



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 05:58 PM UTC

PDB ID : 8QXU / pdb_00008qxu
EMDB ID : EMD-18737
Title : In situ structure average of GroEL14-GroES7 complexes with wide GroEL7 trans ring conformation in Escherichia coli cytosol obtained by cryo electron tomography
Authors : Wagner, J.; Caravajal, A.I.; Beck, F.; Bracher, A.; Wan, W.; Bohn, S.; Kerner, R.; Baumeister, W.; Fernandez-Busnadiego, R.; Hartl, F.U.
Deposited on : 2023-10-25
Resolution : 12.00 Å(reported)
Based on initial models : 1KP8, 8P4M

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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

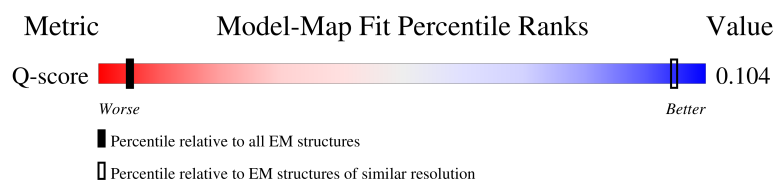
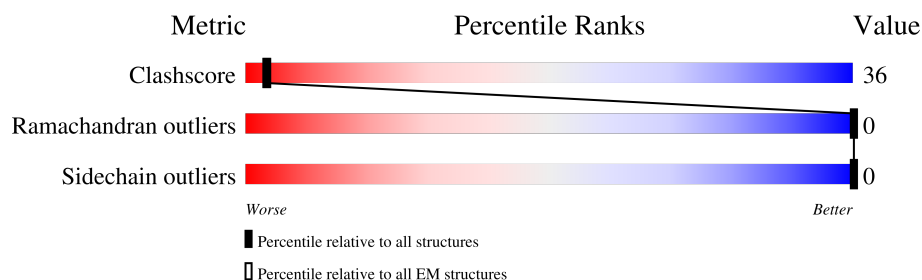
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 12.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	93 (11.50 - 12.50)

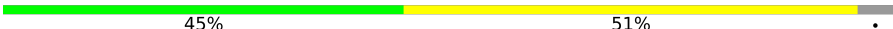
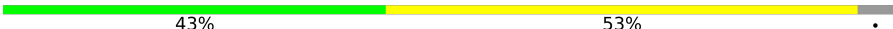
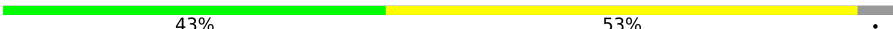
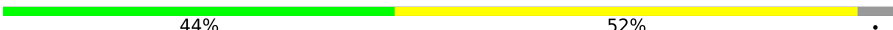
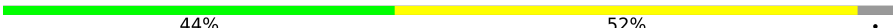
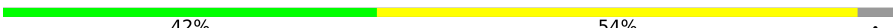
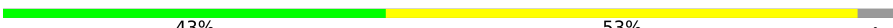
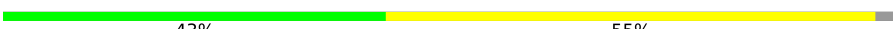
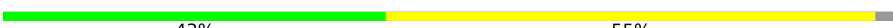
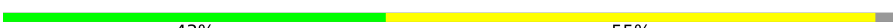
The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment 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 $\leq 5\%$. 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	547	41% 54% .
1	B	547	42% 53% .
1	C	547	42% 54% .

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Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain	
1	D	547		.
1	E	547		.
1	F	547		.
1	G	547		.
1	H	547		.
1	I	547		.
1	J	547		.
1	K	547		.
1	L	547		.
1	M	547		.
1	N	547		.
2	O	97		.
2	P	97		.
2	Q	97		.
2	R	97		.
2	S	97		.
2	T	97		.
2	U	97		.

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 59458 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 Chaperonin GroEL.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	524	Total	C	N	O	S	0	0
			3851	2395	665	771	20		
1	B	524	Total	C	N	O	S	0	0
			3851	2395	665	771	20		
1	C	524	Total	C	N	O	S	0	0
			3851	2395	665	771	20		
1	D	524	Total	C	N	O	S	0	0
			3851	2395	665	771	20		
1	E	524	Total	C	N	O	S	0	0
			3851	2395	665	771	20		
1	F	524	Total	C	N	O	S	0	0
			3851	2395	665	771	20		
1	G	524	Total	C	N	O	S	0	0
			3851	2395	665	771	20		
1	H	525	Total	C	N	O	S	0	0
			3864	2403	667	774	20		
1	I	525	Total	C	N	O	S	0	0
			3864	2403	667	774	20		
1	J	525	Total	C	N	O	S	0	0
			3864	2403	667	774	20		
1	K	525	Total	C	N	O	S	0	0
			3864	2403	667	774	20		
1	L	525	Total	C	N	O	S	0	0
			3864	2403	667	774	20		
1	M	525	Total	C	N	O	S	0	0
			3864	2403	667	774	20		
1	N	525	Total	C	N	O	S	0	0
			3864	2403	667	774	20		

- Molecule 2 is a protein called Co-chaperonin GroES.

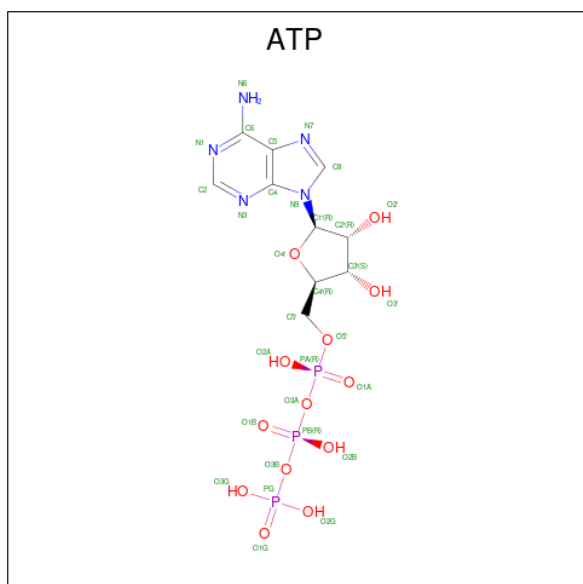
Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	95	Total	C	N	O	S	0	0
			687	430	125	131	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	95	Total	C	N	O	S	0	0
			687	430	125	131	1		
2	Q	95	Total	C	N	O	S	0	0
			687	430	125	131	1		
2	R	95	Total	C	N	O	S	0	0
			687	430	125	131	1		
2	S	95	Total	C	N	O	S	0	0
			687	430	125	131	1		
2	T	95	Total	C	N	O	S	0	0
			687	430	125	131	1		
2	U	95	Total	C	N	O	S	0	0
			687	430	125	131	1		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	B	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	
4	D	1	Total	Mg	0
			1	1	
4	E	1	Total	Mg	0
			1	1	
4	F	1	Total	Mg	0
			1	1	
4	G	1	Total	Mg	0
			1	1	
4	H	1	Total	Mg	0
			1	1	
4	I	1	Total	Mg	0
			1	1	
4	J	1	Total	Mg	0
			1	1	
4	K	1	Total	Mg	0
			1	1	
4	L	1	Total	Mg	0
			1	1	
4	M	1	Total	Mg	0
			1	1	
4	N	1	Total	Mg	0
			1	1	

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

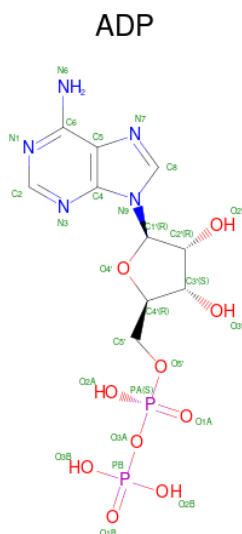
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	K	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total 1	K 1	0
5	C	1	Total 1	K 1	0
5	D	1	Total 1	K 1	0
5	E	1	Total 1	K 1	0
5	F	1	Total 1	K 1	0
5	G	1	Total 1	K 1	0
5	H	1	Total 1	K 1	0
5	I	1	Total 1	K 1	0
5	J	1	Total 1	K 1	0
5	K	1	Total 1	K 1	0
5	L	1	Total 1	K 1	0
5	M	1	Total 1	K 1	0
5	N	1	Total 1	K 1	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
6	H	1	Total 27	C 10	N 5	O 10	P 2	0
6	I	1	Total 27	C 10	N 5	O 10	P 2	0
6	J	1	Total 27	C 10	N 5	O 10	P 2	0
6	K	1	Total 27	C 10	N 5	O 10	P 2	0
6	L	1	Total 27	C 10	N 5	O 10	P 2	0
6	M	1	Total 27	C 10	N 5	O 10	P 2	0
6	N	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 7 is water.

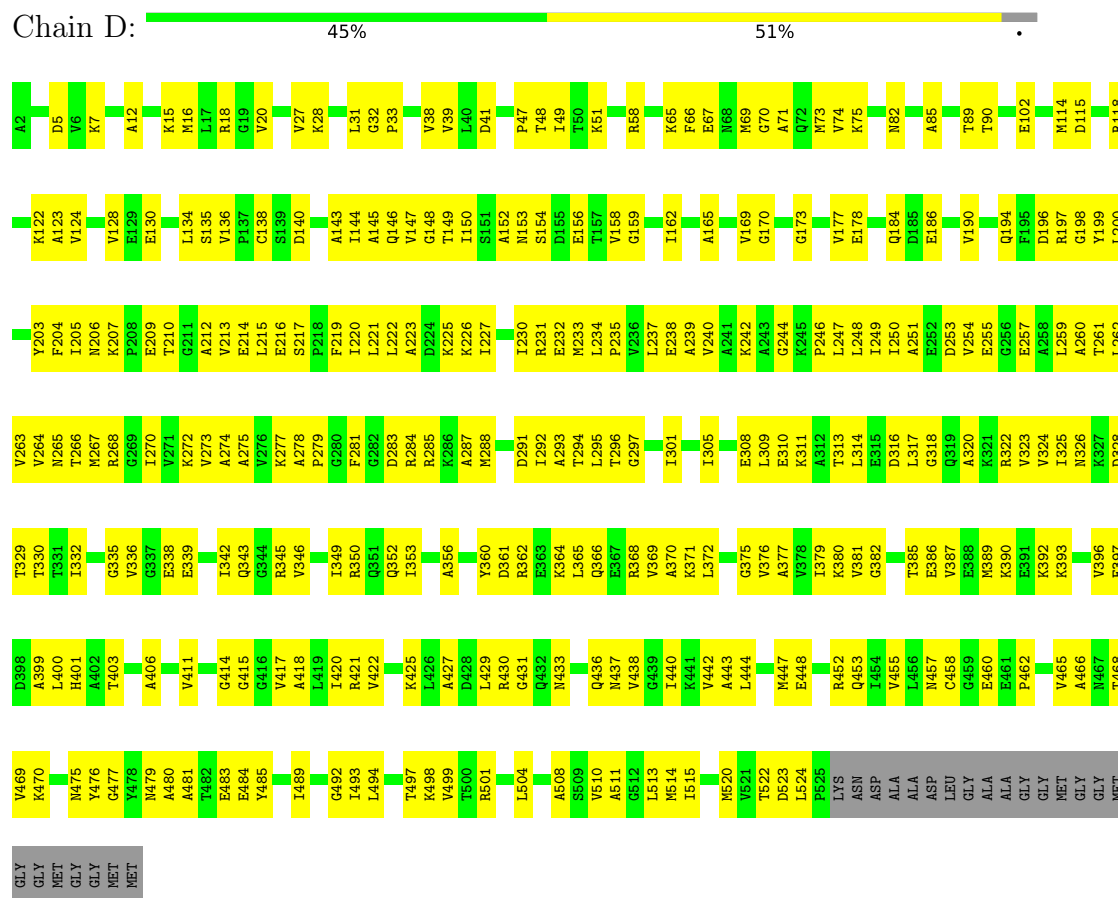
Mol	Chain	Residues	Atoms		AltConf
7	A	30	Total 30	O 30	0
7	B	29	Total 29	O 29	0
7	C	28	Total 28	O 28	0
7	D	30	Total 30	O 30	0
7	E	29	Total 29	O 29	0

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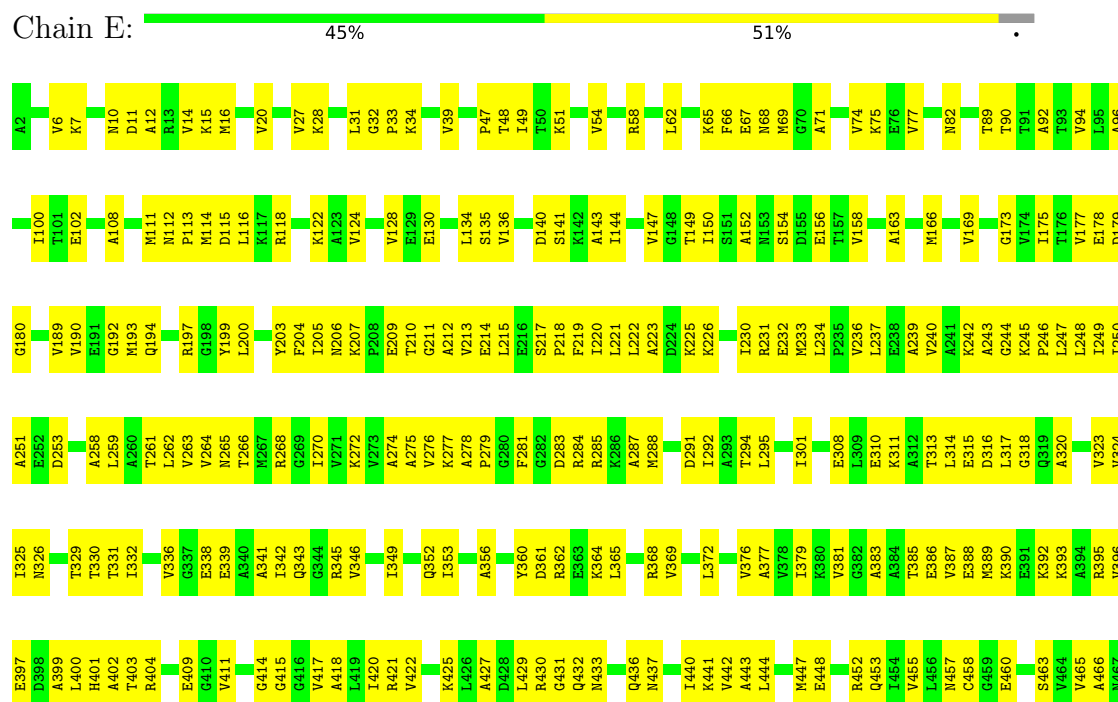
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Mol	Chain	Residues	Atoms		AltConf
7	F	30	Total 30	O 30	0
7	G	27	Total 27	O 27	0
7	H	1	Total 1	O 1	0
7	I	1	Total 1	O 1	0
7	J	1	Total 1	O 1	0
7	K	1	Total 1	O 1	0
7	L	1	Total 1	O 1	0
7	M	1	Total 1	O 1	0
7	N	1	Total 1	O 1	0

