W O R L D W I D E

wwPDB

P R O T E I N D A T A B A N K

wwPDB EM Validation Summary Report (i)

Nov 19, 2022 – 11:27 pm GMT

PDB ID	:	6FKH
EMDB ID	:	EMD-4271
Title	:	Chloroplast F1Fo conformation 2
Authors	:	Hahn, A.; Vonck, J.; Mills, D.J.; Meier, T.; Kuehlbrandt, W.
Deposited on	:	2018-01-24
Resolution	:	4.20 Å(reported)

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 4.20 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	Percentile Ranks	Value
Ramachandran outliers		0.1%
Sidechain outliers		0.0%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures
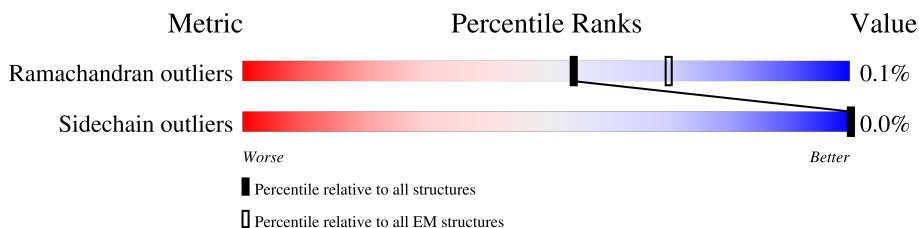
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	247	60% ▬▬▬▬▬ 89% · 10%
2	A	507	5% ▬ 99% ·
2	C	507	· 98% ··
2	E	507	6% ▬ 97% ··
3	B	498	· 96% · ·
3	D	498	· 95% ··
3	F	498	· 95% · ·
4	e	134	23% ▬▬ 98% ·
5	g	364	9% ▬ 87% · 12%

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	G	81	52% ... 96%
6	H	81	62% ... 96%
6	I	81	54% ... 96%
6	J	81	63% ... 96%
6	K	81	52% ... 96%
6	L	81	41% ... 96%
6	M	81	47% ... 96%
6	N	81	56% ... 96%
6	O	81	57% ... 96%
6	P	81	63% ... 96%
6	Q	81	63% ... 96%
6	R	81	70% ... 96%
6	S	81	70% ... 96%
6	T	81	58% ... 96%
7	p	222	42% ... 64% 36%
8	b	184	47% ... 87% 12%
9	d	257	9% 69% 30%

2 Entry composition ⓘ

There are 12 unique types of molecules in this entry. The entry contains 39231 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 a, chloroplastic.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	501	Total	C	N	O	S	0	0
			3851	2423	667	748	13		
2	E	497	Total	C	N	O	S	0	0
			3818	2403	659	743	13		
2	A	502	Total	C	N	O	S	0	0
			3858	2427	668	750	13		

- Molecule 3 is a protein called ATP synthase subunit beta, chloroplastic.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S	79	Total 544	C 355	N 90	O 98	S 1	0	0
6	N	79	Total 544	C 355	N 90	O 98	S 1	0	0
6	O	79	Total 544	C 355	N 90	O 98	S 1	0	0
6	P	79	Total 544	C 355	N 90	O 98	S 1	0	0
6	Q	79	Total 544	C 355	N 90	O 98	S 1	0	0
6	R	79	Total 544	C 355	N 90	O 98	S 1	0	0
6	M	79	Total 544	C 355	N 90	O 98	S 1	0	0
6	T	79	Total 544	C 355	N 90	O 98	S 1	0	0
6	G	79	Total 544	C 355	N 90	O 98	S 1	0	0
6	H	79	Total 544	C 355	N 90	O 98	S 1	0	0
6	L	79	Total 544	C 355	N 90	O 98	S 1	0	0
6	K	79	Total 544	C 355	N 90	O 98	S 1	0	0
6	J	79	Total 544	C 355	N 90	O 98	S 1	0	0
6	I	79	Total 544	C 355	N 90	O 98	S 1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	p	143	Total 1124	C 713	N 182	O 224	S 5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	b	161	Total 1299	C 812	N 236	O 246	S 5	0	0

- Molecule 9 is a protein called ATP synthase delta chain, chloroplastic.

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

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 11 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).
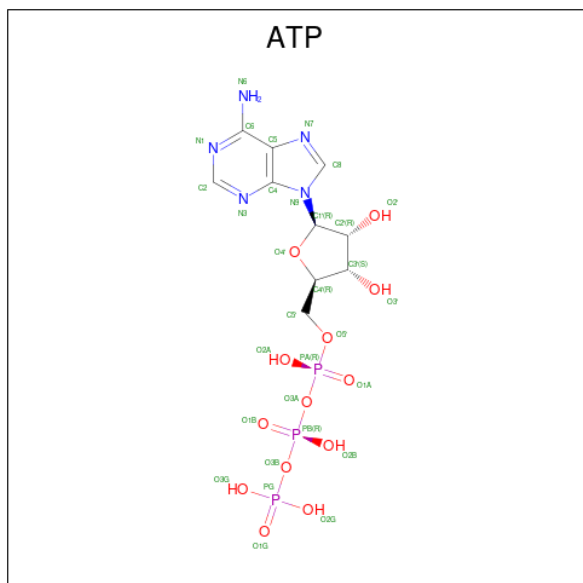
Mol	Chain	Residues	Atoms					AltConf
11	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
11	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
11	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 12 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
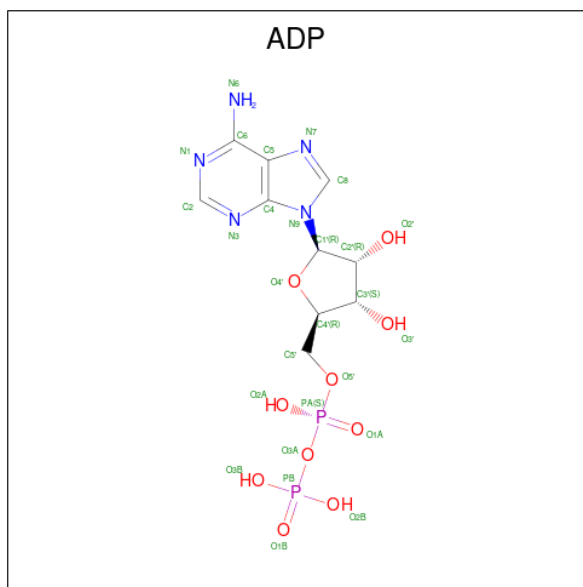
Mol	Chain	Residues	Atoms					AltConf
12	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

3   Residue-property plots ⓘ

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 a, chloroplastic
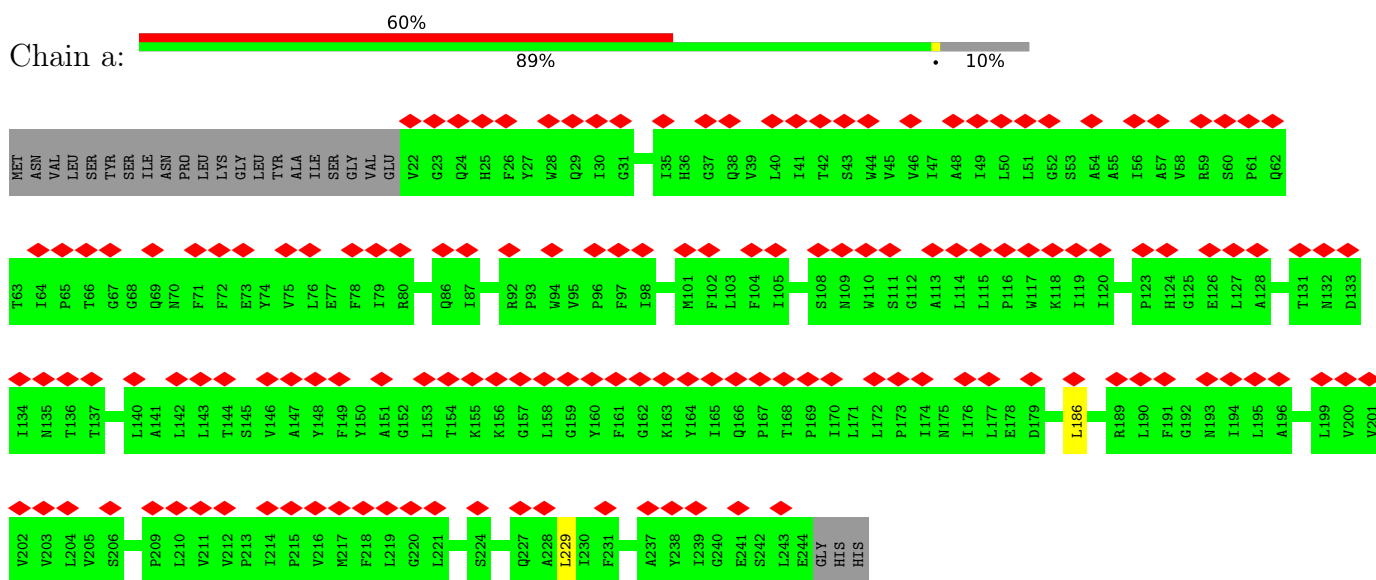
- Molecule 2: ATP synthase subunit alpha, chloroplastic
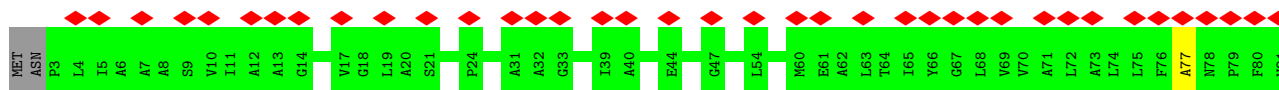

- Molecule 2: ATP synthase subunit alpha, chloroplastic
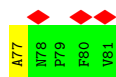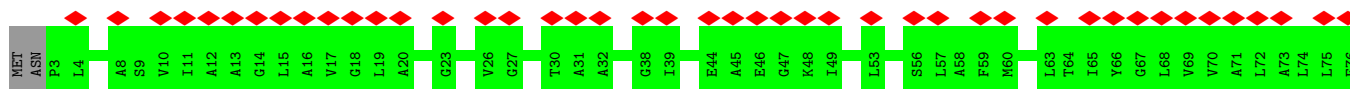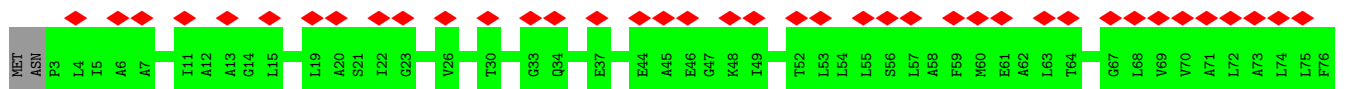
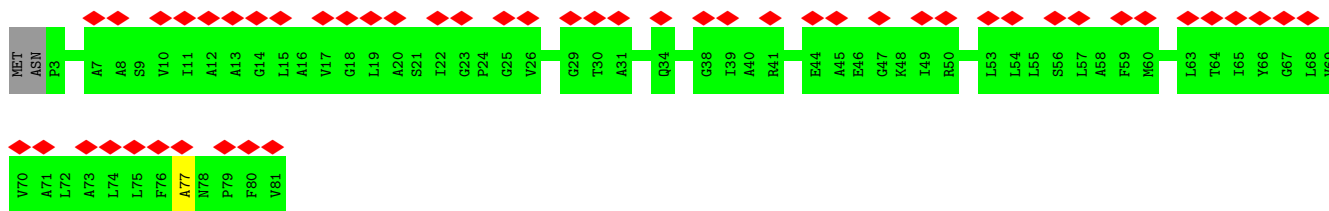- Molecule 2: ATP synthase subunit alpha, chloroplastic

