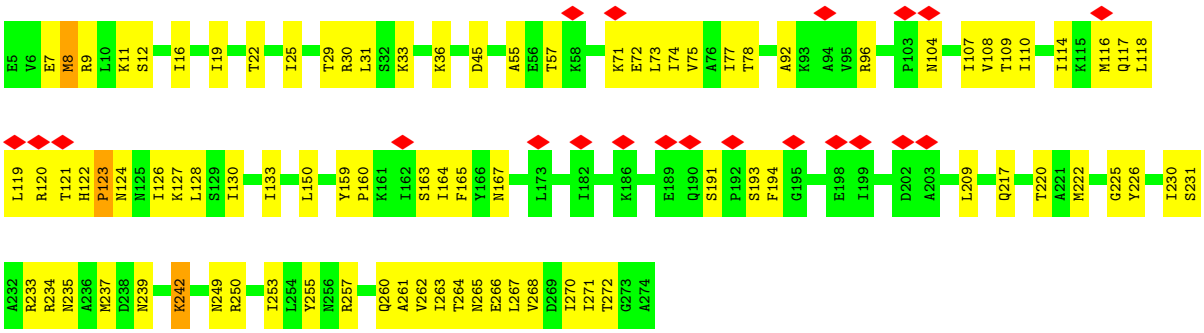
Mol	Chain	Residues	Atoms		AltConf
16	A	1	Total	Mg	0
			1	1	
16	B	1	Total	Mg	0
			1	1	
16	C	1	Total	Mg	0
			1	1	
16	E	1	Total	Mg	0
			1	1	

3 Residue-property plots (i)

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

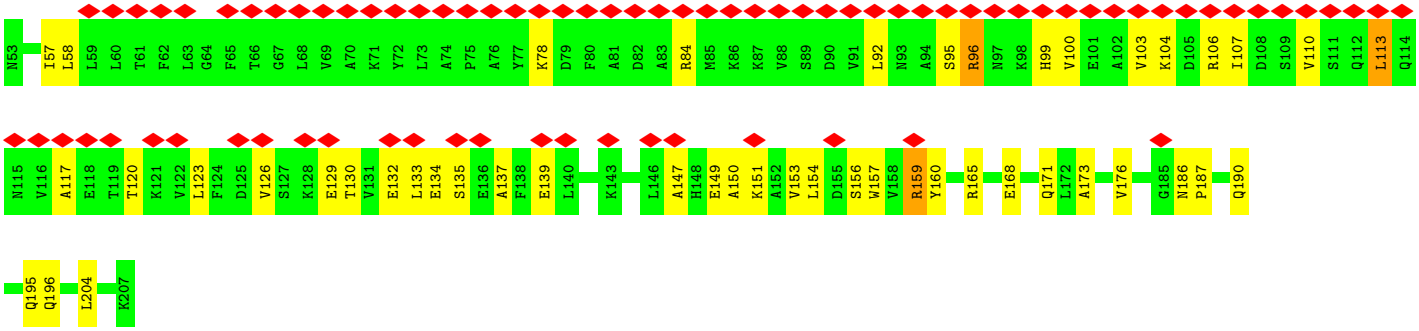
• Molecule 1: ATP synthase subunit gamma, mitochondrial

Chain G:



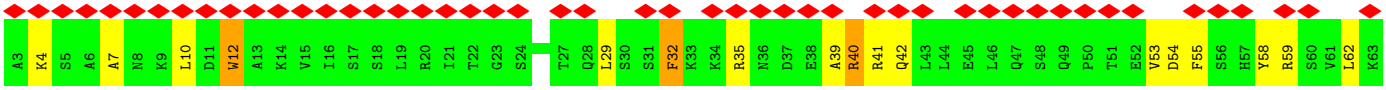
• Molecule 2: ATP synthase subunit 4, mitochondrial

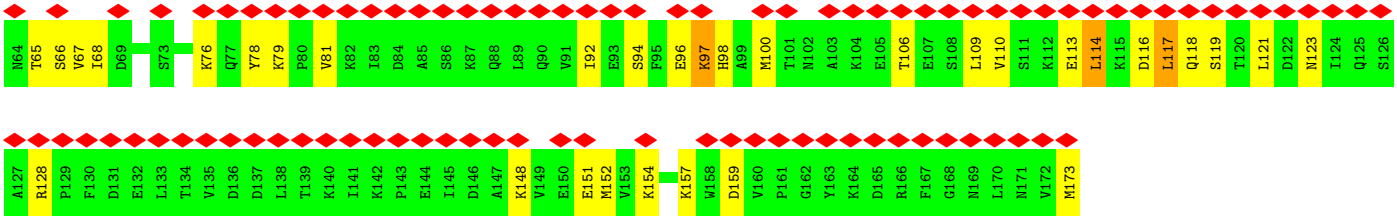
Chain Z:



• Molecule 3: ATP synthase subunit d, mitochondrial

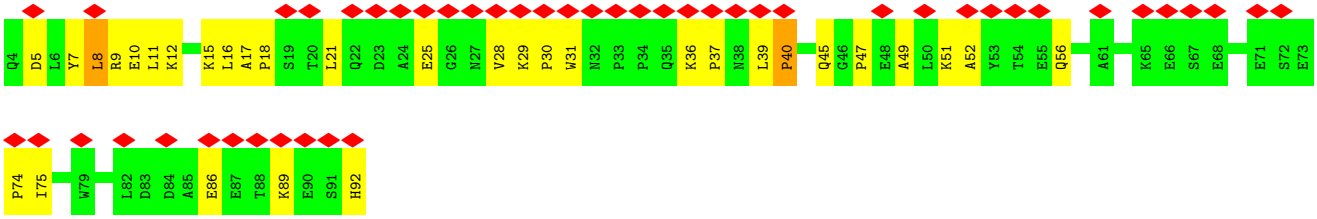
Chain 7:





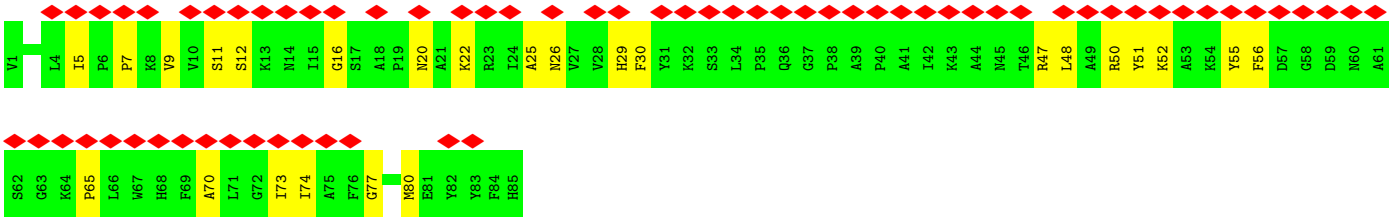
- Molecule 4: ATP synthase subunit H, mitochondrial

Chain 6:



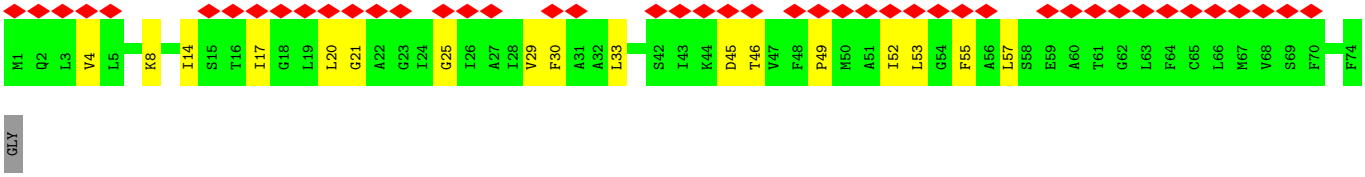
- Molecule 5: ATP synthase subunit f, mitochondrial

Chain U:



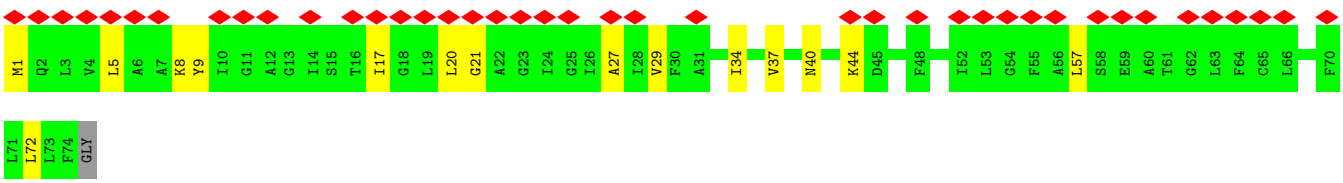
- Molecule 6: ATP synthase subunit 9, mitochondrial

Chain S:



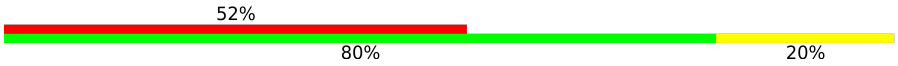
- Molecule 6: ATP synthase subunit 9, mitochondrial

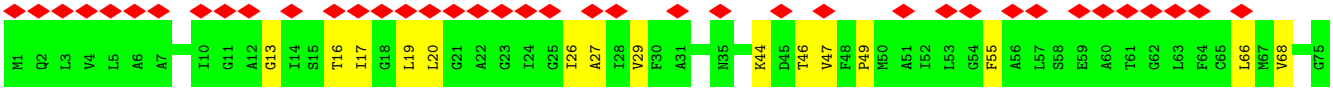
Chain T:



• Molecule 6: ATP synthase subunit 9, mitochondrial

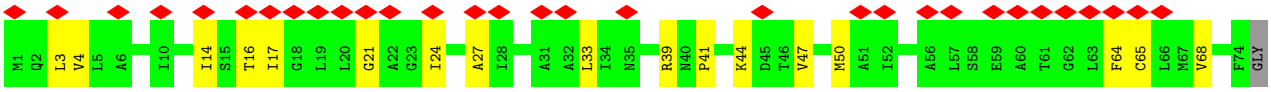
Chain K:





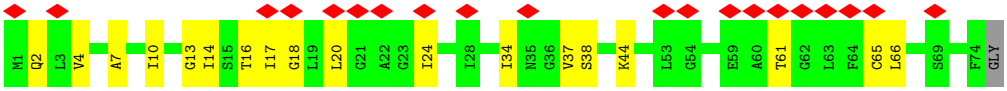
• Molecule 6: ATP synthase subunit 9, mitochondrial

Chain L:



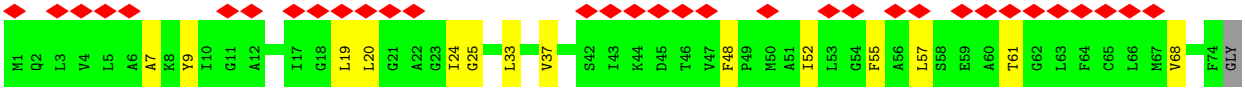
• Molecule 6: ATP synthase subunit 9, mitochondrial

Chain M:



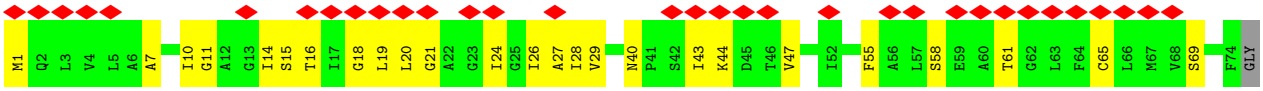
• Molecule 6: ATP synthase subunit 9, mitochondrial

Chain N:



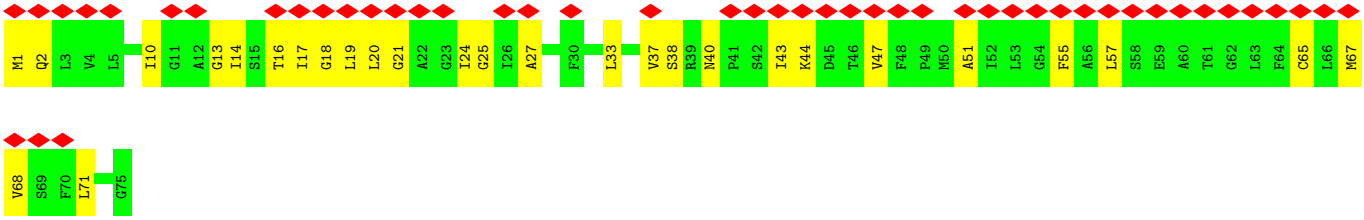
• Molecule 6: ATP synthase subunit 9, mitochondrial

Chain O:



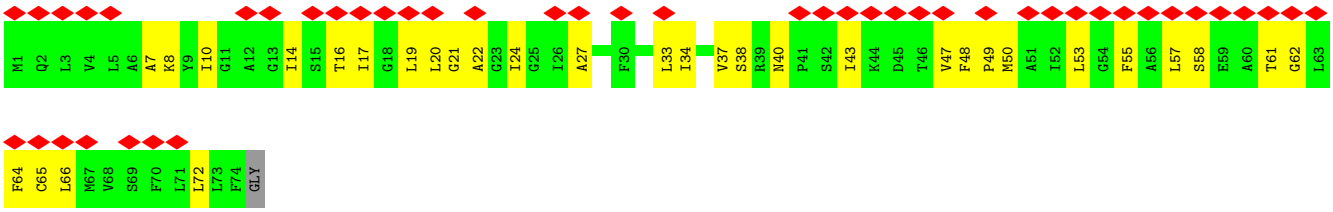
• Molecule 6: ATP synthase subunit 9, mitochondrial

Chain P:



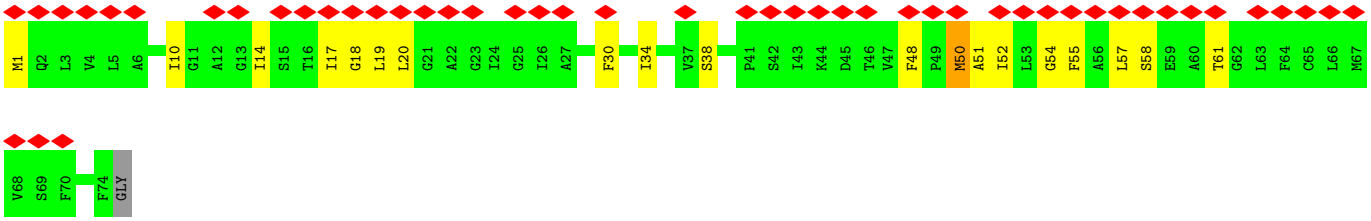
• Molecule 6: ATP synthase subunit 9, mitochondrial

Chain Q:



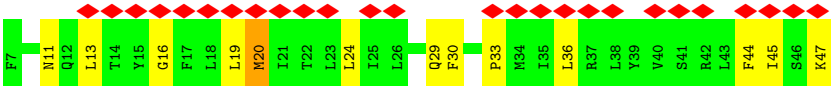
- Molecule 6: ATP synthase subunit 9, mitochondrial

Chain R:



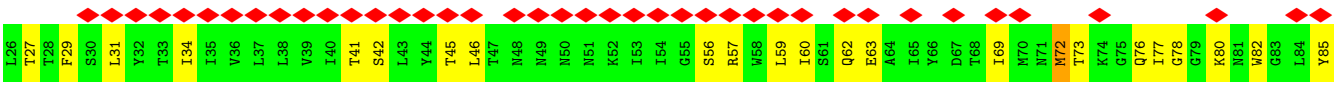
- Molecule 7: ATP synthase protein 8

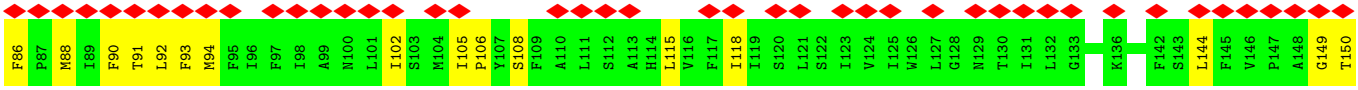
Chain 8:

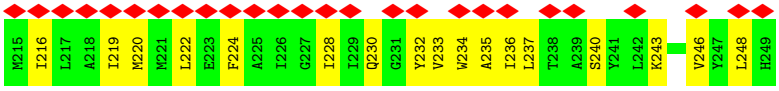


- Molecule 8: ATP synthase subunit a

Chain X:

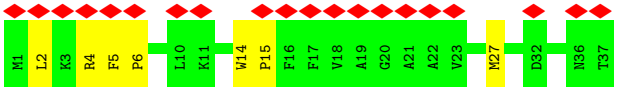






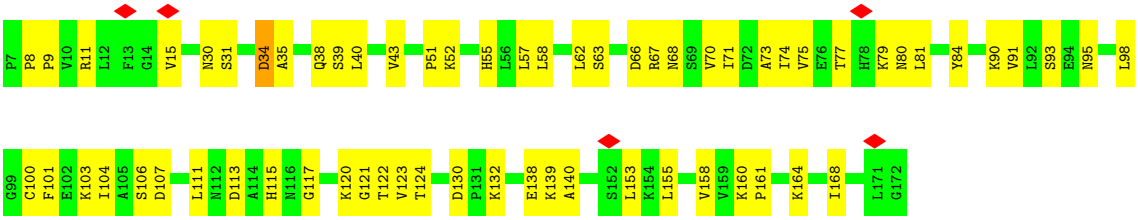
- Molecule 9: ATP synthase subunit J, mitochondrial

Chain J:



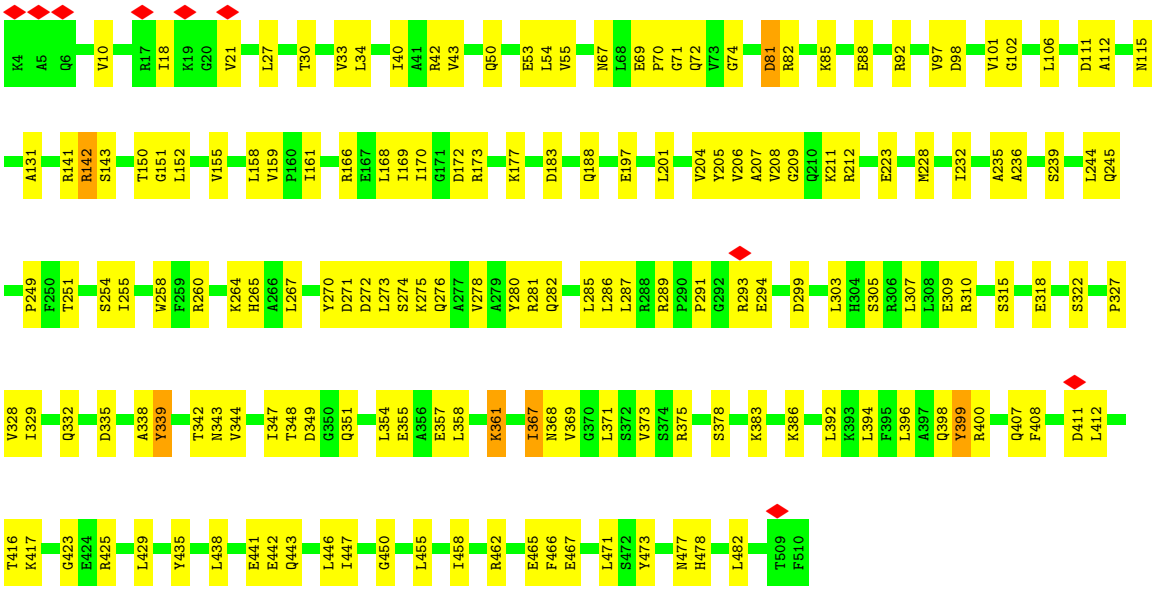
• Molecule 10: ATP synthase subunit 5, mitochondrial

Chain Y:



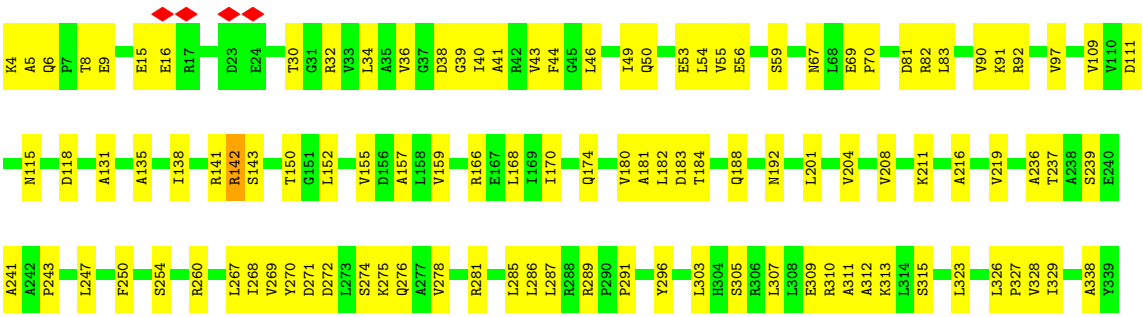
• Molecule 11: ATP synthase subunit alpha, mitochondrial

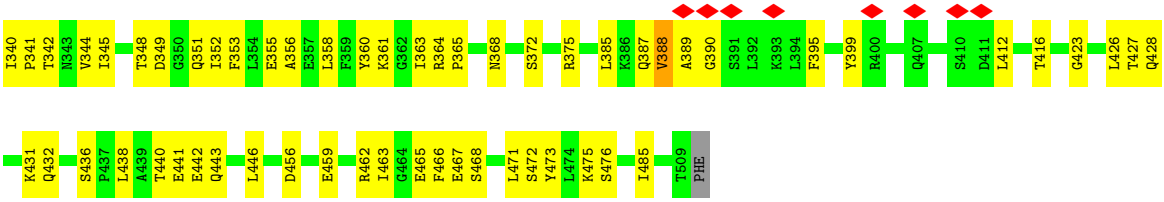
Chain A:



• Molecule 11: ATP synthase subunit alpha, mitochondrial

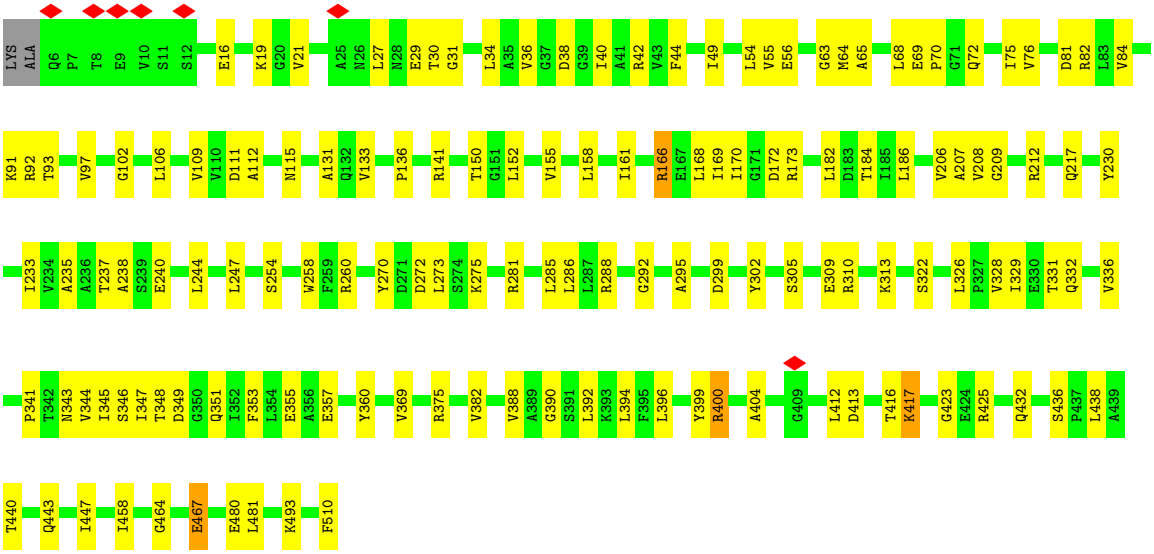
Chain B:





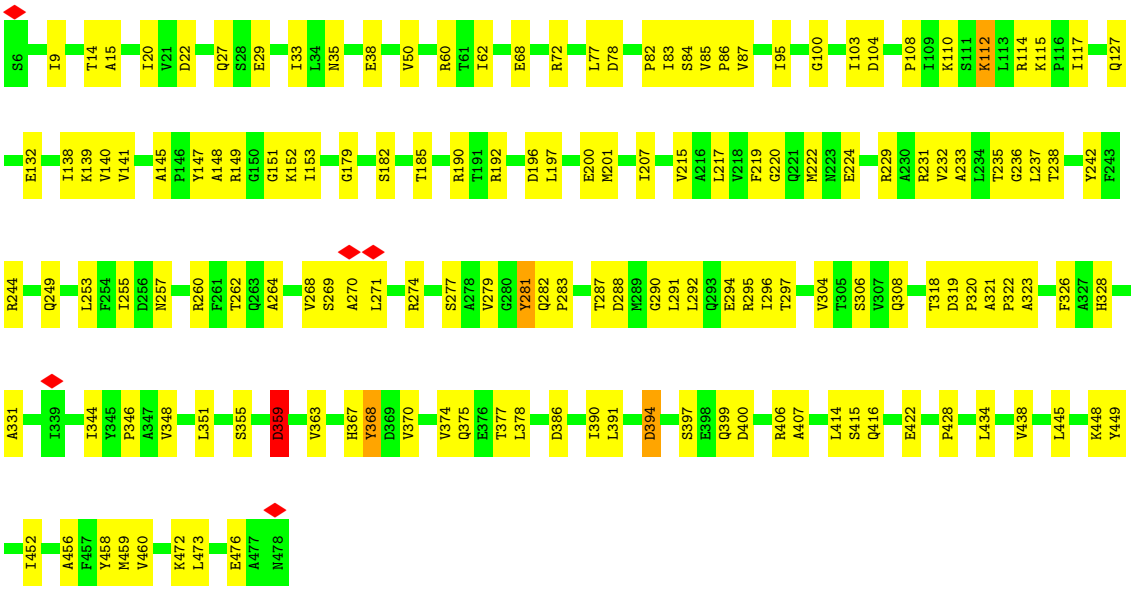
• Molecule 11: ATP synthase subunit alpha, mitochondrial

Chain C:



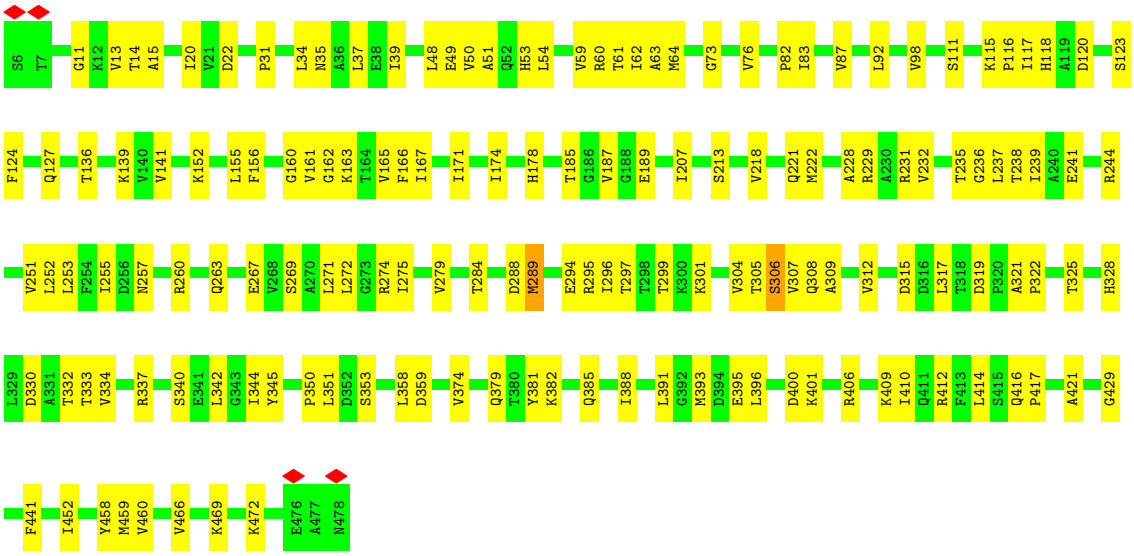
• Molecule 12: ATP synthase subunit beta, mitochondrial

Chain D:



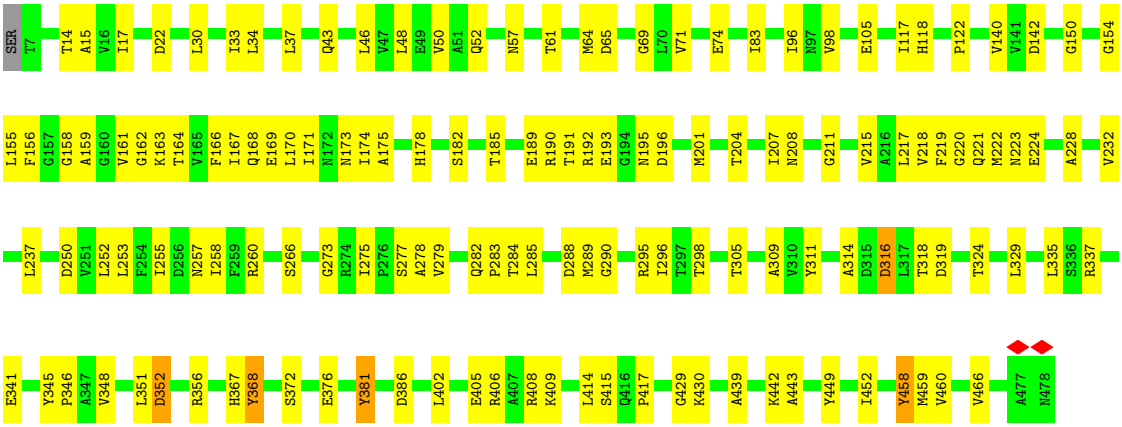
• Molecule 12: ATP synthase subunit beta, mitochondrial

Chain E: 67% 32%



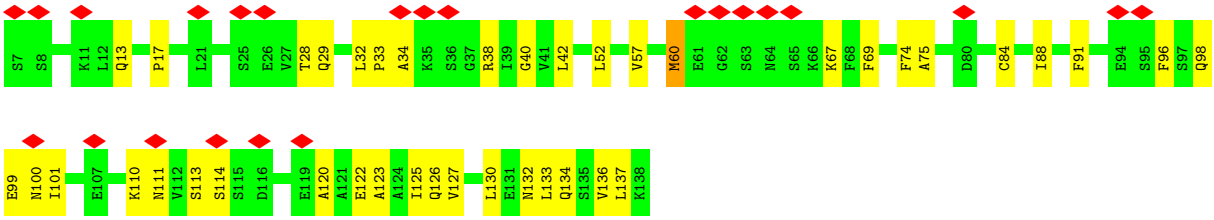
- Molecule 12: ATP synthase subunit beta, mitochondrial

Chain F: 70% 29%



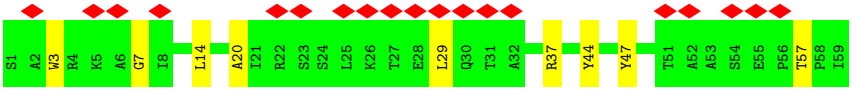
- Molecule 13: ATP synthase subunit delta, mitochondrial

Chain H: 17% 69% 30%



- Molecule 14: ATP synthase subunit epsilon, mitochondrial

Chain I: 32% 85% 15%


S1
A2
W3
R4
K5
A6
G7
I8
L14
A20
I21
R22
S23
S24
L25
K26
T27
E28
L29
Q30
T31
A32
R37
Y44
Y47
T51
A52
A53
S54
E55
P56
T57
P58
I59

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	99780	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 ($e^-/Å^2$)	52	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.078	Depositor
Minimum map value	-0.029	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	256.0, 256.0, 256.0	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	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: MG, 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	G	0.30	1/2057 (0.0%)	0.62	2/2767 (0.1%)
2	Z	0.25	0/1246	0.55	1/1678 (0.1%)
3	7	0.27	0/1382	0.62	2/1858 (0.1%)
4	6	0.27	0/725	0.57	1/988 (0.1%)
5	U	0.25	0/659	0.44	0/895
6	K	0.26	0/545	0.48	0/737
6	L	0.26	0/541	0.45	0/732
6	M	0.26	0/541	0.45	0/732
6	N	0.26	0/541	0.45	0/732
6	O	0.26	0/541	0.41	0/732
6	P	0.26	0/545	0.48	0/737
6	Q	0.28	0/541	0.50	0/732
6	R	0.26	0/541	0.49	0/732
6	S	0.29	0/541	0.53	0/732
6	T	0.27	0/541	0.44	0/732
7	8	0.26	0/366	0.54	0/492
8	X	0.26	0/1820	0.52	1/2483 (0.0%)
9	J	0.26	0/302	0.45	0/410
10	Y	0.27	0/1272	0.57	1/1717 (0.1%)
11	A	0.26	0/3916	0.52	0/5298
11	B	0.26	0/3903	0.54	0/5282
11	C	0.26	0/3902	0.51	0/5280
12	D	0.26	0/3628	0.55	1/4919 (0.0%)
12	E	0.26	0/3628	0.53	0/4919
12	F	0.27	0/3622	0.53	0/4911
13	H	0.25	0/1004	0.49	1/1359 (0.1%)
14	I	0.24	0/398	0.46	0/547
All	All	0.26	1/39248 (0.0%)	0.53	10/53133 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	123	PRO	CG-CD	-5.53	1.32	1.50

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	123	PRO	CA-N-CD	-13.33	92.84	111.50
8	X	72	MET	CA-CB-CG	11.06	132.11	113.30
2	Z	113	LEU	CA-CB-CG	7.60	132.78	115.30
1	G	123	PRO	N-CD-CG	-7.13	92.51	103.20
10	Y	130	ASP	CB-CG-OD2	6.84	124.46	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2032	0	2093	69	0
2	Z	1232	0	1256	48	0
3	7	1363	0	1389	50	0
4	6	710	0	668	31	0
5	U	639	0	615	16	0
6	K	537	0	582	13	0
6	L	533	0	579	20	0
6	M	533	0	579	23	0
6	N	533	0	579	14	0
6	O	533	0	579	23	0
6	P	537	0	582	29	0
6	Q	533	0	579	37	0
6	R	533	0	579	21	0
6	S	533	0	579	25	0
6	T	533	0	579	25	0
7	8	356	0	379	11	0
8	X	1772	0	1873	58	0
9	J	292	0	298	5	0
10	Y	1254	0	1318	46	0
11	A	3858	0	3941	133	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	B	3846	0	3932	133	0
11	C	3844	0	3923	105	0
12	D	3572	0	3638	114	0
12	E	3572	0	3638	124	0
12	F	3566	0	3633	108	0
13	H	990	0	999	30	0
14	I	392	0	306	8	0
15	A	27	0	12	0	0
15	B	27	0	12	2	0
15	C	27	0	12	0	0
15	E	27	0	12	7	0
15	F	27	0	12	3	0
16	A	1	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	E	1	0	0	0	0
All	All	38767	0	39755	1106	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 14.

