



wwPDB EM Validation Summary Report ⓘ

Aug 25, 2026 – 11:47 am BST

PDB ID : 8BA8 / pdb_00008ba8
EMDB ID : EMD-15940
Title : CryoEM structure of GroEL-ADP.BeF3-Rubisco.
Authors : Gardner, S.; Saibil, H.R.
Deposited on : 2022-10-11
Resolution : 3.40 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 ⓘ 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:

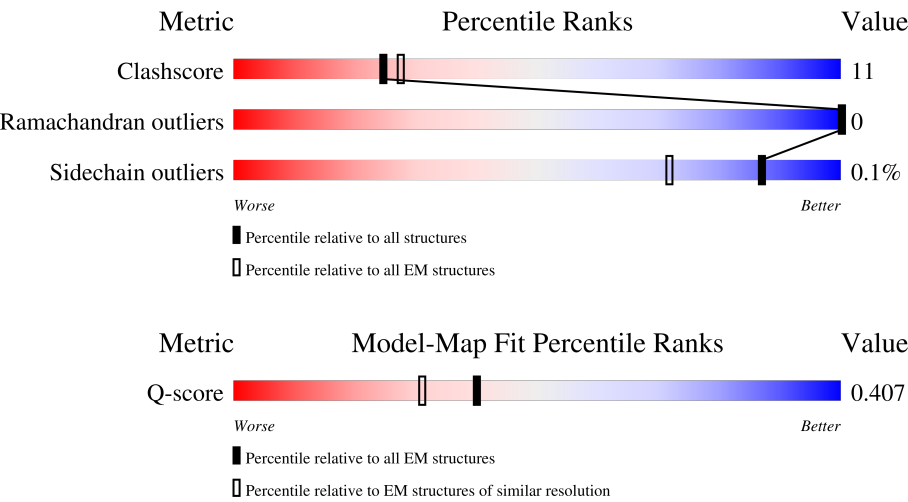
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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)
Validation Pipeline (wwPDB-VP) : 2.50

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 3.40 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	14717 (2.90 - 3.90)

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	548	
1	B	548	
1	C	548	
1	D	548	

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Mol	Chain	Length	Quality of chain
1	E	548	
1	F	548	
1	G	548	
1	H	548	
1	I	548	
1	J	548	
1	K	548	
1	L	548	
1	M	548	
1	N	548	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BEF	B	603	-	-	X	-
2	BEF	C	603	-	-	X	-
2	BEF	F	601	-	-	X	-
2	BEF	G	603	-	-	X	-

2 Entry composition

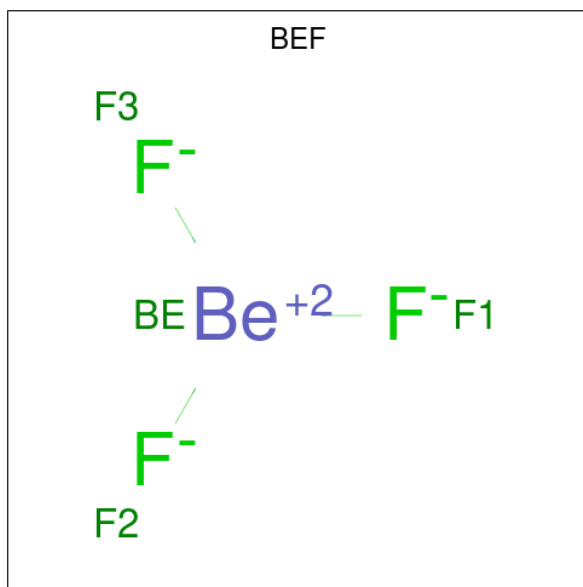
There are 6 unique types of molecules in this entry. The entry contains 110327 atoms, of which 55902 are hydrogens and 0 are deuteriums.

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.

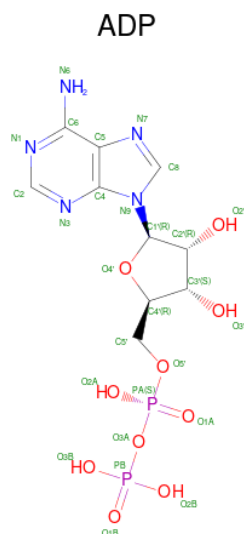
Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	525	Total	C	H	N	O	S	0	0
			7854	2403	3990	667	774	20		
1	B	525	Total	C	H	N	O	S	0	0
			7854	2403	3990	667	774	20		
1	C	525	Total	C	H	N	O	S	0	0
			7854	2403	3990	667	774	20		
1	D	525	Total	C	H	N	O	S	0	0
			7854	2403	3990	667	774	20		
1	E	525	Total	C	H	N	O	S	0	0
			7854	2403	3990	667	774	20		
1	F	525	Total	C	H	N	O	S	0	0
			7854	2403	3990	667	774	20		
1	G	525	Total	C	H	N	O	S	0	0
			7854	2403	3990	667	774	20		
1	H	523	Total	C	H	N	O	S	0	0
			7818	2392	3970	664	772	20		
1	I	523	Total	C	H	N	O	S	0	0
			7818	2392	3970	664	772	20		
1	J	523	Total	C	H	N	O	S	0	0
			7818	2392	3970	664	772	20		
1	K	523	Total	C	H	N	O	S	0	0
			7818	2392	3970	664	772	20		
1	L	523	Total	C	H	N	O	S	0	0
			7818	2392	3970	664	772	20		
1	M	523	Total	C	H	N	O	S	0	0
			7818	2392	3970	664	772	20		
1	N	523	Total	C	H	N	O	S	0	0
			7818	2392	3970	664	772	20		

- Molecule 2 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃).



Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	Be	F	0
			4	1	3	
2	B	1	Total	Be	F	0
			4	1	3	
2	C	1	Total	Be	F	0
			4	1	3	
2	D	1	Total	Be	F	0
			4	1	3	
2	E	1	Total	Be	F	0
			4	1	3	
2	F	1	Total	Be	F	0
			4	1	3	
2	G	1	Total	Be	F	0
			4	1	3	

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	B	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	C	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	D	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	E	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	F	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	G	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	H	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	I	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	J	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	K	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	L	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	M	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	N	1	Total 39	C 10	H 12	N 5	O 10	P 2	0

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

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

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

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

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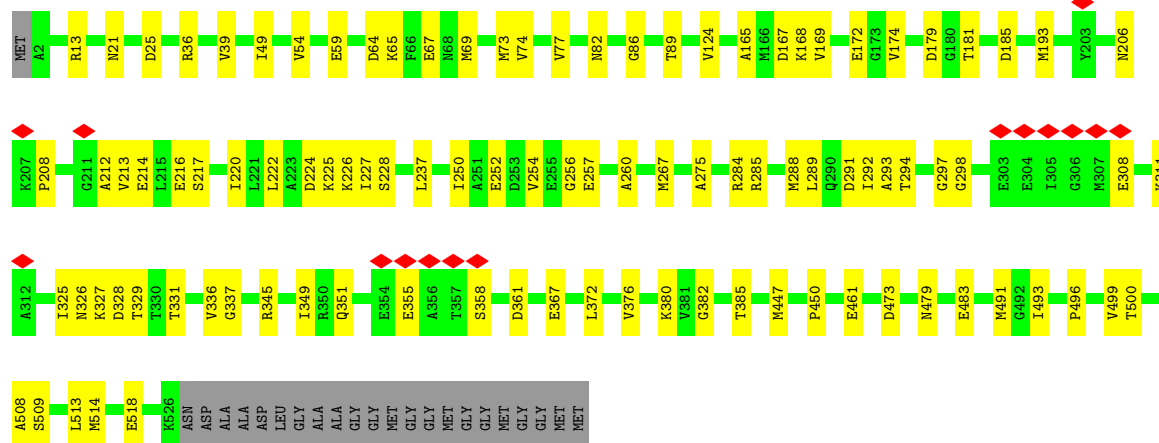
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Mol	Chain	Residues	Atoms		AltConf
5	F	1	Total 1	K 1	0
5	G	1	Total 1	K 1	0
5	H	1	Total 1	K 1	0
5	I	1	Total 1	K 1	0
5	J	1	Total 1	K 1	0
5	K	1	Total 1	K 1	0
5	L	1	Total 1	K 1	0
5	M	1	Total 1	K 1	0
5	N	1	Total 1	K 1	0

- Molecule 6 is water.

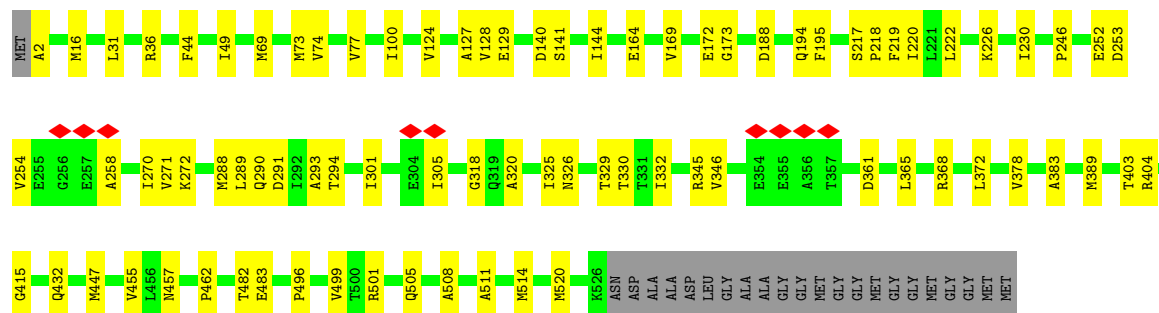
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total 3	H 2	O 1	0
6	B	1	Total 3	H 2	O 1	0
6	C	1	Total 3	H 2	O 1	0
6	D	1	Total 3	H 2	O 1	0
6	E	1	Total 3	H 2	O 1	0
6	F	1	Total 3	H 2	O 1	0
6	G	1	Total 3	H 2	O 1	0

Chain C:  78% 18%



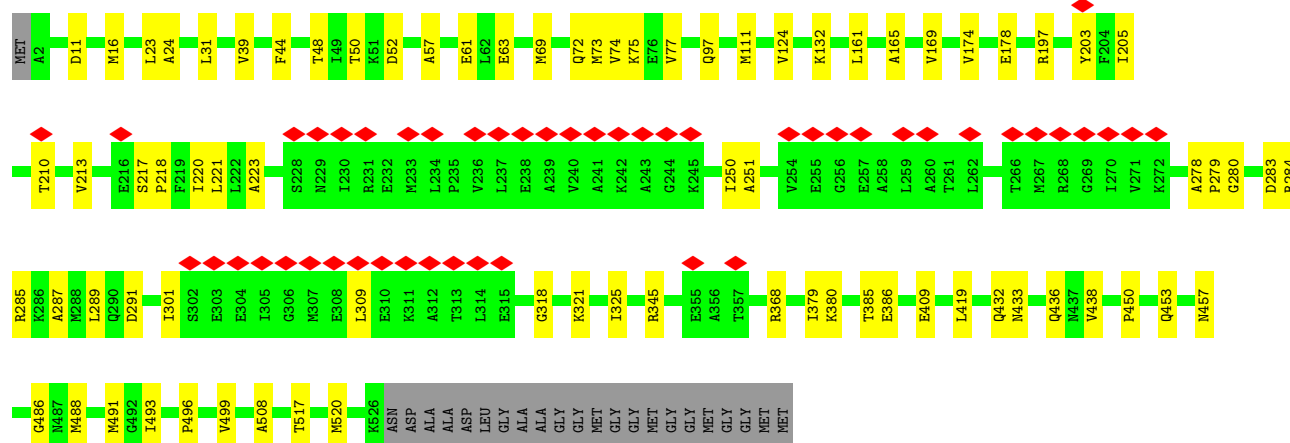
• Molecule 1: Chaperonin GroEL

Chain D:  81% 15%



• Molecule 1: Chaperonin GroEL

Chain E:  9% 82% 14%



• Molecule 1: Chaperonin GroEL

Category A	P525	T329	D185	MET
	K526	D334	E186	A2
	ASN	D348	L187	G9
	ASP	I349	D188	A12
	ALA	R350	Q194	R18
	ASP	R351	Y203	V39
	LEU	G352	N206	L40
	GLY		P207	D41
	ALA	A356	E209	I49
	GLY	T357	V213	V54
Category B	MET	D361	E214	D64
	GLY	R362	L215	E67
	MET	R363	E216	N68
	GLY	K364	S217	M69
	GLY	L365	P218	M73
	MET	R366	D224	V74
	GLY	E367	S228	E76
	GLY	R368	N229	V77
	GLY	V369	L230	N82
	MET	A370	R231	T89
Category C		K371	E232	A96
		K380	A239	I100
		T403	A260	T101
		I420	V264	E102
		R421		V124
		V422	M447	E130
			P450	S139
			L451	T144
			Y478	A145
			M479	T149
Category D		E483	L289	L161
		M491	Q290	K171
		P496	D291	E172
		V499	I292	G173
		A508	A293	V174
		I515	T294	E178
		T516	S302	D179
		T517	M307	
		E518	K311	
		C519	L314	
Category E	M520	N326	K327	
	E524	P328	D329	