Chain A:

- Molecule 3: ATP synthase subunit beta, chloroplastic
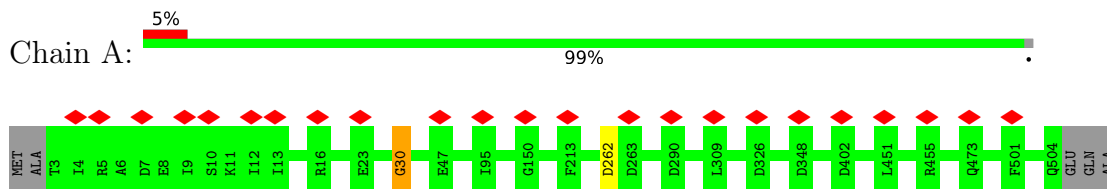
Chain D:
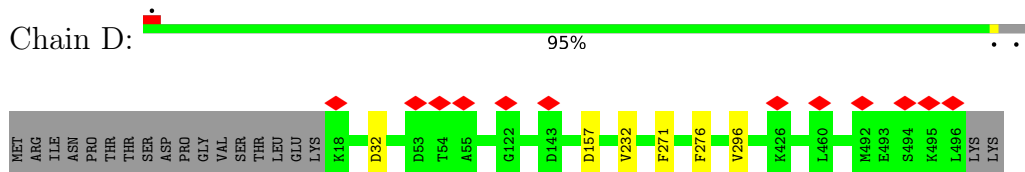
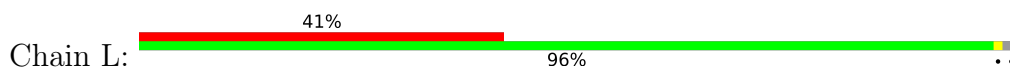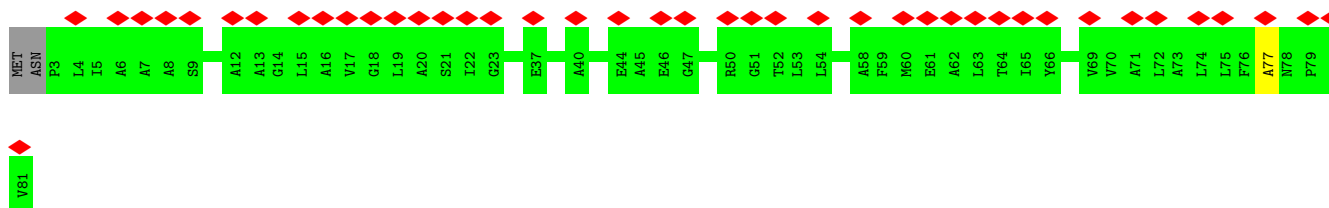- Molecule 3: ATP synthase subunit beta, chloroplastic
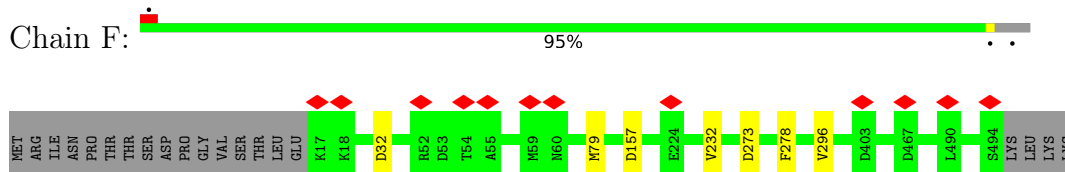
Chain F:

- Molecule 3: ATP synthase subunit beta, chloroplastic
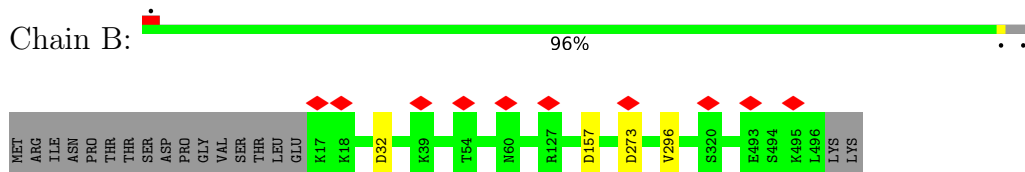
Chain B:

- Molecule 4: ATP synthase epsilon chain, chloroplastic
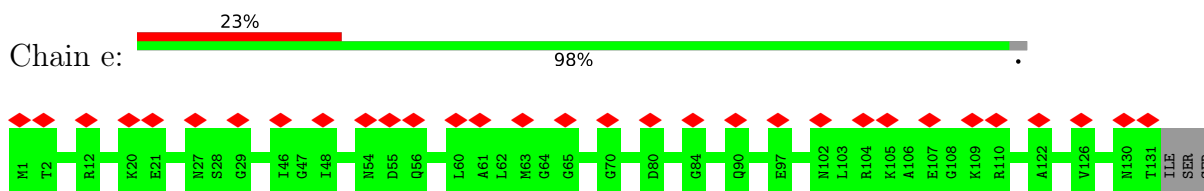
Chain e:

- Molecule 5: ATP synthase gamma chain, chloroplastic

Chain g:

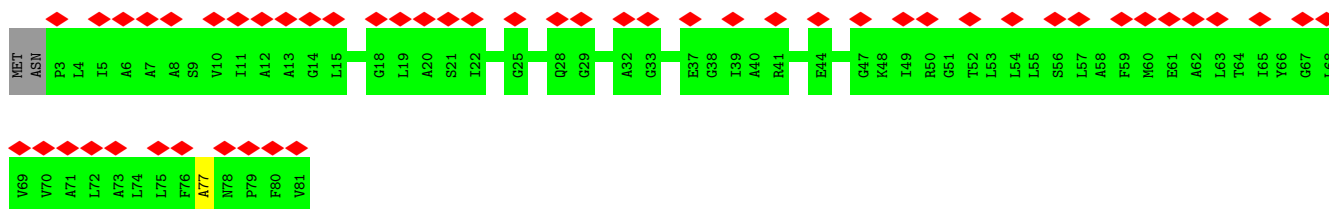- Molecule 6: ATP synthase subunit c, chloroplastic

Chain S:

70%

96%

MET ASN P3 L4 I5 A6 A7 A8 S9 V10 I11 A12 A13 G14 L15 A16 V17 G18 L19 A20 S21 I22 G23 V26 G27 Q28 Q29 T30 A31 A32 A35 V36 A40 R41 E44 A45 E46 I49 R50 G51 T52 L53 L54 L55 S56 L57 A58 F59 M60 E61 A62 L63 T64 I65 Y66

G67 L68 V69 V70 A71 L72 A73 L74 L75 F76 A77 N78 P79 F80 V81

• Molecule 6: ATP synthase subunit c, chloroplastic

Chain N:

56%

96%

MET ASN P3 L4 I5 A6 A7 A8 S9 V10 I11 A12 A13 G14 L15 A16 V17 G18 L19 A20 S21 P24 G25 Q28 Q29 T30 A31 A32 I39 A40 R41 E44 G47 G51 T52 L53 L54 A58 F59 M60 E61 A62 L63 T64 I65 L68 V69 V70 A71 L72 A73 L74

L75 F76 A77 N78 P79 F80 V81

• Molecule 6: ATP synthase subunit c, chloroplastic

Chain O:

57%

96%

MET ASN P3 L4 I5 A6 A7 V10 I11 A12 A13 G14 L15 A16 V17 G18 L19 A20 S21 I22 G23 P24 Q28 I39 A40 R41 Q42 P43 E44 A45 E46 G47 K48 I49 R50 G51 L54 L55 S56 L57 A58 F59 M60 E61 A62 L63 Y66 G67 L68 V69 V70 A71 L72 A73 L74

L75 F76 A77 N78 P79 F80 V81

• Molecule 6: ATP synthase subunit c, chloroplastic

Chain P:

63%

96%

MET ASN P3 L4 I5 A6 A7 A8 S9 V10 I11 A12 A13 G14 L15 A16 V17 G18 L19 A20 S21 I22 G27 Q28 Q34 A35 I39 A40 R41 Q42 P43 E44 A45 E46 G47 K48 G51 T52 L53 L54 L55 S56 L57 A58 E61 A62 L63 T64 I65 Y66 G67 L68 V69 V70 A71

L72 A73 L74 L75 F76 A77 N78 P79 F80 V81

• Molecule 6: ATP synthase subunit c, chloroplastic

Chain Q:

63%

96%

MET ASN P3 L4 I5 A6 A7 A8 S9 V10 I11 A12 A13 G14 L15 A16 V17 G18 L19 A20 S21 I22 G23 V26 G27 Q28 Q29 T30 A31 A32 G33 Q34 A35 I39 Q42 P43 E44 A45 E46 G47 K48 I49 T52 L53 S56 F59 M60 L63 T64 I65 Y66 G67 L68

• Molecule 6: ATP synthase subunit c, chloroplastic

Chain R:

• Molecule 6: ATP synthase subunit c, chloroplastic

Chain M:

• Molecule 6: ATP synthase subunit c, chloroplastic

Chain T:

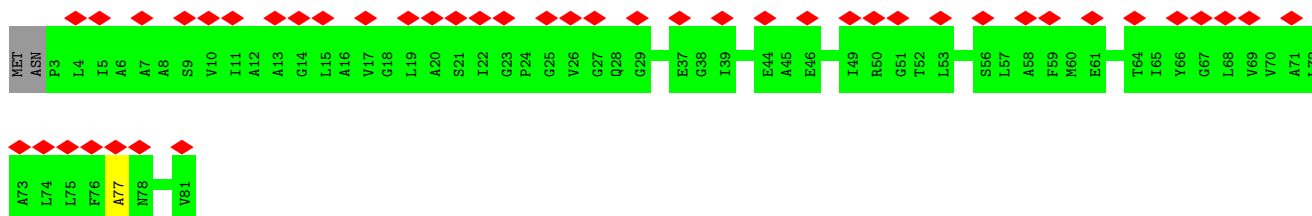• Molecule 6: ATP synthase subunit c, chloroplastic

Chain G:

• Molecule 6: ATP synthase subunit c, chloroplastic

Chain H:

- Molecule 6: ATP synthase subunit c, chloroplastic

Chain L:

- Molecule 6: ATP synthase subunit c, chloroplastic

Chain K:

- Molecule 6: ATP synthase subunit c, chloroplastic

Chain J:

- Molecule 6: ATP synthase subunit c, chloroplastic

Chain I:

- Molecule 7: ATP synthase subunit b', chloroplastic

Chain p:

• Molecule 8: ATP synthase subunit b, chloroplastic

Chain b:

• Molecule 9: ATP synthase delta chain, chloroplastic

Chain d:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	15395	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/Å^2)$	25	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	132953	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.270	Depositor
Minimum map value	-0.181	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	368.55, 368.55, 368.55	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.053, 1.053, 1.053	Depositor

5   Model quality ⓘ

5.1   Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z| > 5$	RMSZ	#$|Z| > 5$
1	a	0.47	0/1792	0.71	2/2454 (0.1%)
2	A	0.77	1/3907 (0.0%)	0.72	1/5286 (0.0%)
2	C	0.78	1/3900 (0.0%)	0.75	5/5276 (0.1%)
2	E	0.77	1/3867 (0.0%)	0.80	4/5232 (0.1%)
3	B	0.74	0/3693	0.69	2/5005 (0.0%)
3	D	0.80	2/3684 (0.1%)	0.74	3/4994 (0.1%)
3	F	0.71	0/3676	0.71	5/4983 (0.1%)
4	e	0.43	0/1019	0.65	0/1381
5	g	0.56	1/2526 (0.0%)	0.69	4/3412 (0.1%)
6	G	0.36	0/551	0.59	0/750
6	H	0.36	0/551	0.59	0/750
6	I	0.36	0/551	0.59	0/750
6	J	0.36	0/551	0.59	0/750
6	K	0.36	0/551	0.59	0/750
6	L	0.36	0/551	0.59	0/750
6	M	0.36	0/551	0.59	0/750
6	N	0.36	0/551	0.59	0/750
6	O	0.36	0/551	0.59	0/750
6	P	0.36	0/551	0.59	0/750
6	Q	0.36	0/551	0.59	0/750
6	R	0.36	0/551	0.59	0/750
6	S	0.36	0/551	0.59	0/750
6	T	0.36	0/551	0.59	0/750
7	p	0.41	1/1134 (0.1%)	0.63	2/1519 (0.1%)
8	b	0.32	0/1309	0.55	1/1754 (0.1%)
9	d	0.43	0/1399	0.59	0/1898
All	All	0.64	7/39620 (0.0%)	0.69	29/53694 (0.1%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	2
2	C	0	2
2	E	0	2
3	B	0	1
6	G	0	1
6	H	0	1
6	I	0	1
6	J	0	1
6	K	0	1
6	L	0	1
6	M	0	1
6	N	0	1
6	O	0	1
6	P	0	1
6	Q	0	1
6	R	0	1
6	S	0	1
6	T	0	1
7	p	0	1
8	b	0	1
All	All	0	23

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	30	GLY	C-N	17.17	1.73	1.34
3	D	276	PHE	C-N	-15.91	0.97	1.34
2	E	30	GLY	C-N	13.02	1.64	1.34
5	g	84	PRO	N-CD	12.70	1.65	1.47
2	A	30	GLY	C-N	10.56	1.58	1.34

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	30	GLY	O-C-N	20.02	154.73	122.70
2	E	30	GLY	CA-C-N	-16.40	81.12	117.20
2	C	30	GLY	O-C-N	-15.11	98.52	122.70
2	E	30	GLY	C-N-CA	-14.64	85.10	121.70
2	C	30	GLY	CA-C-N	9.81	138.78	117.20

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	30	GLY	Mainchain
2	C	10	SER	Peptide
2	C	262	ASP	Peptide
2	E	226	ALA	Peptide
2	E	262	ASP	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	221/247 (90%)	211 (96%)	10 (4%)	0	100	100
2	A	500/507 (99%)	483 (97%)	17 (3%)	0	100	100
2	C	499/507 (98%)	483 (97%)	16 (3%)	0	100	100
2	E	495/507 (98%)	480 (97%)	15 (3%)	0	100	100
3	B	478/498 (96%)	463 (97%)	14 (3%)	1 (0%)	47	80
3	D	477/498 (96%)	463 (97%)	13 (3%)	1 (0%)	47	80
3	F	476/498 (96%)	445 (94%)	30 (6%)	1 (0%)	47	80
4	e	129/134 (96%)	122 (95%)	7 (5%)	0	100	100
5	g	319/364 (88%)	306 (96%)	13 (4%)	0	100	100
6	G	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
6	H	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
6	I	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
6	J	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
6	K	77/81 (95%)	74 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	L	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
6	M	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
6	N	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
6	O	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
6	P	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
6	Q	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
6	R	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
6	S	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
6	T	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
7	p	141/222 (64%)	130 (92%)	11 (8%)	0	100	100
8	b	157/184 (85%)	151 (96%)	6 (4%)	0	100	100
9	d	177/257 (69%)	170 (96%)	6 (3%)	1 (1%)	25	64
All	All	5147/5557 (93%)	4943 (96%)	200 (4%)	4 (0%)	54	85

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	d	217	LEU
3	F	296	VAL
3	D	296	VAL
3	B	296	VAL

5.3.2   Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	187/207 (90%)	187 (100%)	0	100	100
2	A	411/414 (99%)	411 (100%)	0	100	100
2	C	410/414 (99%)	410 (100%)	0	100	100
2	E	407/414 (98%)	406 (100%)	1 (0%)	93	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	B	391/408 (96%)	391 (100%)	0	100	100
3	D	390/408 (96%)	390 (100%)	0	100	100
3	F	389/408 (95%)	388 (100%)	1 (0%)	92	95
4	e	109/112 (97%)	109 (100%)	0	100	100
5	g	276/315 (88%)	276 (100%)	0	100	100
6	G	51/53 (96%)	51 (100%)	0	100	100
6	H	51/53 (96%)	51 (100%)	0	100	100
6	I	51/53 (96%)	51 (100%)	0	100	100
6	J	51/53 (96%)	51 (100%)	0	100	100
6	K	51/53 (96%)	51 (100%)	0	100	100
6	L	51/53 (96%)	51 (100%)	0	100	100
6	M	51/53 (96%)	51 (100%)	0	100	100
6	N	51/53 (96%)	51 (100%)	0	100	100
6	O	51/53 (96%)	51 (100%)	0	100	100
6	P	51/53 (96%)	51 (100%)	0	100	100
6	Q	51/53 (96%)	51 (100%)	0	100	100
6	R	51/53 (96%)	51 (100%)	0	100	100
6	S	51/53 (96%)	51 (100%)	0	100	100
6	T	51/53 (96%)	51 (100%)	0	100	100
7	p	124/197 (63%)	124 (100%)	0	100	100
8	b	142/161 (88%)	142 (100%)	0	100	100
9	d	156/220 (71%)	156 (100%)	0	100	100
All	All	4106/4420 (93%)	4104 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	165	ARG
3	F	278	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	187	GLN
9	d	141	HIS
5	g	228	HIS
8	b	165	HIS
6	K	42	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 ⓘ

Of 10 ligands modelled in this entry, 5 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	#$|Z| > 2$
12	ADP	F	600	10	24,29,29	1.09	1 (4%)	29,45,45	1.48	4 (13%)
12	ADP	B	501	10	24,29,29	1.32	3 (12%)	29,45,45	1.48	4 (13%)
11	ATP	E	600	10	26,33,33	1.07	1 (3%)	31,52,52	1.36	4 (12%)
11	ATP	C	602	10	26,33,33	1.20	3 (11%)	31,52,52	1.53	7 (22%)
11	ATP	A	600	10	26,33,33	0.96	1 (3%)	31,52,52	1.52	6 (19%)

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
12	ADP	F	600	10	-	5/12/32/32	0/3/3/3
12	ADP	B	501	10	-	5/12/32/32	0/3/3/3
11	ATP	E	600	10	-	3/18/38/38	0/3/3/3
11	ATP	C	602	10	-	4/18/38/38	0/3/3/3
11	ATP	A	600	10	-	0/18/38/38	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	501	ADP	C2'-C1'	-2.73	1.49	1.53
11	C	602	ATP	C2'-C1'	-2.57	1.49	1.53
12	F	600	ADP	C2'-C1'	-2.35	1.50	1.53
12	B	501	ADP	PB-O3B	-2.24	1.46	1.54
11	C	602	ATP	PG-O2G	-2.18	1.46	1.54

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	602	ATP	N3-C2-N1	-3.95	122.51	128.68
12	B	501	ADP	N3-C2-N1	-3.86	122.64	128.68
11	E	600	ATP	N3-C2-N1	-3.47	123.25	128.68
11	A	600	ATP	N3-C2-N1	-3.46	123.26	128.68
12	F	600	ADP	C3'-C2'-C1'	3.27	105.90	100.98

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	F	600	ADP	C5'-O5'-PA-O2A
12	B	501	ADP	C5'-O5'-PA-O1A
12	B	501	ADP	C5'-O5'-PA-O2A
12	F	600	ADP	O4'-C4'-C5'-O5'
12	F	600	ADP	C3'-C4'-C5'-O5'