The worst 5 of 1106 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)
3:7:39:ALA:O	3:7:42:GLN:NE2	2.07	0.87
6:N:25:GLY:HA2	6:O:27:ALA:HB2	1.60	0.83
12:E:237:LEU:HD13	12:E:295:ARG:HB2	1.61	0.82
12:D:270:ALA:HB2	12:D:282:GLN:HA	1.61	0.81
1:G:242:LYS:HE3	11:A:407:GLN:HB3	1.61	0.81

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	G	257/261 (98%)	239 (93%)	17 (7%)	1 (0%)	34	72
2	Z	153/155 (99%)	148 (97%)	5 (3%)	0	100	100
3	7	169/171 (99%)	161 (95%)	8 (5%)	0	100	100
4	6	87/89 (98%)	78 (90%)	9 (10%)	0	100	100
5	U	83/85 (98%)	78 (94%)	5 (6%)	0	100	100
6	K	73/75 (97%)	73 (100%)	0	0	100	100
6	L	72/75 (96%)	70 (97%)	2 (3%)	0	100	100
6	M	72/75 (96%)	69 (96%)	3 (4%)	0	100	100
6	N	72/75 (96%)	71 (99%)	1 (1%)	0	100	100
6	O	72/75 (96%)	71 (99%)	1 (1%)	0	100	100
6	P	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
6	Q	72/75 (96%)	70 (97%)	2 (3%)	0	100	100
6	R	72/75 (96%)	72 (100%)	0	0	100	100
6	S	72/75 (96%)	72 (100%)	0	0	100	100
6	T	72/75 (96%)	70 (97%)	2 (3%)	0	100	100
7	8	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
8	X	222/224 (99%)	201 (90%)	20 (9%)	1 (0%)	29	68
9	J	35/37 (95%)	35 (100%)	0	0	100	100
10	Y	164/166 (99%)	145 (88%)	17 (10%)	2 (1%)	13	50
11	A	505/507 (100%)	477 (94%)	27 (5%)	1 (0%)	47	81
11	B	504/507 (99%)	477 (95%)	25 (5%)	2 (0%)	34	72
11	C	503/507 (99%)	487 (97%)	16 (3%)	0	100	100
12	D	471/473 (100%)	448 (95%)	22 (5%)	1 (0%)	47	81
12	E	471/473 (100%)	437 (93%)	31 (7%)	3 (1%)	25	64
12	F	470/473 (99%)	451 (96%)	19 (4%)	0	100	100
13	H	130/132 (98%)	112 (86%)	18 (14%)	0	100	100
14	I	57/59 (97%)	51 (90%)	6 (10%)	0	100	100
All	All	5042/5110 (99%)	4771 (95%)	260 (5%)	11 (0%)	50	81

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	A	367	ILE
11	B	388	VAL
8	X	176	ARG
12	E	161	VAL
1	G	57	THR

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	G	224/224 (100%)	220 (98%)	4 (2%)	59	81
2	Z	137/138 (99%)	135 (98%)	2 (2%)	65	84
3	7	154/156 (99%)	149 (97%)	5 (3%)	39	69
4	6	79/79 (100%)	78 (99%)	1 (1%)	69	86
5	U	60/68 (88%)	60 (100%)	0	100	100
6	K	55/55 (100%)	55 (100%)	0	100	100
6	L	55/55 (100%)	55 (100%)	0	100	100
6	M	55/55 (100%)	55 (100%)	0	100	100
6	N	55/55 (100%)	55 (100%)	0	100	100
6	O	55/55 (100%)	54 (98%)	1 (2%)	59	81
6	P	55/55 (100%)	54 (98%)	1 (2%)	59	81
6	Q	55/55 (100%)	53 (96%)	2 (4%)	35	66
6	R	55/55 (100%)	53 (96%)	2 (4%)	35	66
6	S	55/55 (100%)	55 (100%)	0	100	100
6	T	55/55 (100%)	55 (100%)	0	100	100
7	8	40/40 (100%)	38 (95%)	2 (5%)	24	58
8	X	193/193 (100%)	191 (99%)	2 (1%)	76	88
9	J	30/30 (100%)	30 (100%)	0	100	100
10	Y	139/139 (100%)	135 (97%)	4 (3%)	42	71
11	A	410/410 (100%)	401 (98%)	9 (2%)	52	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	B	409/410 (100%)	407 (100%)	2 (0%)	88	94
11	C	409/410 (100%)	402 (98%)	7 (2%)	60	82
12	D	382/382 (100%)	376 (98%)	6 (2%)	62	83
12	E	382/382 (100%)	381 (100%)	1 (0%)	92	97
12	F	381/382 (100%)	376 (99%)	5 (1%)	69	86
13	H	111/111 (100%)	109 (98%)	2 (2%)	59	81
14	I	25/46 (54%)	24 (96%)	1 (4%)	31	64
All	All	4115/4150 (99%)	4056 (99%)	59 (1%)	68	85

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	A	172	ASP
12	F	458	TYR
11	B	142	ARG
12	F	381	TYR
12	D	394	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
4	6	56	GLN
6	M	2	GLN
12	F	195	ASN
6	P	40	ASN
10	Y	115	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
15	ADP	E	501	16	24,29,29	0.97	1 (4%)	29,45,45	1.36	3 (10%)
15	ADP	A	601	16	24,29,29	0.95	1 (4%)	29,45,45	1.34	4 (13%)
15	ADP	F	600	-	24,29,29	0.94	1 (4%)	29,45,45	1.51	4 (13%)
15	ADP	C	601	16	24,29,29	0.96	1 (4%)	29,45,45	1.47	4 (13%)
15	ADP	B	601	16	24,29,29	0.95	1 (4%)	29,45,45	1.46	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
15	ADP	E	501	16	-	5/12/32/32	0/3/3/3
15	ADP	A	601	16	-	0/12/32/32	0/3/3/3
15	ADP	F	600	-	-	4/12/32/32	0/3/3/3
15	ADP	C	601	16	-	3/12/32/32	0/3/3/3
15	ADP	B	601	16	-	5/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	E	501	ADP	C5-C4	2.60	1.47	1.40
15	A	601	ADP	C5-C4	2.51	1.47	1.40
15	F	600	ADP	C5-C4	2.50	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	601	ADP	C5-C4	2.50	1.47	1.40
15	B	601	ADP	C5-C4	2.47	1.47	1.40

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	F	600	ADP	PA-O3A-PB	-3.72	120.05	132.83
15	F	600	ADP	C3'-C2'-C1'	3.65	106.47	100.98
15	C	601	ADP	PA-O3A-PB	-3.59	120.50	132.83
15	E	501	ADP	PA-O3A-PB	-3.49	120.86	132.83
15	B	601	ADP	C3'-C2'-C1'	3.45	106.17	100.98

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	B	601	ADP	C5'-O5'-PA-O2A
15	B	601	ADP	C5'-O5'-PA-O3A
15	B	601	ADP	O4'-C4'-C5'-O5'
15	C	601	ADP	C5'-O5'-PA-O1A
15	E	501	ADP	C5'-O5'-PA-O1A

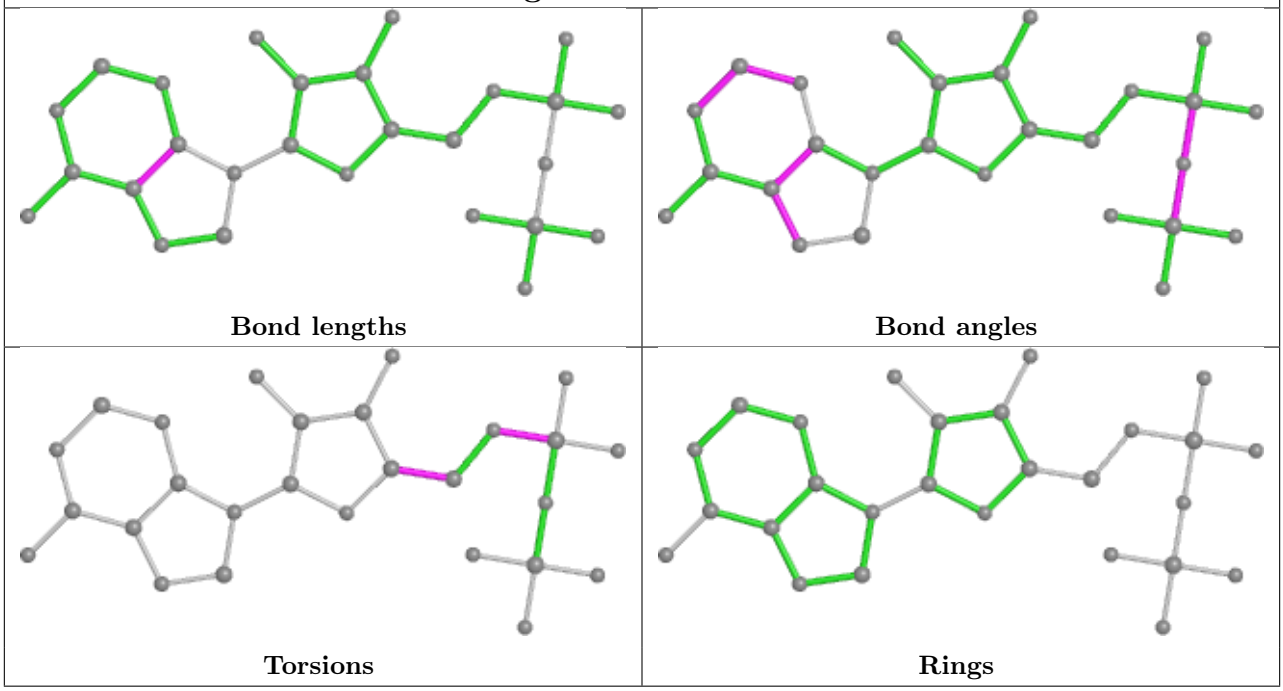
There are no ring outliers.

3 monomers are involved in 12 short contacts:

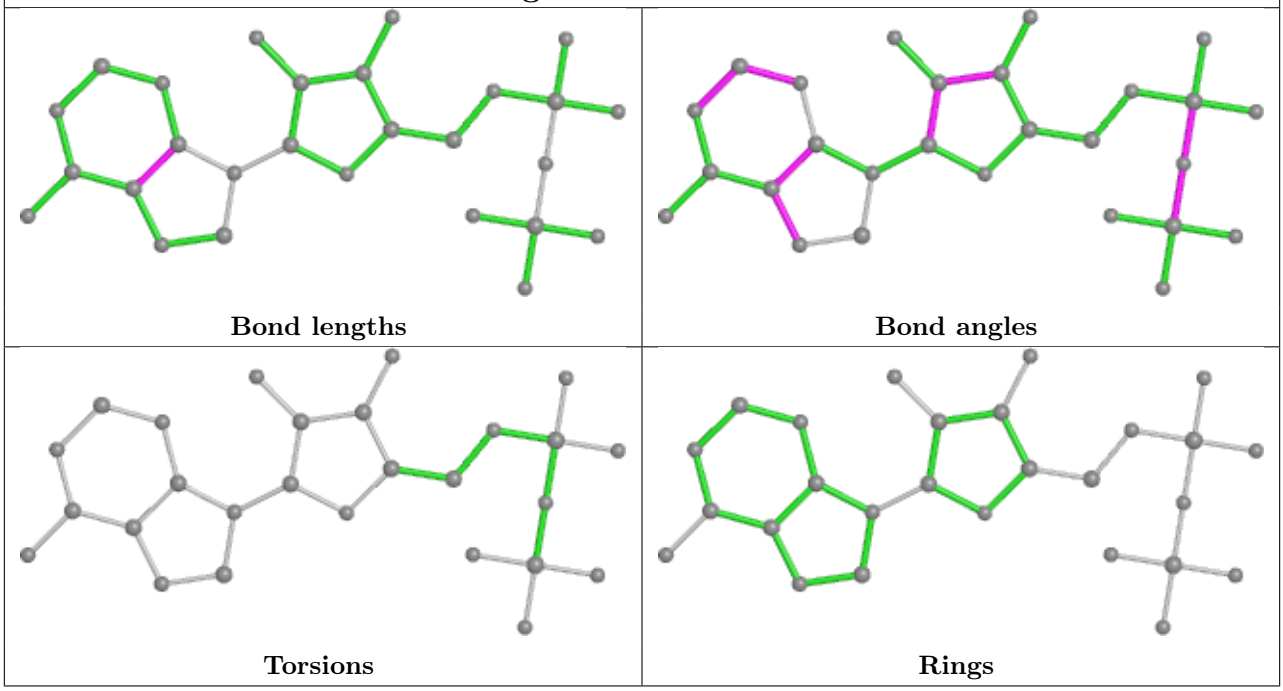
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	E	501	ADP	7	0
15	F	600	ADP	3	0
15	B	601	ADP	2	0