Chain G: 5% 77% 18%

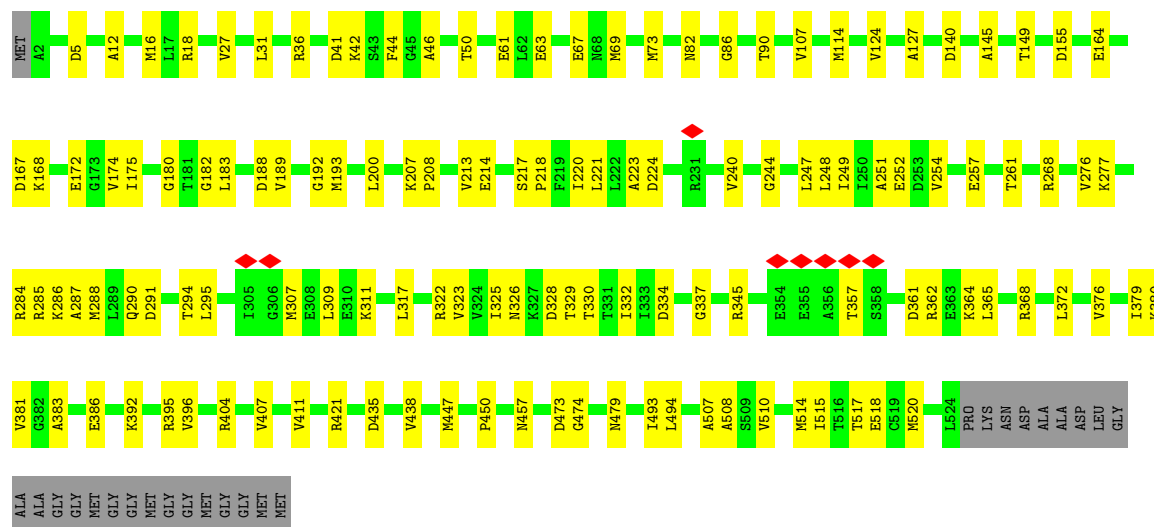
V438	L444	M447	E448	R452	Q453	M457	A480	M488	I493	K498	A508	T517	E518	G519	M520	L524	P525	K526	ASN	ASP	ALA	ALA	ASP	LEU	GLY	ALA	ALA	GLY	GLY	GLY	MET	MET																	
I301	S302	E303	E304	I305	G306	M307	E308	L309	L314	E315	D316	L317	G318	K321	R322	V323	V324	I325	T330	V336	G337	T342	Q343	G344	R345	V346	A347	Q348	I349	Q352	E355	A356	D359	R362	V369	V376	V381	K393	A394	R395	A406	E409	G410						
L215	E216	S217	P218	F219	T220	L221	L222	L227	S228	W229	T230	R231	E232	W233	A241	K242	A243	G244	L247	L248	V254	E255	G256	E257	A258	L259	L262	V263	T266	T267	R268	G269	I270	V271	K272	K277	A278	P279	G280	R285	Q290	D291	T292	T293	T294	L295	G298	T299	V299
MET	A2	D5	G9	N10	D11	M16	L17	R18	K28	L31	K34	V39	F44	D52	E61	M69	M11	N112	V124	V128	I150	S151	A152	D155	L161	E172	G173	V174	E178	E186	L187	M193	Q194	R197	L200														

Chain H: 73% 22% 5%

L456	L457	L458	G459	G474	M475	T482	E483	E484	M488	I489	G492	I493	L494	D495	P496	T497	K498	V499	T500	R501	Q505	A508	T516	M520	V521	T522	D523	L524	PRO	LYS	ASN	ASP	ALA	ALA	ASP	LEU	GLY	ALA	ALA	GLY	GLY	MET	GLY	GLY	GLY	GLY	MET
N326	T329	T330	L333	I342	R345	V346	A347	Q348	I353	E354	E355	A356	T357	S358	D359	R362	E363	K364	Q366	V369	L372	A373	R376	A377	V381	T385	E386	V387	E388	M389	K390	F391	K392	V396	T403	V411	L419	T420	R421	V422	D428						
K207	A212	V213	E214	L215	E216	S217	P218	L221	L222	R231	L234	P235	V240	G244	K245	P246	L247	L248	L249	T261	L262	V263	K267	R268	G269	I270	V276	K277	D283	Q290	D291	I292	A293	T296	G297	T305	G306	K307	E310	D316	L317	E318	T325				
MET	A2	D5	A12	R13	L31	D52	G53	V54	N82	D83	A84	A85	G86	E102	V124	E129	E130	D140	S141	I144	A152	D155	V169	E172	G173	V174	G180	T181	D188	V189	V190	M193	Q194	F195	D196	L200	S201	P202	Y203	N206							

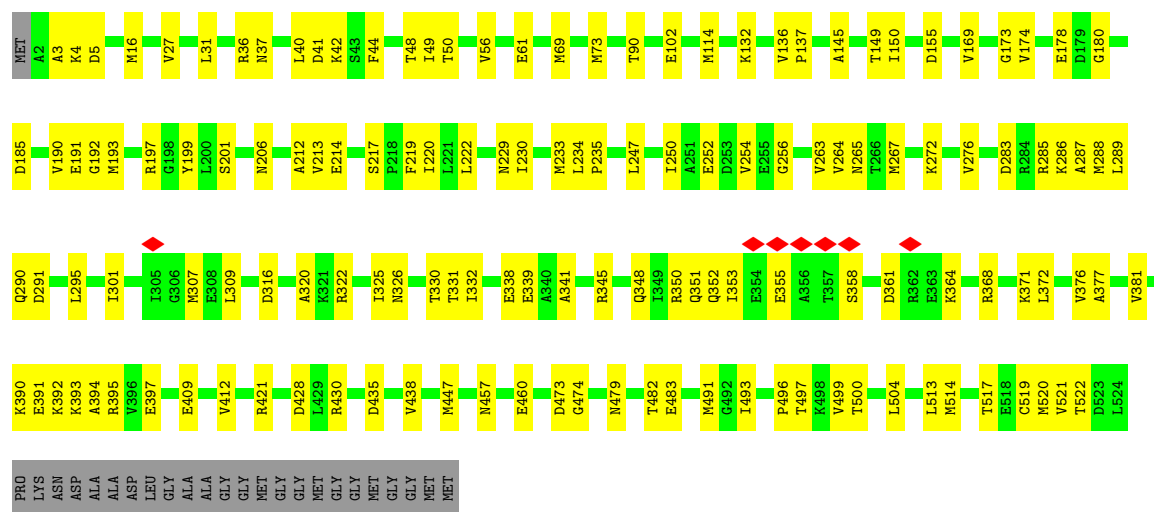
- Molecule 1: Chaperonin GroEL

Chain I:



- Molecule 1: Chaperonin GroEL

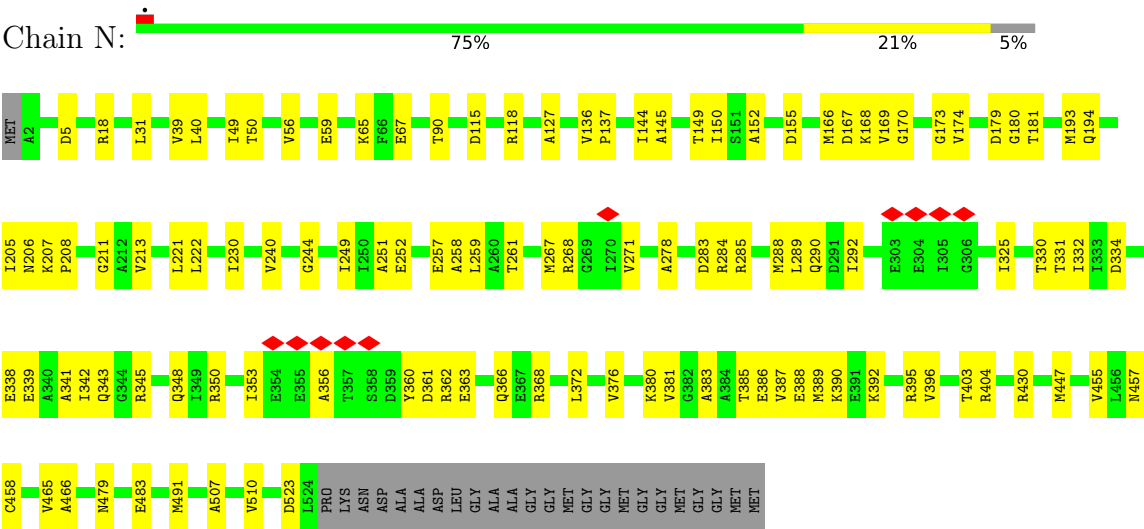
Chain J:



- Molecule 1: Chaperonin GroEL

Chain K:





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	202582	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 ($e^-/\text{\AA}^2$)	40.2	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.159	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0218	Depositor
Map size (Å)	546.2912, 546.2912, 546.2912	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2194, 1.2194, 1.2194	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, MG, BEF, K

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	0.16	0/3892	0.42	0/5254
1	B	0.14	0/3892	0.37	0/5254
1	C	0.16	0/3892	0.42	2/5254 (0.0%)
1	D	0.15	0/3892	0.32	0/5254
1	E	0.14	0/3892	0.32	0/5254
1	F	0.15	0/3892	0.37	0/5254
1	G	0.15	0/3892	0.39	0/5254
1	H	0.15	0/3875	0.40	0/5231
1	I	0.15	0/3875	0.39	0/5231
1	J	0.16	0/3875	0.40	0/5231
1	K	0.16	0/3875	0.43	0/5231
1	L	0.16	0/3875	0.42	0/5231
1	M	0.16	0/3875	0.40	0/5231
1	N	0.15	0/3875	0.41	1/5231 (0.0%)
All	All	0.15	0/54369	0.39	3/73395 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	367	GLU	CA-C-N	7.89	130.70	120.44
1	C	367	GLU	C-N-CA	7.89	130.70	120.44
1	N	390	LYS	CD-CE-NZ	-6.97	89.60	111.90

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	3864	3990	3987	99	0
1	B	3864	3990	3987	66	0
1	C	3864	3990	3987	76	0
1	D	3864	3990	3988	66	0
1	E	3864	3990	3987	57	0
1	F	3864	3990	3988	86	0
1	G	3864	3990	3987	75	0
1	H	3848	3970	3969	93	0
1	I	3848	3970	3969	101	0
1	J	3848	3970	3969	103	0
1	K	3848	3970	3969	92	0
1	L	3848	3970	3969	111	0
1	M	3848	3970	3969	85	0
1	N	3848	3970	3969	91	0
2	A	4	0	0	1	0
2	B	4	0	0	3	0
2	C	4	0	0	2	0
2	D	4	0	0	1	0
2	E	4	0	0	1	0
2	F	4	0	0	2	0
2	G	4	0	0	2	0
3	A	27	12	12	1	0
3	B	27	12	12	2	0
3	C	27	12	12	2	0
3	D	27	12	12	2	0
3	E	27	12	12	1	0
3	F	27	12	12	2	0
3	G	27	12	12	2	0
3	H	27	12	12	1	0
3	I	27	12	12	1	0
3	J	27	12	12	1	0
3	K	27	12	12	1	0
3	L	27	12	12	0	0
3	M	27	12	12	1	0
3	N	27	12	12	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	A	1	2	0	0	0
6	B	1	2	0	1	0
6	C	1	2	0	0	0
6	D	1	2	0	0	0
6	E	1	2	0	1	0
6	F	1	2	0	0	0
6	G	1	2	0	1	0
All	All	54425	55902	55862	1165	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 11.

The worst 5 of 1165 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:H:482:THR:OG1	1:H:484:GLU:OE1	1.79	1.01
1:M:290:GLN:NE2	1:M:291:ASP:OD1	2.04	0.91
1:D:291:ASP:OD1	1:D:345:ARG:NH1	2.05	0.90
1:G:178:GLU:N	1:G:178:GLU:OE1	2.07	0.87
1:M:364:LYS:O	1:M:368:ARG:NH2	2.07	0.87

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	523/548 (95%)	479 (92%)	44 (8%)	0	100	100
1	B	523/548 (95%)	490 (94%)	33 (6%)	0	100	100
1	C	523/548 (95%)	495 (95%)	28 (5%)	0	100	100
1	D	523/548 (95%)	500 (96%)	23 (4%)	0	100	100
1	E	523/548 (95%)	500 (96%)	23 (4%)	0	100	100
1	F	523/548 (95%)	503 (96%)	20 (4%)	0	100	100
1	G	523/548 (95%)	492 (94%)	31 (6%)	0	100	100
1	H	521/548 (95%)	497 (95%)	24 (5%)	0	100	100
1	I	521/548 (95%)	488 (94%)	33 (6%)	0	100	100
1	J	521/548 (95%)	501 (96%)	20 (4%)	0	100	100
1	K	521/548 (95%)	483 (93%)	38 (7%)	0	100	100
1	L	521/548 (95%)	473 (91%)	48 (9%)	0	100	100
1	M	521/548 (95%)	492 (94%)	29 (6%)	0	100	100
1	N	521/548 (95%)	493 (95%)	28 (5%)	0	100	100
All	All	7308/7672 (95%)	6886 (94%)	422 (6%)	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	405/415 (98%)	405 (100%)	0	100	100
1	B	405/415 (98%)	405 (100%)	0	100	100
1	C	405/415 (98%)	404 (100%)	1 (0%)	87	85
1	D	405/415 (98%)	405 (100%)	0	100	100
1	E	405/415 (98%)	405 (100%)	0	100	100
1	F	405/415 (98%)	405 (100%)	0	100	100
1	G	405/415 (98%)	405 (100%)	0	100	100
1	H	403/415 (97%)	401 (100%)	2 (0%)	81	81
1	I	403/415 (97%)	403 (100%)	0	100	100
1	J	403/415 (97%)	403 (100%)	0	100	100
1	K	403/415 (97%)	402 (100%)	1 (0%)	87	85
1	L	403/415 (97%)	403 (100%)	0	100	100
1	M	403/415 (97%)	403 (100%)	0	100	100
1	N	403/415 (97%)	403 (100%)	0	100	100
All	All	5656/5810 (97%)	5652 (100%)	4 (0%)	87	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	500	THR
1	H	333	ILE
1	H	482	THR
1	K	87	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	290	GLN
1	N	401	HIS

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Mol	Chain	Res	Type
1	F	453	GLN
1	M	206	ASN
1	F	352	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 49 ligands modelled in this entry, 28 are monoatomic - leaving 21 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	$\# Z > 2$
2	BEF	B	603	3	0,3,3	-	-	-		
3	ADP	H	603	5,4	27,29,29	1.29	5 (18%)	42,45,45	2.02	11 (26%)
3	ADP	A	602	2,4,5	27,29,29	1.31	4 (14%)	42,45,45	2.05	11 (26%)
3	ADP	C	601	2,4,5	27,29,29	1.32	4 (14%)	42,45,45	2.04	12 (28%)
2	BEF	F	601	3	0,3,3	-	-	-		
3	ADP	D	604	2,4,5	27,29,29	1.33	4 (14%)	42,45,45	2.04	12 (28%)
3	ADP	N	601	4	27,29,29	1.29	5 (18%)	42,45,45	2.04	11 (26%)
2	BEF	E	601	3	0,3,3	-	-	-		
3	ADP	J	601	5,4	27,29,29	1.28	4 (14%)	42,45,45	2.04	12 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	I	601	5,4	27,29,29	1.32	5 (18%)	42,45,45	1.91	11 (26%)
3	ADP	B	604	5,4,2	27,29,29	1.30	4 (14%)	42,45,45	2.04	13 (30%)
2	BEF	G	603	3	0,3,3	-	-	-	-	-
3	ADP	E	604	2,4,5	27,29,29	1.31	4 (14%)	42,45,45	2.03	11 (26%)
3	ADP	G	601	2,4,5	27,29,29	1.33	4 (14%)	42,45,45	2.05	12 (28%)
3	ADP	K	2002	5,4	27,29,29	1.30	5 (18%)	42,45,45	1.99	11 (26%)
3	ADP	F	602	2,4,5	27,29,29	1.29	4 (14%)	42,45,45	2.07	13 (30%)
3	ADP	L	601	5,4	27,29,29	1.31	4 (14%)	42,45,45	2.03	12 (28%)
2	BEF	C	603	3	0,3,3	-	-	-	-	-
2	BEF	A	601	3	0,3,3	-	-	-	-	-
2	BEF	D	601	3	0,3,3	-	-	-	-	-
3	ADP	M	603	5,4	27,29,29	1.31	4 (14%)	42,45,45	1.99	11 (26%)