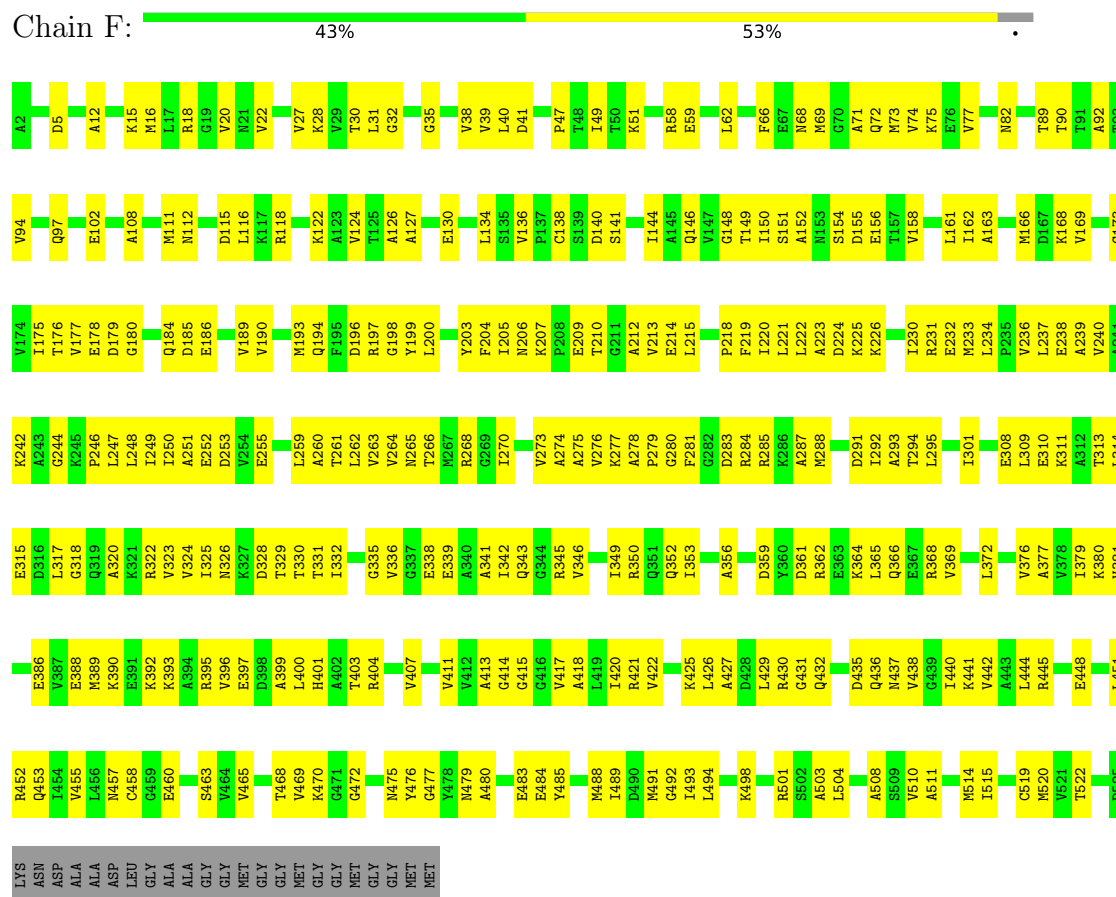
• Molecule 1: Chaperonin GroEL



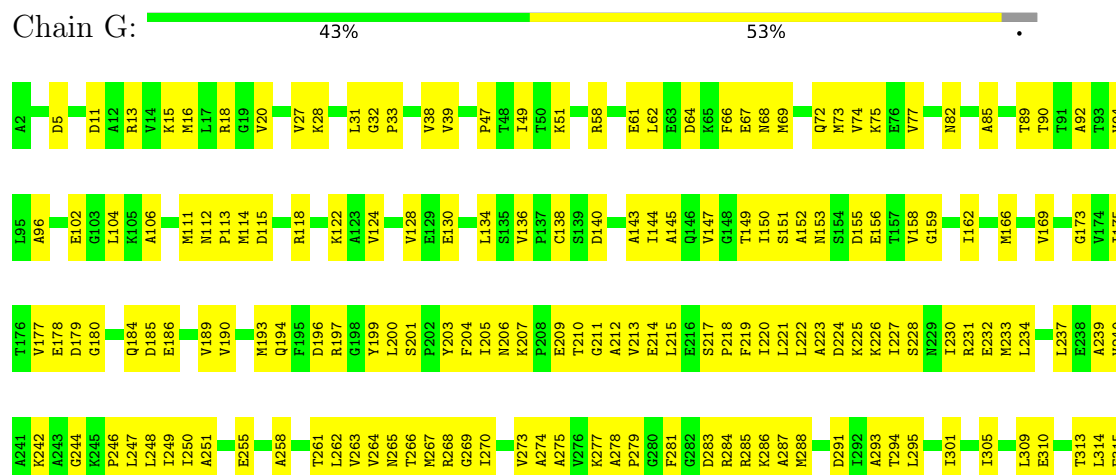
• Molecule 1: Chaperonin GroEL



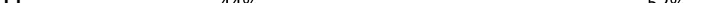
- Molecule 1: Chaperonin GroEL

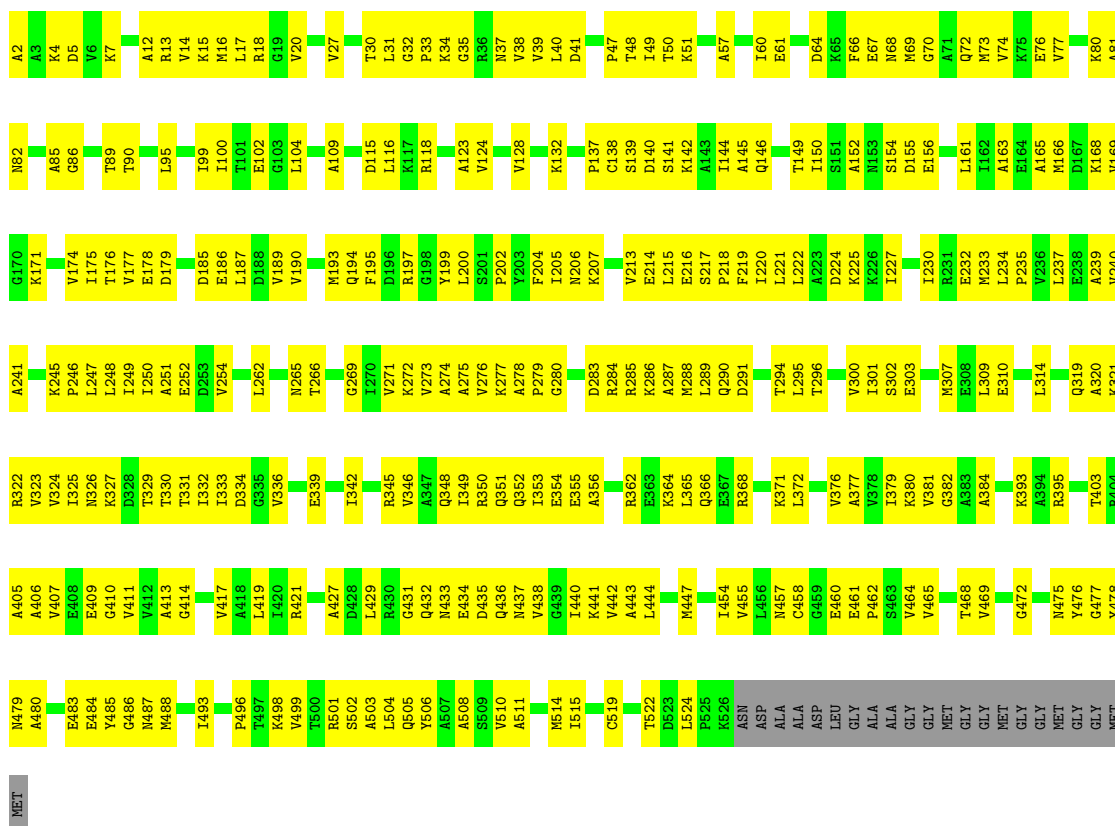


- Molecule 1: Chaperonin GroEL

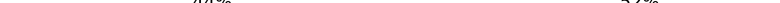


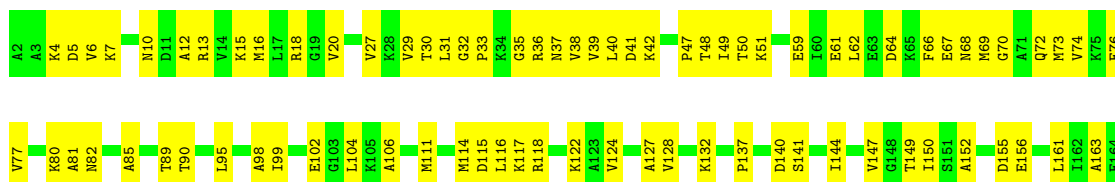
- Molecule 1: Chaperonin GroEL

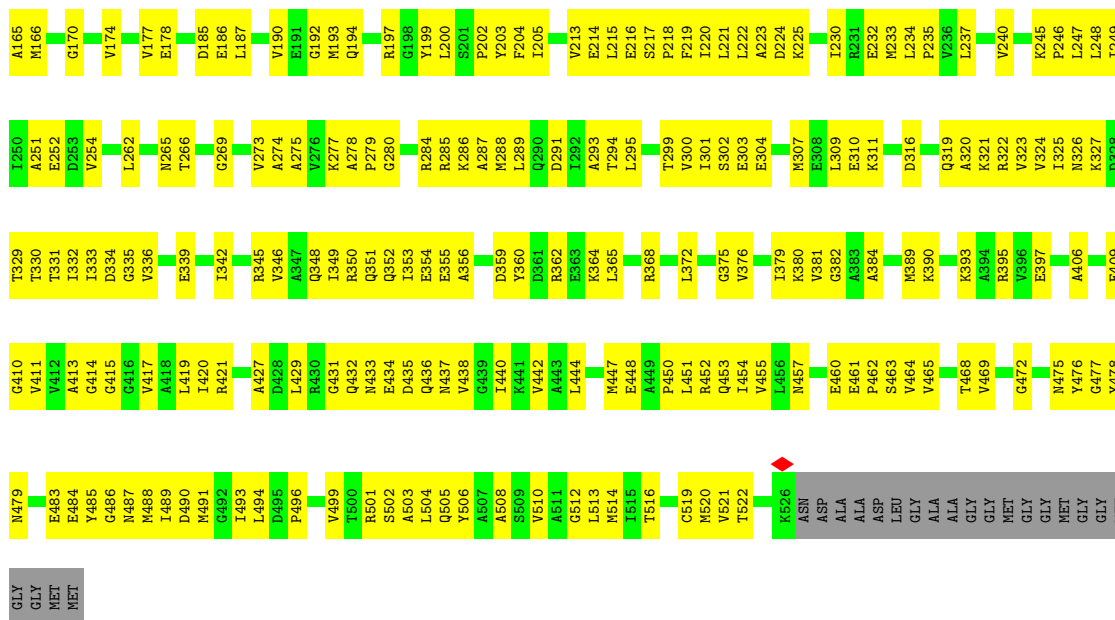
Chain H:  44% 52%



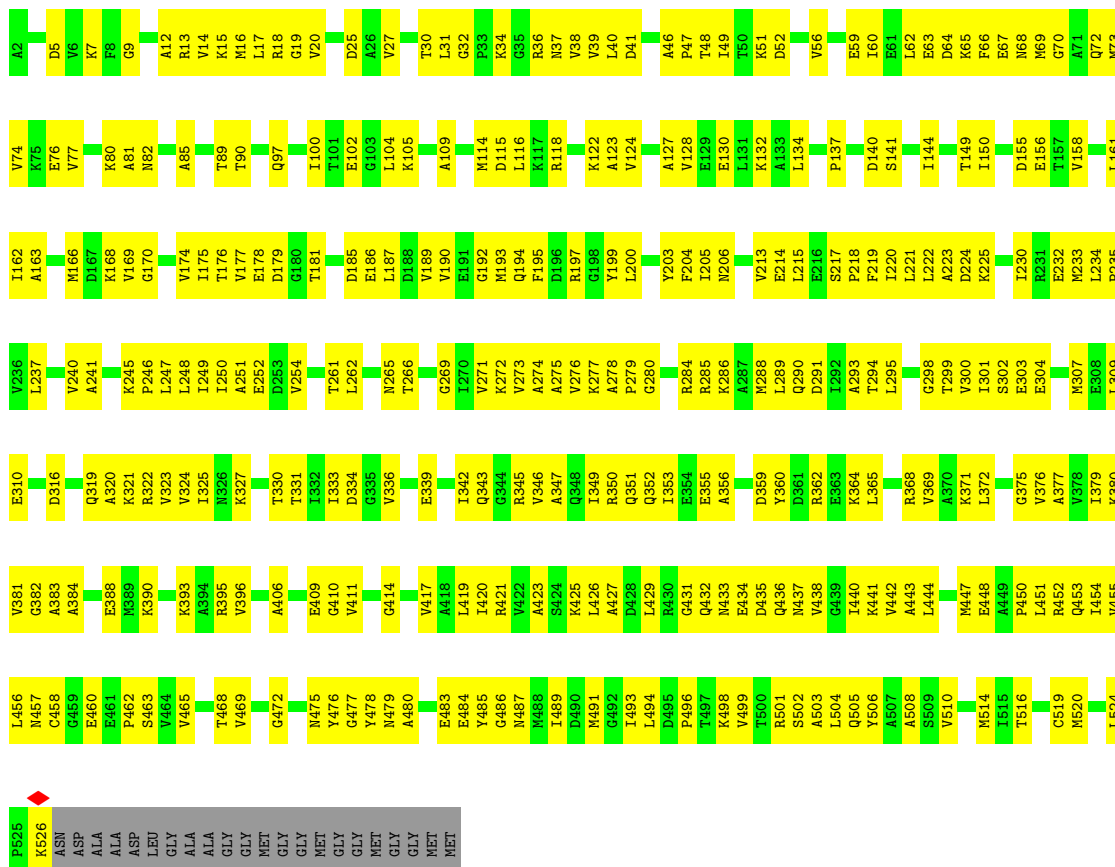
- Molecule 1: Chaperonin GroEL

Chain I:  44% 52% .





- Molecule 1: Chaperonin GroEL



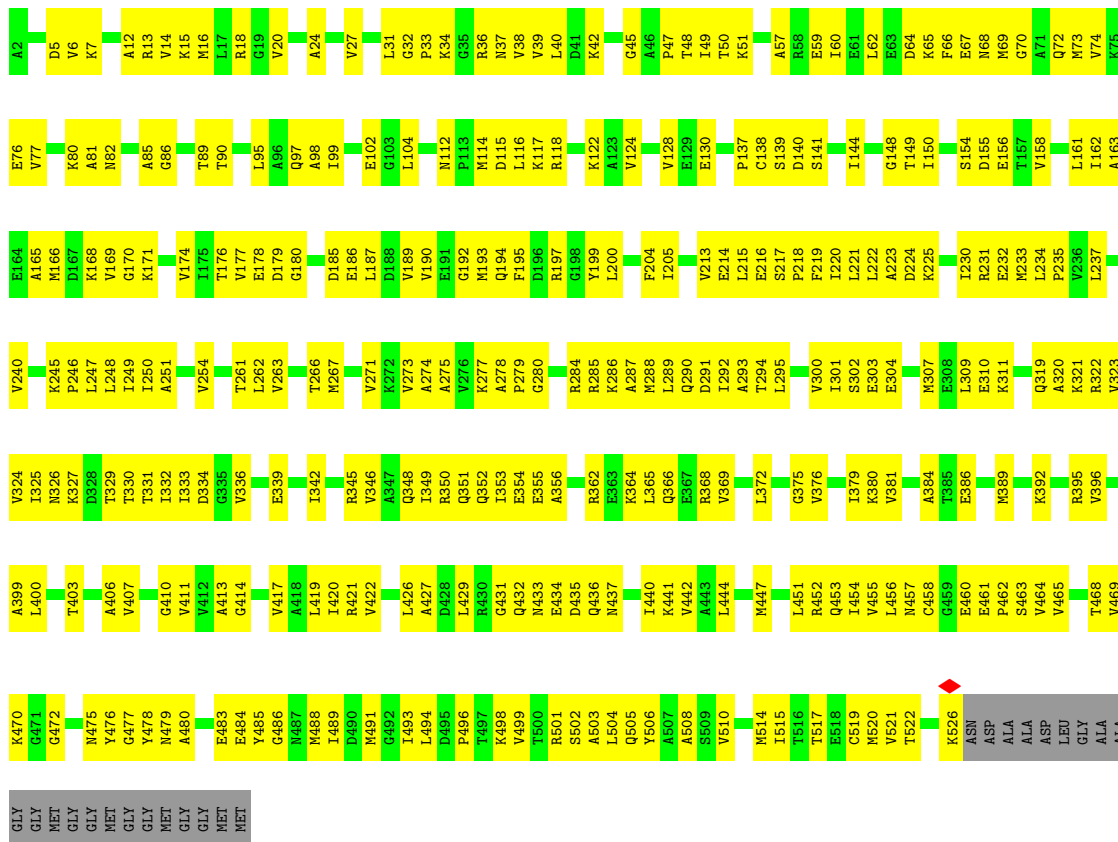
- Molecule 1: Chaperonin GroEL

LEU	V465	A394	V323	P246	M166	D83	A2
	GLY	R395	V324	P247	D167	A84	A3
	ALA	V396	I325	L247	K168	A85	K4
	ALA	V469	I326	L248	G96	G86	D5
	GLY	T403	K327	I249	K171		V6
	GLY	G472	I328	I250	T89		K7
	MET	A406	T329	A251	T90		F8
	GLY	N475	T330	E252	V174		G9
	GLY	V476	T331	D253	T176		N10
	MET	G477	I332	V254	I177		D11
GLY	V478	V411	I333		E178		A12
	GLY	N479	D334	T261			R13
	MET	A480	G335	L262	T181		V14
	GLY	G415	V336				K15
	GLY	E483	G416	N265	D185		M16
	GLY	E484	T266	T266	E186		L17
	MET	V485	E339		L104		R18
	MET	G486	A418		L187		G19
	MET	N487	L419		D188		
	MET	N488	I420	G269	V189		V27
GLY	I489	V422	R345	V271	V190		T30
	D490	G423	A346	K272	E191		L31
	G491	L426	V347	V273	G192		G32
	M492	A427	I348	A274	M193		P33
	GLY	D428	T349	A275	Q194		
	GLY	I493	R350	V276	F195		
	GLY	L494	I351	K277	D196		
	GLY	D495	K352	A278	R197		
	GLY	P496	I353	T279	G198		
	GLY	T497	Q432	G280	V199		
GLY	K498	M433	A356		L200		V38
	V499	E434	T357	R284	S201		V39
	T500	D435	S358	R285	P202		L40
	R501	Q436		K286	V203		D41
	E502	N437	R362	A287	F204		
	A503	V438	E363	M288	I205		
	L504	G439	K364	L289	E130		
	Q505	I440	L365	G290	K132		
	V506	K441	A366	D291	E214		
	V507	V442	E367		L215		
GLY	A508	A443	R368	T294	E216		
	S509	L444	V369	L295	G138		
	V510	R445			S139		
	A511	A446	L372	V300	P218		
	G512	N447		I301	F219		
	L513	E448	G375	S302	L221		
	N514	A449	V376	E303	L222		
	I515	P450	A377		Q146		
		L451	V378	M307	D224		
			T379	E308	K225		
ASN	E518		I379	R309	T230		
	C519	I454	K380	E310	E231		
	N520	V455	V381	K311	S154		
	V521	L456	G382		D155		
	T522	N457	A383		E156		
		C458		L314	M233		
		G459	E386		L234		
	K526	E460	M389	G318	T236		
	ASP	E461	P462	Q319	V236		
	ALA	A462		A320	L237		
ALA		S463	K392	K321	I162		
		V463	T393	P222	V200		
					A155		A81
							N82