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 ADP F 600

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP E 600

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP C 602

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP A 600

Bond lengths	Bond angles
Torsions	Rings
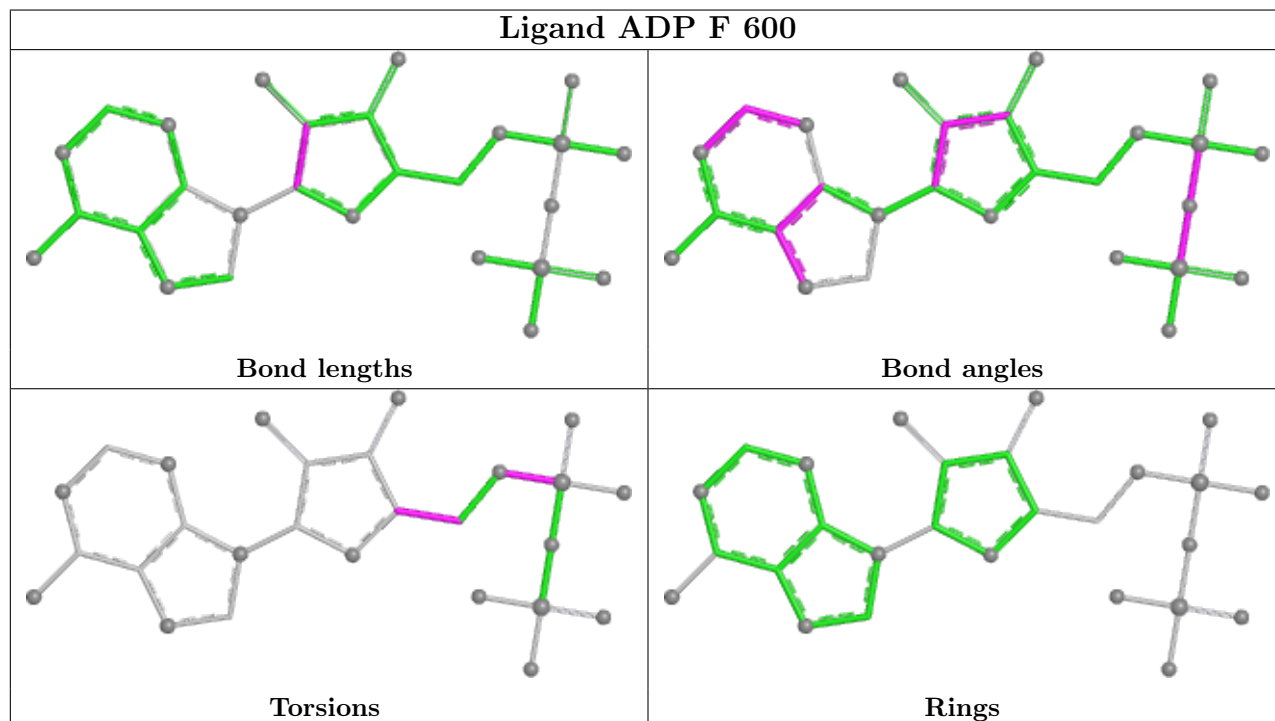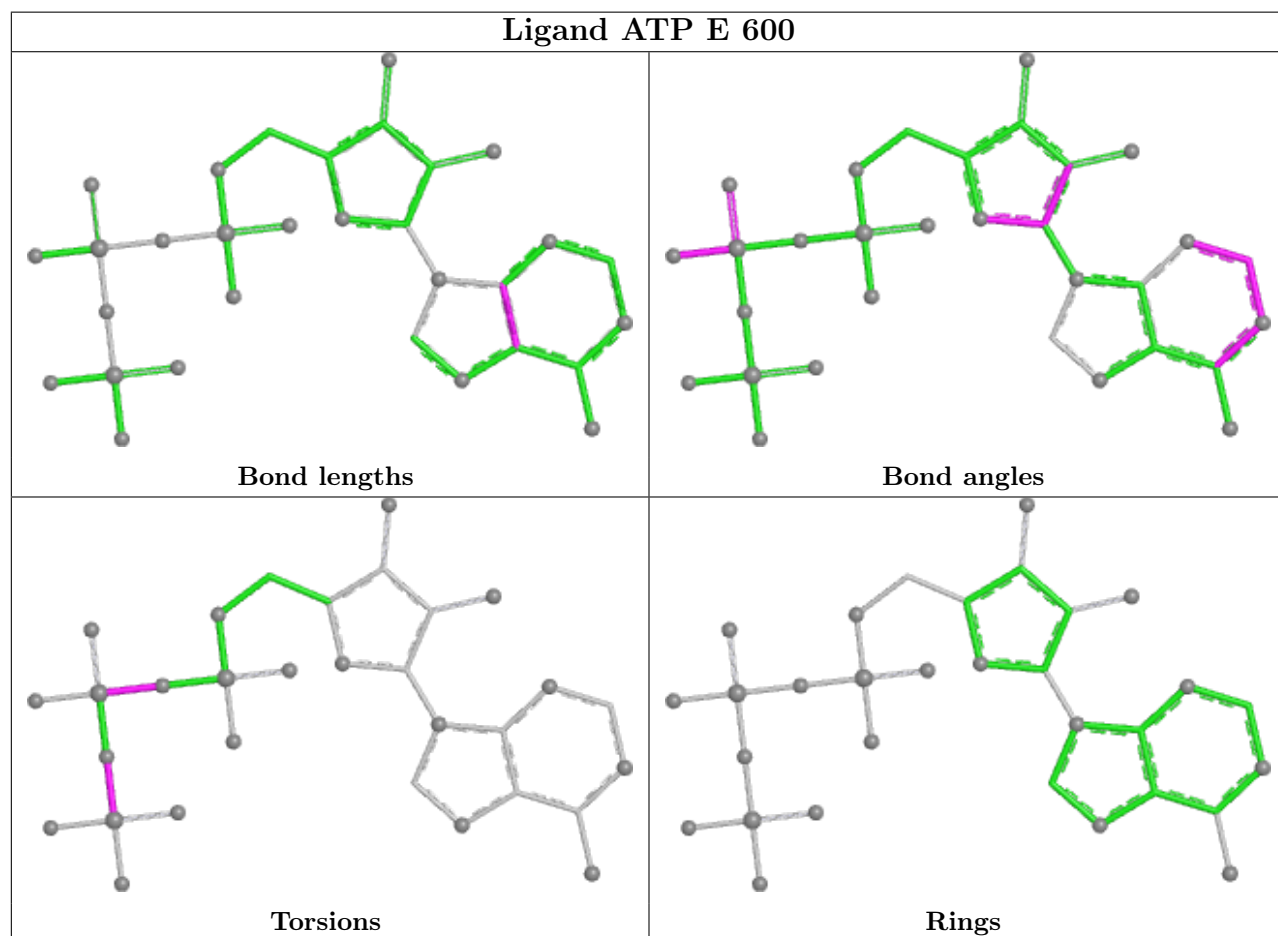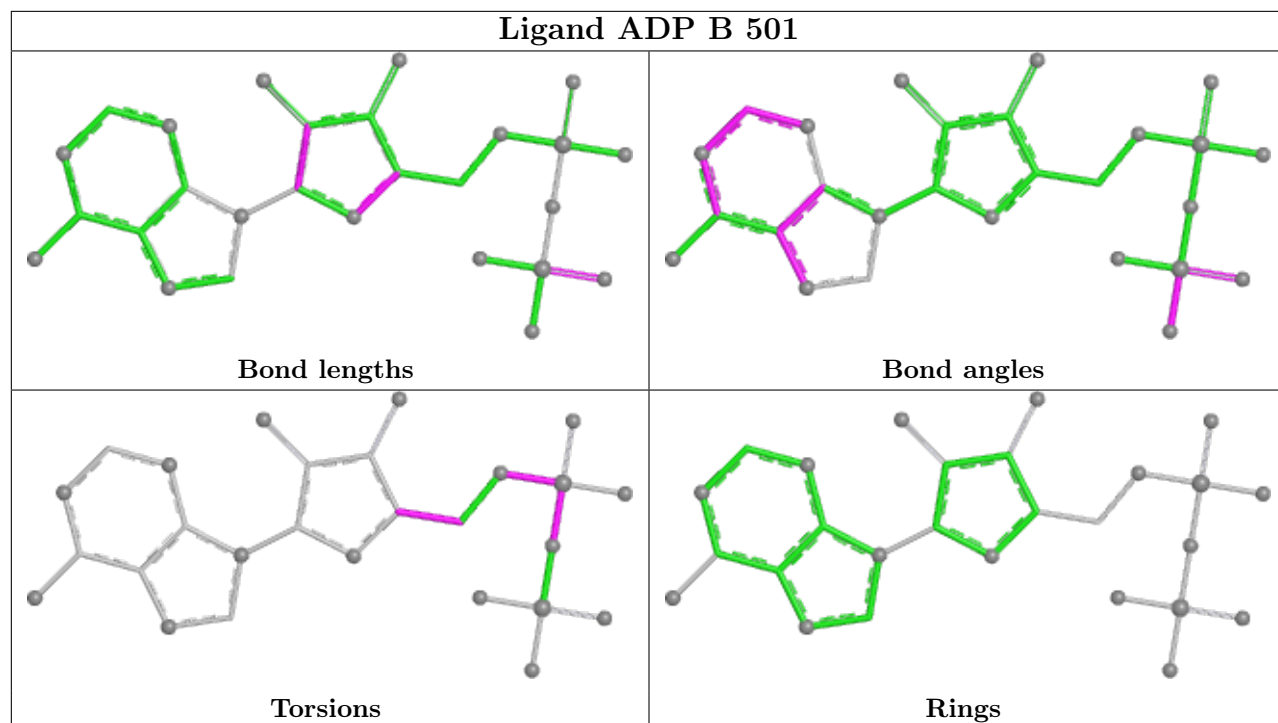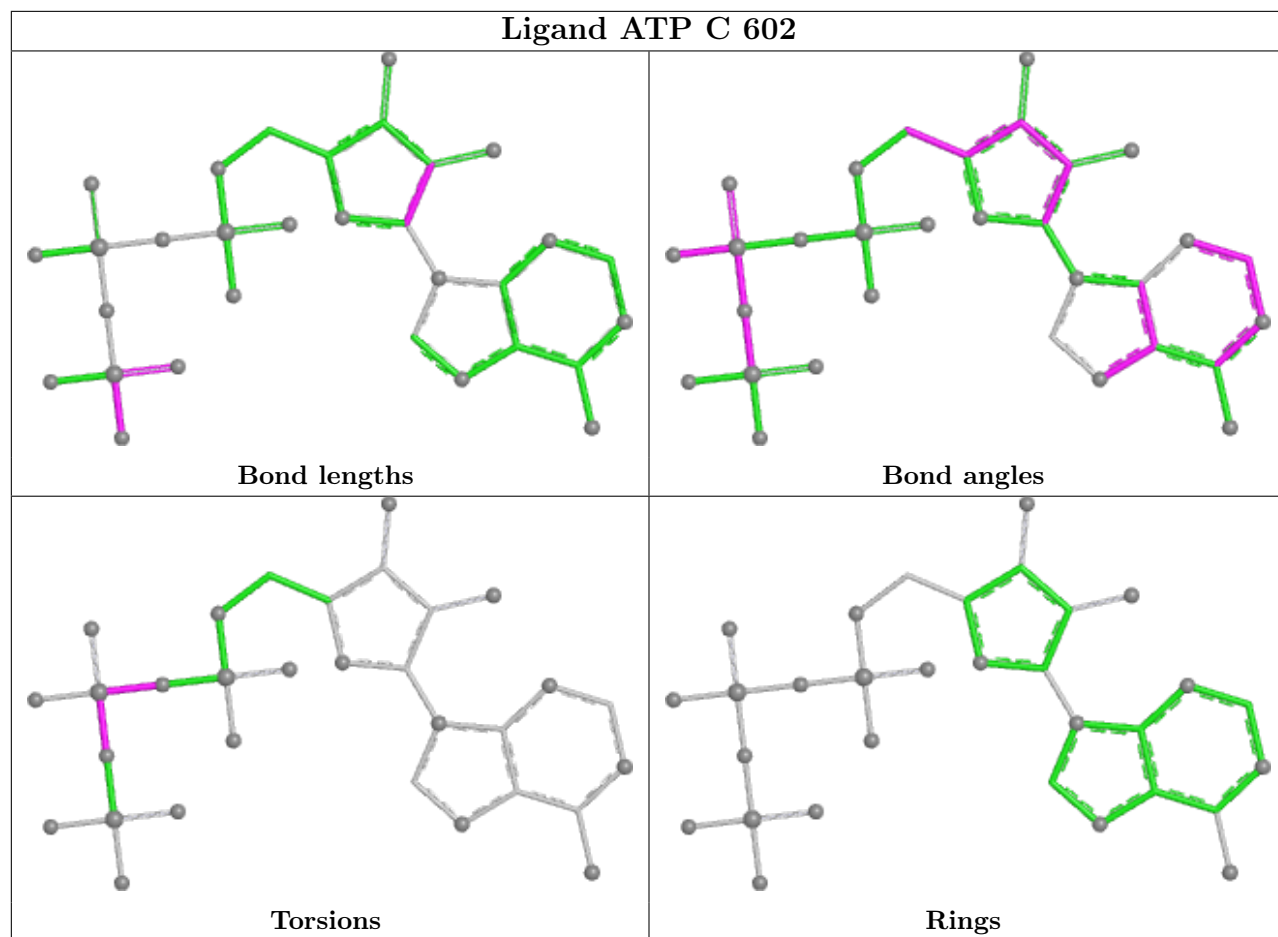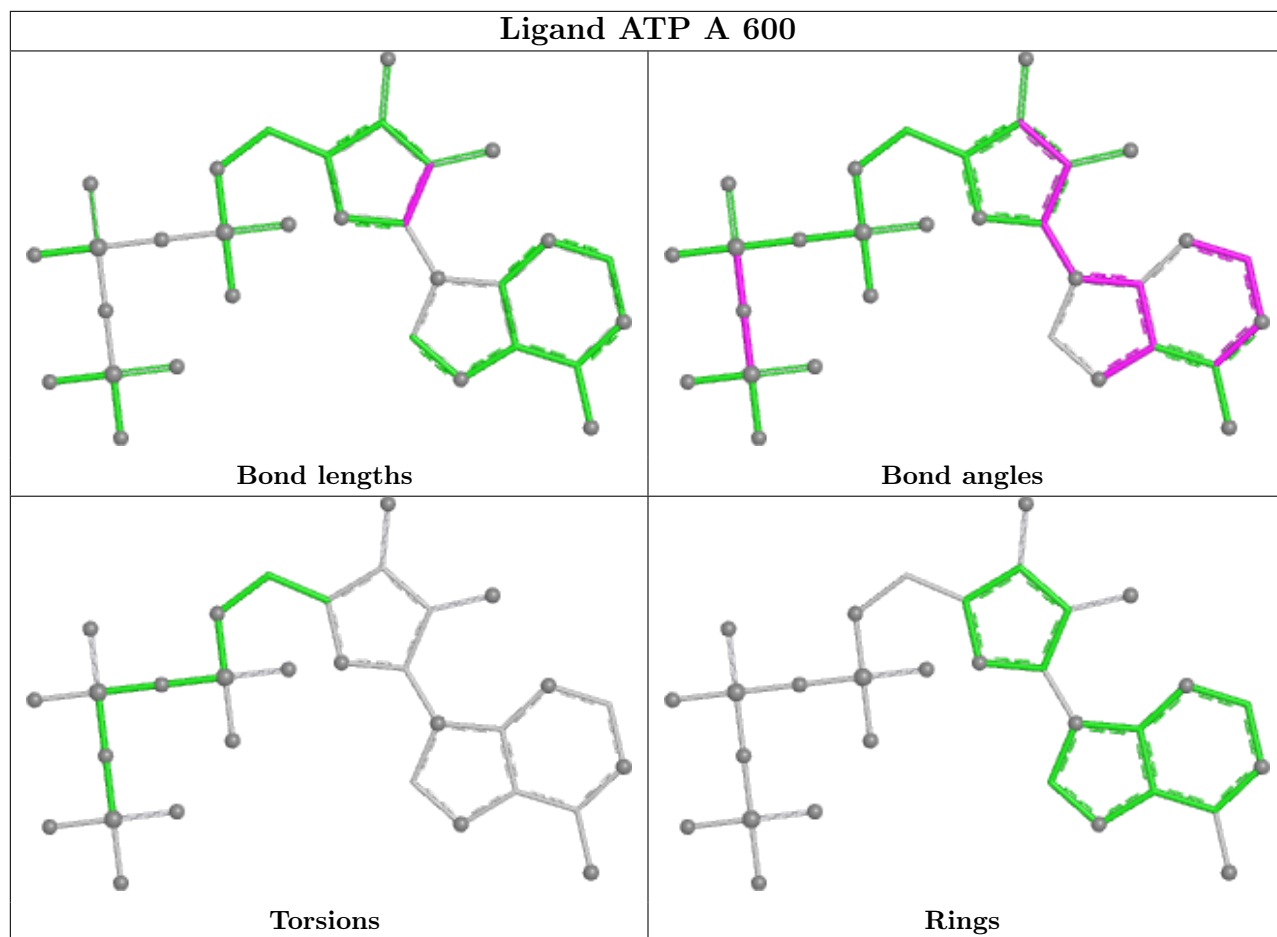
5.7 Other polymers (i)