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	ADP	D	604	2,4,5	-	1/16/32/32	0/3/3/3
3	ADP	H	603	5,4	-	0/16/32/32	0/3/3/3
3	ADP	N	601	4	-	4/16/32/32	0/3/3/3
3	ADP	B	604	5,4,2	-	3/16/32/32	0/3/3/3
3	ADP	F	602	2,4,5	-	2/16/32/32	0/3/3/3
3	ADP	L	601	5,4	-	1/16/32/32	0/3/3/3
3	ADP	A	602	2,4,5	-	0/16/32/32	0/3/3/3
3	ADP	C	601	2,4,5	-	1/16/32/32	0/3/3/3
3	ADP	E	604	2,4,5	-	3/16/32/32	0/3/3/3
3	ADP	K	2002	5,4	-	1/16/32/32	0/3/3/3
3	ADP	G	601	2,4,5	-	3/16/32/32	0/3/3/3
3	ADP	J	601	5,4	-	3/16/32/32	0/3/3/3
3	ADP	I	601	5,4	-	1/16/32/32	0/3/3/3
3	ADP	M	603	5,4	-	3/16/32/32	0/3/3/3

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	604	ADP	C5-C4	4.17	1.46	1.39
3	M	603	ADP	C5-C4	4.16	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	601	ADP	C5-C4	4.14	1.46	1.39
3	C	601	ADP	C5-C4	4.12	1.46	1.39
3	A	602	ADP	C5-C4	4.10	1.46	1.39

The worst 5 of 163 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	ADP	C5-C4-N3	-6.20	118.66	126.75
3	D	604	ADP	C5-C4-N3	-6.17	118.70	126.75
3	M	603	ADP	C5-C4-N3	-6.12	118.76	126.75
3	E	604	ADP	C5-C4-N3	-6.09	118.81	126.75
3	C	601	ADP	C5-C4-N3	-6.07	118.83	126.75

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	602	ADP	PA-O3A-PB-O3B
3	B	604	ADP	PA-O3A-PB-O1B
3	J	601	ADP	PA-O3A-PB-O1B
3	I	601	ADP	PA-O3A-PB-O3B
3	L	601	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

20 monomers are involved in 20 short contacts:

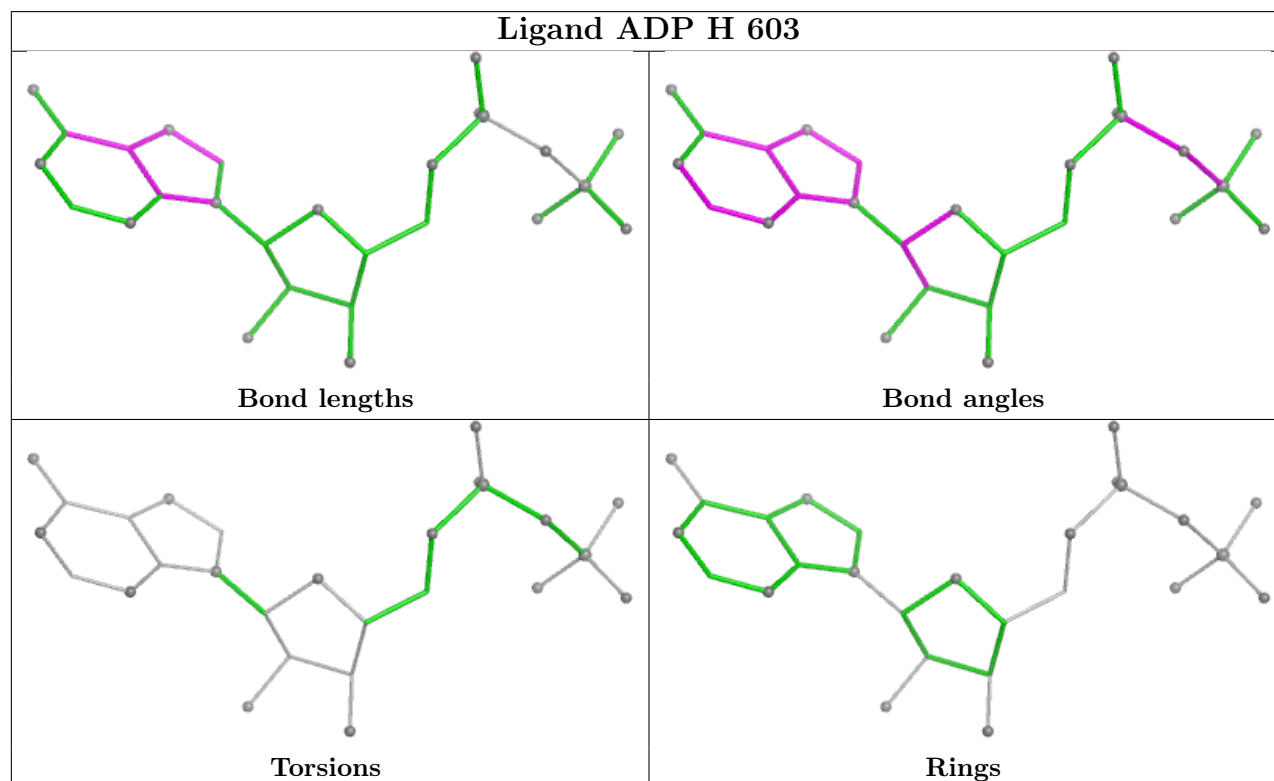
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	603	BEF	3	0
3	H	603	ADP	1	0
3	A	602	ADP	1	0
3	C	601	ADP	2	0
2	F	601	BEF	2	0
3	D	604	ADP	2	0
3	N	601	ADP	2	0
2	E	601	BEF	1	0
3	J	601	ADP	1	0
3	I	601	ADP	1	0
3	B	604	ADP	2	0
2	G	603	BEF	2	0
3	E	604	ADP	1	0
3	G	601	ADP	2	0

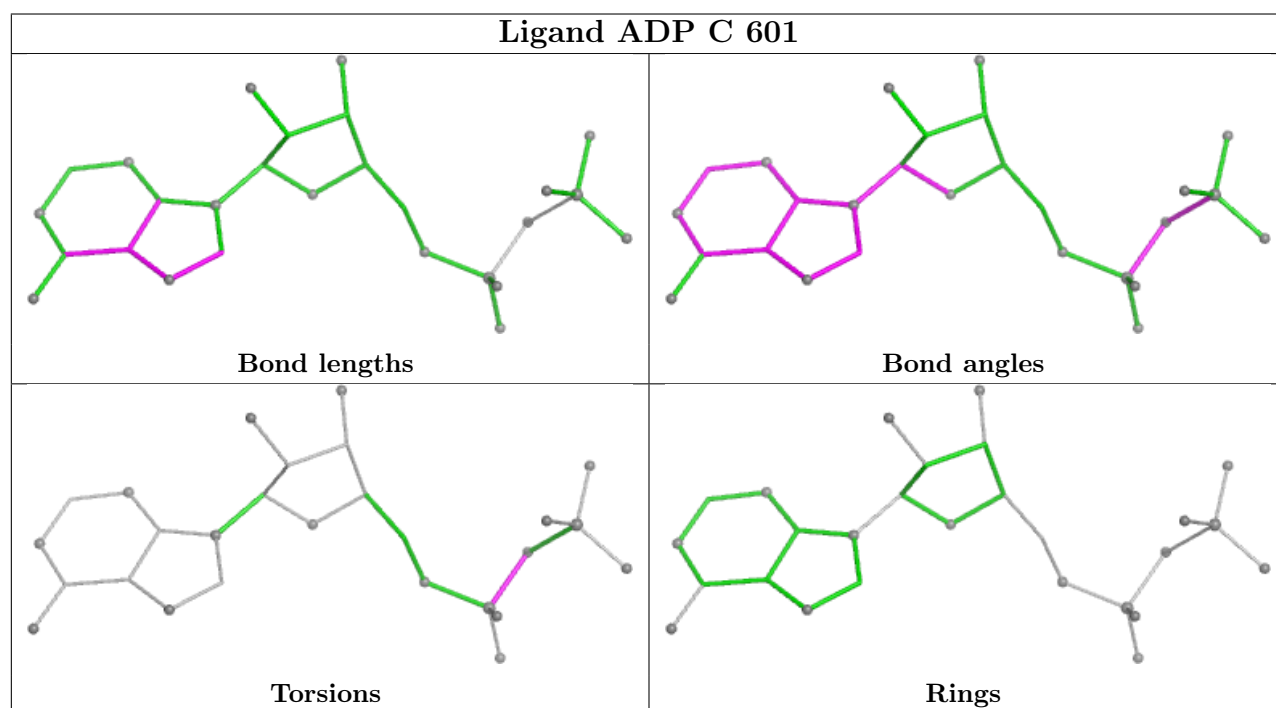
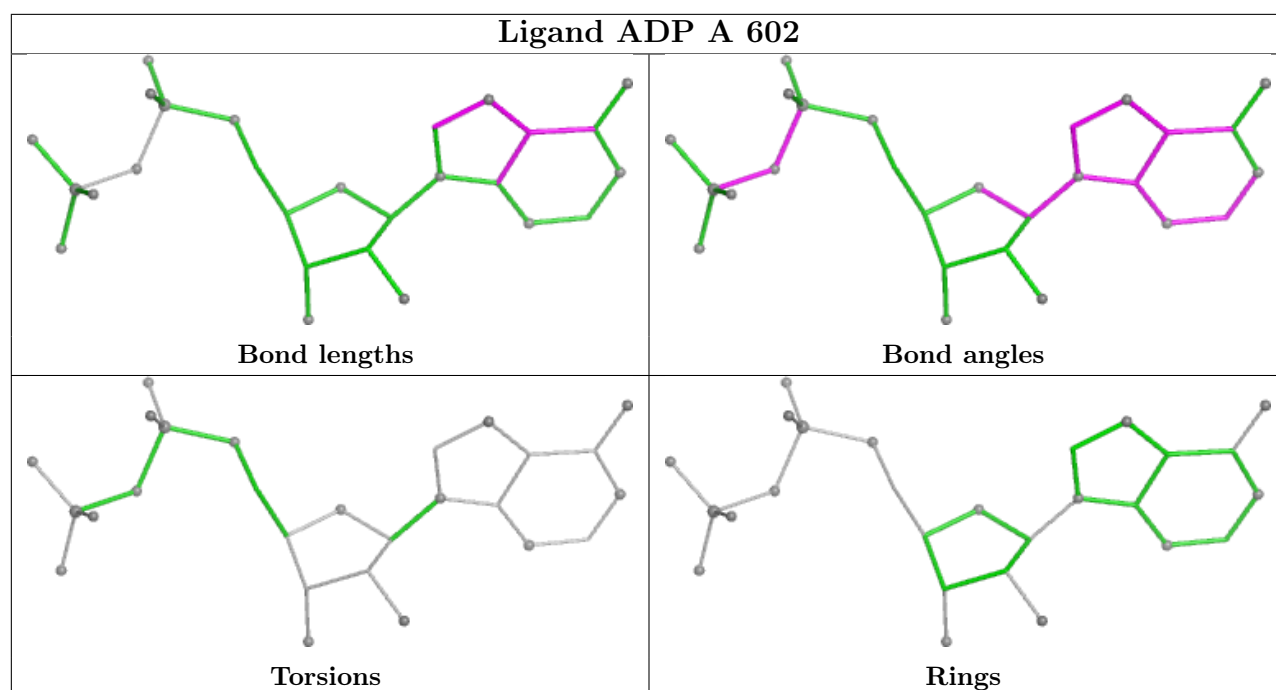
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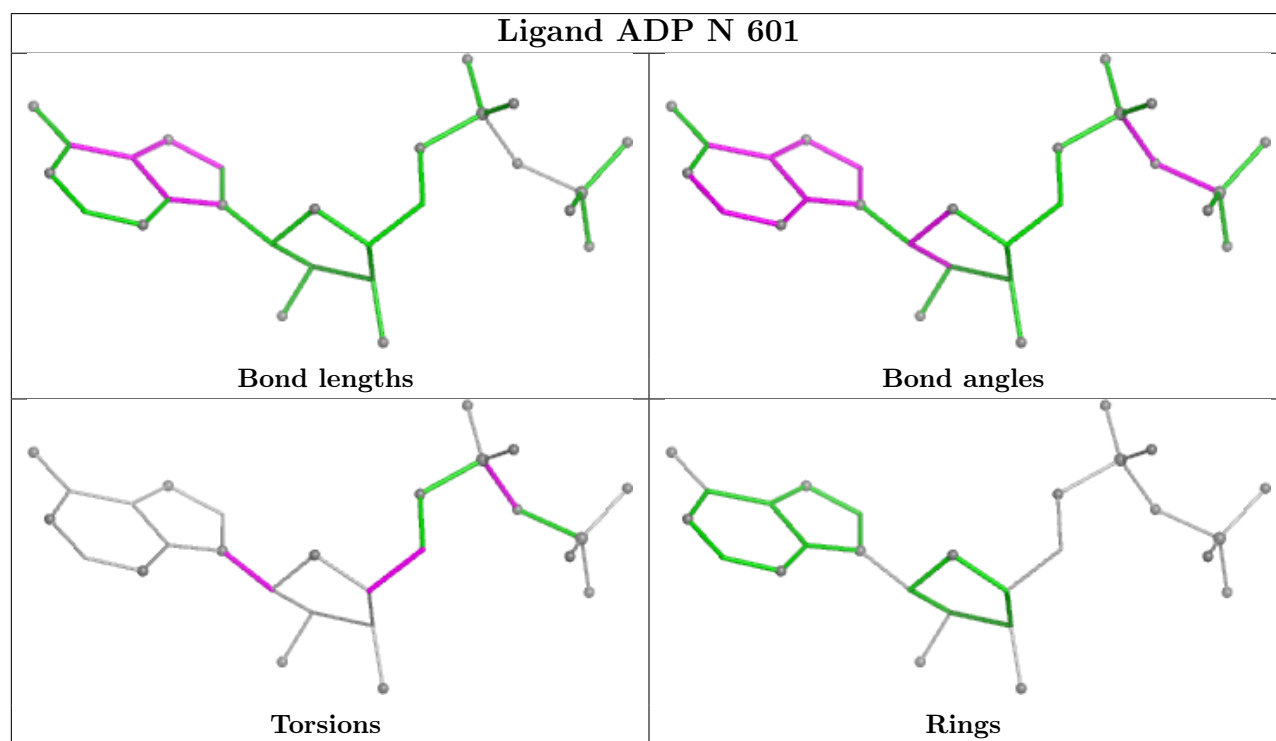
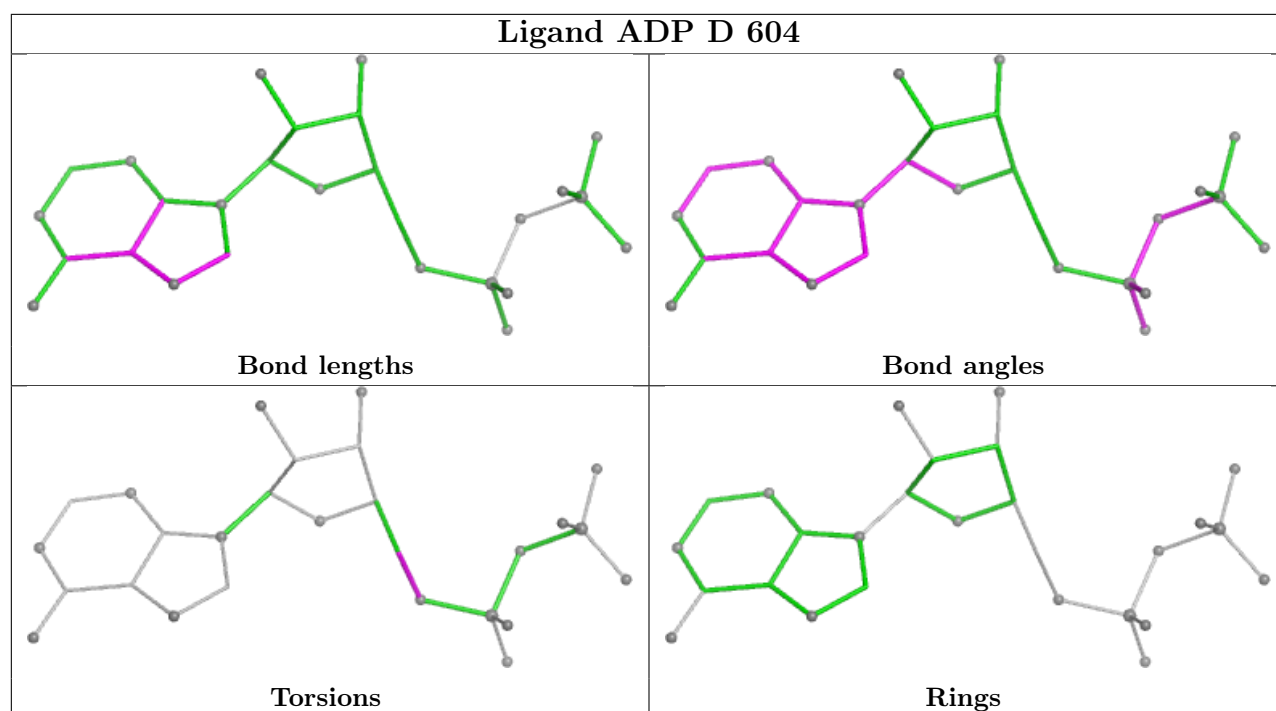
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	2002	ADP	1	0
3	F	602	ADP	2	0
2	C	603	BEF	2	0
2	A	601	BEF	1	0
2	D	601	BEF	1	0
3	M	603	ADP	1	0