K390	L314	E238	A163	K80	A12
K393	E315	A239	M166	A81	D6
A394	D316	V240		N82	V6
K395				D83	K7
V396	Q319	K245		A84	
	K321	P246		A85	
A399	K322	L247	G170	T89	A12
L400	V323	L249		T90	R13
A406	V324	L250	V174	L95	K15
V407	K325	A251	T176	A96	M16
	K327	V254	T178	Q97	L17
E408			E178	A98	R18
A409	T330	L259	D179	T99	G19
V411	T331	A260	G180	E102	N21
	I332	T261		G103	
G414	I333	L262	D186	L104	V27
	D334	V263			
V417	G335	V264	K105	A106	T30
A418	V336	N265	V189	V107	L31
L419		T266	V190		G32
L420	E339	M267	E191	M111	P33
R421		K268	G192	M112	K34
V422	I342	G269	M193	P113	G35
A423	Q343		Q194		
	G344	V273	F195	M114	
L426	R345	A274	D196	D115	N37
A427	V346	A275	R197	L116	V38
	A347	V276	G198	K117	V39
V428	Q348	T277	Y199	R118	L40
L429	L349	A278	L200		D41
R430	R349	T279	S201	V124	
G431	R350	P279	G202		G45
Q432	Q351	G280	Y203	V128	A46
K433	Q352		F204	E129	P47
E434	I353	R284	T205	E130	T48
A435	E354	R285		L131	I49
Q436	E355	K286	V213	K132	T50
N437	R362	A287	E214		K51
	E363	T288	L215	P137	
L440	K364	R289	E216	C138	A57
V441	L365	Q290	S217	S139	E58
A443	K368	D291	F218	D140	E59
L444	V369	T292	F219	S141	I60
		A293	T220		E61
V447		T294	L221	I144	D64
E448	L372	L295	L222	A145	K65
			A223		F66
L451	G376	T299	D224	T148	E67
R452	V376	V300	K225	M68	M69
Q453	A377	S302			
I454	K378	E303	T230	S154	Q72
V455	I379		R231	D155	M73
L456	K380	M307	E232	E156	V74
N457	V381	E308	K233	T157	K75
C458		L309	L234	V158	E76
	A384	E310	P235	G159	
V459		K311	V236		V77
E460			L237	L162	
L461	V389				

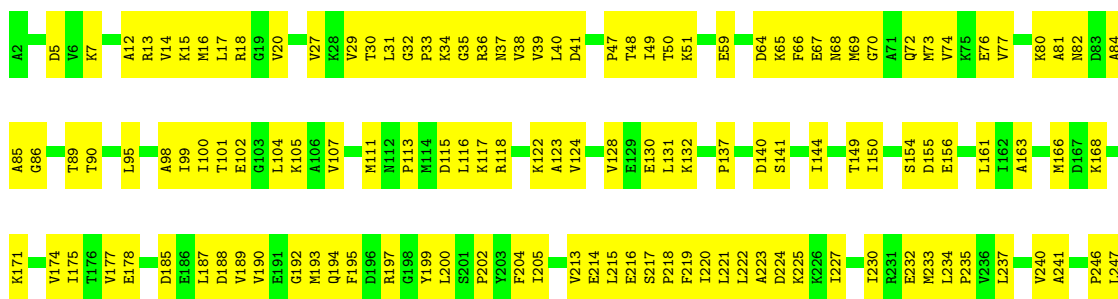
- Molecule 1: Chaperonin GroEL

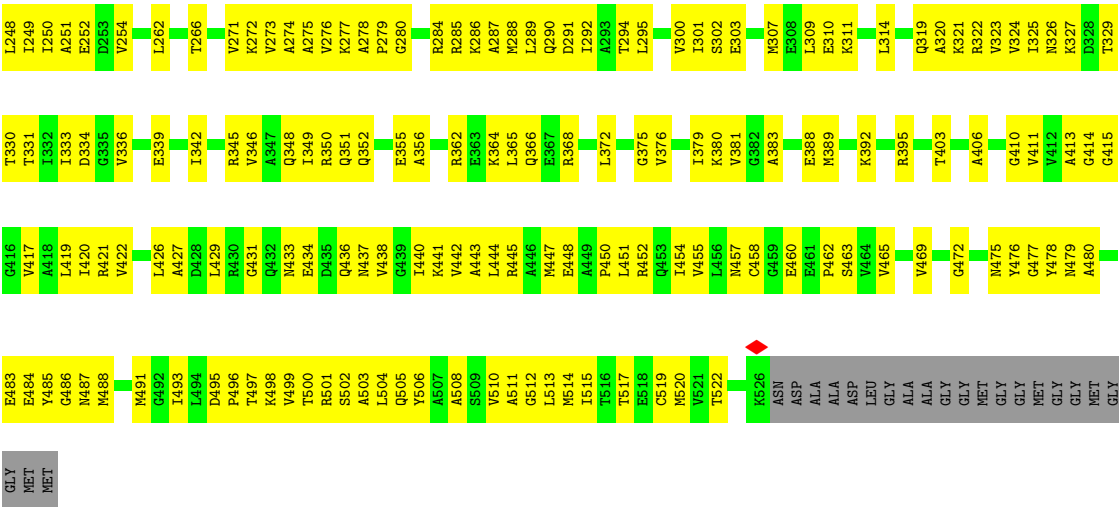
Chain M: 41% 55% .



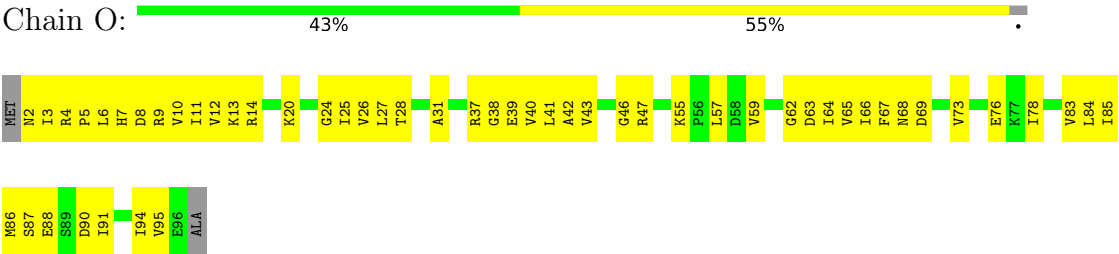
- Molecule 1: Chaperonin GroEL

Chain N: 43% 53% .

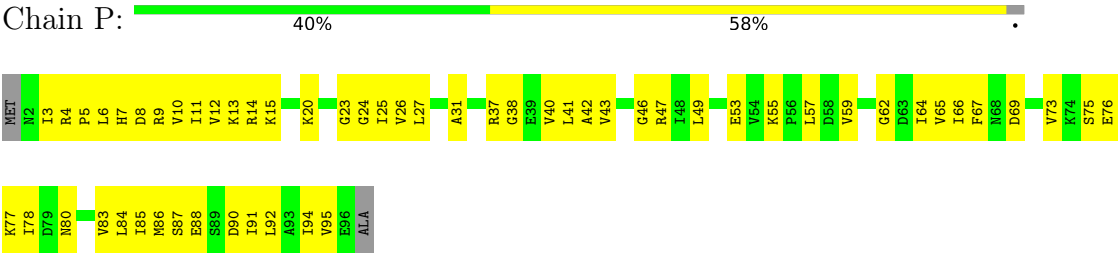




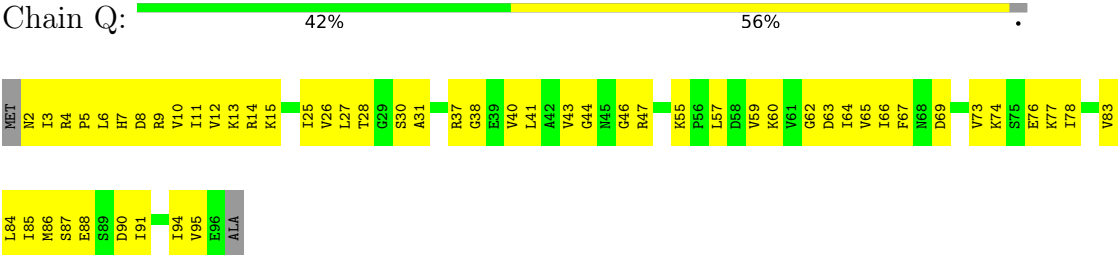
● Molecule 2: Co-chaperonin GroES



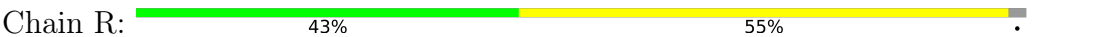
● Molecule 2: Co-chaperonin GroES



● Molecule 2: Co-chaperonin GroES



● Molecule 2: Co-chaperonin GroES

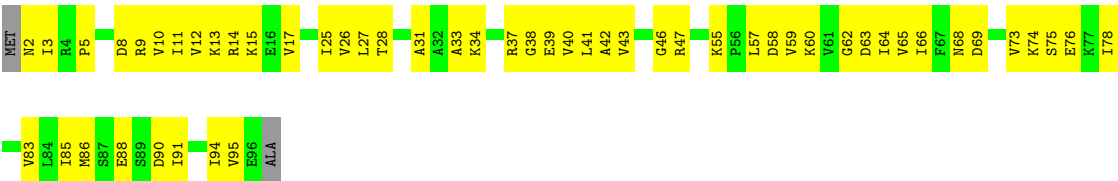




• Molecule 2: Co-chaperonin GroES



• Molecule 2: Co-chaperonin GroES



• Molecule 2: Co-chaperonin GroES



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C7	Depositor
Number of subtomograms used	10130	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 ($e^-/\text{\AA}^2$)	120	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.512	Depositor
Minimum map value	-0.283	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.0981	Depositor
Map size (Å)	450.56, 450.56, 450.56	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	3.52, 3.52, 3.52	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, K, MG, 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	0.20	0/3879	0.42	0/5238
1	B	0.20	0/3879	0.43	0/5238
1	C	0.20	0/3879	0.41	0/5238
1	D	0.20	0/3879	0.43	0/5238
1	E	0.20	0/3879	0.42	0/5238
1	F	0.19	0/3879	0.42	0/5238
1	G	0.20	0/3879	0.43	0/5238
1	H	0.20	0/3892	0.42	0/5254
1	I	0.21	0/3892	0.43	0/5254
1	J	0.20	0/3892	0.42	0/5254
1	K	0.20	0/3892	0.42	0/5254
1	L	0.20	0/3892	0.45	0/5254
1	M	0.20	0/3892	0.45	0/5254
1	N	0.20	0/3892	0.41	0/5254
2	O	0.23	0/690	0.44	0/930
2	P	0.22	0/690	0.45	0/930
2	Q	0.22	0/690	0.45	0/930
2	R	0.23	0/690	0.46	0/930
2	S	0.21	0/690	0.41	0/930
2	T	0.22	0/690	0.45	0/930
2	U	0.23	0/690	0.45	0/930
All	All	0.20	0/59227	0.43	0/79954

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3851	0	3970	286	0
1	B	3851	0	3971	288	0
1	C	3851	0	3971	284	0
1	D	3851	0	3970	268	0
1	E	3851	0	3970	274	0
1	F	3851	0	3970	290	0
1	G	3851	0	3970	271	0
1	H	3864	0	3989	282	0
1	I	3864	0	3989	285	0
1	J	3864	0	3989	292	0
1	K	3864	0	3989	301	0
1	L	3864	0	3989	283	0
1	M	3864	0	3989	298	0
1	N	3864	0	3989	292	0
2	O	687	0	718	65	0
2	P	687	0	718	69	0
2	Q	687	0	718	66	0
2	R	687	0	718	66	0
2	S	687	0	718	64	0
2	T	687	0	718	66	0
2	U	687	0	718	60	0
3	A	31	0	12	6	0
3	B	31	0	12	8	0
3	C	31	0	12	6	0
3	D	31	0	12	6	0
3	E	31	0	12	8	0
3	F	31	0	12	6	0
3	G	31	0	12	7	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0
5	N	1	0	0	0	0
6	H	27	0	12	4	0
6	I	27	0	12	4	0
6	J	27	0	12	5	0
6	K	27	0	12	5	0
6	L	27	0	12	4	0
6	M	27	0	12	4	0
6	N	27	0	12	7	0
7	A	30	0	0	2	0
7	B	29	0	0	2	0
7	C	28	0	0	1	0
7	D	30	0	0	4	0
7	E	29	0	0	2	0
7	F	30	0	0	4	0
7	G	27	0	0	2	0
7	H	1	0	0	0	0
7	I	1	0	0	0	0
7	J	1	0	0	0	0
7	K	1	0	0	0	0
7	L	1	0	0	0	0
7	M	1	0	0	0	0
7	N	1	0	0	0	0
All	All	59458	0	60909	4276	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 36.

The worst 5 of 4276 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:ALA:HA	1:D:520:MET:HE2	1.42	1.02
1:B:12:ALA:HA	1:B:520:MET:HE2	1.46	0.98
1:D:233:MET:HB3	1:D:237:LEU:HD23	1.49	0.95
1:L:166:MET:HB3	1:L:175:ILE:HD11	1.50	0.93
1:F:16:MET:HE2	1:F:520:MET:HE2	1.49	0.93

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	522/547 (95%)	504 (97%)	18 (3%)	0	100	100
1	B	522/547 (95%)	509 (98%)	13 (2%)	0	100	100
1	C	522/547 (95%)	506 (97%)	16 (3%)	0	100	100
1	D	522/547 (95%)	510 (98%)	12 (2%)	0	100	100
1	E	522/547 (95%)	507 (97%)	15 (3%)	0	100	100
1	F	522/547 (95%)	507 (97%)	15 (3%)	0	100	100
1	G	522/547 (95%)	510 (98%)	12 (2%)	0	100	100
1	H	523/547 (96%)	500 (96%)	23 (4%)	0	100	100
1	I	523/547 (96%)	500 (96%)	23 (4%)	0	100	100
1	J	523/547 (96%)	500 (96%)	23 (4%)	0	100	100
1	K	523/547 (96%)	500 (96%)	23 (4%)	0	100	100
1	L	523/547 (96%)	499 (95%)	24 (5%)	0	100	100
1	M	523/547 (96%)	504 (96%)	19 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	523/547 (96%)	502 (96%)	21 (4%)	0	100	100
2	O	93/97 (96%)	87 (94%)	6 (6%)	0	100	100
2	P	93/97 (96%)	88 (95%)	5 (5%)	0	100	100
2	Q	93/97 (96%)	89 (96%)	4 (4%)	0	100	100
2	R	93/97 (96%)	87 (94%)	6 (6%)	0	100	100
2	S	93/97 (96%)	85 (91%)	8 (9%)	0	100	100
2	T	93/97 (96%)	90 (97%)	3 (3%)	0	100	100
2	U	93/97 (96%)	89 (96%)	4 (4%)	0	100	100
All	All	7966/8337 (96%)	7673 (96%)	293 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	403/414 (97%)	403 (100%)	0	100	100
1	B	403/414 (97%)	403 (100%)	0	100	100
1	C	403/414 (97%)	403 (100%)	0	100	100
1	D	403/414 (97%)	403 (100%)	0	100	100
1	E	403/414 (97%)	403 (100%)	0	100	100
1	F	403/414 (97%)	403 (100%)	0	100	100
1	G	403/414 (97%)	403 (100%)	0	100	100
1	H	405/414 (98%)	405 (100%)	0	100	100
1	I	405/414 (98%)	405 (100%)	0	100	100
1	J	405/414 (98%)	405 (100%)	0	100	100
1	K	405/414 (98%)	405 (100%)	0	100	100
1	L	405/414 (98%)	405 (100%)	0	100	100
1	M	405/414 (98%)	405 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	405/414 (98%)	405 (100%)	0	100	100
2	O	73/80 (91%)	73 (100%)	0	100	100
2	P	73/80 (91%)	73 (100%)	0	100	100
2	Q	73/80 (91%)	73 (100%)	0	100	100
2	R	73/80 (91%)	73 (100%)	0	100	100
2	S	73/80 (91%)	73 (100%)	0	100	100
2	T	73/80 (91%)	73 (100%)	0	100	100
2	U	73/80 (91%)	73 (100%)	0	100	100
All	All	6167/6356 (97%)	6167 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	72	GLN
1	L	72	GLN
1	I	487	ASN
1	L	10	ASN
1	L	343	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 42 ligands modelled in this entry, 28 are monoatomic - leaving 14 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$
3	ATP	D	601	4,5	32,33,33	0.27	0	48,52,52	0.29	0
6	ADP	I	601	4,5	28,29,29	1.37	4 (14%)	43,45,45	1.88	9 (20%)
6	ADP	N	601	4,5	28,29,29	1.39	5 (17%)	43,45,45	1.85	10 (23%)
3	ATP	G	601	4,5	32,33,33	0.26	0	48,52,52	0.29	0
6	ADP	J	601	4,5	28,29,29	1.40	4 (14%)	43,45,45	1.86	10 (23%)
3	ATP	B	601	4,5	32,33,33	0.27	0	48,52,52	0.29	0
3	ATP	F	601	4,5	32,33,33	0.28	0	48,52,52	0.29	0
3	ATP	C	601	5	32,33,33	0.27	0	48,52,52	0.29	0
3	ATP	A	601	4,5	32,33,33	0.27	0	48,52,52	0.28	0
6	ADP	K	601	4,5	28,29,29	1.39	4 (14%)	43,45,45	1.84	10 (23%)
6	ADP	H	601	4,5	28,29,29	1.39	4 (14%)	43,45,45	1.86	10 (23%)
6	ADP	M	601	4,5	28,29,29	1.38	4 (14%)	43,45,45	1.88	9 (20%)
3	ATP	E	601	4,5	32,33,33	0.27	0	48,52,52	0.29	0
6	ADP	L	601	4,5	28,29,29	1.40	5 (17%)	43,45,45	1.84	10 (23%)

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
3	ATP	D	601	4,5	-	5/22/38/38	0/3/3/3
6	ADP	I	601	4,5	-	6/16/32/32	0/3/3/3
6	ADP	N	601	4,5	-	5/16/32/32	0/3/3/3
3	ATP	G	601	4,5	-	6/22/38/38	0/3/3/3
6	ADP	J	601	4,5	-	6/16/32/32	0/3/3/3
3	ATP	B	601	4,5	-	4/22/38/38	0/3/3/3
3	ATP	F	601	4,5	-	4/22/38/38	0/3/3/3
3	ATP	C	601	5	-	4/22/38/38	0/3/3/3
3	ATP	A	601	4,5	-	2/22/38/38	0/3/3/3
6	ADP	K	601	4,5	-	6/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ADP	H	601	4,5	-	5/16/32/32	0/3/3/3
6	ADP	M	601	4,5	-	6/16/32/32	0/3/3/3
3	ATP	E	601	4,5	-	3/22/38/38	0/3/3/3
6	ADP	L	601	4,5	-	5/16/32/32	0/3/3/3

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	601	ADP	C5-C4	4.60	1.47	1.39
6	L	601	ADP	C5-C4	4.57	1.47	1.39
6	M	601	ADP	C5-C4	4.57	1.47	1.39
6	N	601	ADP	C5-C4	4.56	1.47	1.39
6	I	601	ADP	C5-C4	4.55	1.47	1.39

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	601	ADP	C5-C4-N3	-5.89	118.61	126.72
6	J	601	ADP	C5-C4-N3	-5.86	118.65	126.72
6	H	601	ADP	C5-C4-N3	-5.83	118.69	126.72
6	K	601	ADP	C5-C4-N3	-5.80	118.74	126.72
6	N	601	ADP	C5-C4-N3	-5.76	118.78	126.72

There are no chirality outliers.