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
8	b	1
2	C	1
2	E	1
7	p	1
3	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	b	77:GLN	C	78:LEU	N	2.25

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	30:GLY	C	31:THR	N	1.73
1	E	30:GLY	C	31:THR	N	1.64
1	p	105:ASP	C	106:LYS	N	1.17
1	D	276:PHE	C	277:ARG	N	0.97

6   Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4271. 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
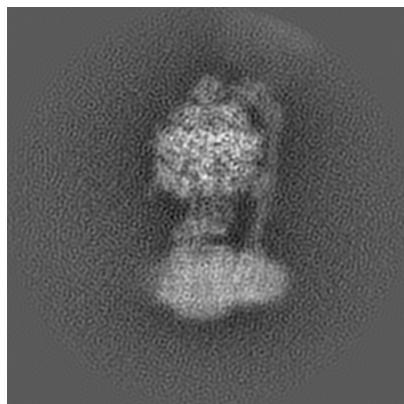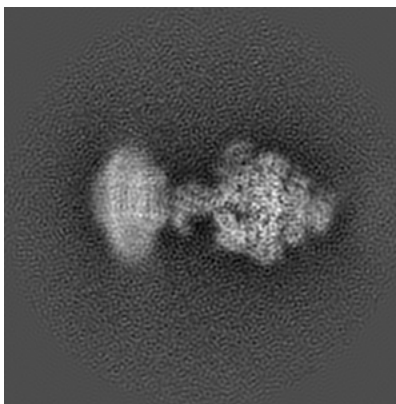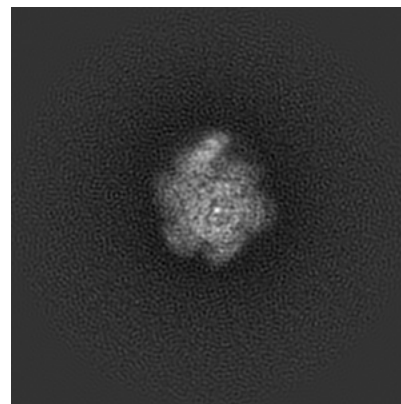
X   Y   Z

6.1.2   Raw map

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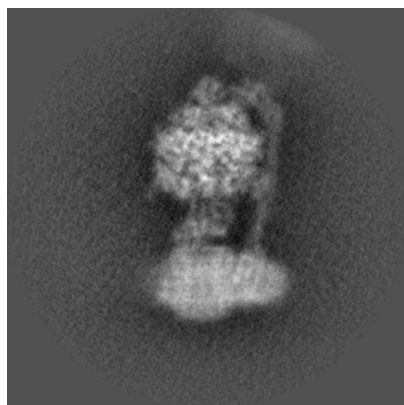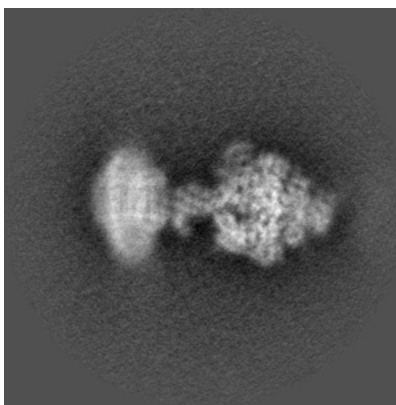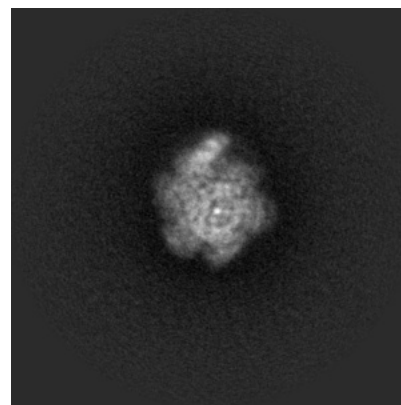
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
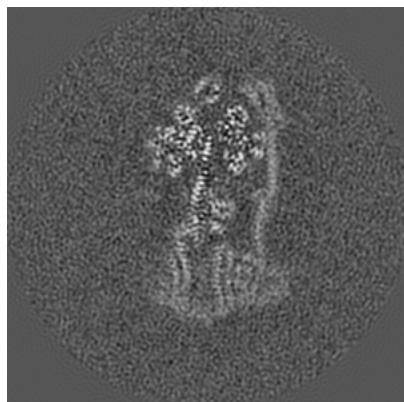
6.2.1 Primary map
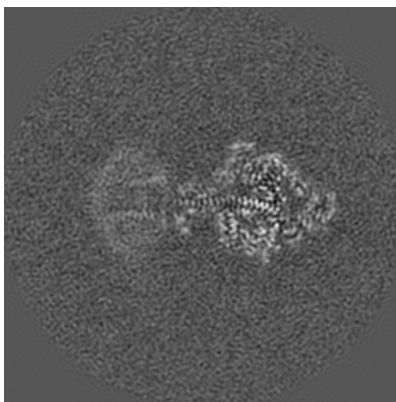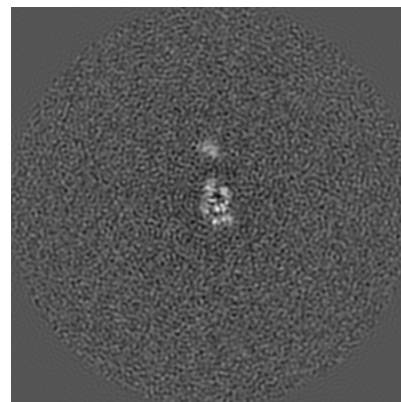
X Index: 175   Y Index: 175   Z Index: 175