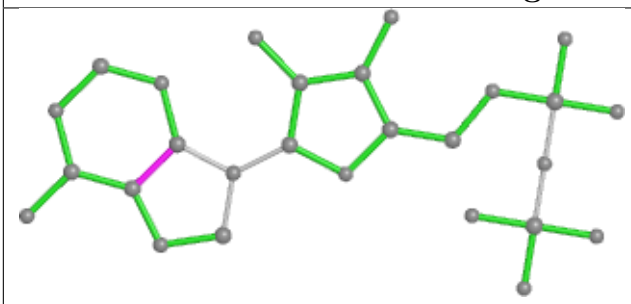
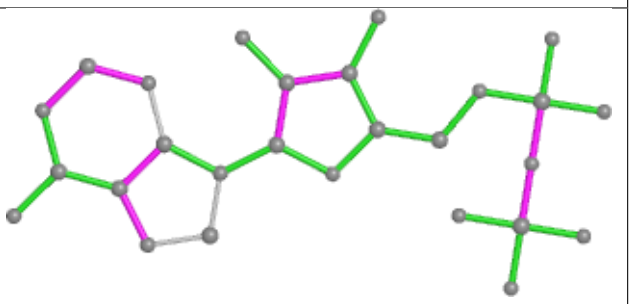
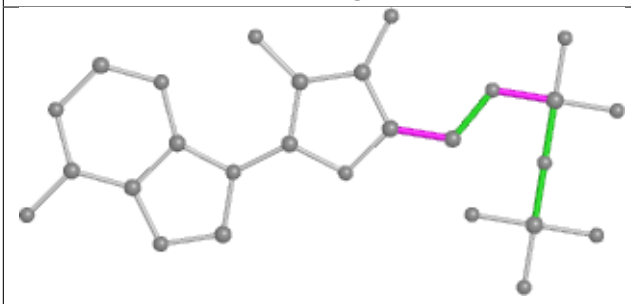
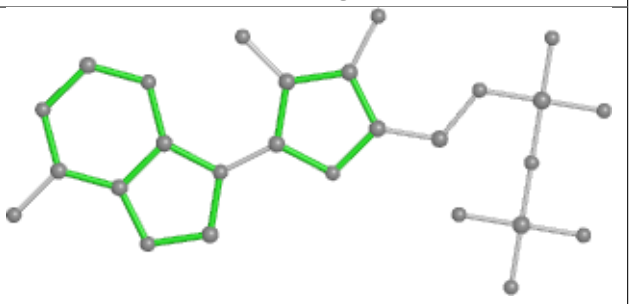
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

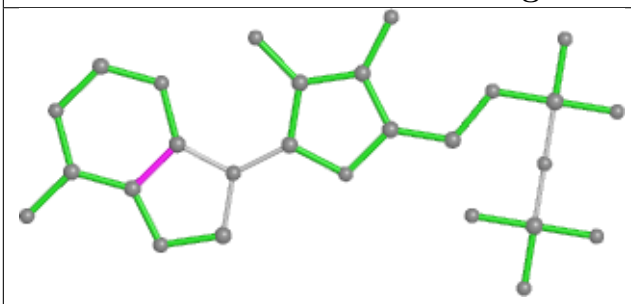
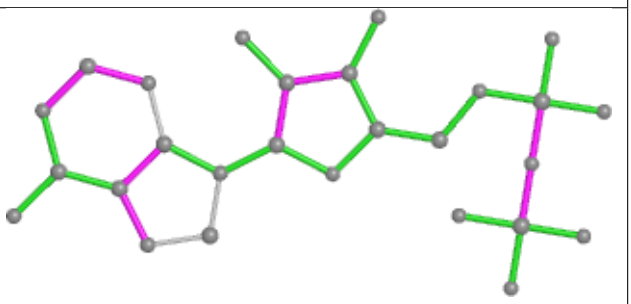
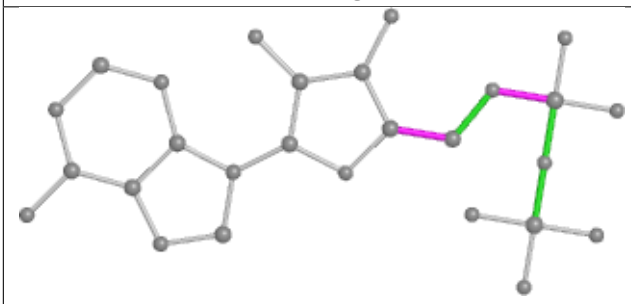
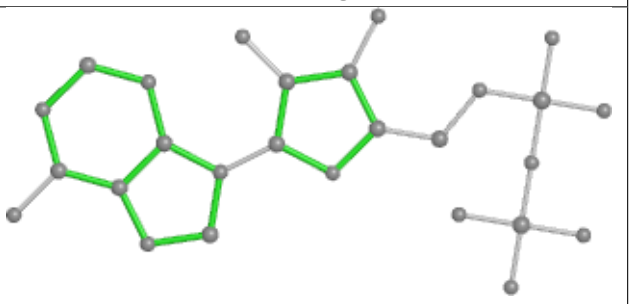
Ligand ADP E 501

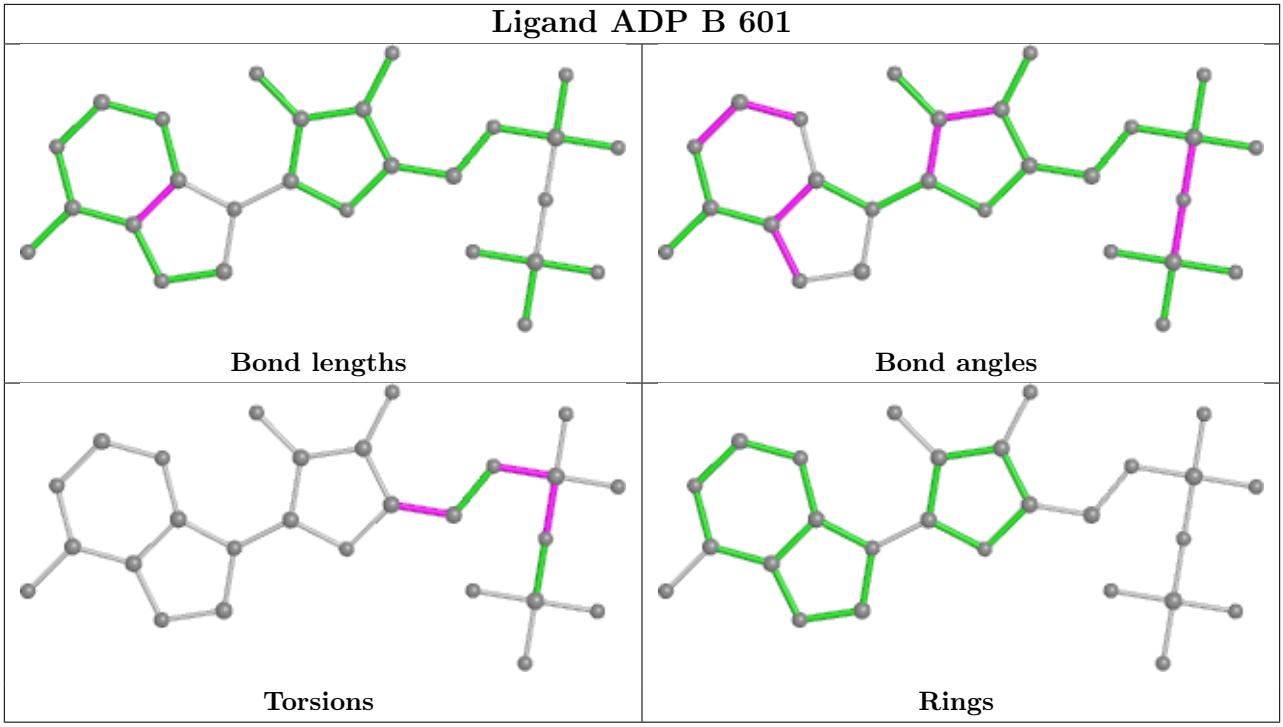


Ligand ADP A 601



Ligand ADP F 600	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP C 601	
 Bond lengths	 Bond angles
 Torsions	 Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	61:ASP	C	71:LYS	N	12.83

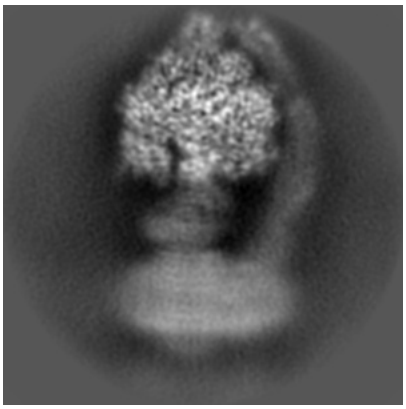
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-28835. These allow visual inspection of the internal detail of the map and identification of artifacts.

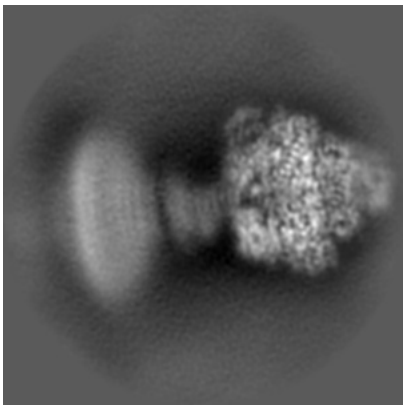
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