5 of 67 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	601	ATP	C5'-O5'-PA-O2A
6	H	601	ADP	C5'-O5'-PA-O3A
6	I	601	ADP	C5'-O5'-PA-O1A
6	I	601	ADP	C5'-O5'-PA-O3A
6	J	601	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

14 monomers are involved in 80 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	601	ATP	6	0
6	I	601	ADP	4	0
6	N	601	ADP	7	0

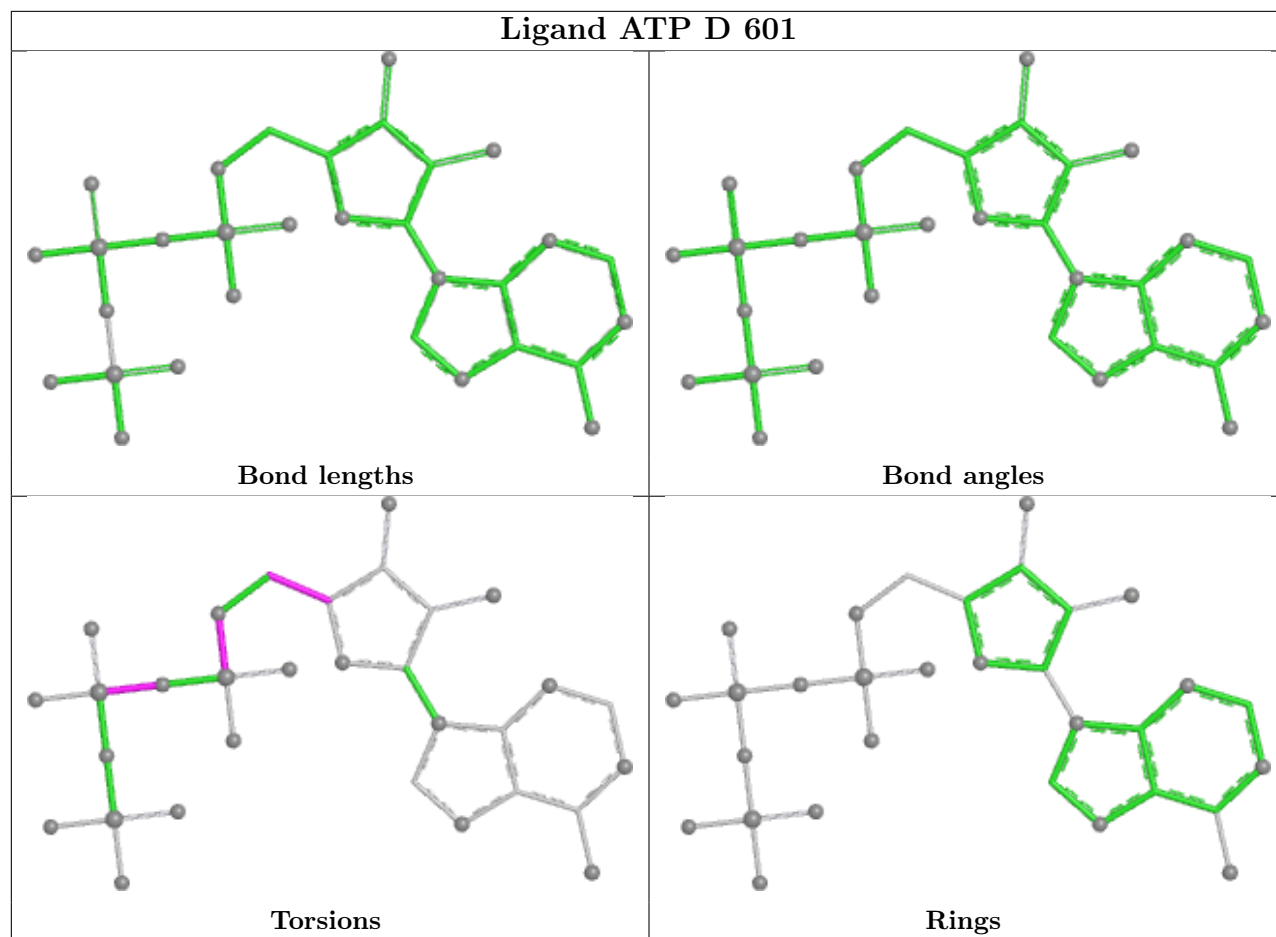
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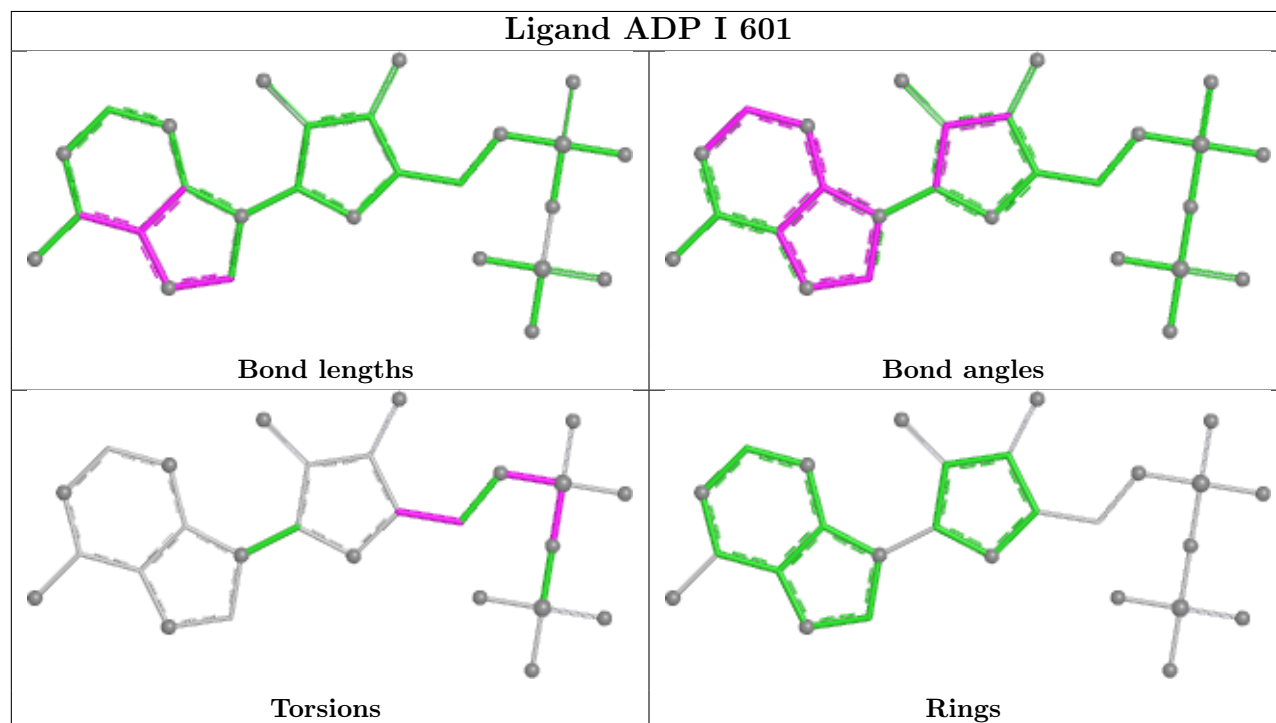
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	601	ATP	7	0
6	J	601	ADP	5	0
3	B	601	ATP	8	0
3	F	601	ATP	6	0
3	C	601	ATP	6	0
3	A	601	ATP	6	0
6	K	601	ADP	5	0
6	H	601	ADP	4	0
6	M	601	ADP	4	0
3	E	601	ATP	8	0
6	L	601	ADP	4	0

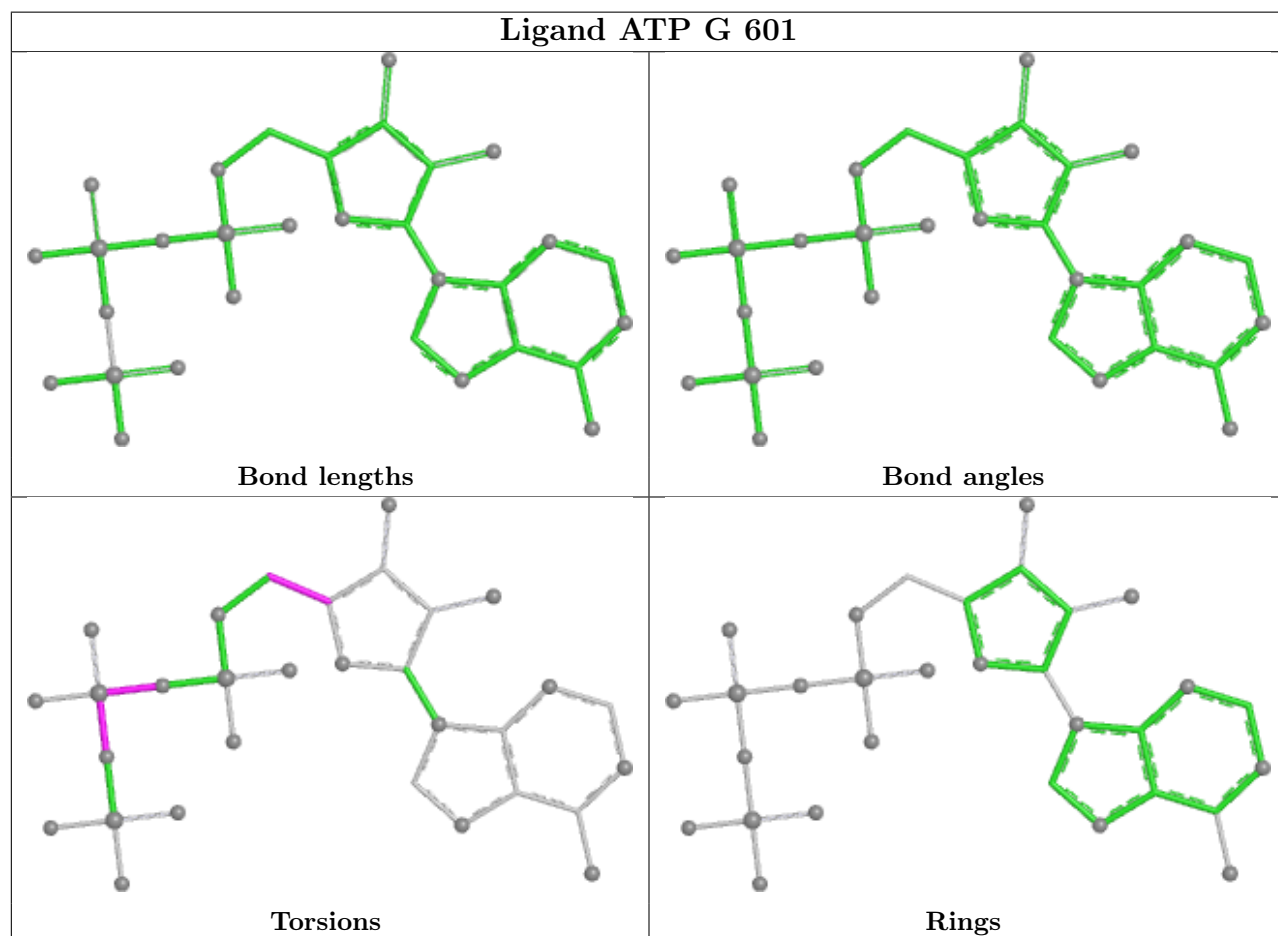
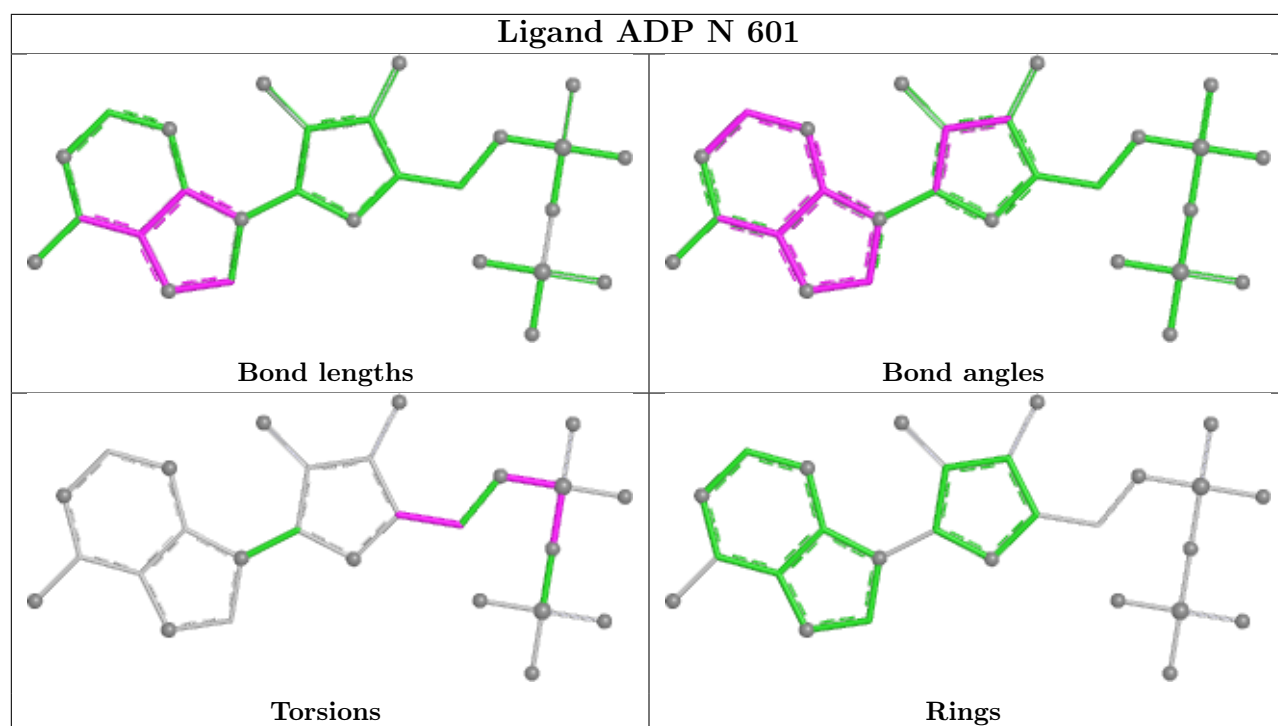
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