6.2.2 Raw map
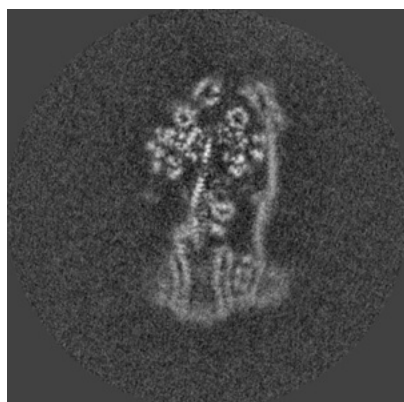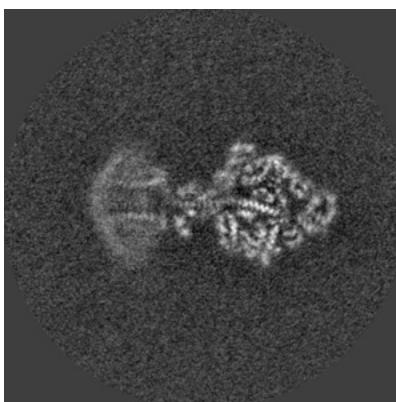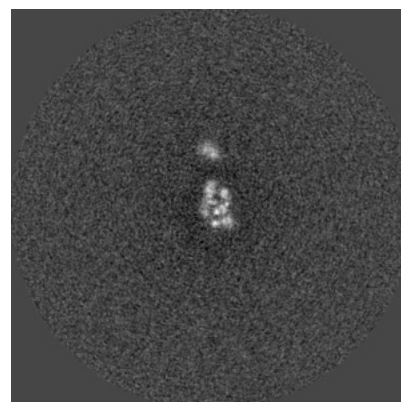
X Index: 175   Y Index: 175   Z Index: 175

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

6.3   Largest variance slices ⓘ
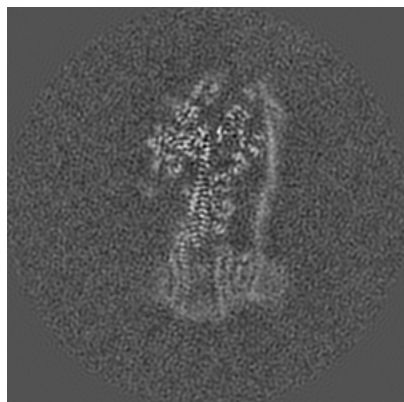
6.3.1   Primary map
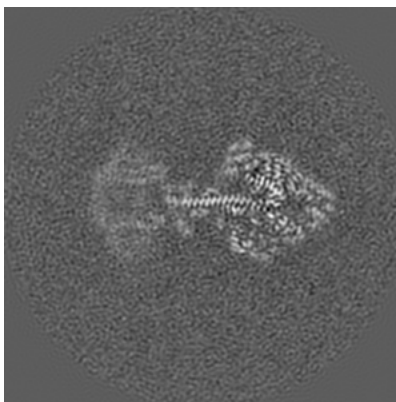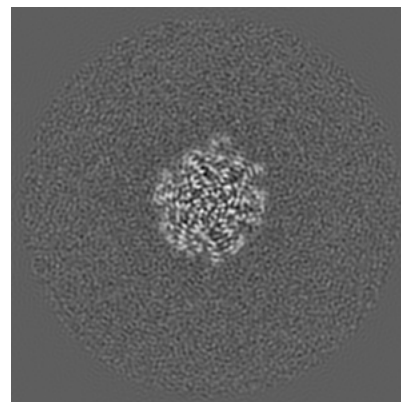
X Index: 177   Y Index: 171   Z Index: 234

6.3.2   Raw map
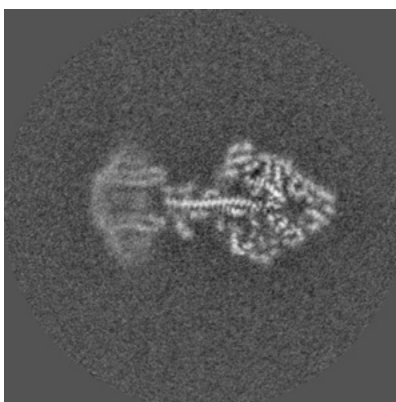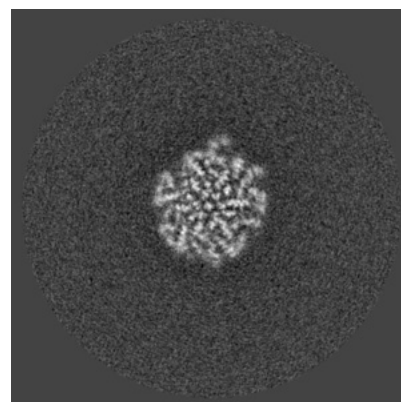
X Index: 177   Y Index: 171   Z Index: 235

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

X	Y	Z
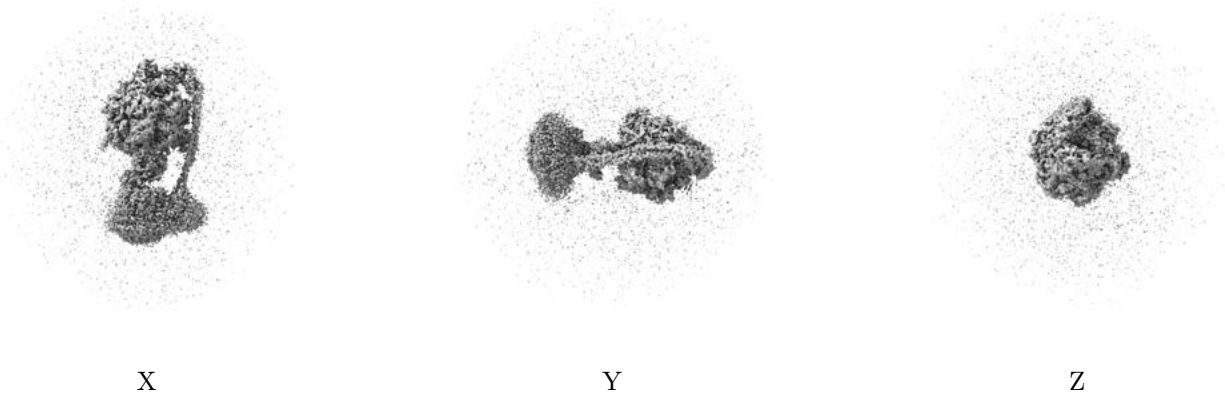
The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X	Y	Z
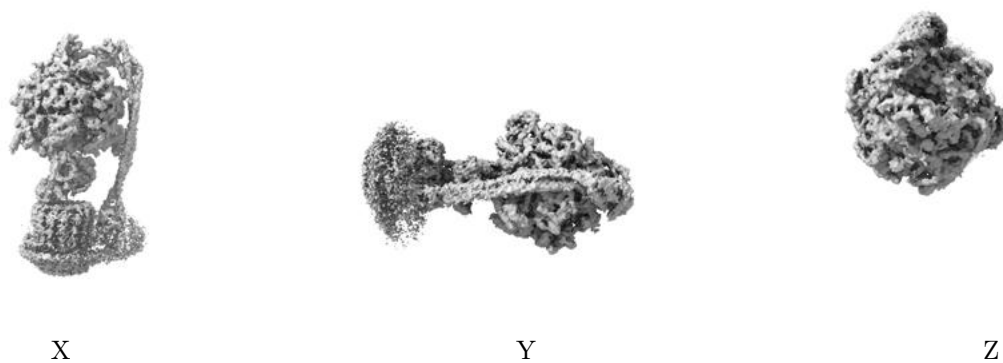
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.5 Mask visualisation ⓘ

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure

- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

6.5.1 emd_4271_msk_1.map ⓘ
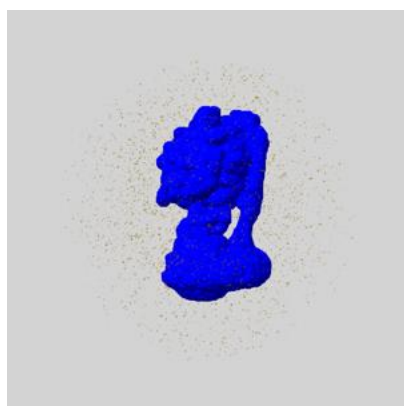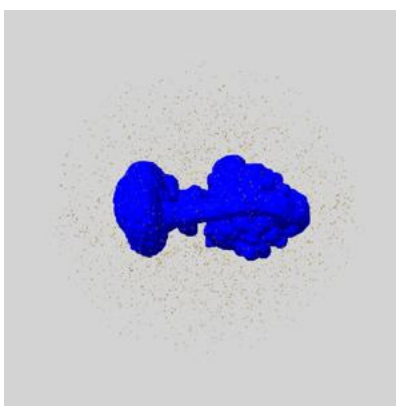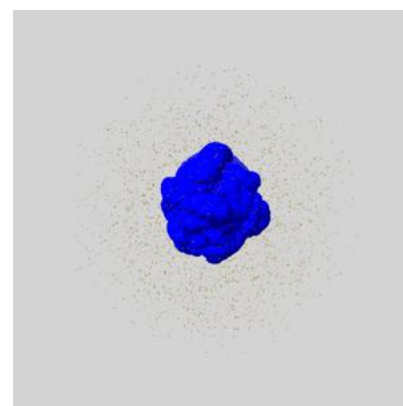
X Y Z