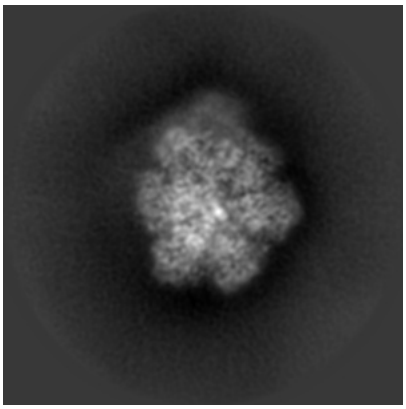
6.1.1 Primary map



X

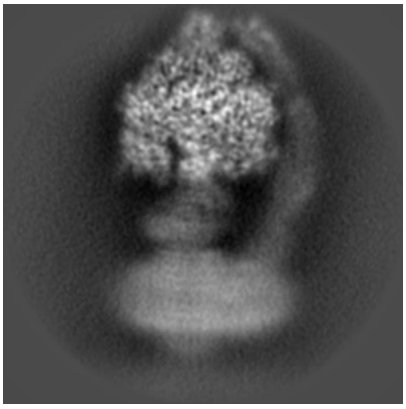


Y

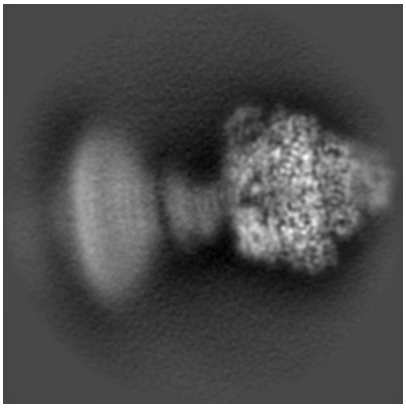


Z

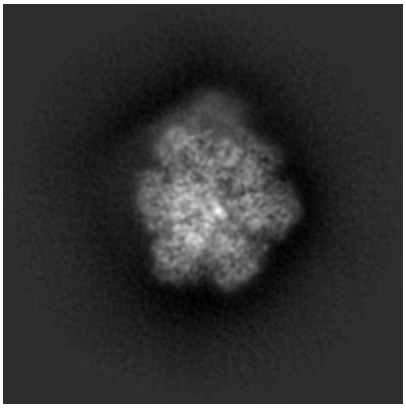
6.1.2 Raw map



X



Y

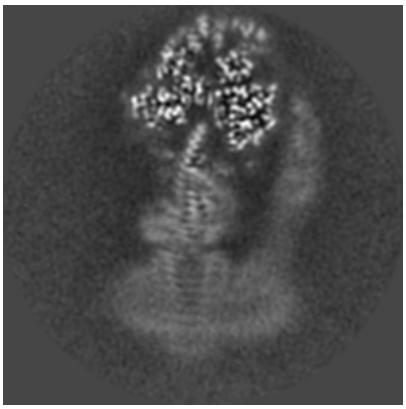


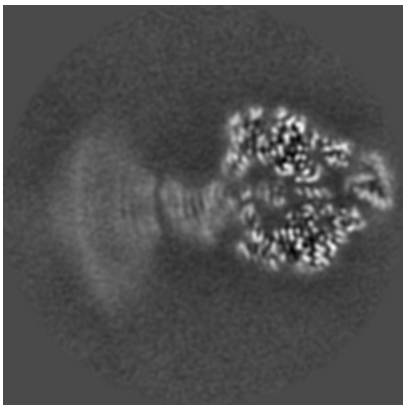
Z

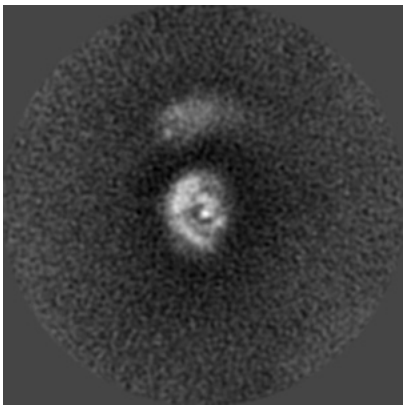
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

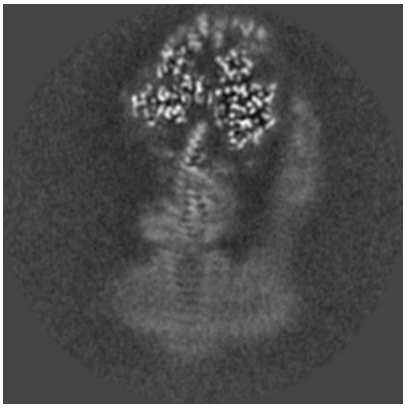
6.2.1 Primary map

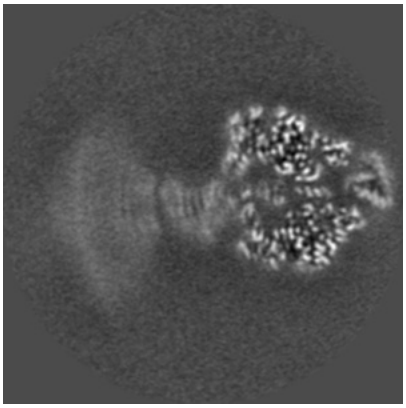

X Index: 128

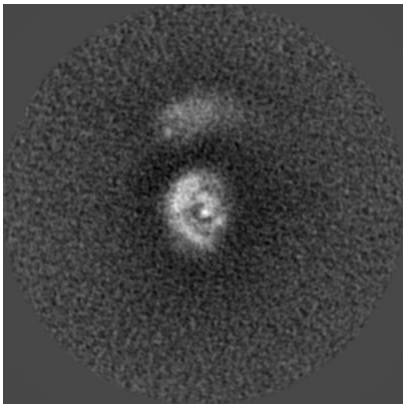

Y Index: 128


Z Index: 128

6.2.2 Raw map


X Index: 128

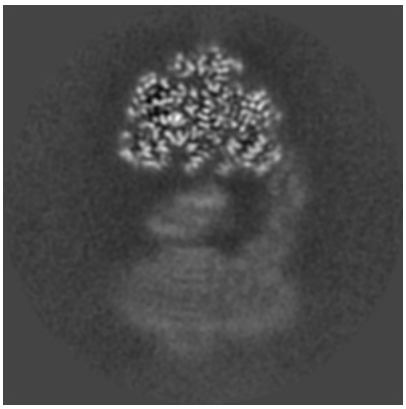

Y Index: 128

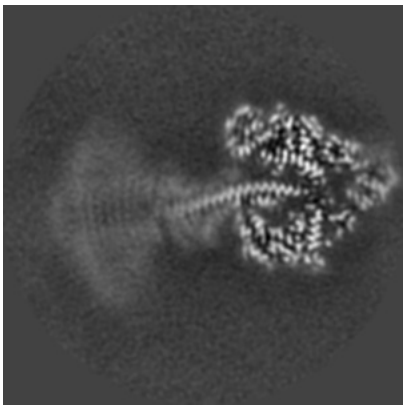

Z Index: 128

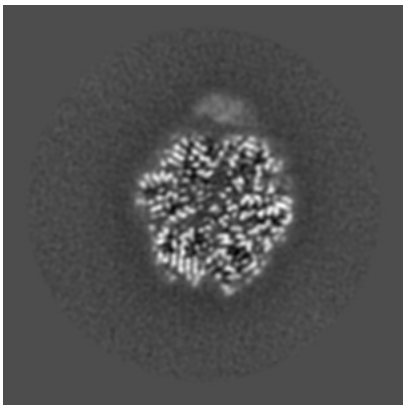
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

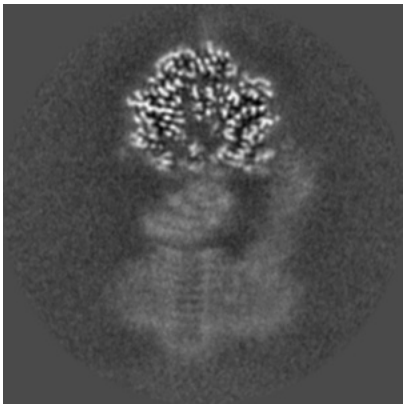
6.3.1 Primary map

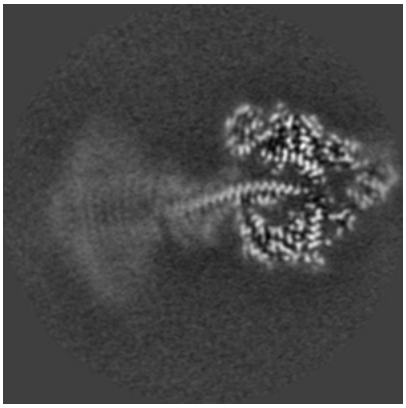

X Index: 111

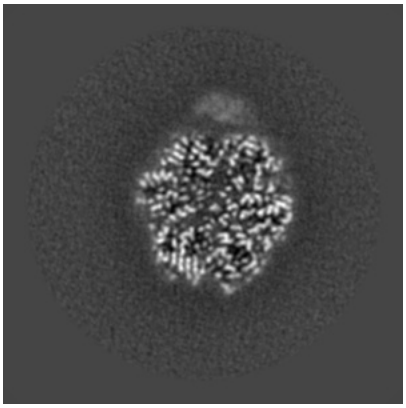

Y Index: 122


Z Index: 191

6.3.2 Raw map


X Index: 118

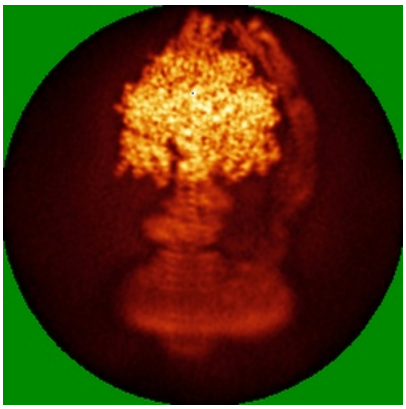

Y Index: 122

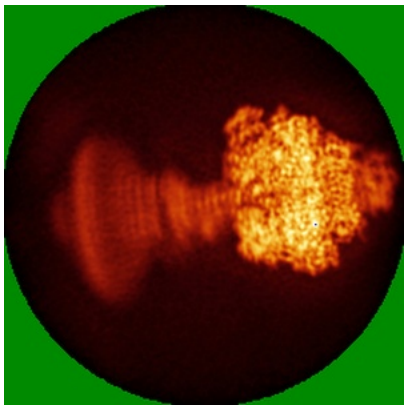

Z Index: 191

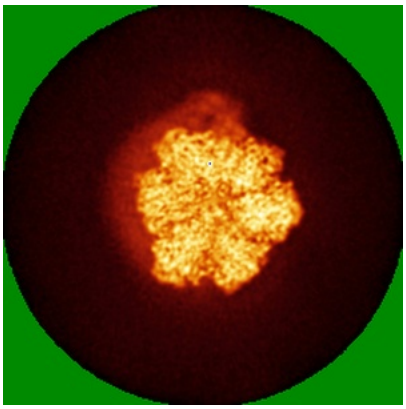
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

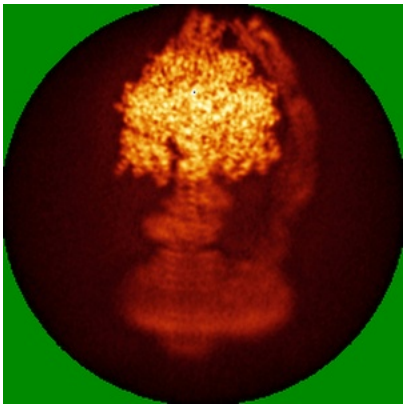
6.4.1 Primary map

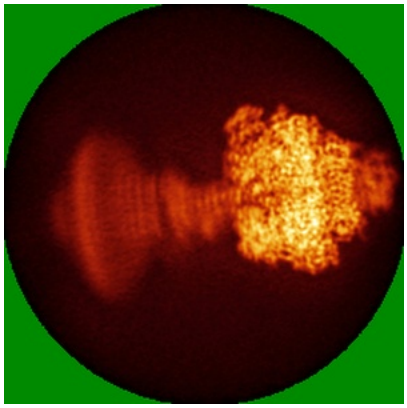

X

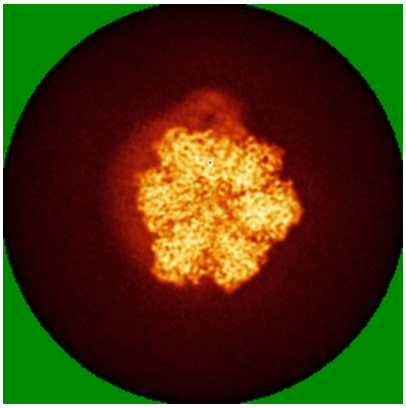

Y


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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.009. 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

X Y Z

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.