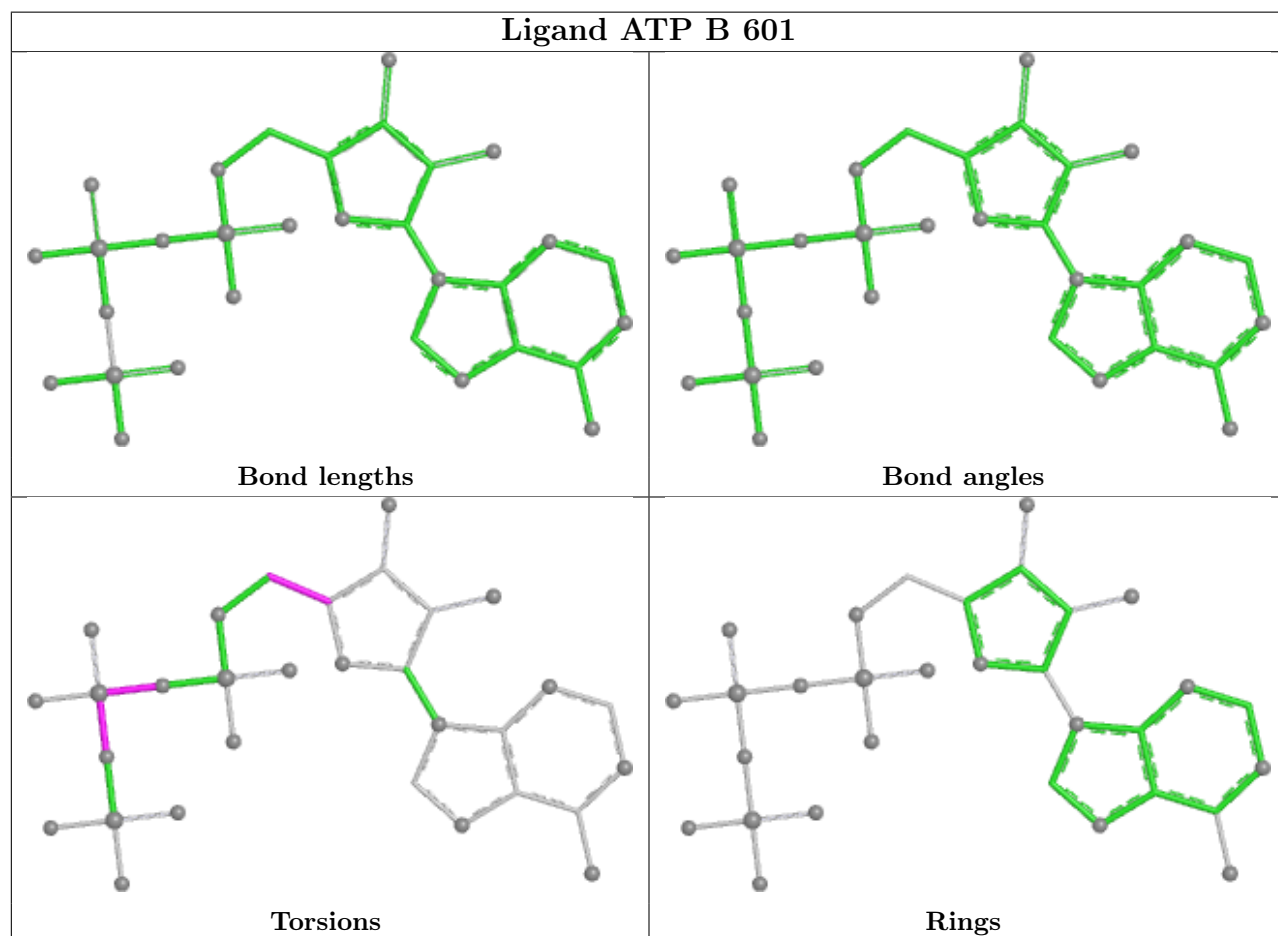
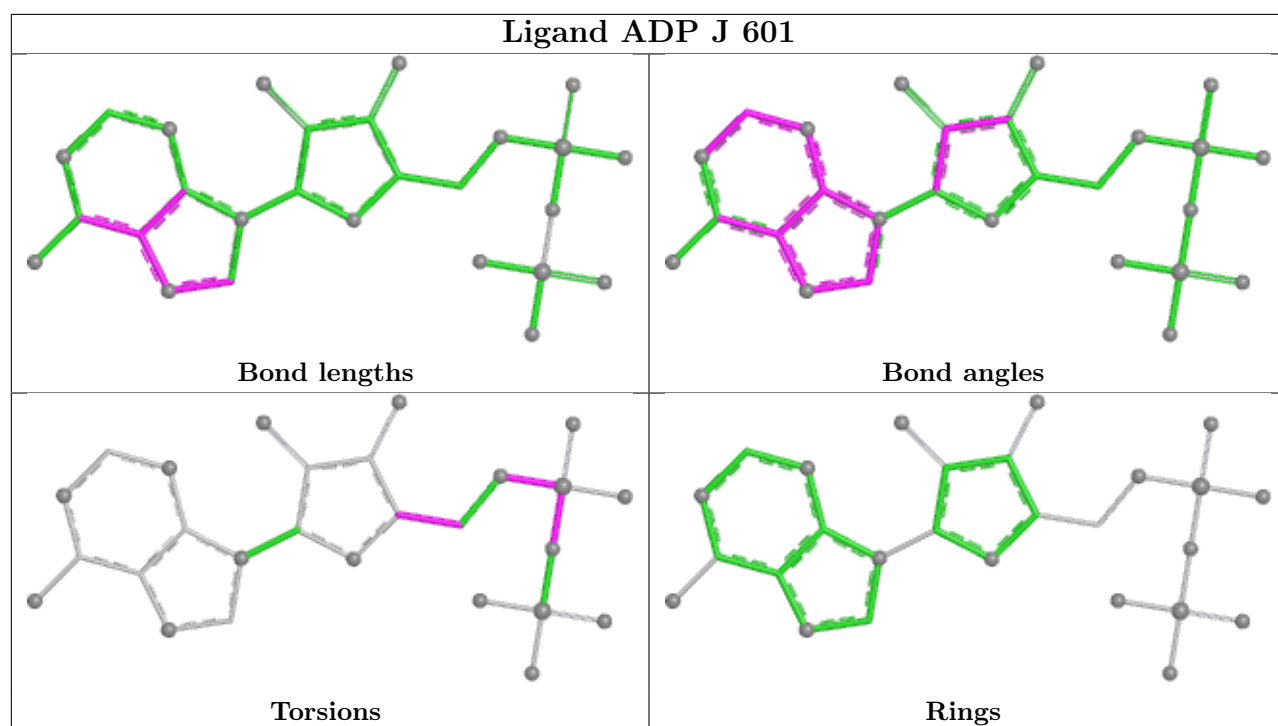
Ligand ATP D 601