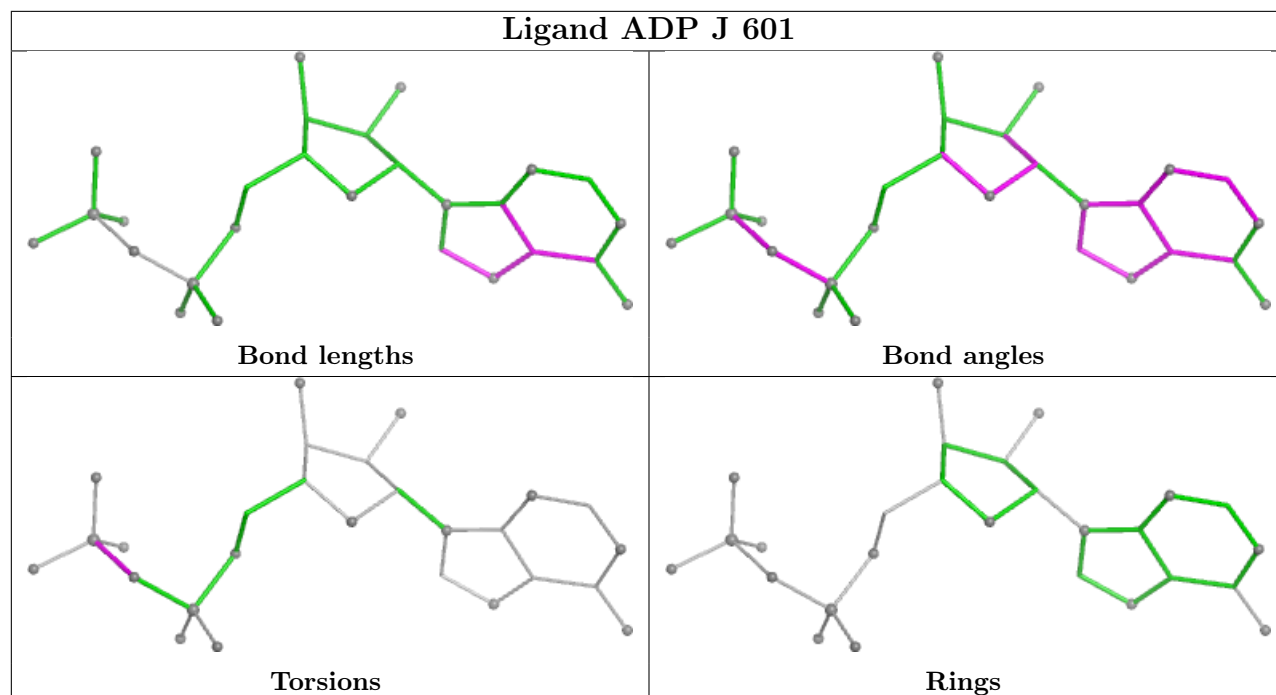
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



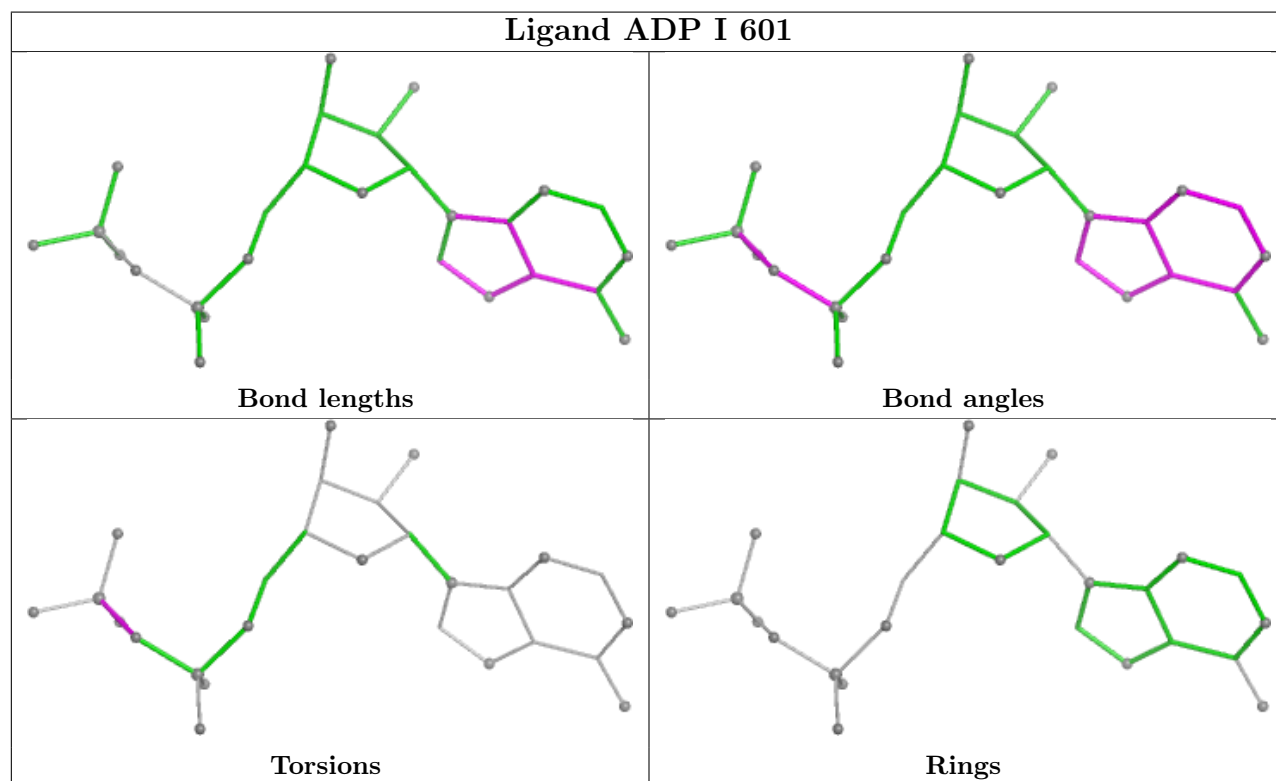


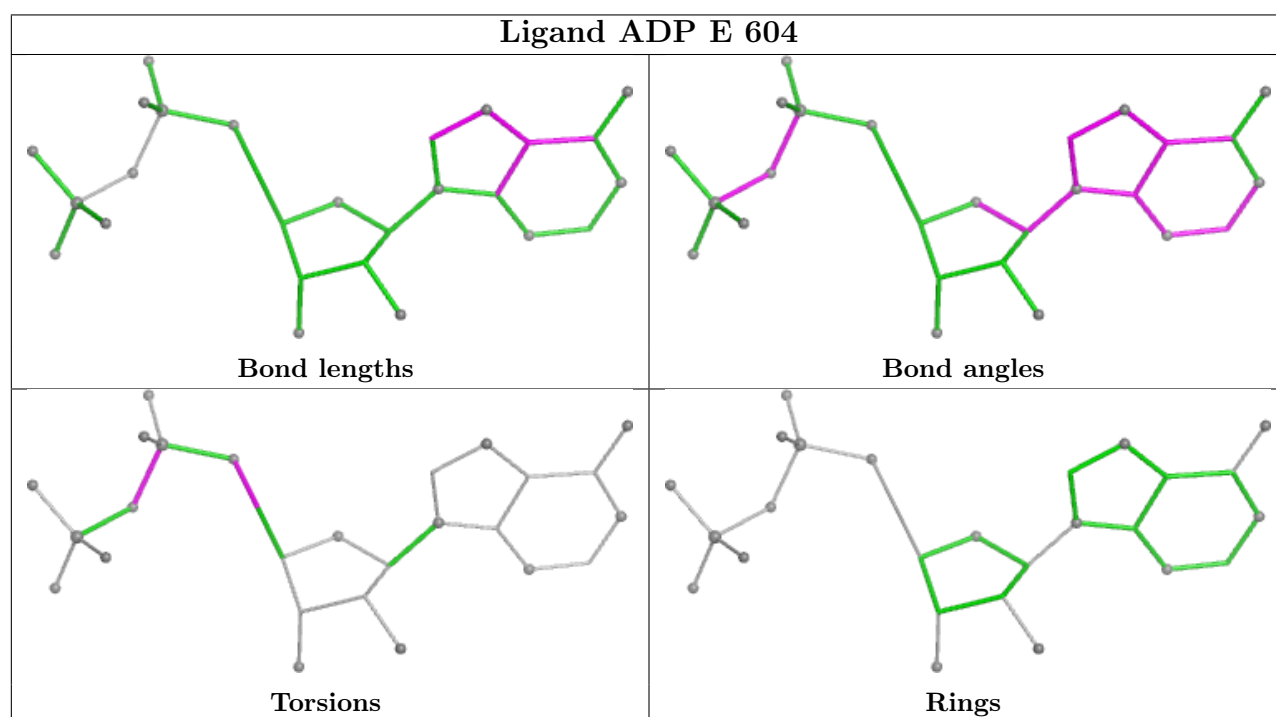
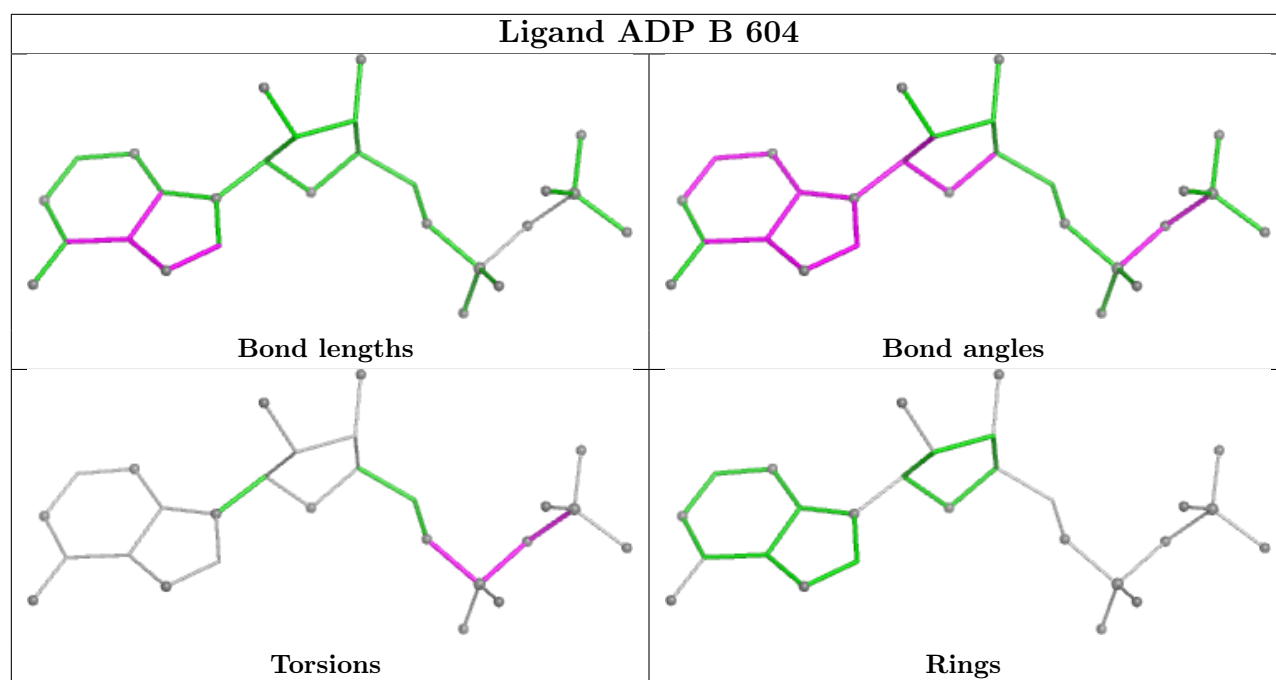