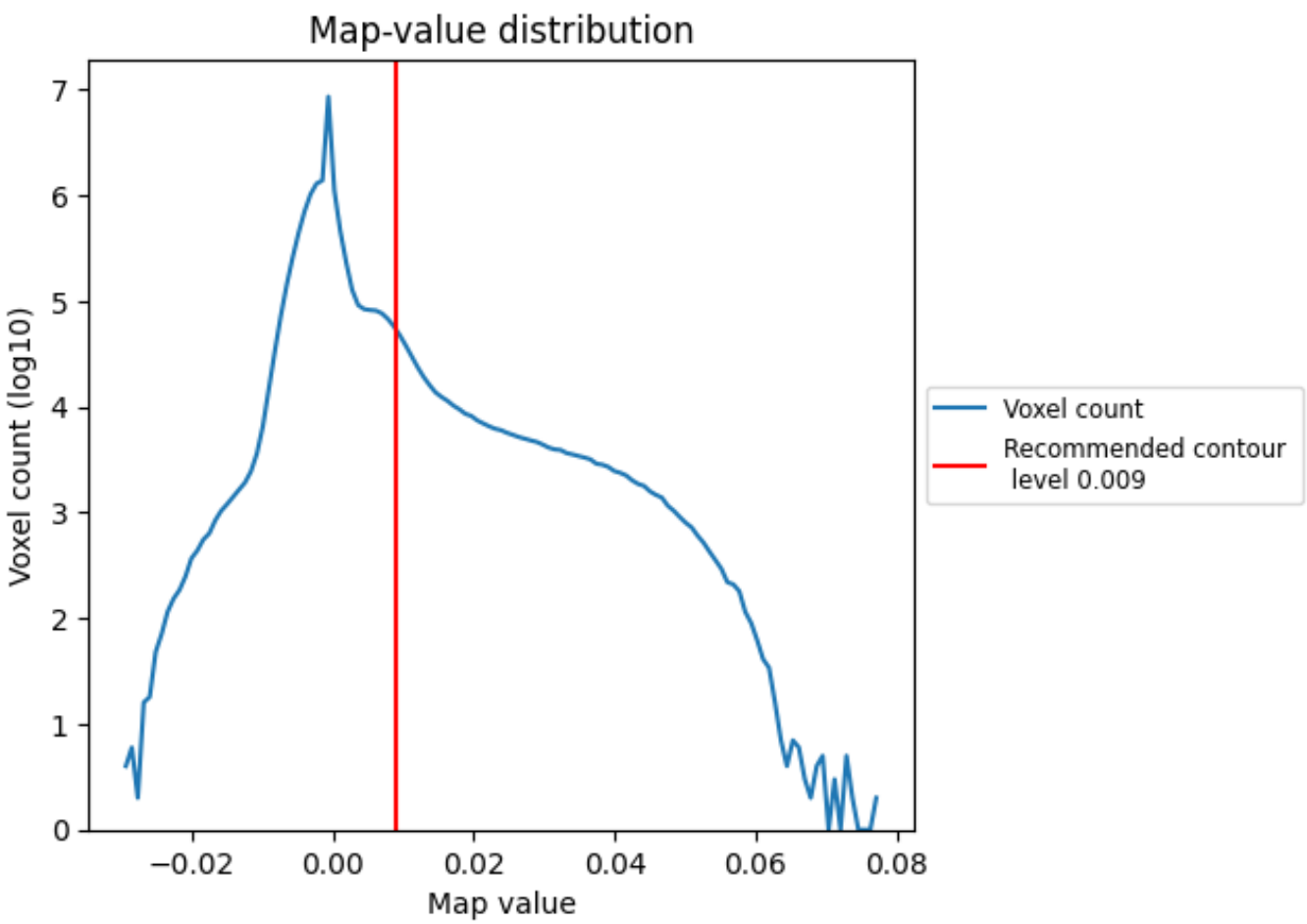
6.6 Mask visualisation (i)

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

7 Map analysis (i)

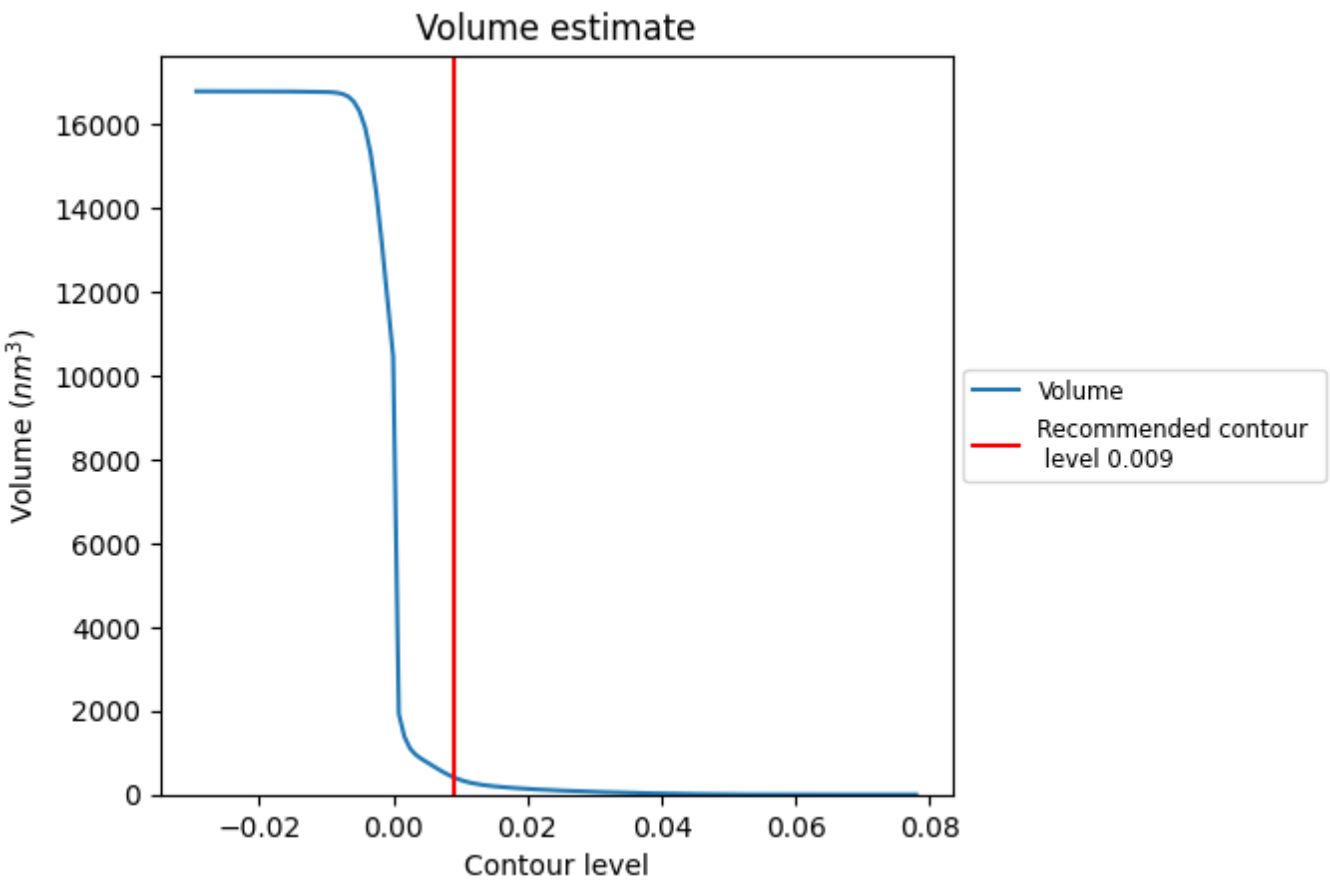
This section contains the results of statistical analysis of the map.

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.

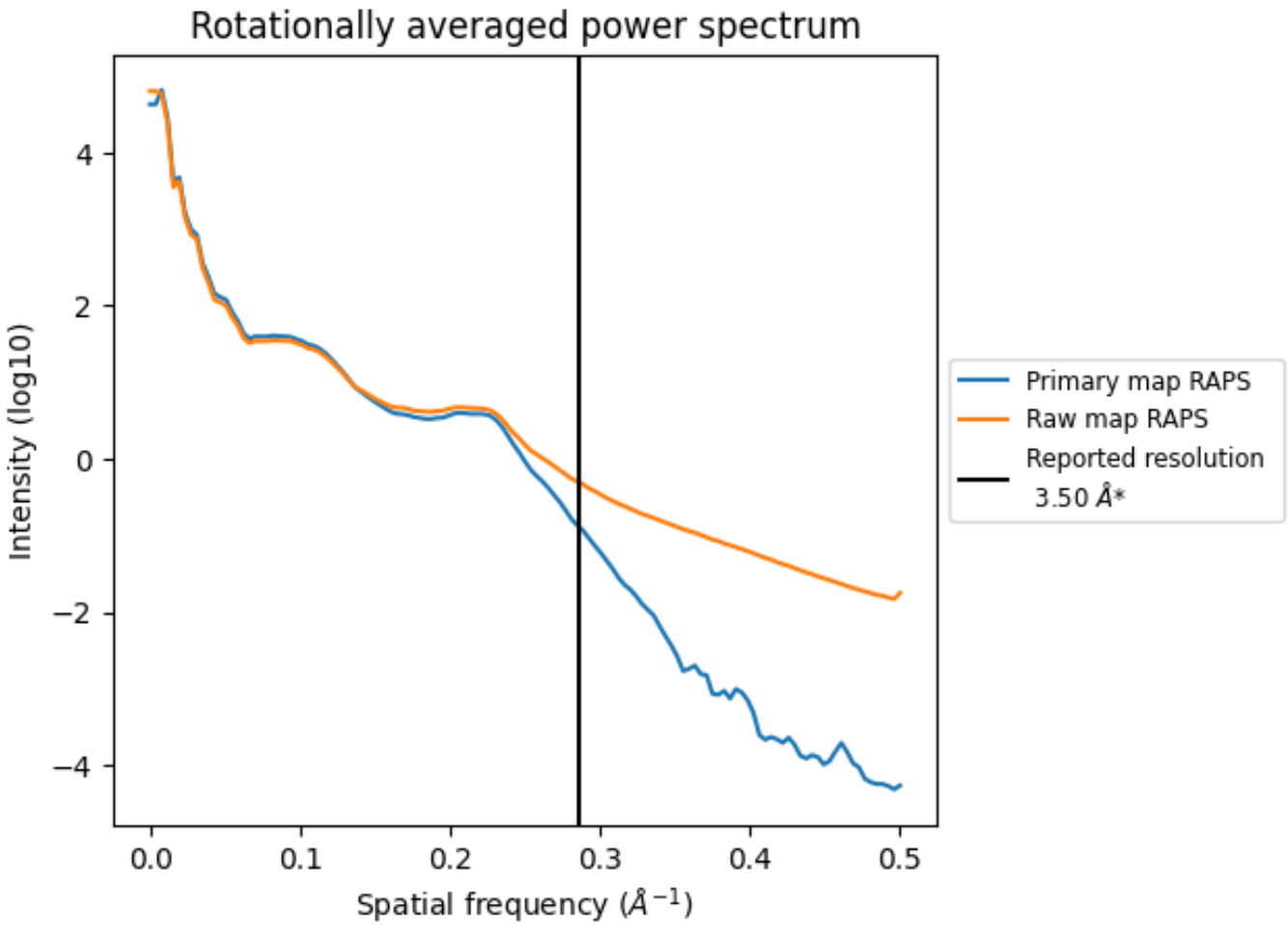
7.2 Volume estimate (i)



The volume at the recommended contour level is 414 nm^3; this corresponds to an approximate mass of 374 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)