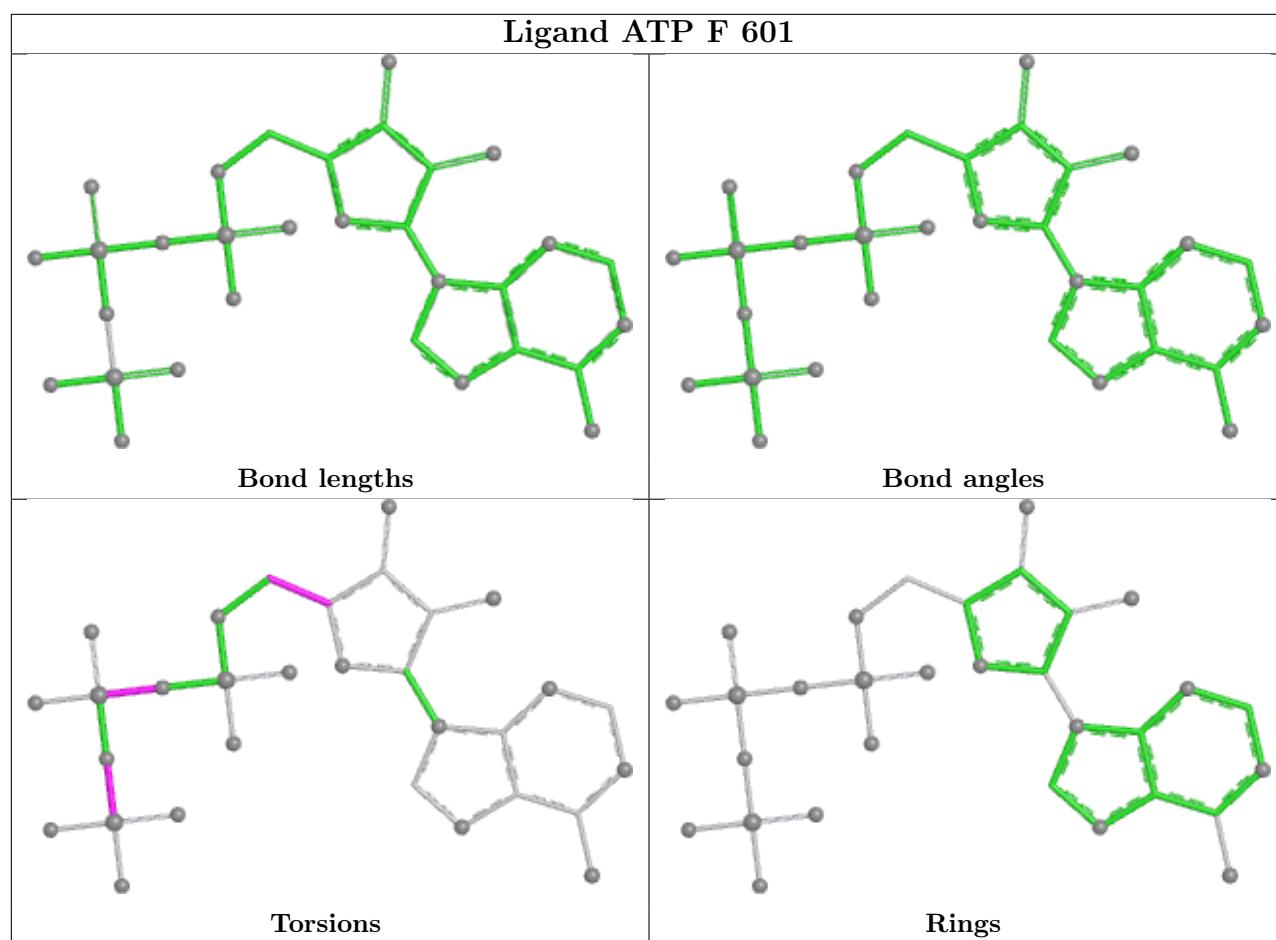


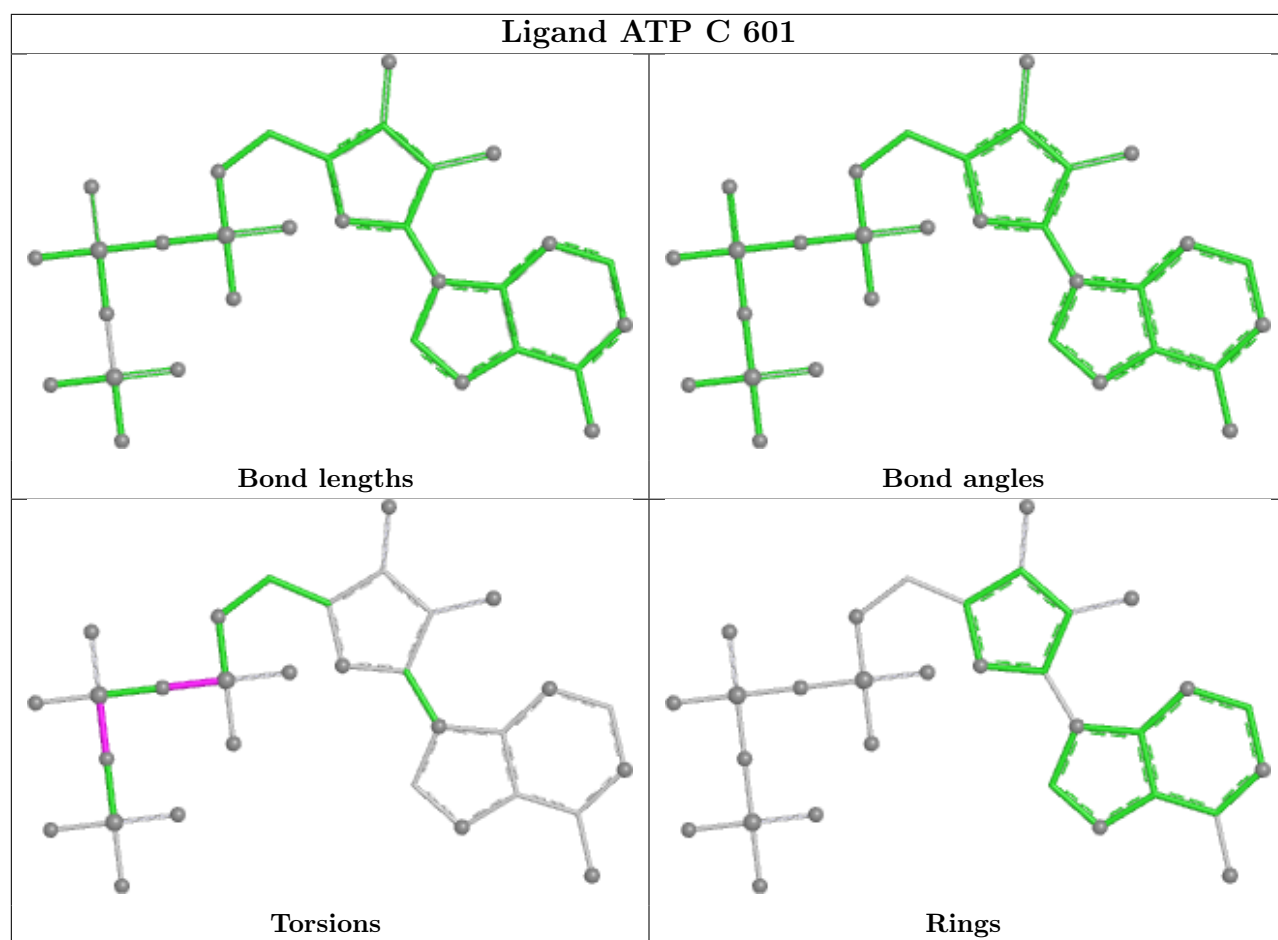
Ligand ADP I 601



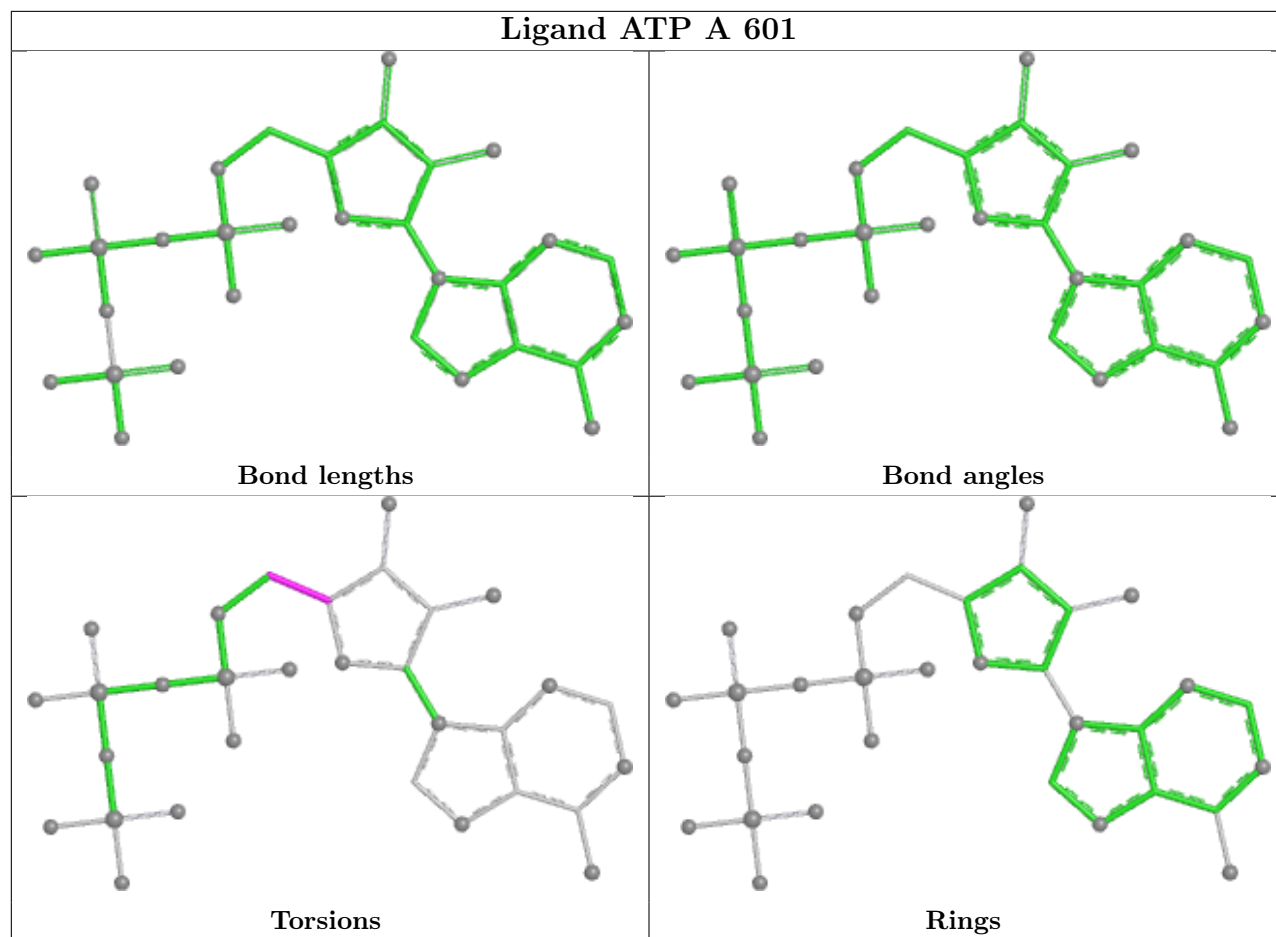




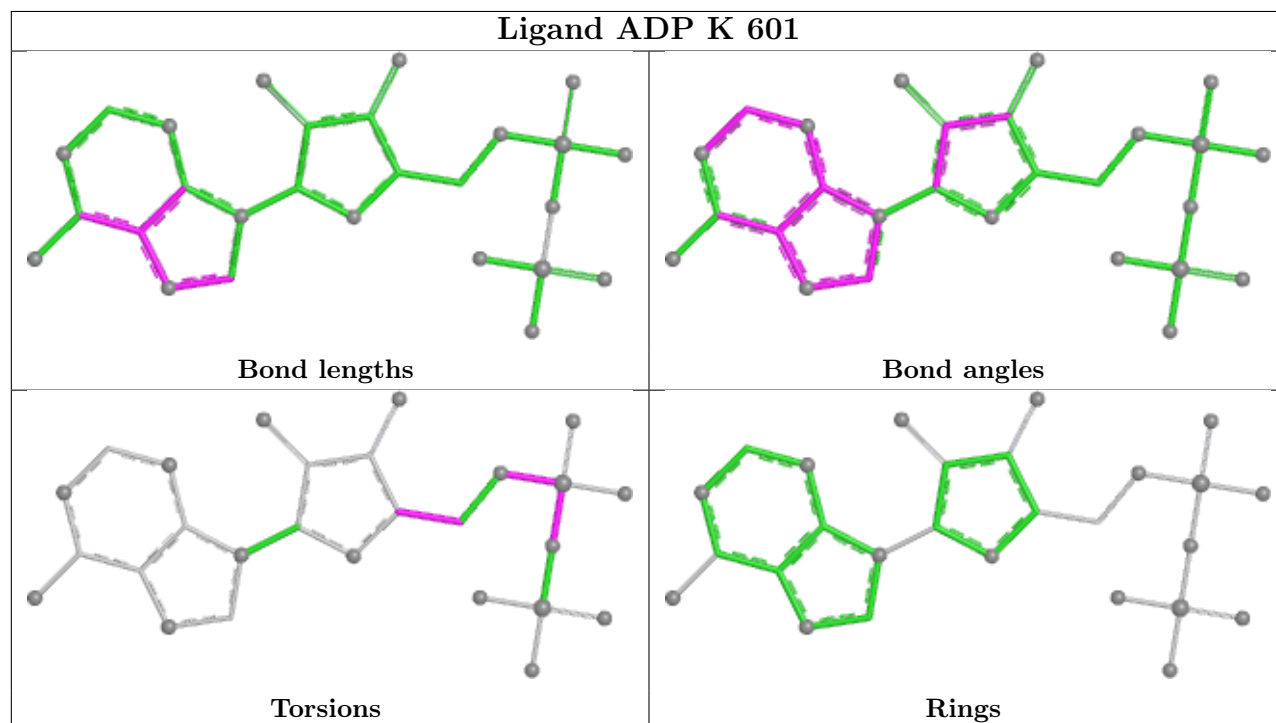


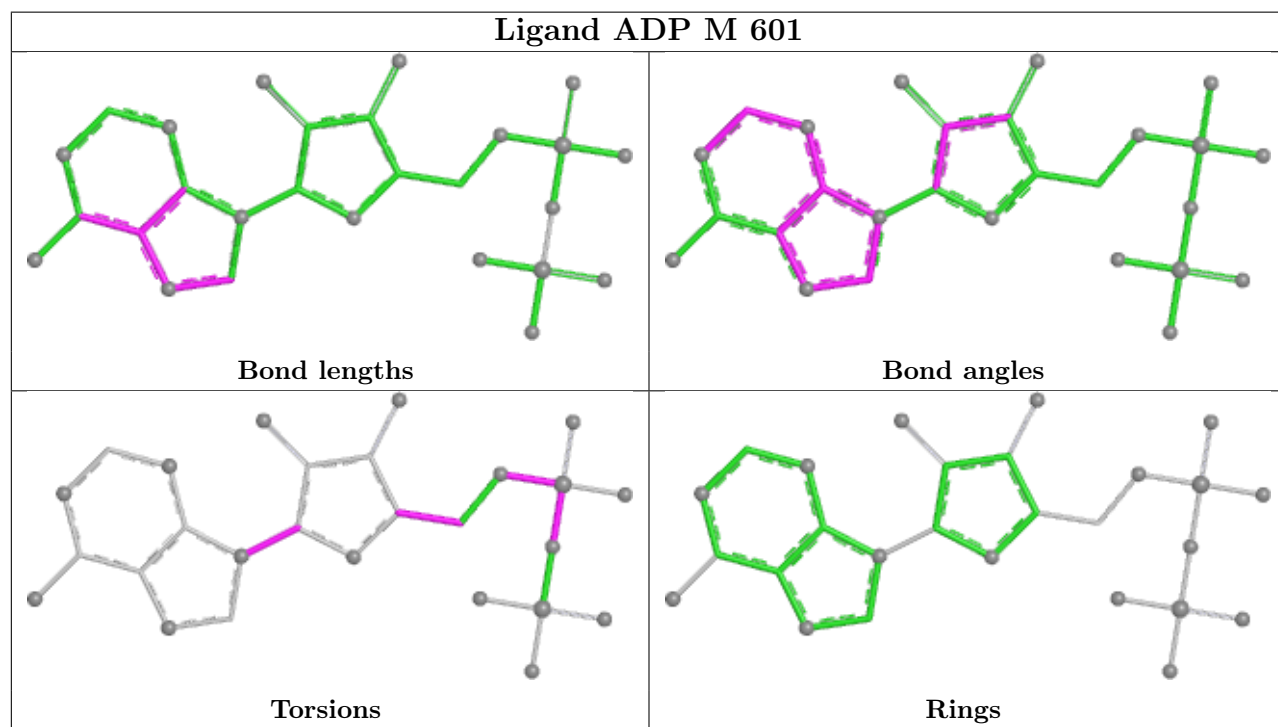
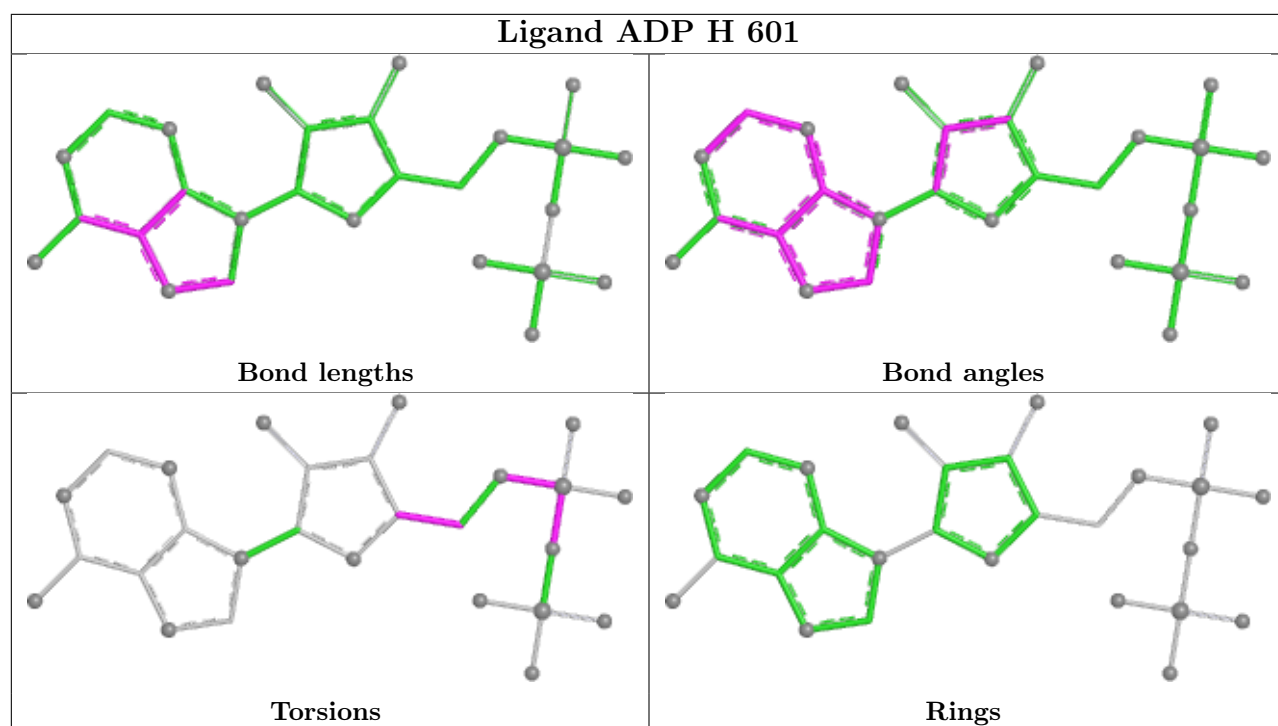


Ligand ATP A 601

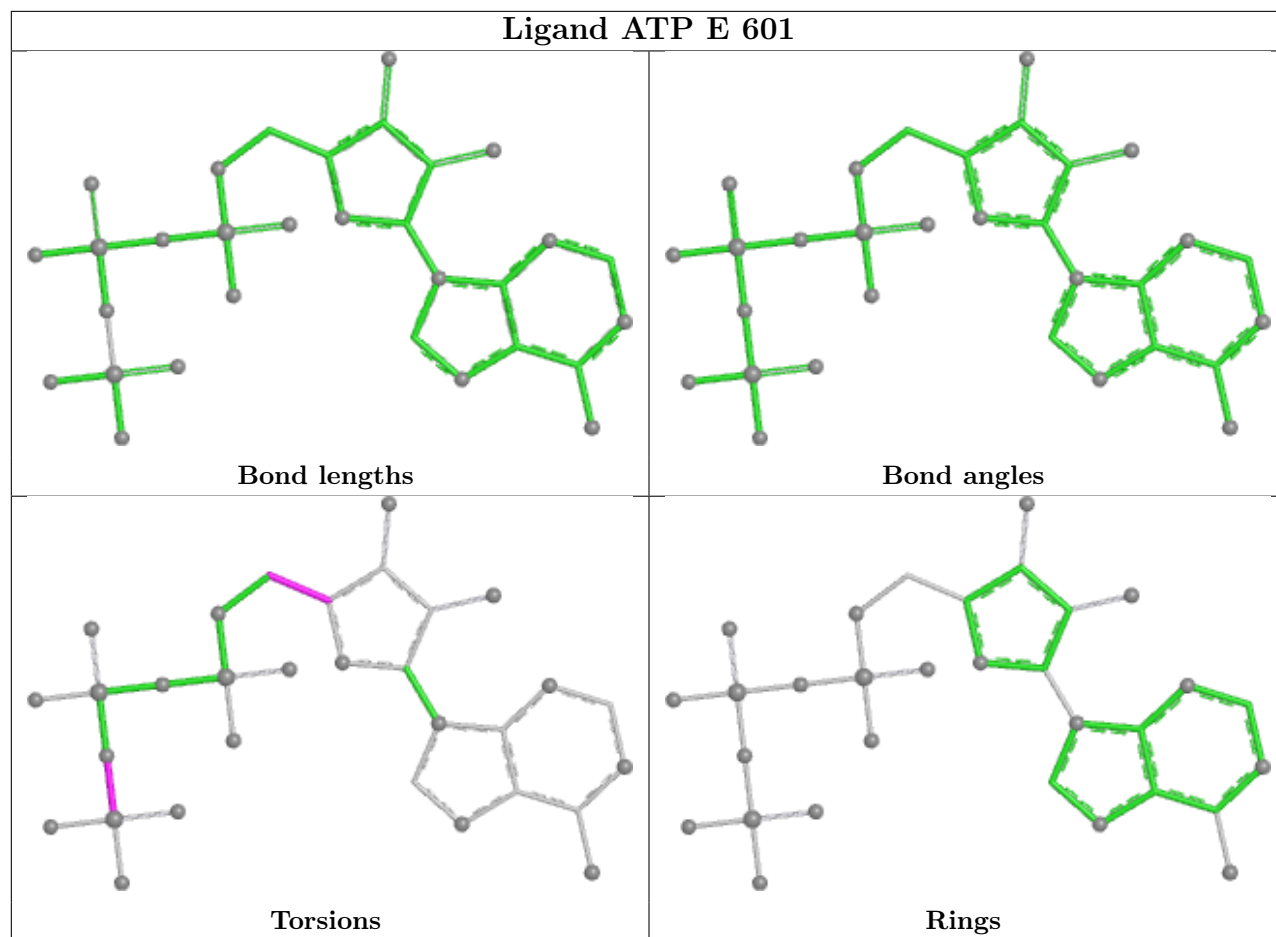


Ligand ADP K 601

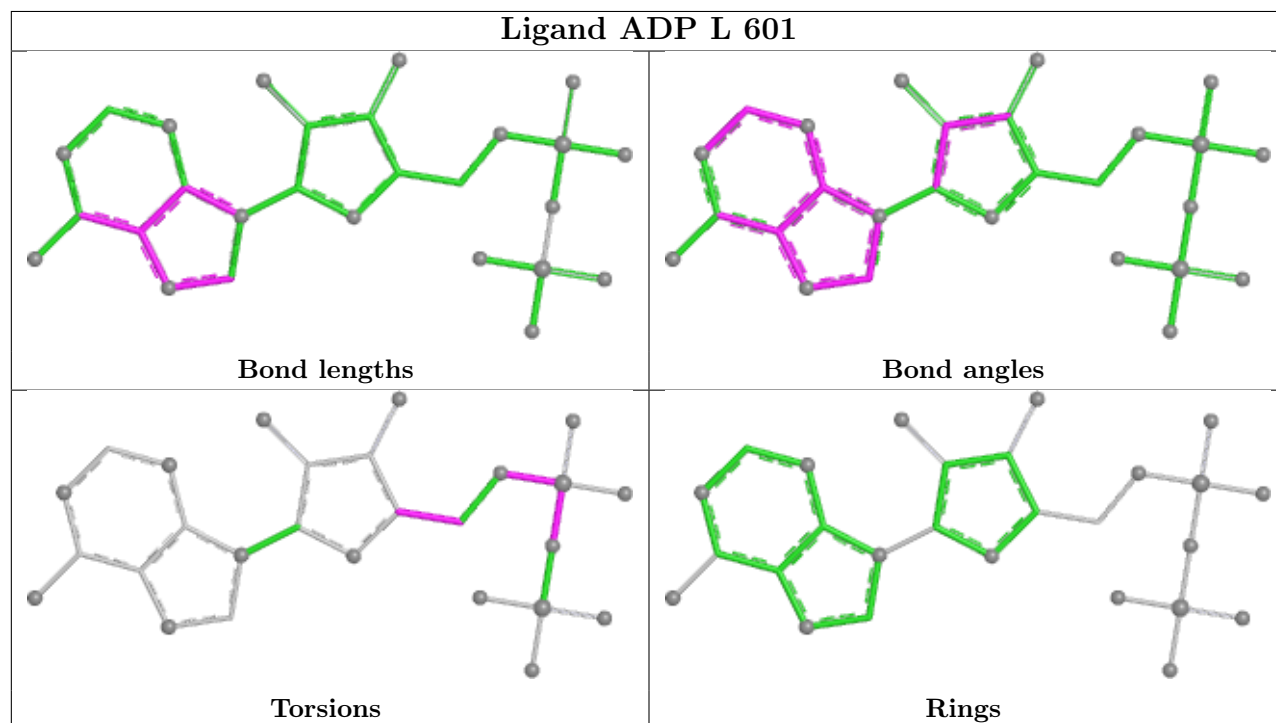




Ligand ATP E 601



Ligand ADP L 601



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.

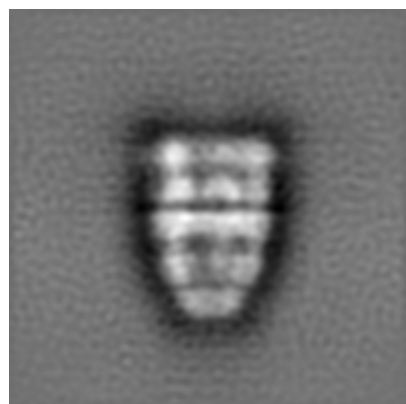
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18737. These allow visual inspection of the internal detail of the map and identification of artifacts.

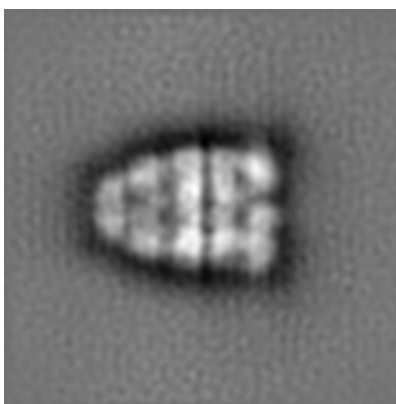
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

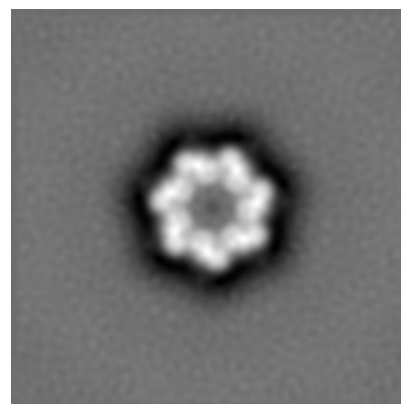
6.1.1 Primary map



X

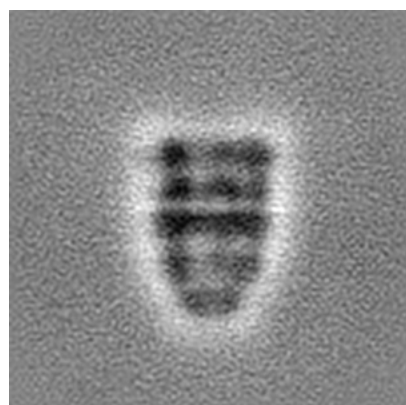


Y

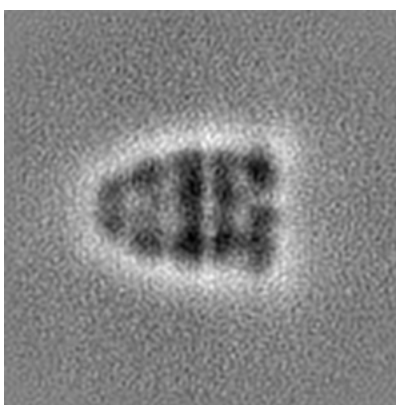


Z

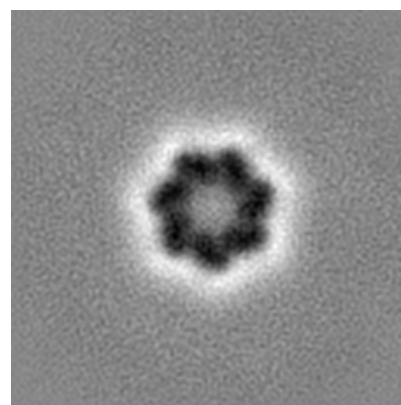
6.1.2 Raw map



X



Y

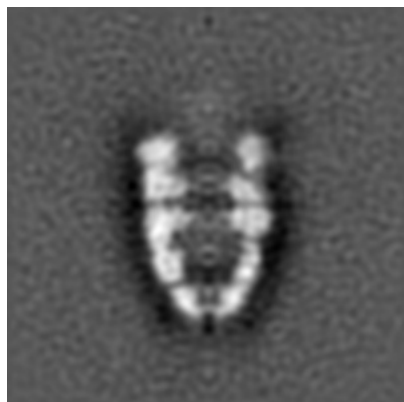


Z

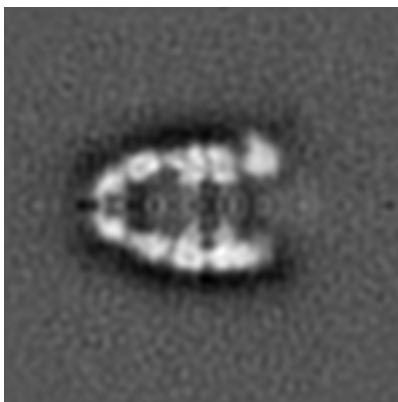
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