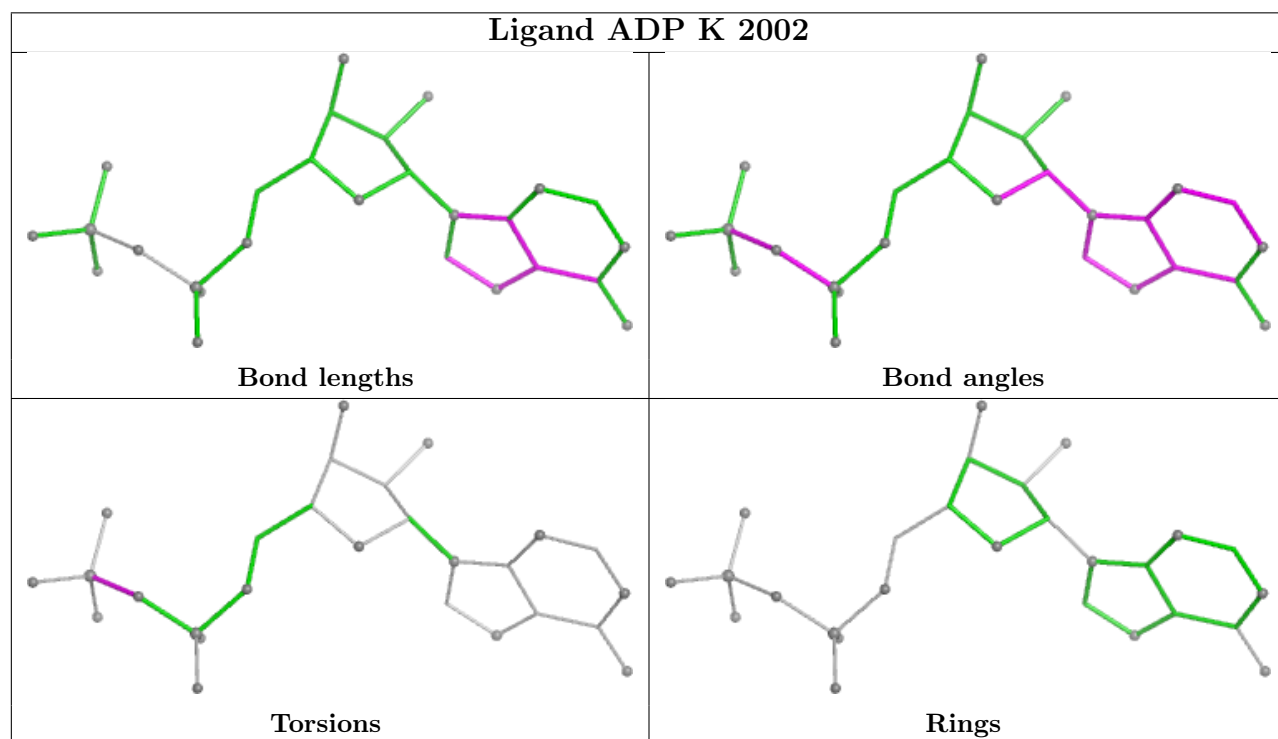
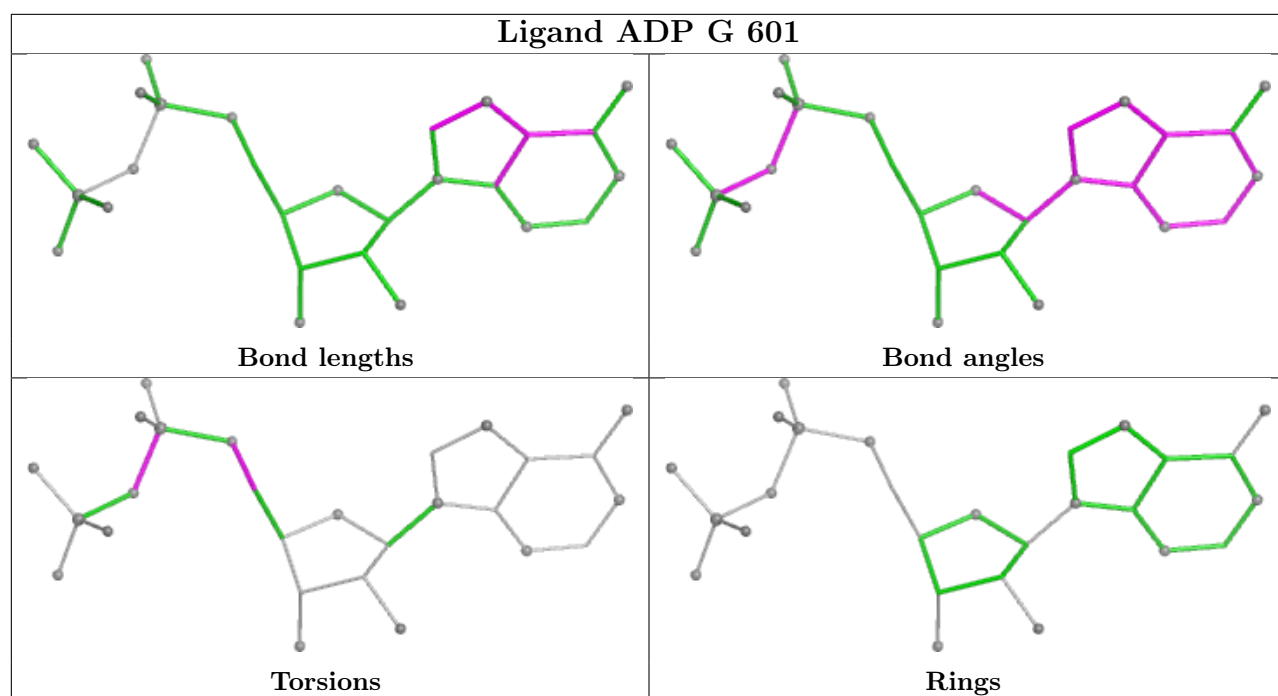
Ligand ADP J 601

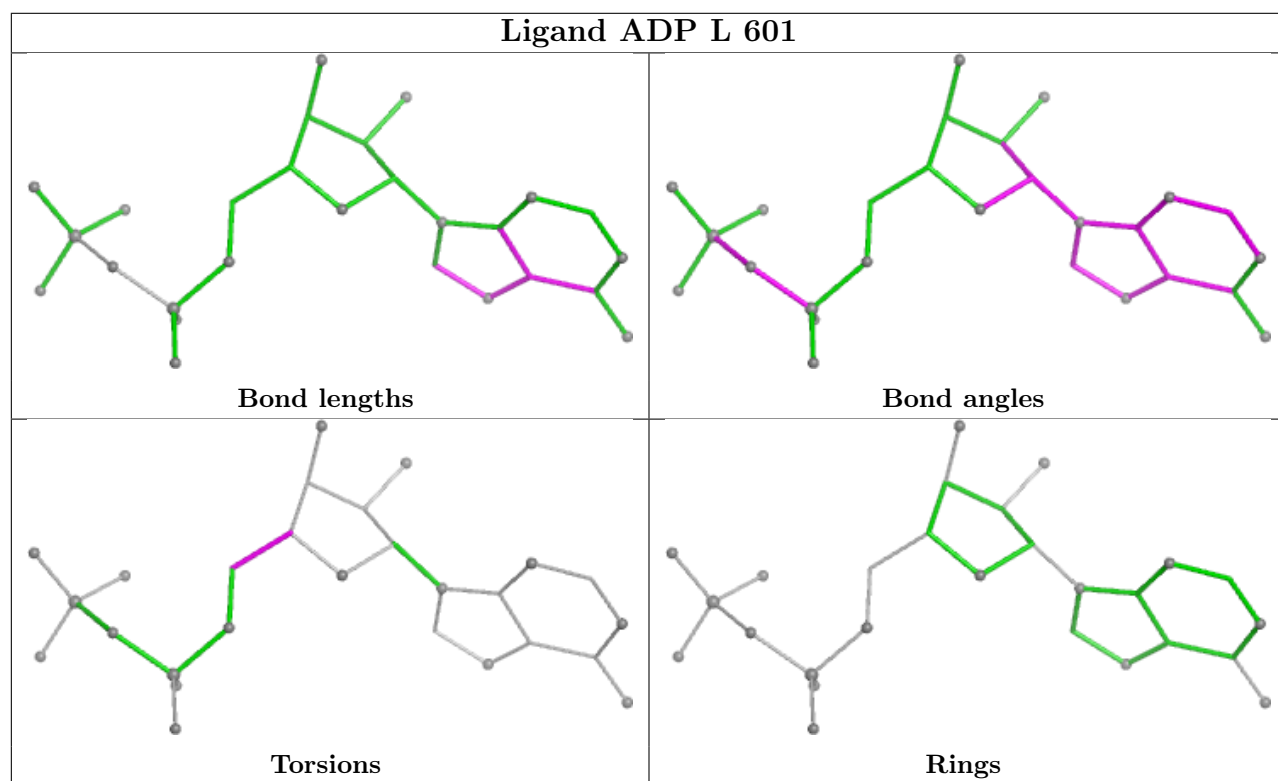
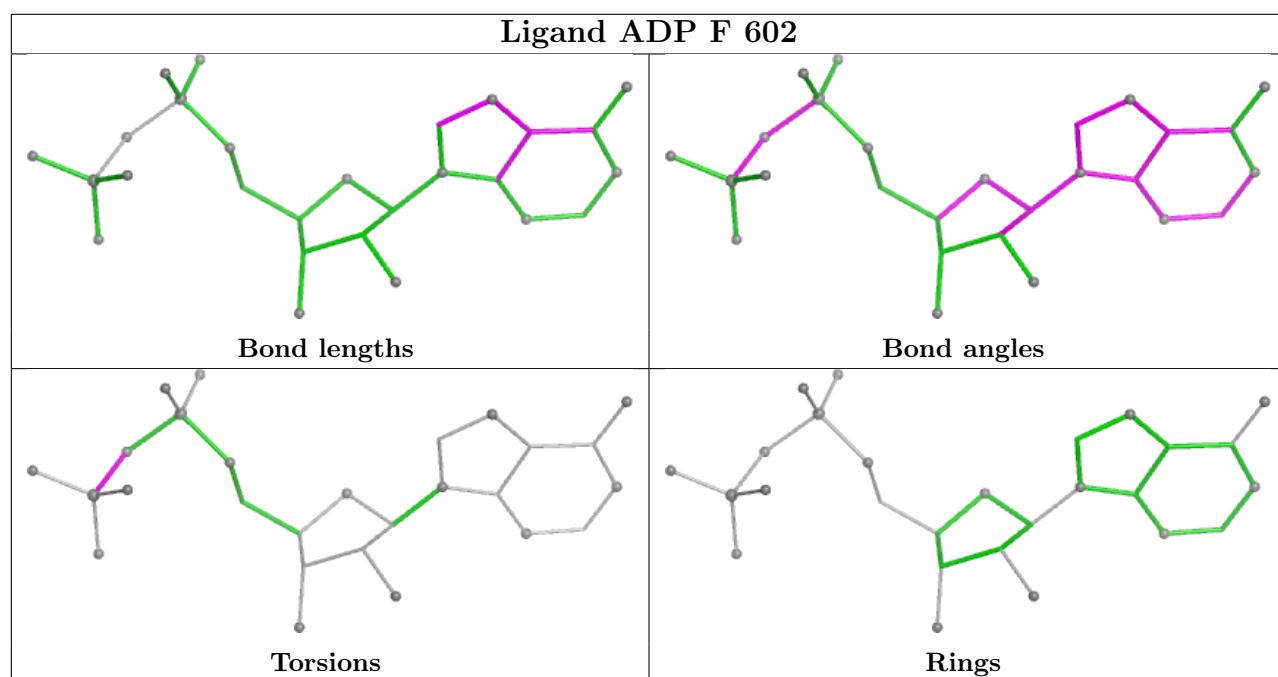


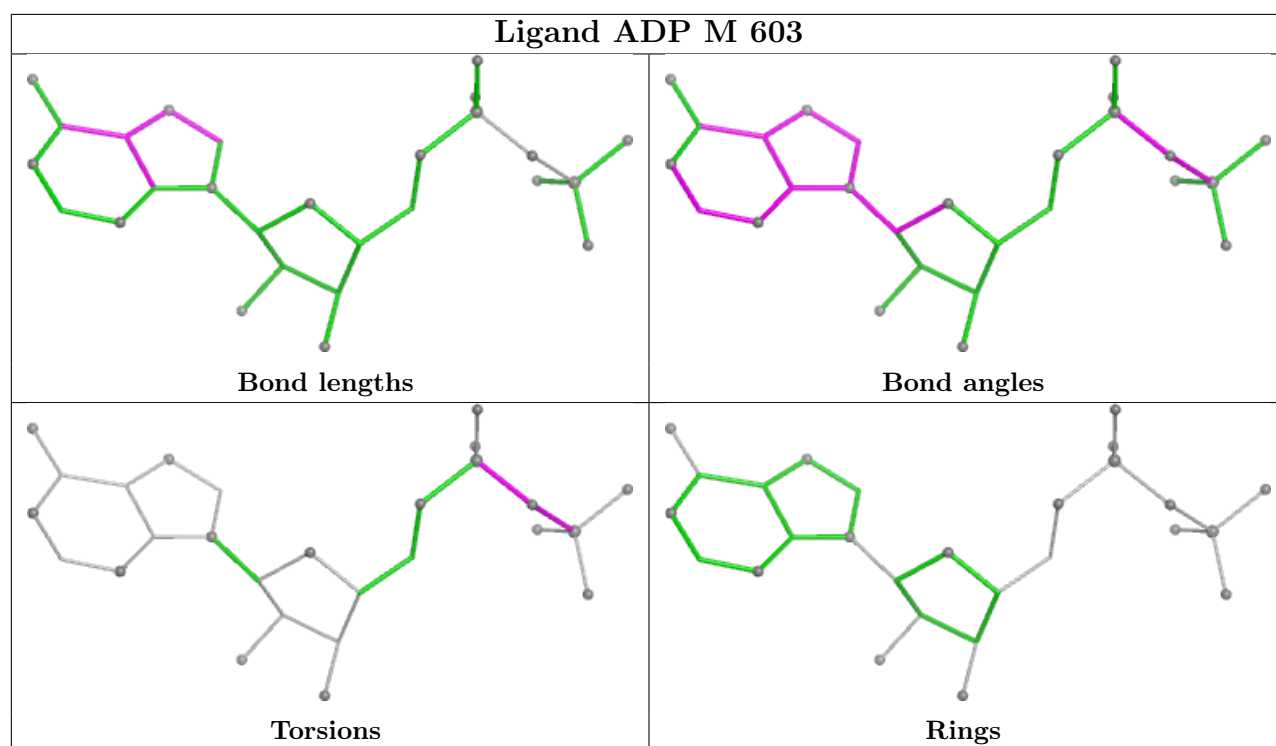
Ligand ADP I 601











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-15940. These allow visual inspection of the internal detail of the map and identification of artifacts.