7   Map analysis (i)

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

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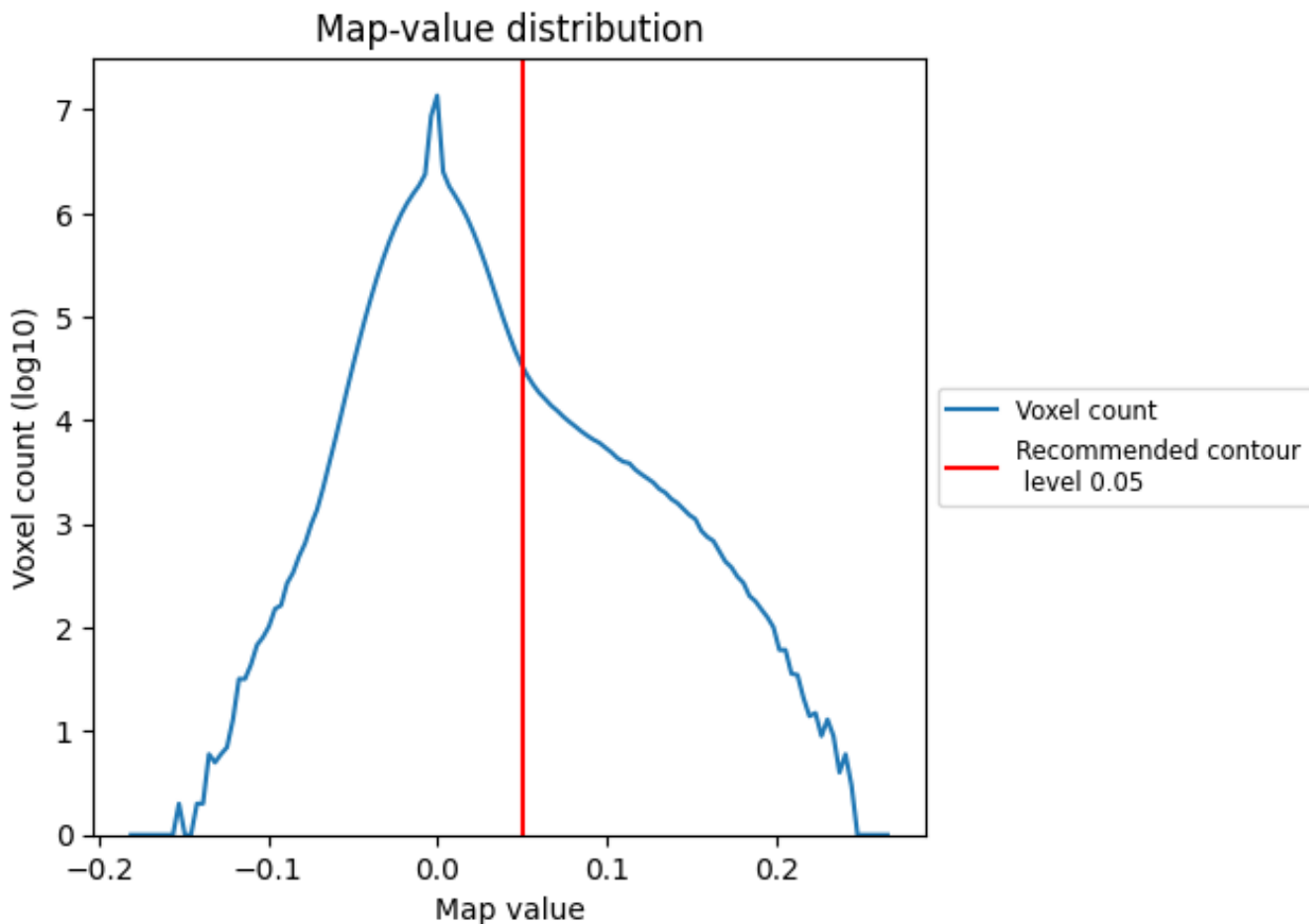
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
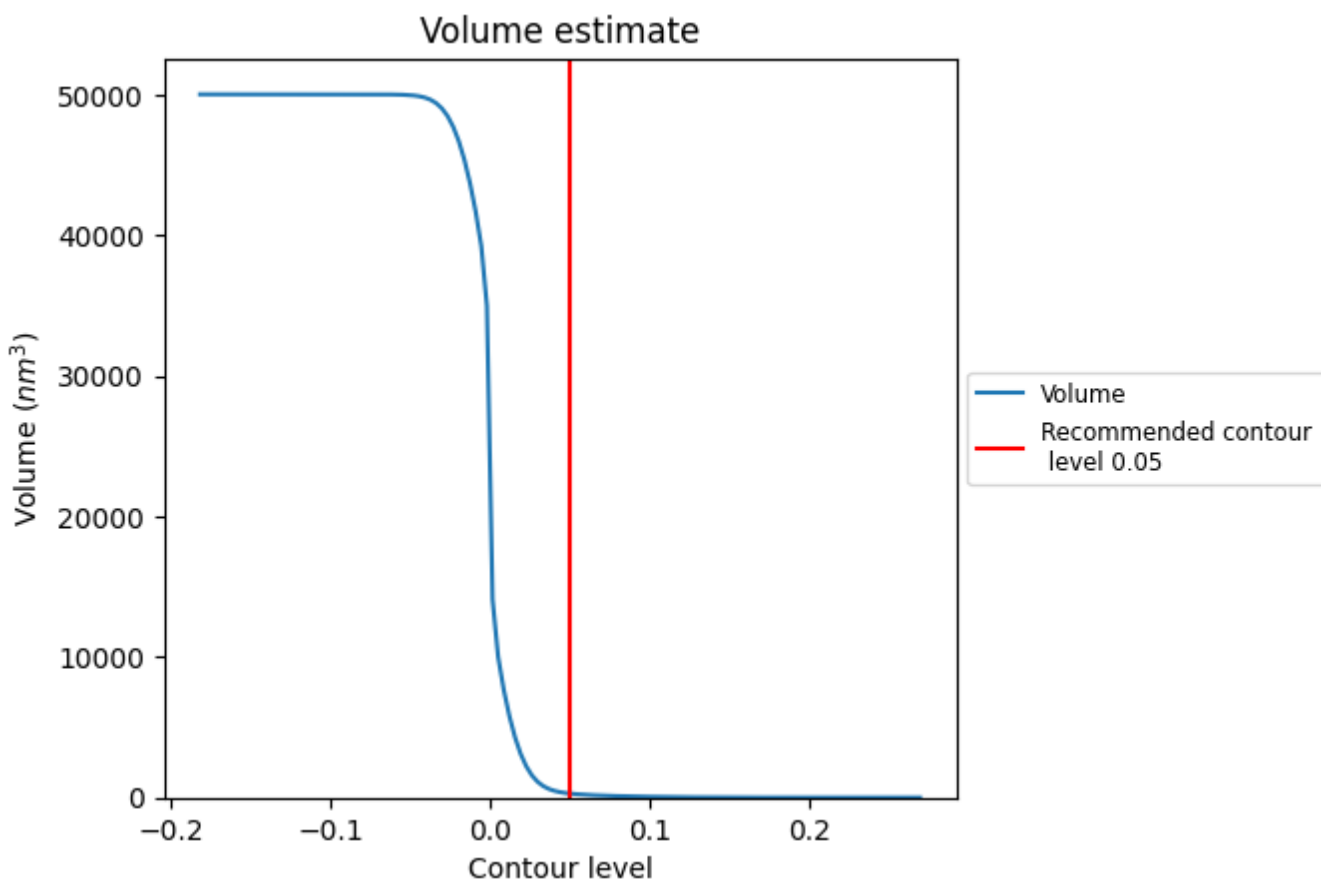
The volume at the recommended contour level is 291 nm^3; this corresponds to an approximate mass of 263 kDa.

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 ⓘ
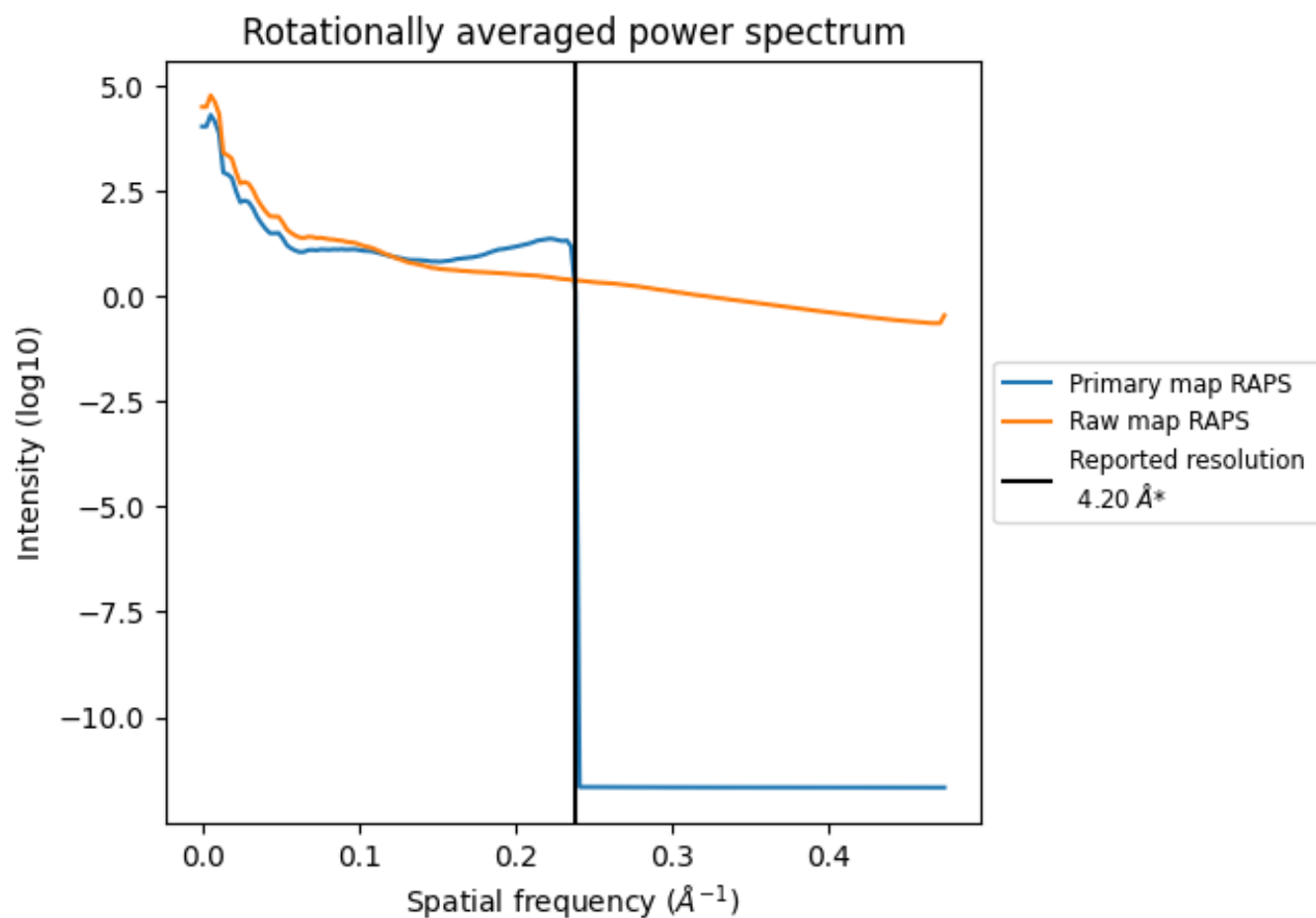
*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