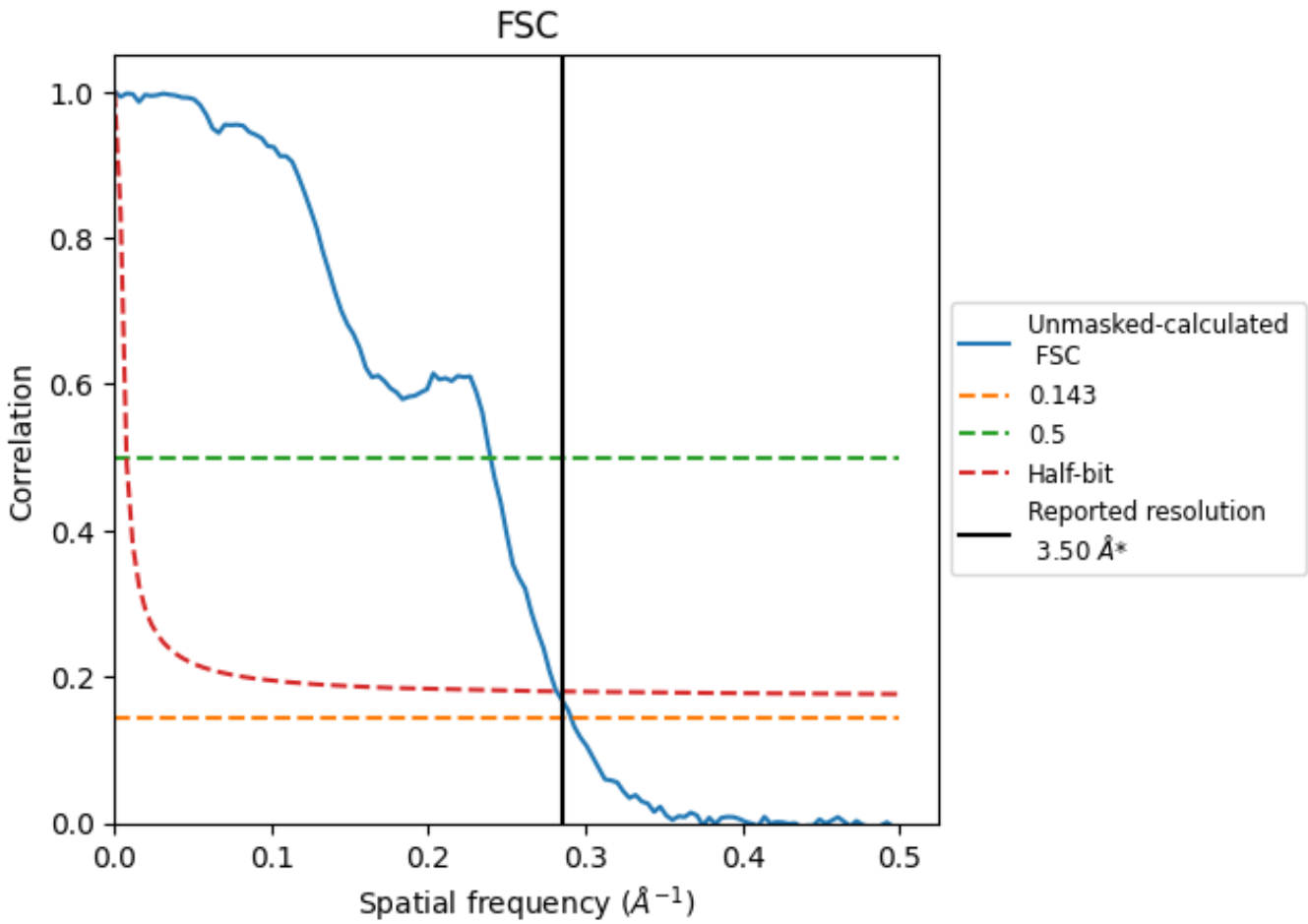


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8.2 Resolution estimates (i)

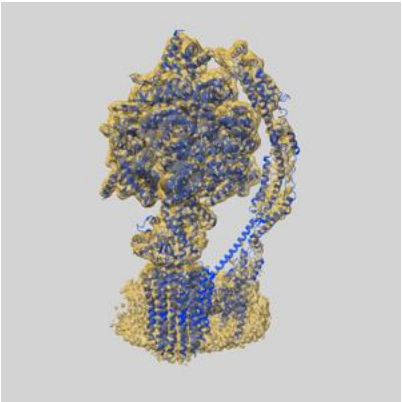
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.44	4.18	3.55

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

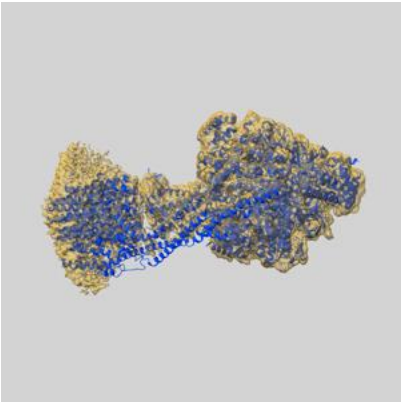
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-28835 and PDB model 8F39. Per-residue inclusion information can be found in section 3 on page 8.

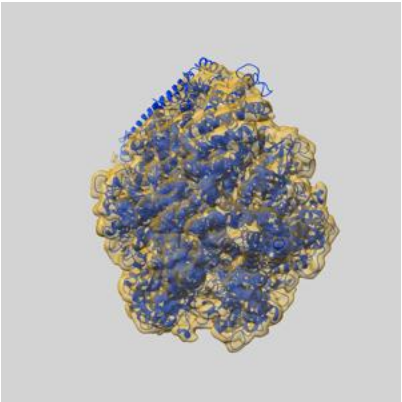
9.1 Map-model overlay (i)



X



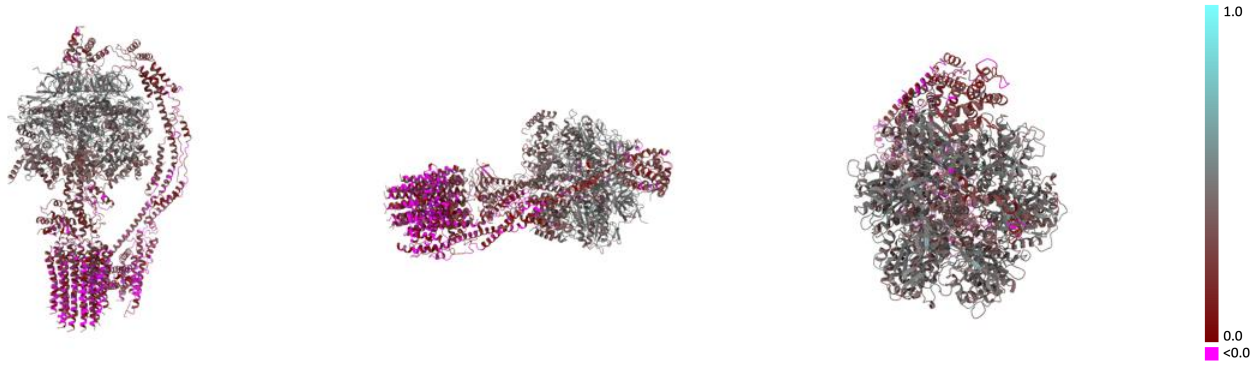
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.009 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.

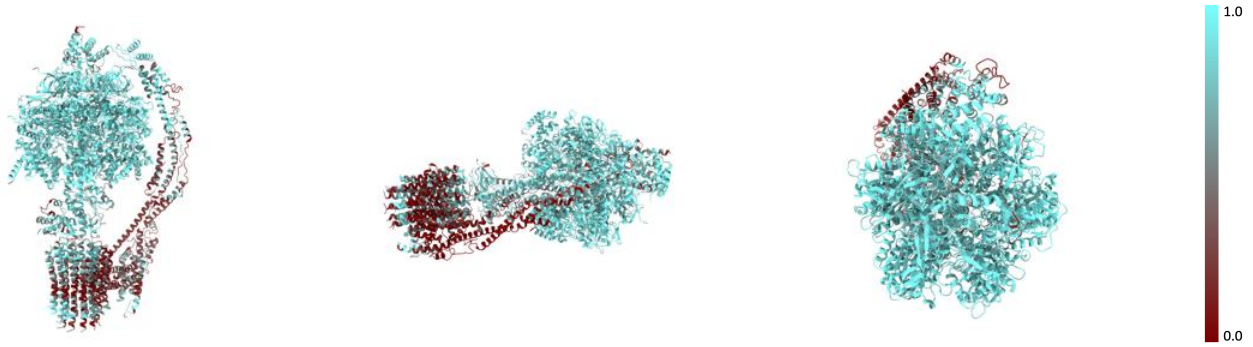
9.2 Q-score mapped to coordinate model (i)



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.

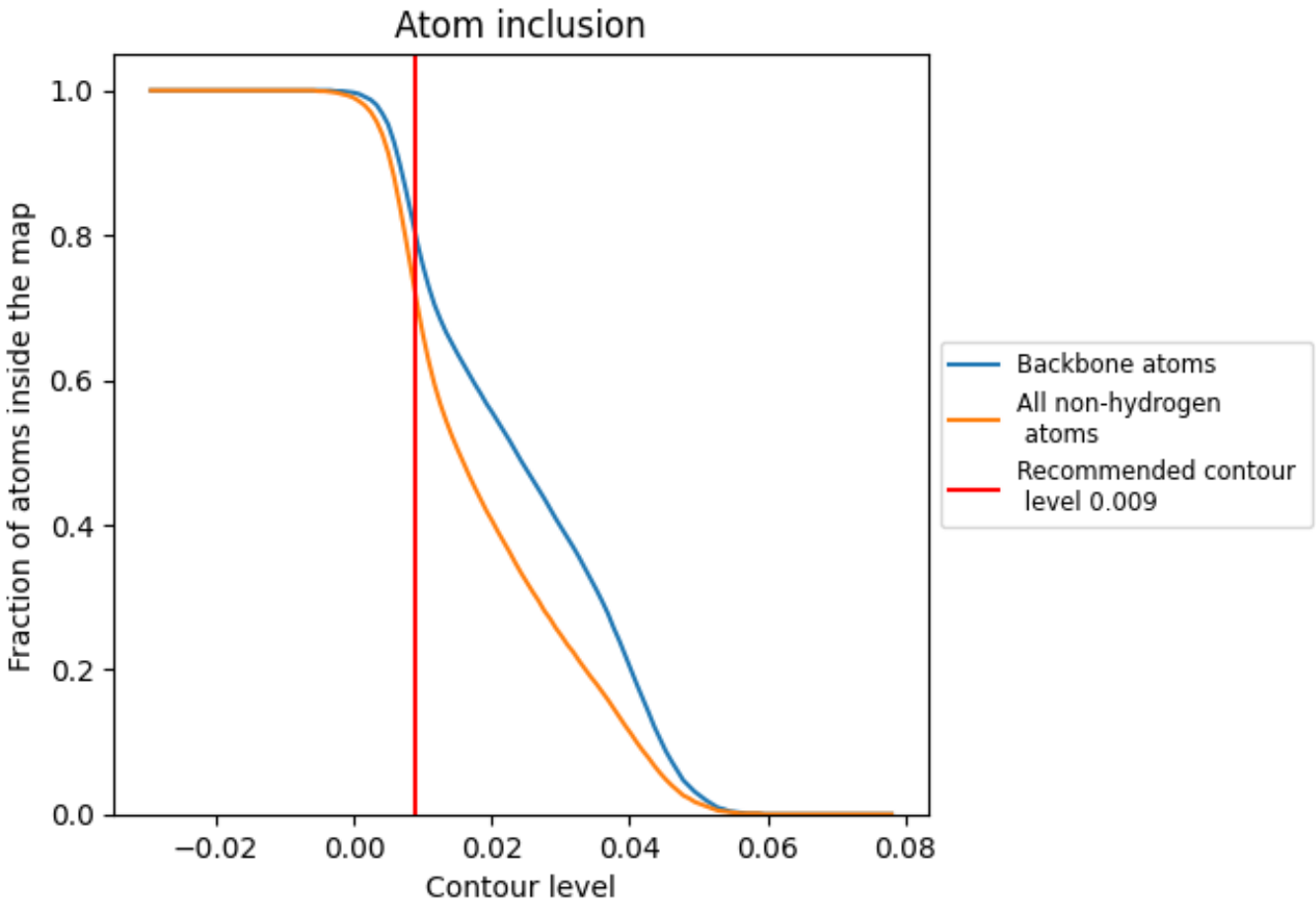
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.009).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7170	0.3010
6	0.3860	0.1050
7	0.2030	0.1580
8	0.3610	0.0320
A	0.8930	0.4080
B	0.8630	0.4050
C	0.8950	0.4300
D	0.8860	0.4220
E	0.8810	0.4370
F	0.8850	0.4350
G	0.8070	0.2230
H	0.7490	0.1720
I	0.6530	0.1540
J	0.3780	0.0110
K	0.4940	0.1190
L	0.5450	0.0780
M	0.6430	0.1090
N	0.4830	0.0850
O	0.4490	0.1050
P	0.3390	0.0490
Q	0.3380	0.0550
R	0.3170	0.0700
S	0.3530	0.0830
T	0.4170	0.0840
U	0.2370	0.0860
X	0.2750	0.0710
Y	0.8410	0.2840
Z	0.4450	0.1840