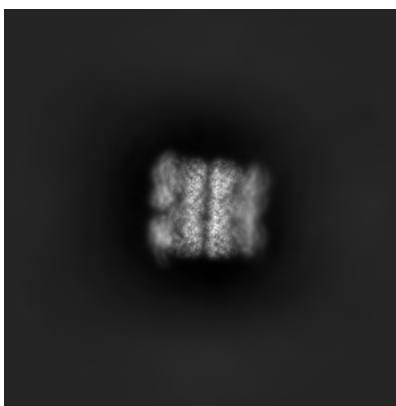
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

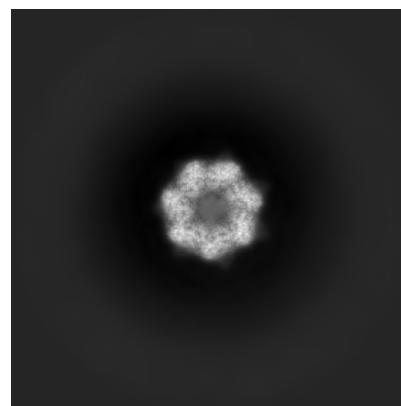
6.1.1 Primary map



X

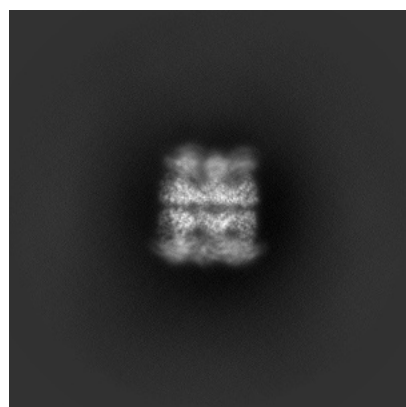


Y

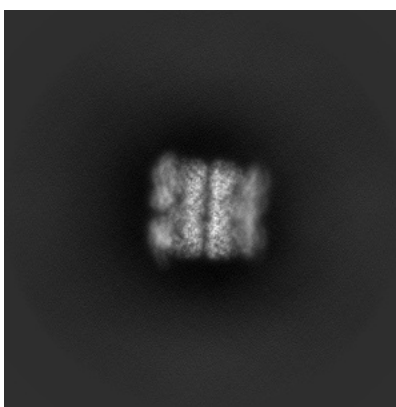


Z

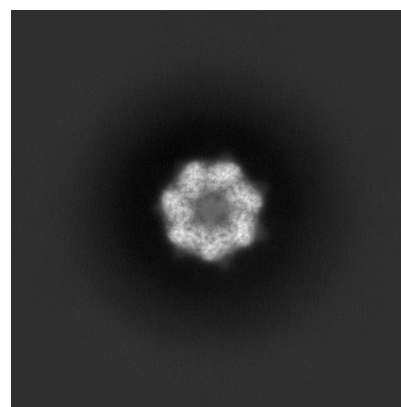
6.1.2 Raw map



X



Y

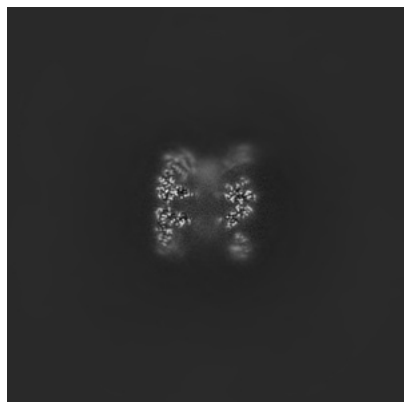


Z

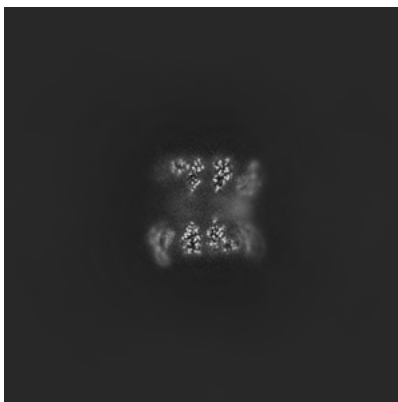
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

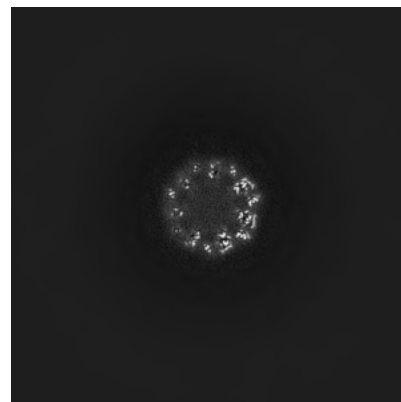
6.2.1 Primary map



X Index: 224

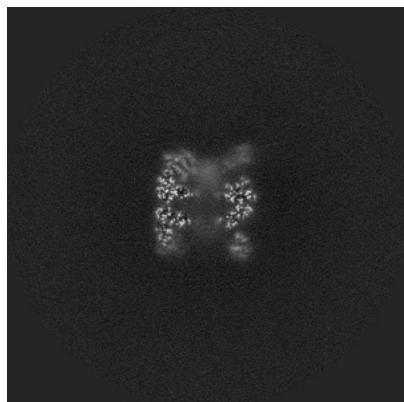


Y Index: 224

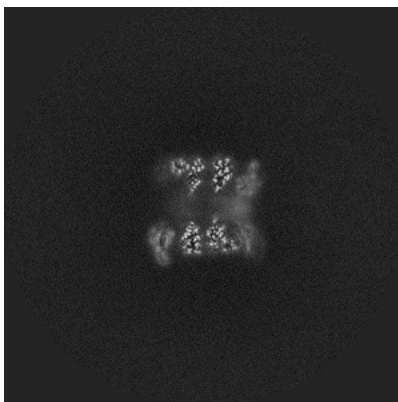


Z Index: 224

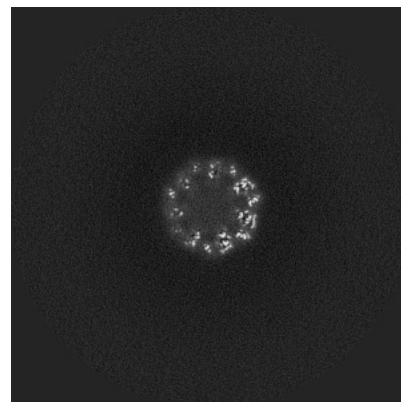
6.2.2 Raw map



X Index: 224



Y Index: 224

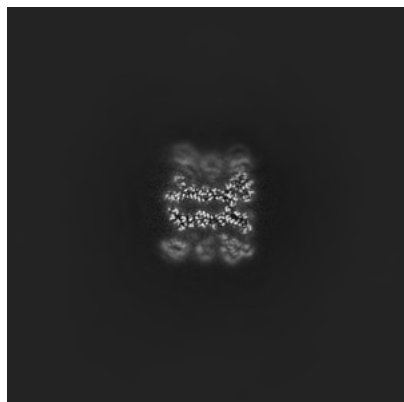


Z Index: 224

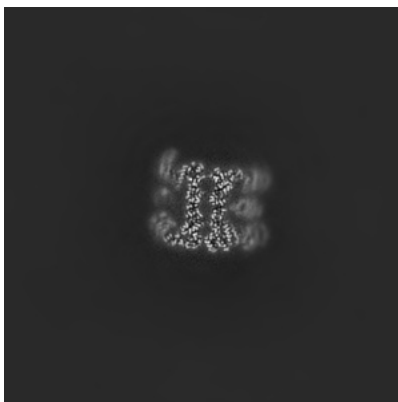
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

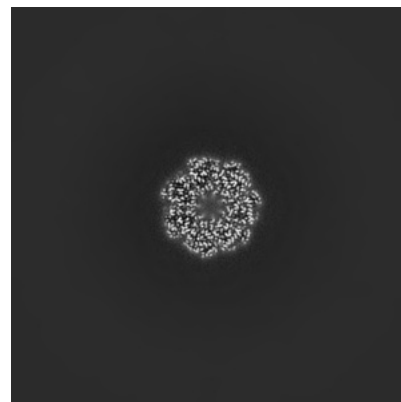
6.3.1 Primary map



X Index: 198

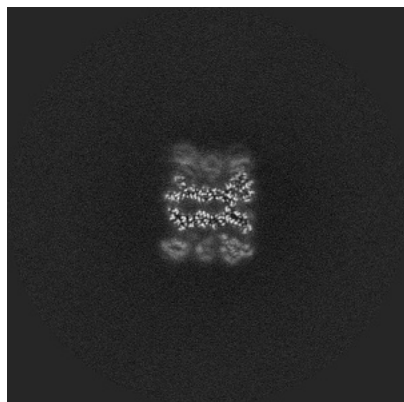


Y Index: 197

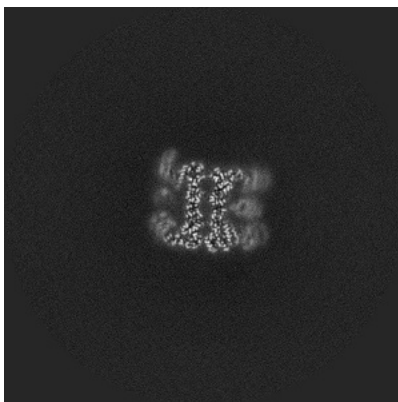


Z Index: 237

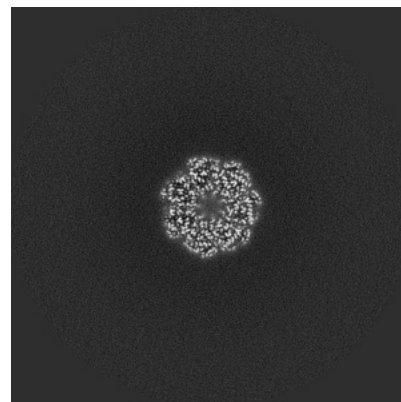
6.3.2 Raw map



X Index: 198



Y Index: 197



Z Index: 237

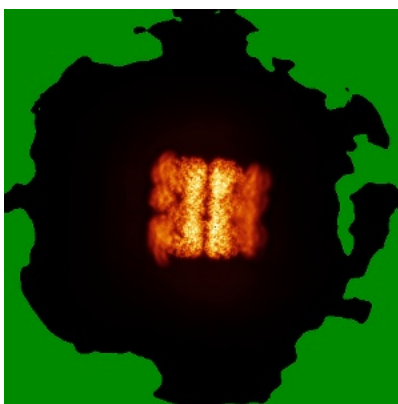
The images above show the largest variance slices of the map in three orthogonal directions.

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

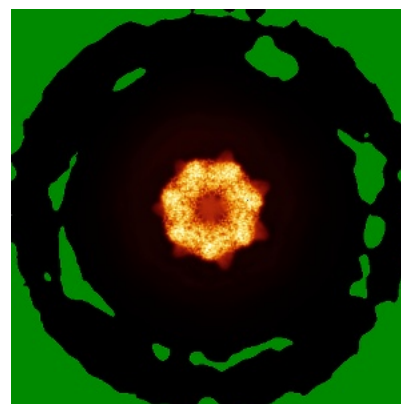
6.4.1 Primary map



X

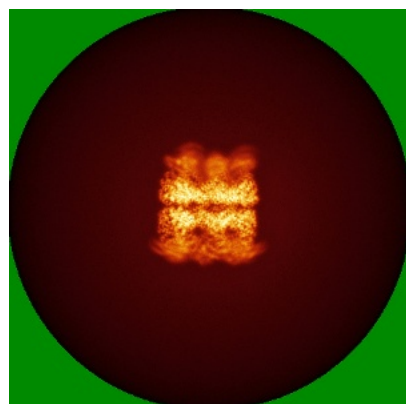


Y

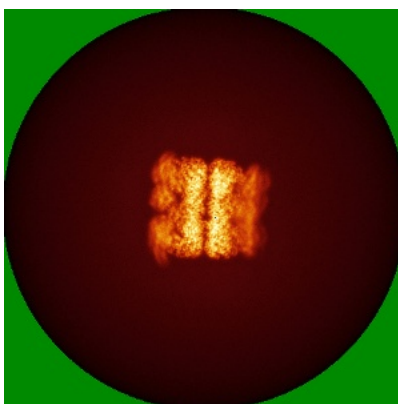


Z

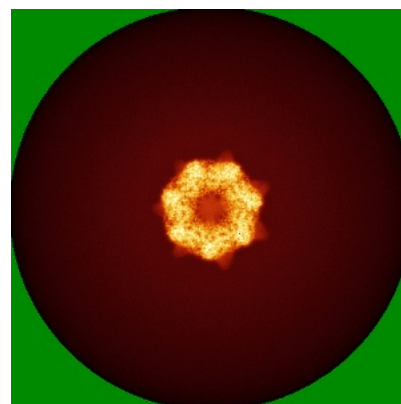
6.4.2 Raw map



X



Y

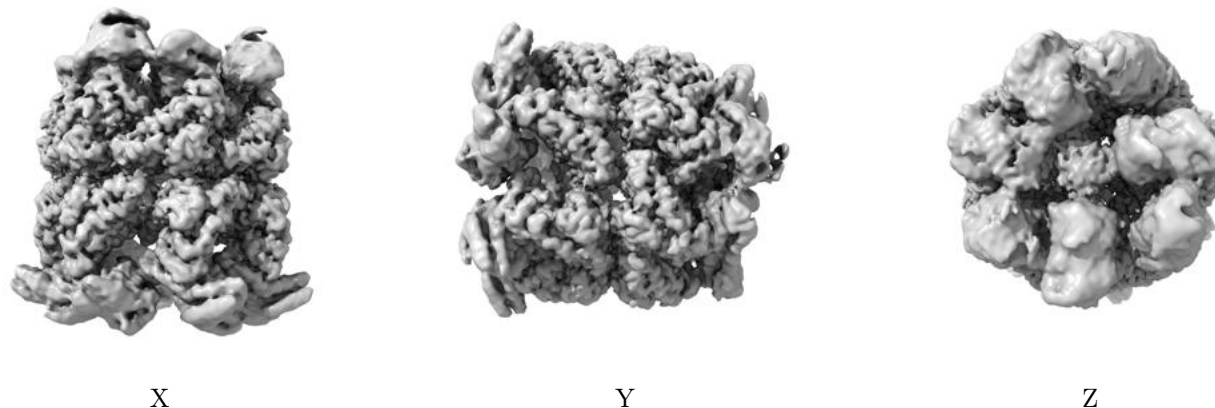


Z

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.