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　ⓘ
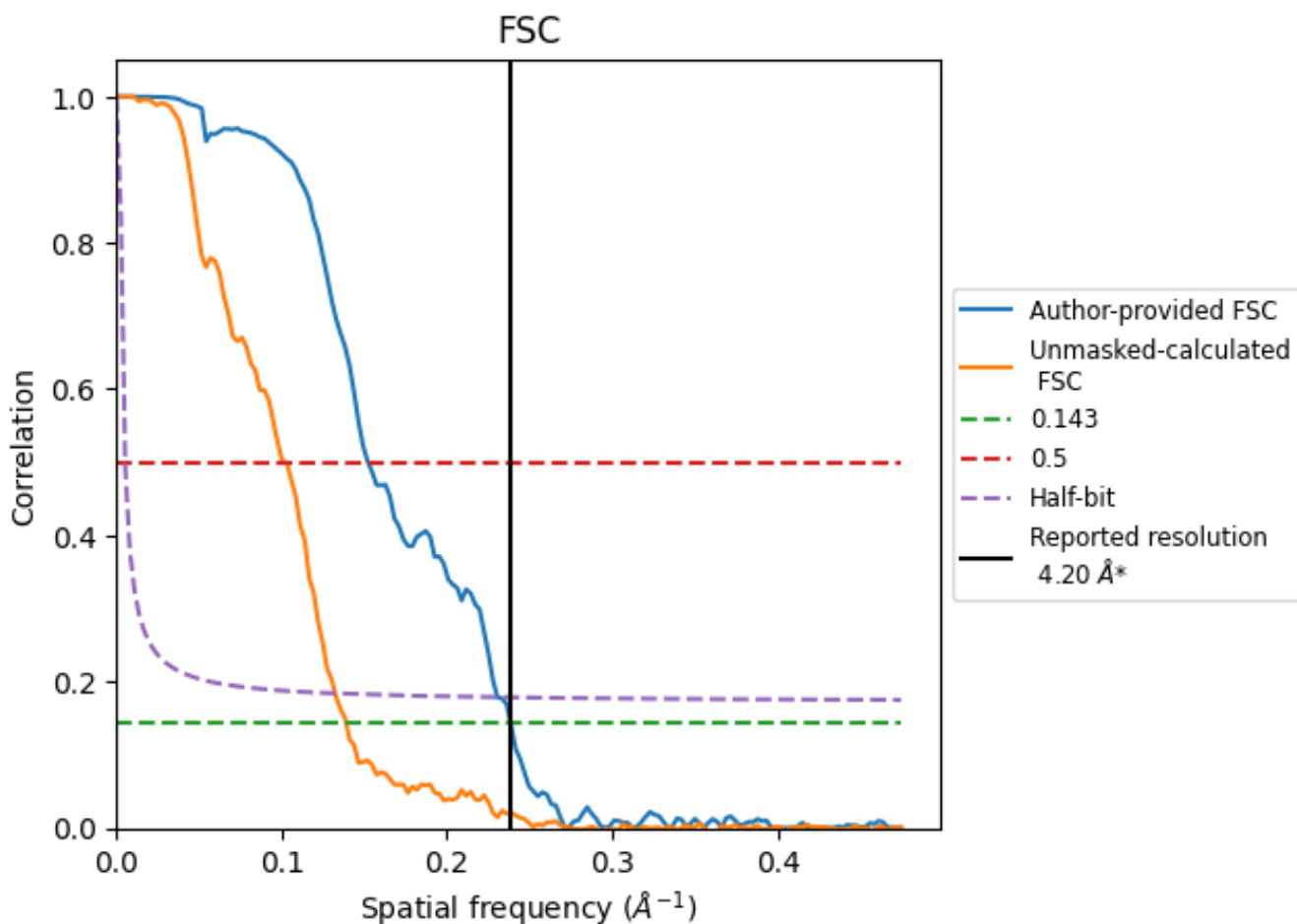
*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8.2　Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.19	6.57	4.33
Unmasked-calculated*	7.19	9.79	7.55

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.19 differs from the reported value 4.2 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-4271 and PDB model 6FKH. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay ⓘ

X	Y	Z
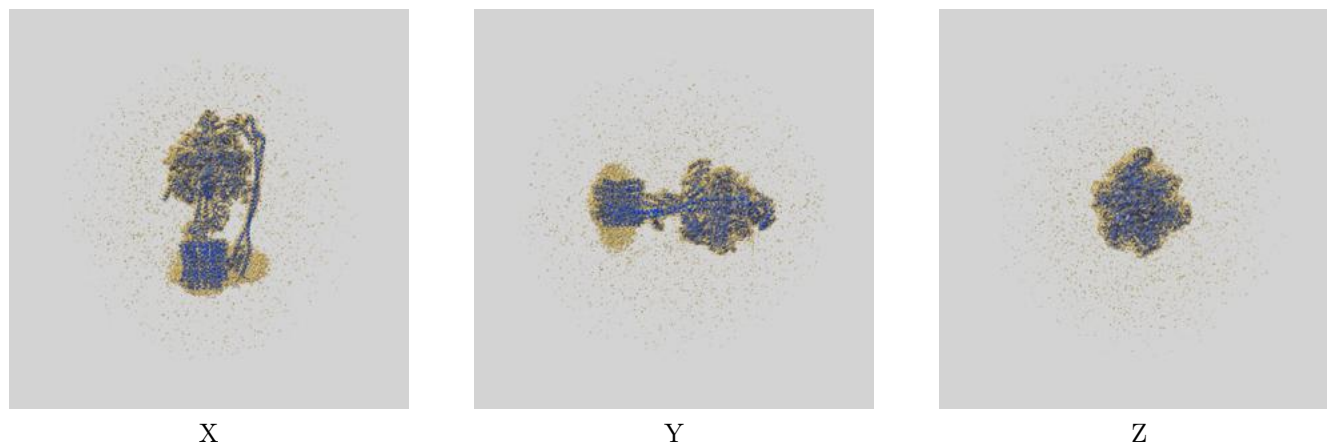
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model   ⓘ

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   ⓘ
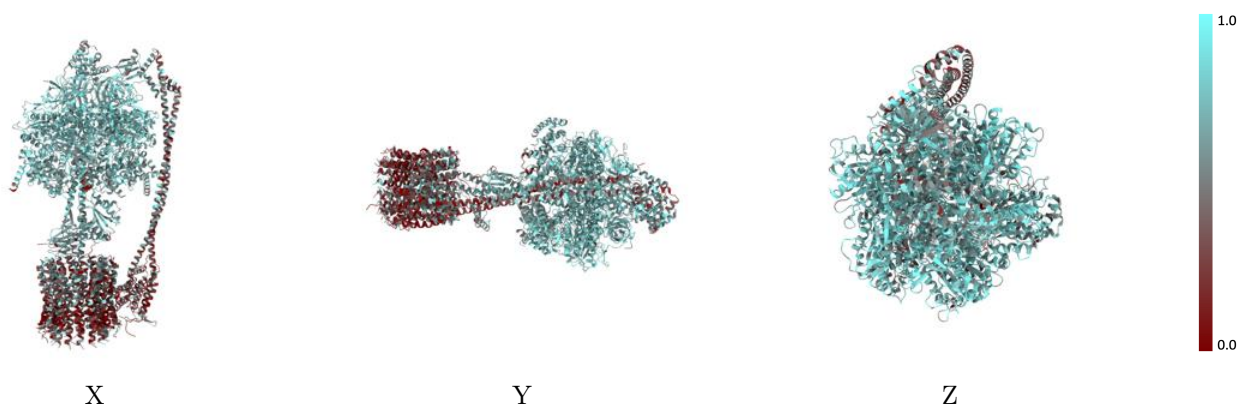
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4   Atom inclusion (i)
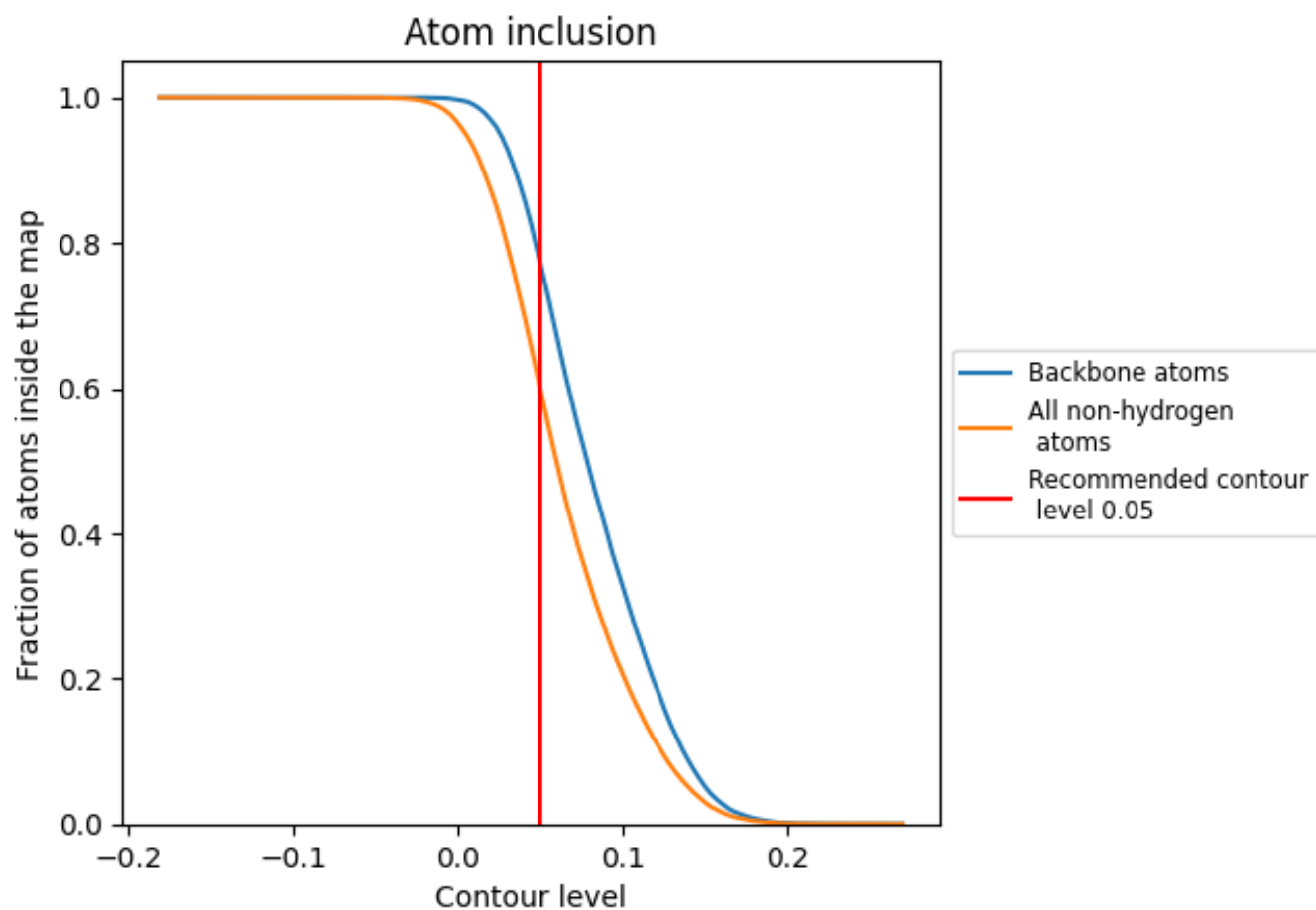
At the recommended contour level, 77% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5956	0.2790
A	0.6984	0.3490
B	0.7368	0.3700
C	0.7142	0.3530
D	0.7346	0.3630
E	0.6903	0.3270
F	0.7272	0.3760
G	0.4193	0.2070
H	0.3618	0.1460
I	0.3618	0.1840
J	0.3228	0.1620
K	0.3878	0.1670
L	0.4378	0.1970
M	0.4286	0.1620
N	0.4063	0.1570
O	0.3748	0.1420
P	0.3692	0.1520
Q	0.3191	0.1260
R	0.2709	0.0930
S	0.2894	0.1190
T	0.3655	0.1760
a	0.3151	0.1120
b	0.3940	0.0880
d	0.6167	0.2870
e	0.5730	0.2070
g	0.6381	0.2910
p	0.3169	0.0760

1.0

0.0
<0.0