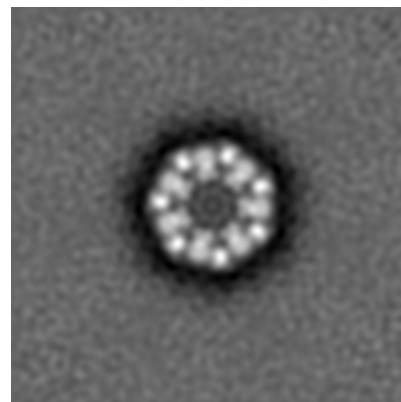
6.2.1 Primary map



X Index: 64



Y Index: 64

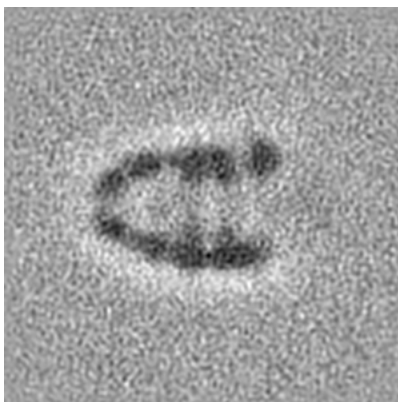


Z Index: 64

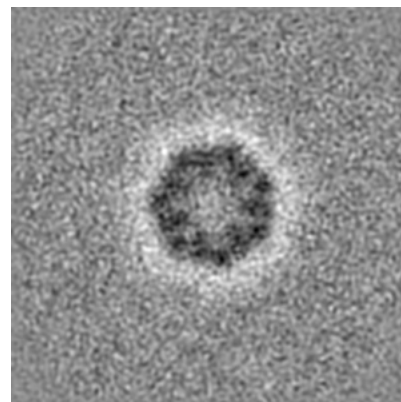
6.2.2 Raw map



X Index: 64



Y Index: 64

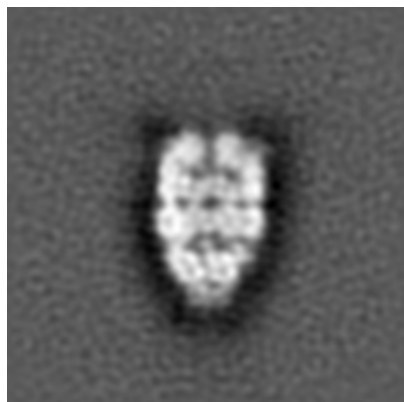


Z Index: 64

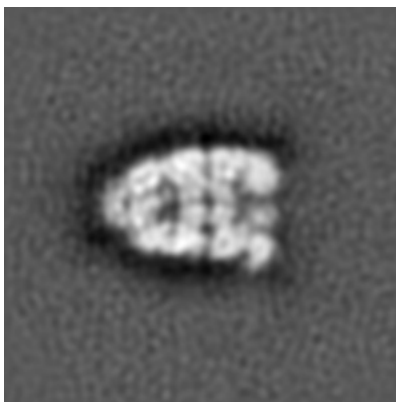
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

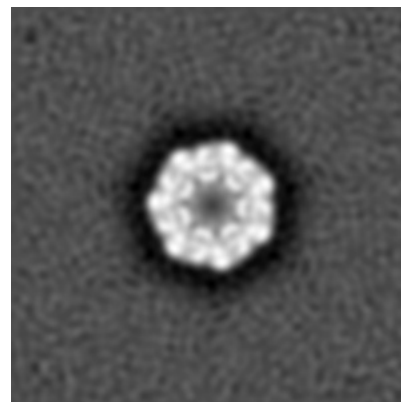
6.3.1 Primary map



X Index: 53



Y Index: 54

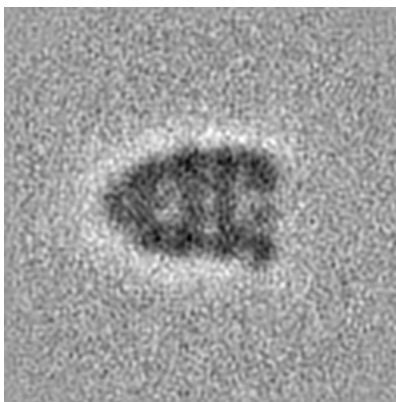


Z Index: 61

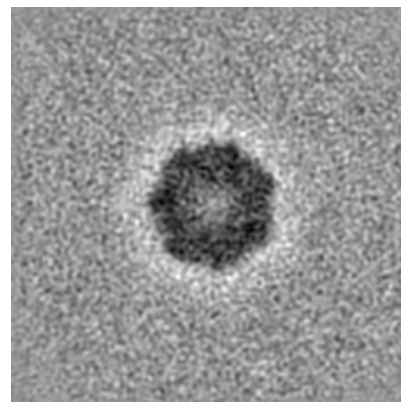
6.3.2 Raw map



X Index: 52



Y Index: 54

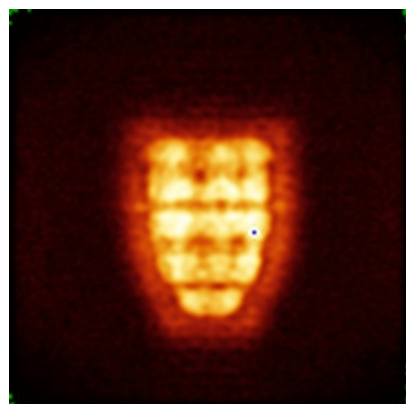


Z Index: 60

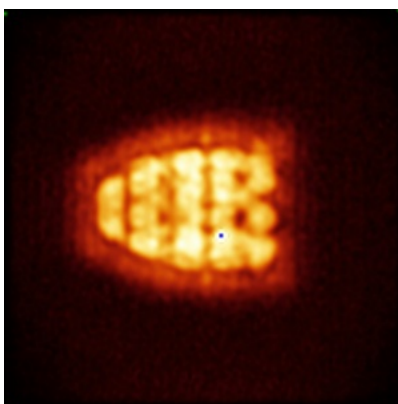
The images above show the largest variance slices of the map in three orthogonal directions.

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

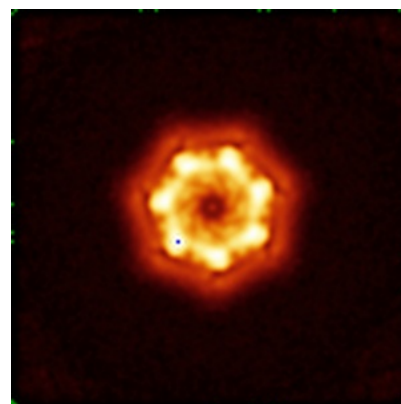
6.4.1 Primary map



X

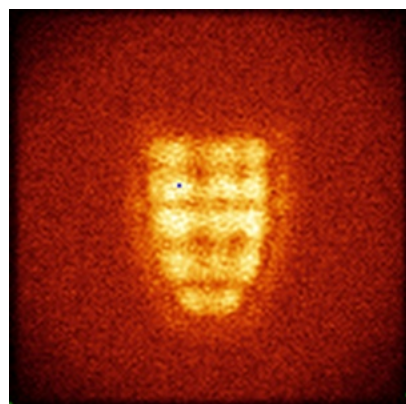


Y

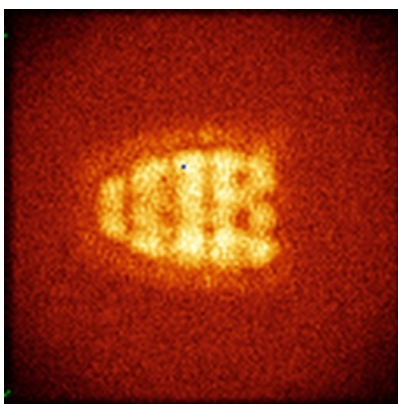


Z

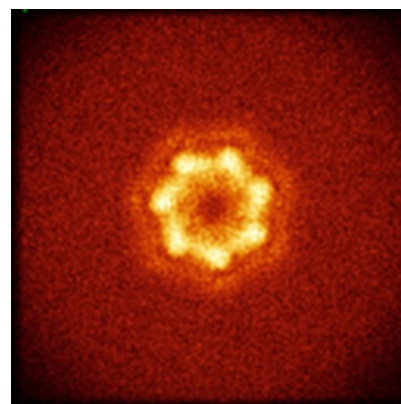
6.4.2 Raw map



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](#)

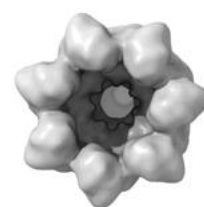
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0981. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

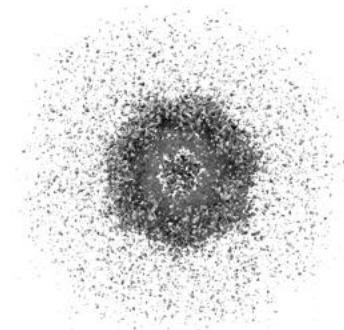
6.5.2 Raw map



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.

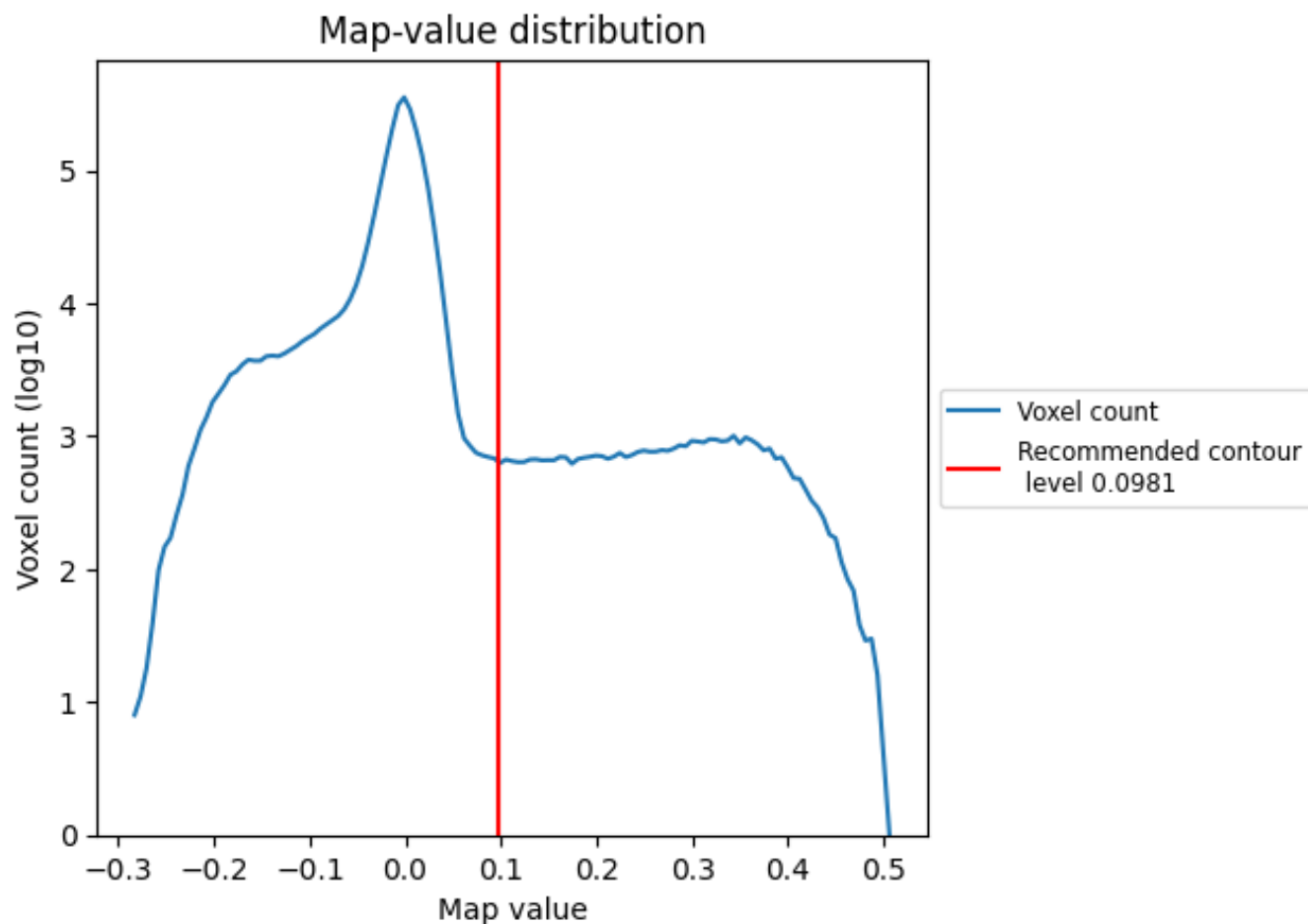
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

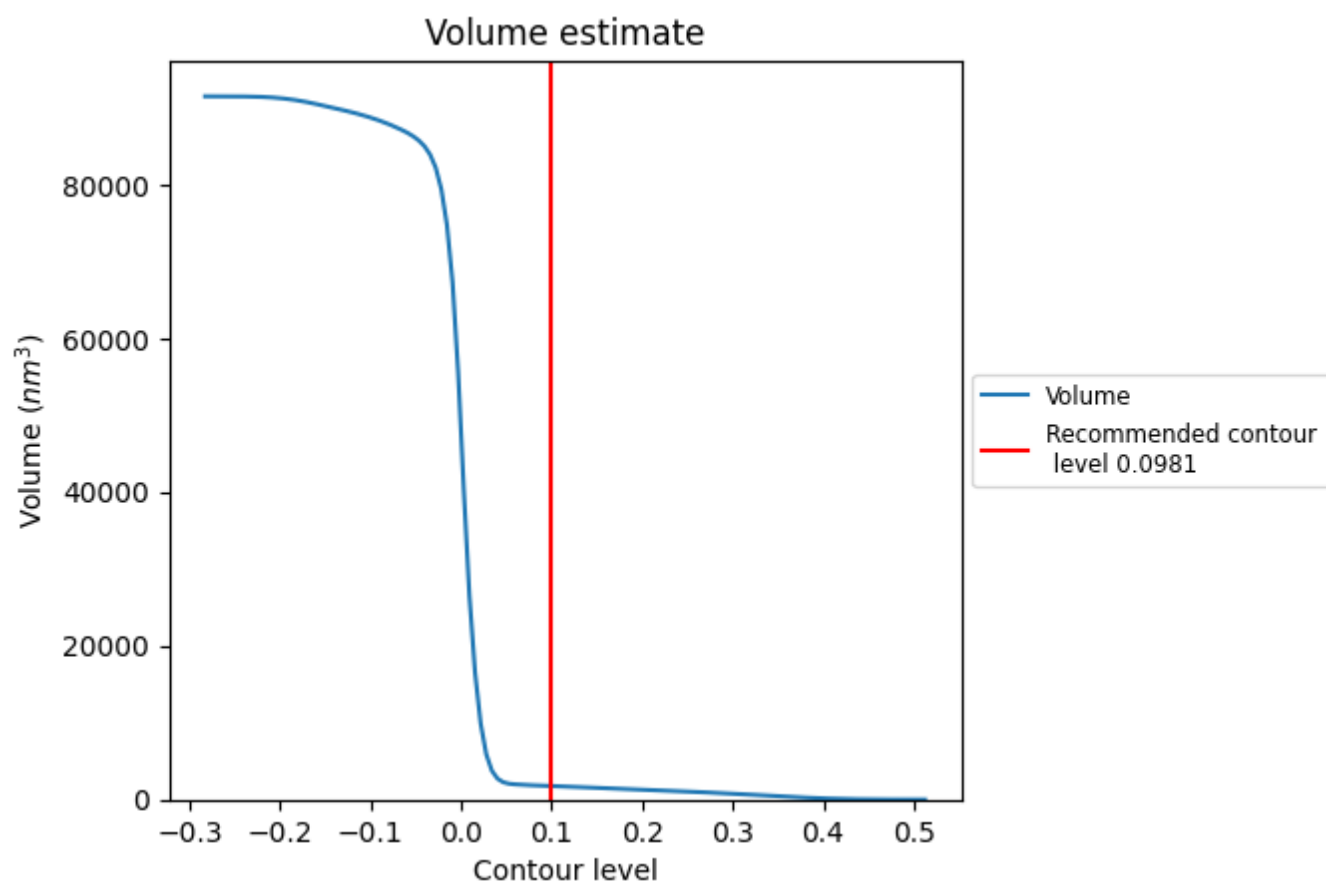
This section contains the results of statistical analysis of the map.

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.