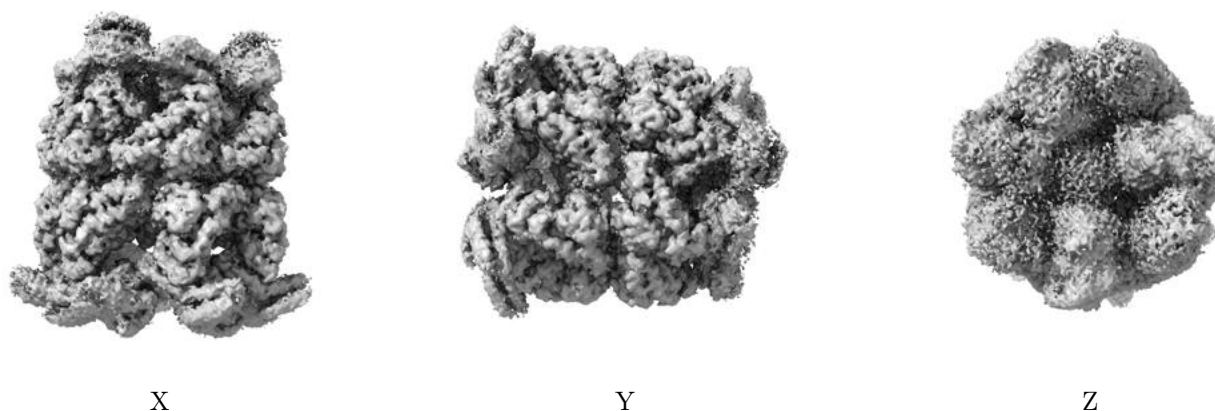
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0218. 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



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.

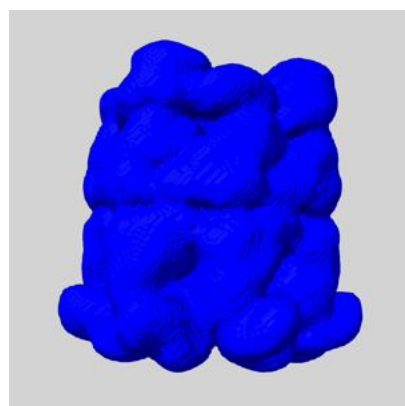
6.6 Mask visualisation [i](#)

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

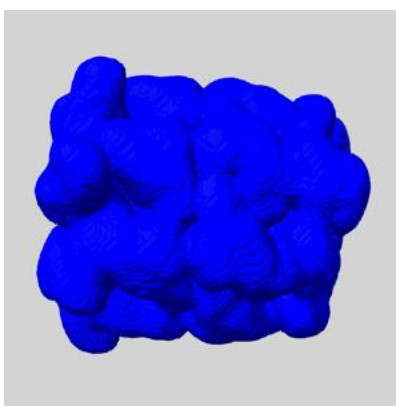
A mask typically either:

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

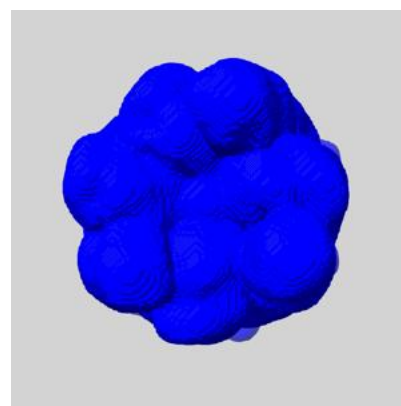
6.6.1 emd_15940_msk_1.map [i](#)



X



Y

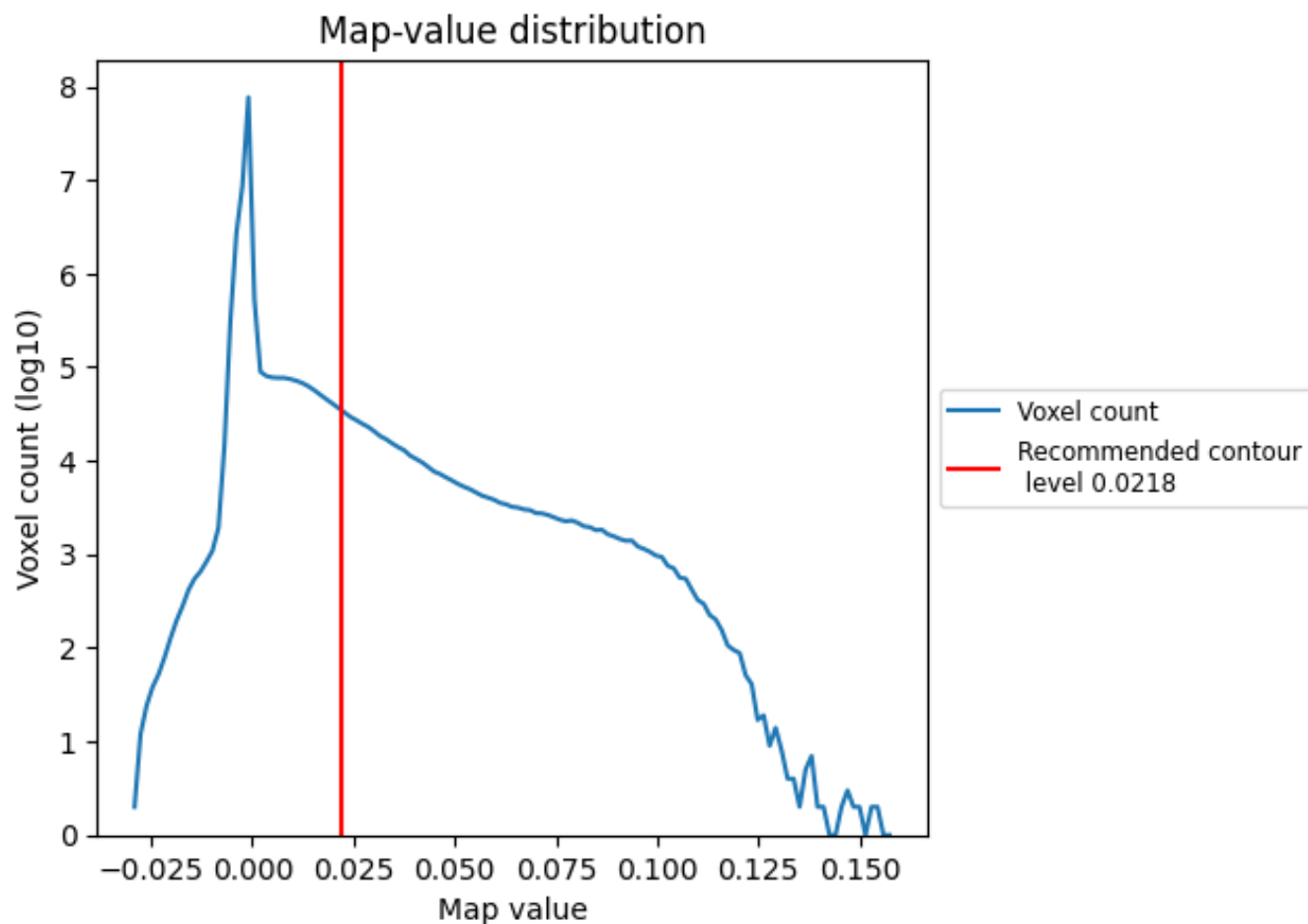


Z

7 Map analysis [i](#)

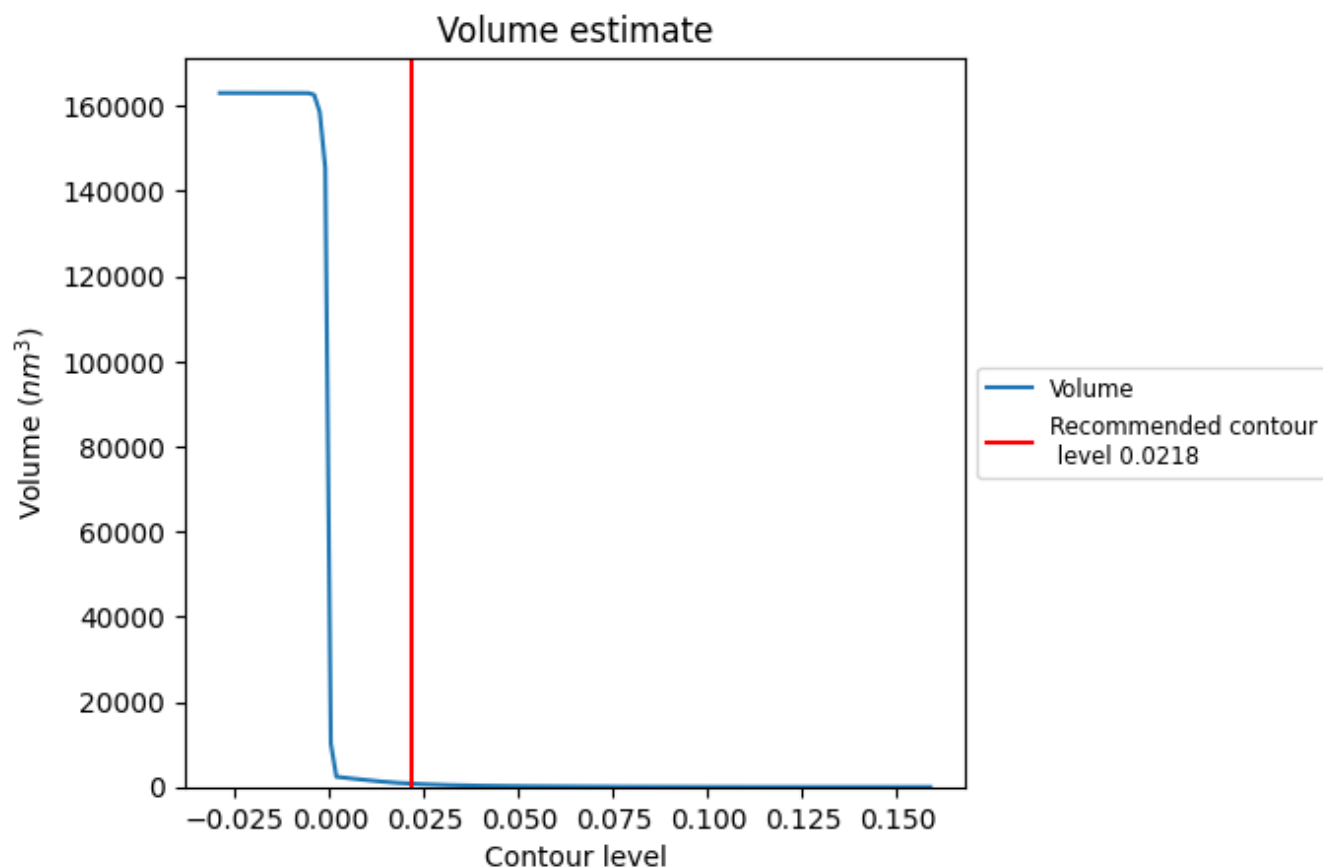
This section contains the results of statistical analysis of the map.

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.

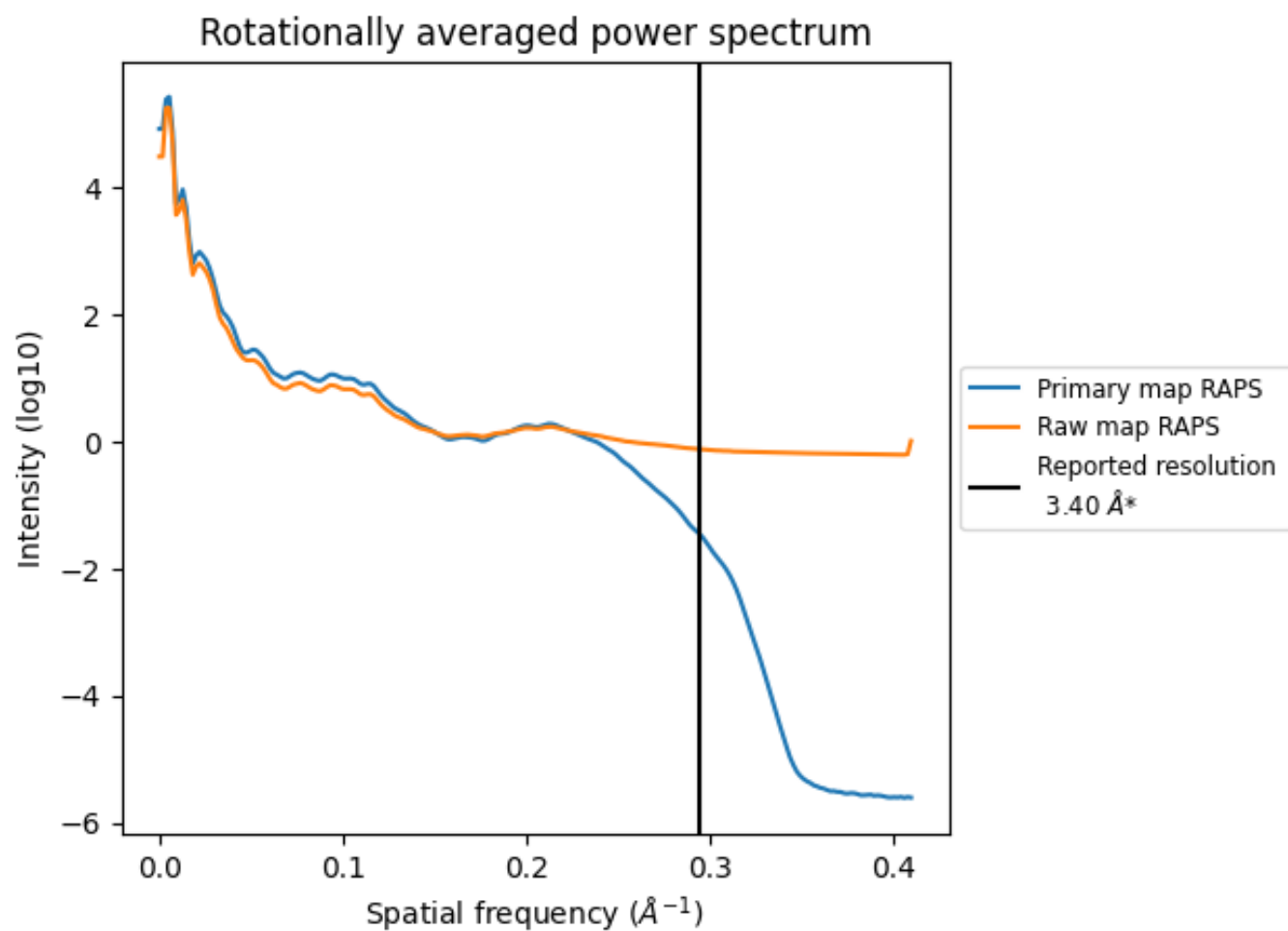
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 765 nm^3 ; this corresponds to an approximate mass of 691 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 ⓘ

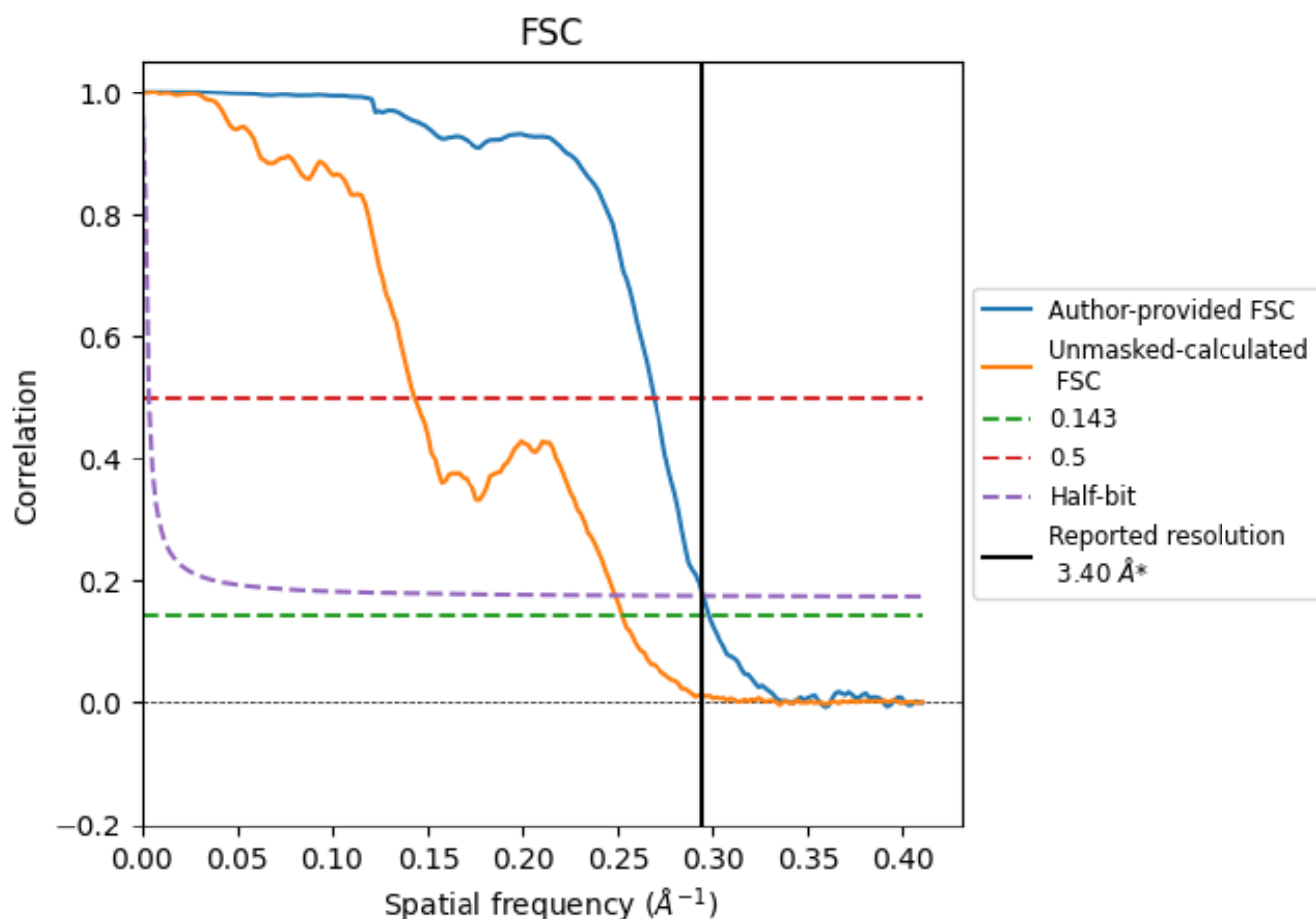


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

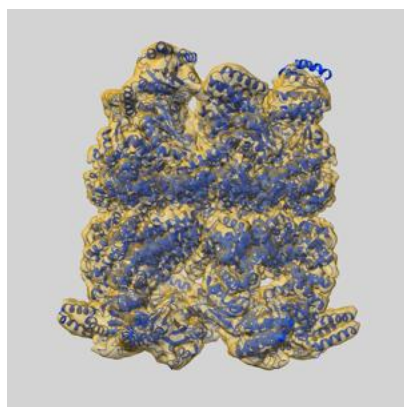
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.35	3.72	3.39
Unmasked-calculated*	3.97	7.00	4.02

*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 3.97 differs from the reported value 3.4 by more than 10 %

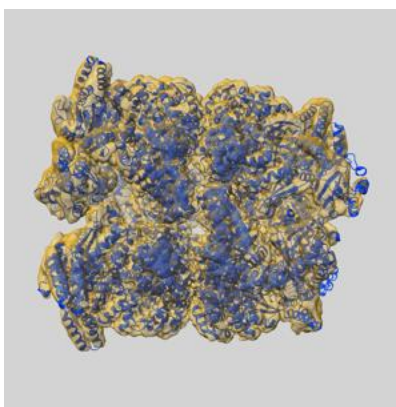
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15940 and PDB model 8BA8. Per-residue inclusion information can be found in section [3](#) on page [9](#).

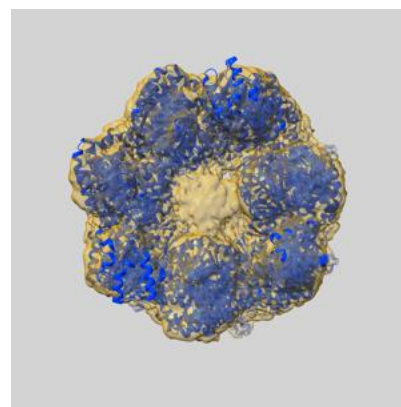
9.1 Map-model overlay [i](#)



X



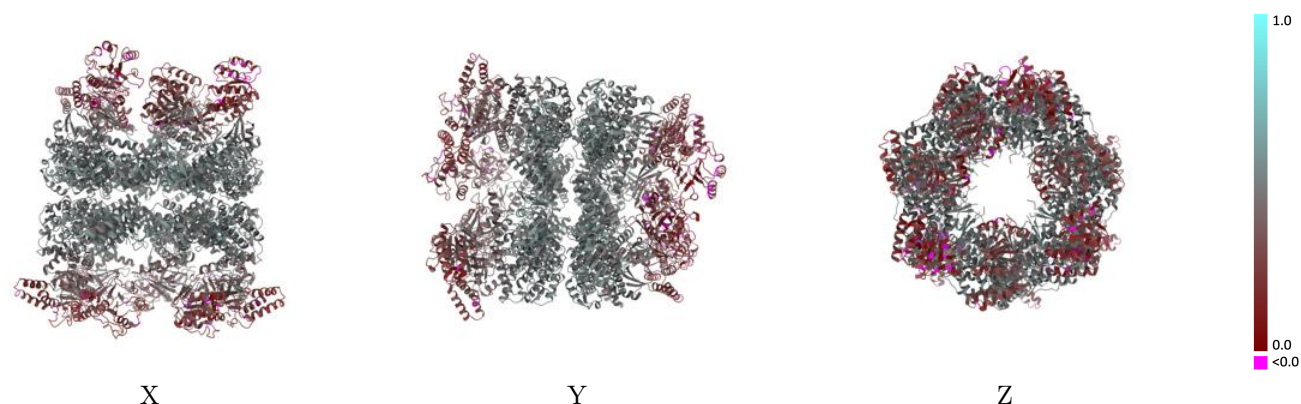
Y



Z

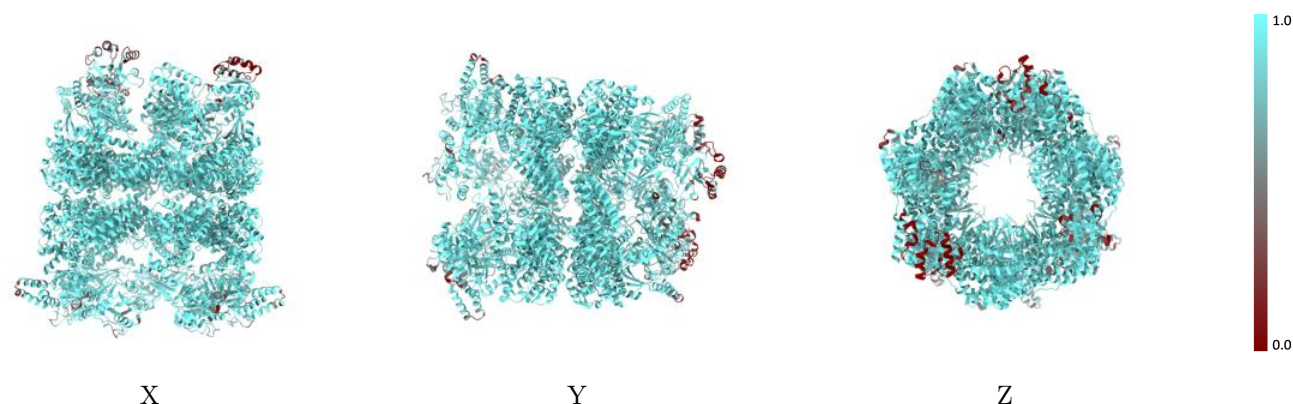
The images above show the 3D surface view of the map at the recommended contour level 0.0218 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



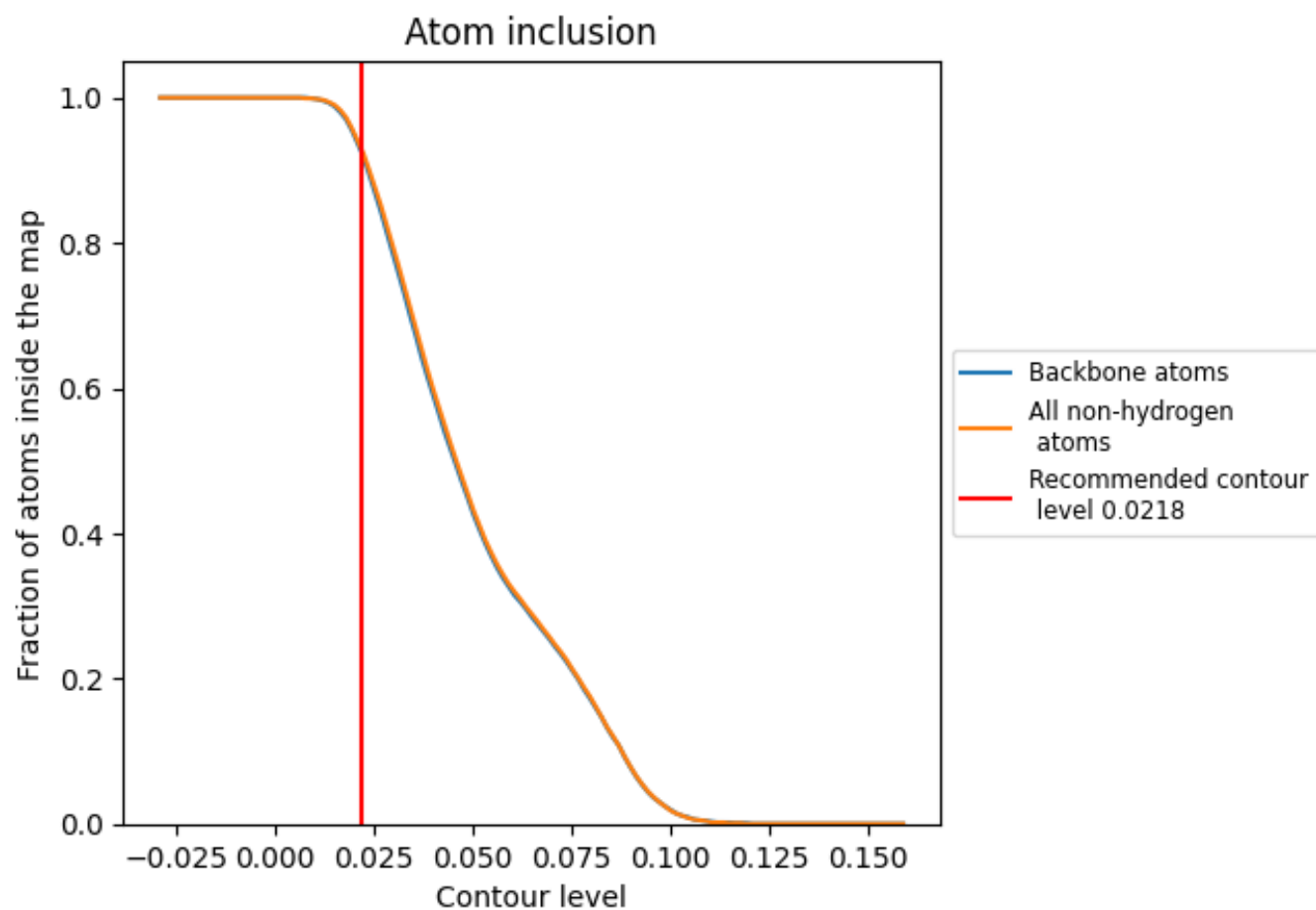
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0218).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 93% 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 (0.0218) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9290	 0.4070
A	 0.9750	 0.4220
B	 0.8390	 0.3800
C	 0.9240	 0.4090
D	 0.9430	 0.4030
E	 0.8740	 0.3870
F	 0.9740	 0.4260
G	 0.9030	 0.3870
H	 0.9480	 0.4030
I	 0.9470	 0.4110
J	 0.9470	 0.4090
K	 0.9390	 0.4070
L	 0.9410	 0.4170
M	 0.9480	 0.4190
N	 0.9430	 0.4130