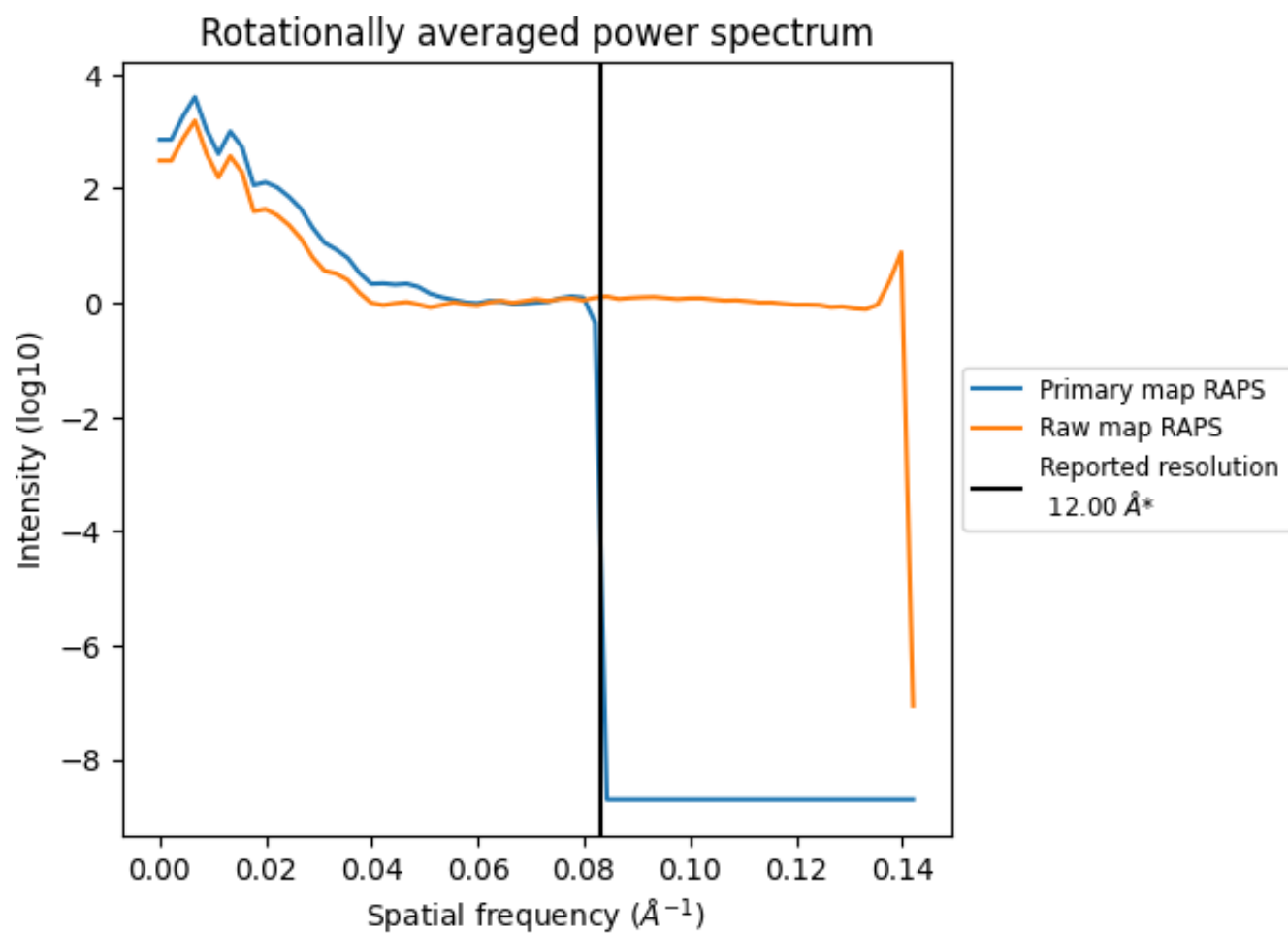
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1763 nm³; this corresponds to an approximate mass of 1593 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 ⓘ

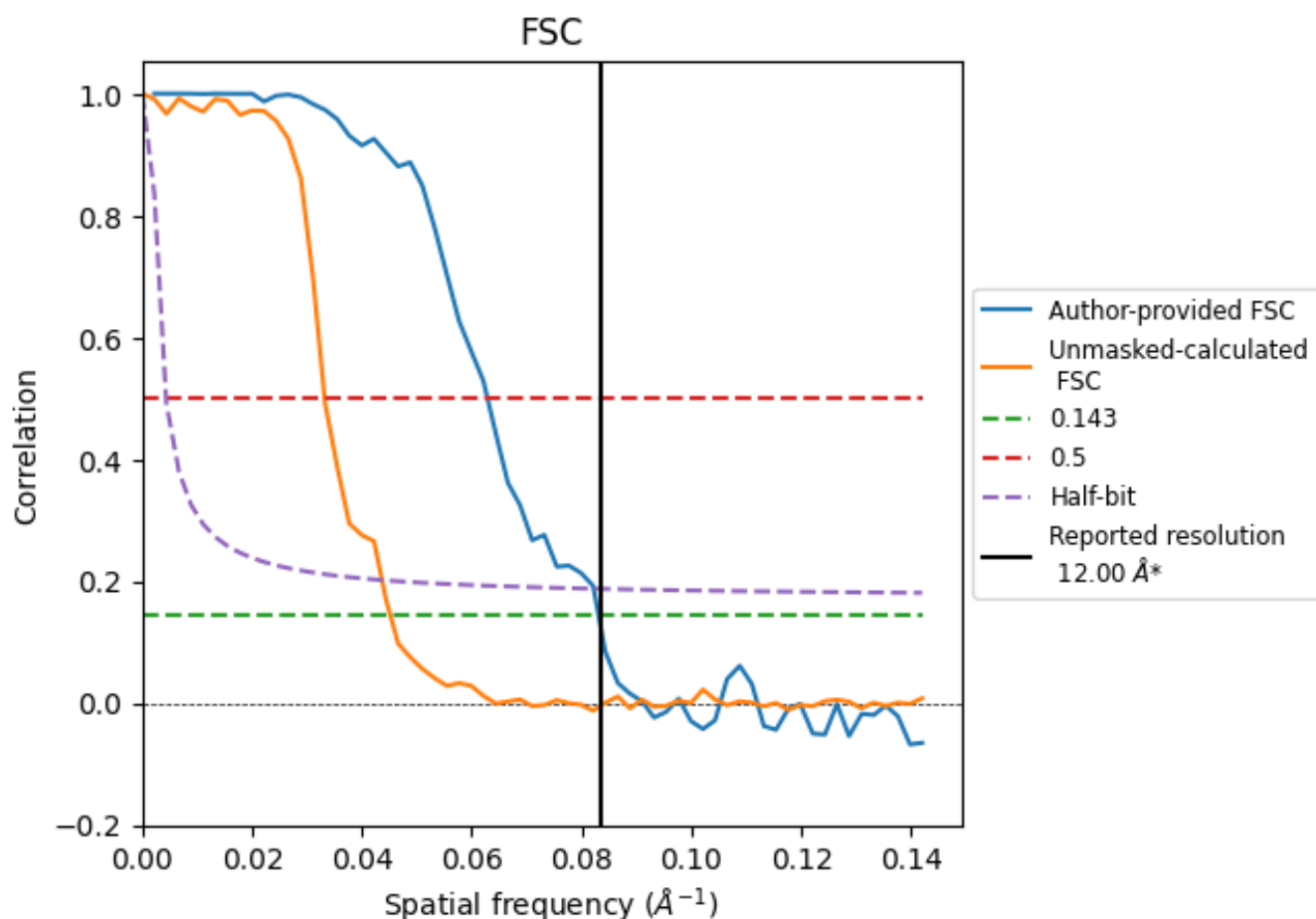


*Reported resolution corresponds to spatial frequency of $0.083 \text{ \AA}^{-1}$

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 0.083 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

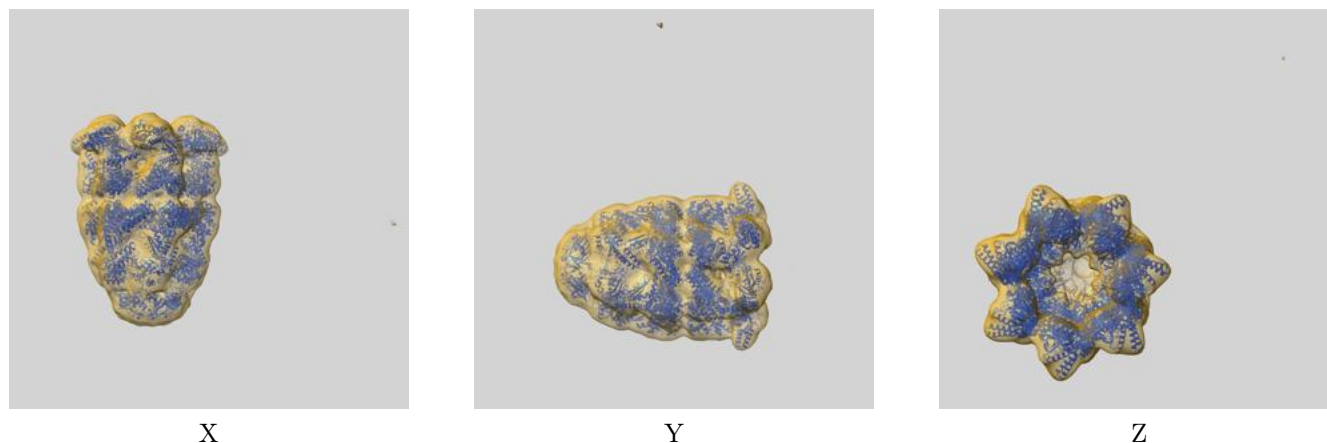
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	12.00	-	-
Author-provided FSC curve	12.03	15.90	12.17
Unmasked-calculated*	22.12	30.12	22.94

*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 22.12 differs from the reported value 12.0 by more than 10 %

9 Map-model fit [i](#)

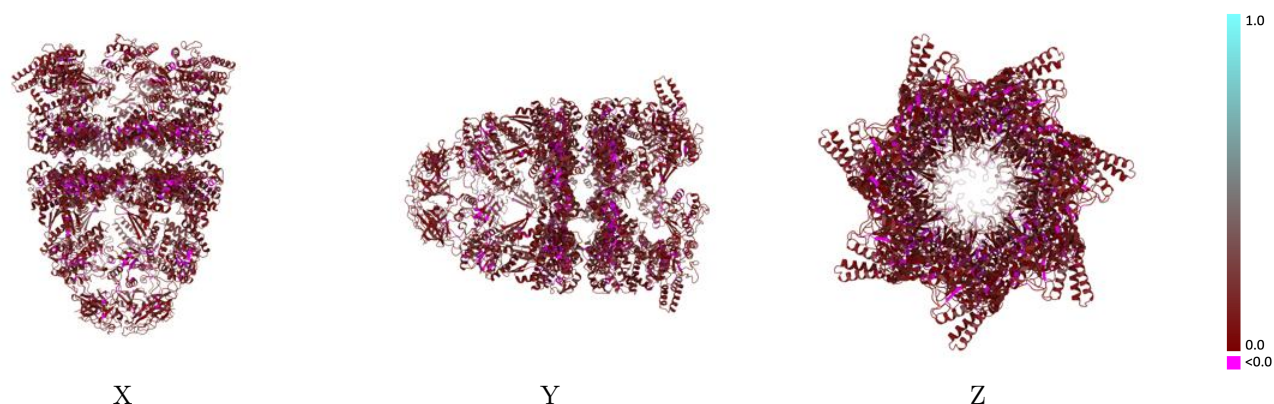
This section contains information regarding the fit between EMDB map EMD-18737 and PDB model 8QXU. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



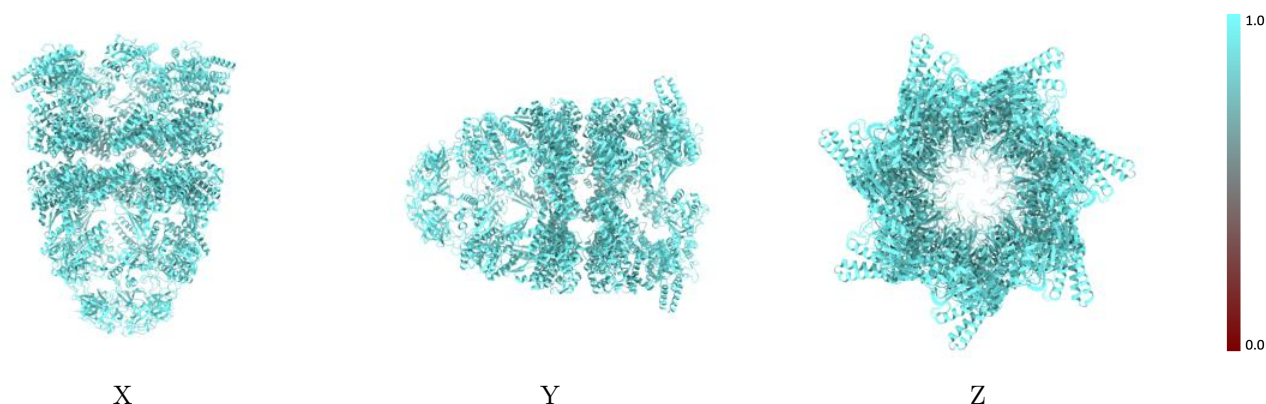
The images above show the 3D surface view of the map at the recommended contour level 0.0981 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



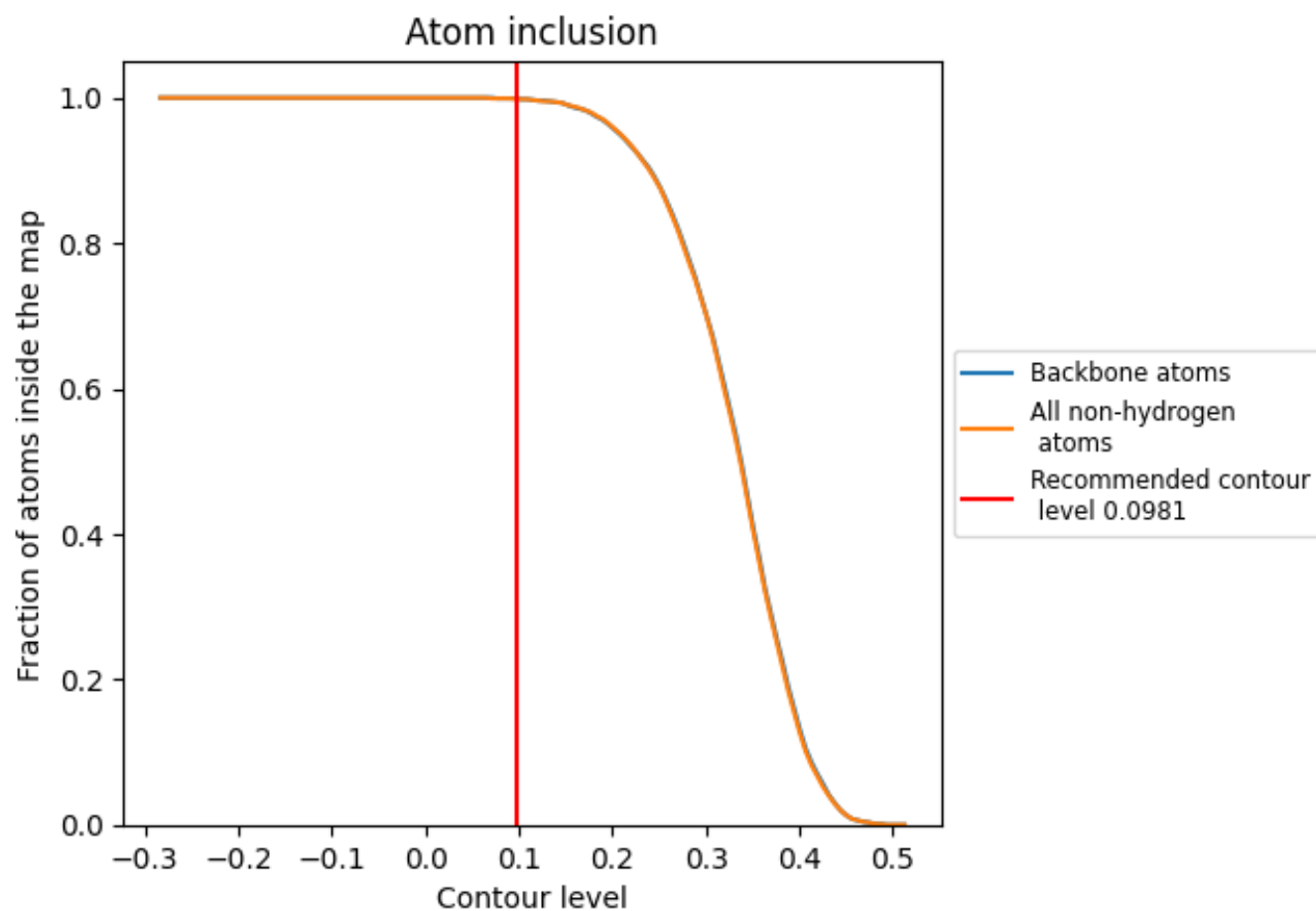
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0981).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.0981) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9980	 0.1040
A	 1.0000	 0.1080
B	 1.0000	 0.1060
C	 1.0000	 0.1070
D	 1.0000	 0.1040
E	 1.0000	 0.1040
F	 1.0000	 0.1040
G	 1.0000	 0.1070
H	 0.9970	 0.1010
I	 0.9960	 0.1000
J	 0.9960	 0.1030
K	 0.9960	 0.1010
L	 0.9960	 0.1000
M	 0.9960	 0.1020
N	 0.9960	 0.1040
O	 1.0000	 0.1090
P	 1.0000	 0.1080
Q	 1.0000	 0.1030
R	 1.0000	 0.1090
S	 1.0000	 0.1090
T	 1.0000	 0.1070
U	 1.0000	 0.1040

