



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 09:33 PM UTC

PDB ID : 8UAE / pdb_00008uae
EMDB ID : EMD-42061
Title : E. coli Sir2_HerA complex (12:6) with ATPgamaS
Authors : Shen, Z.F.; Lin, Q.P.; Fu, T.M.
Deposited on : 2023-09-20
Resolution : 3.25 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.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)
Validation Pipeline (wwPDB-VP) : 2.49

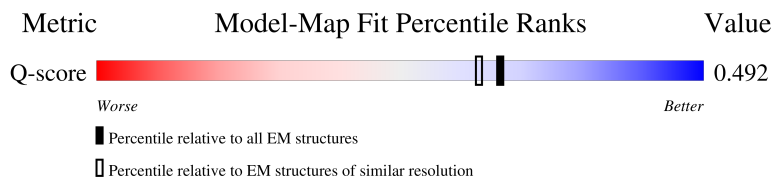
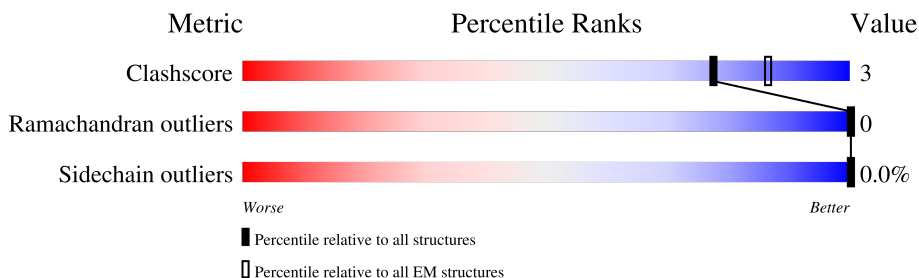
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.25 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.



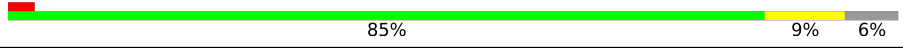
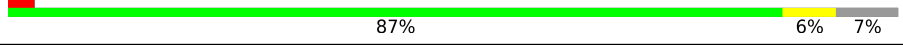
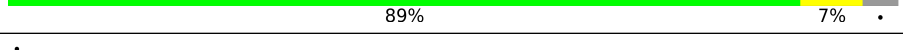
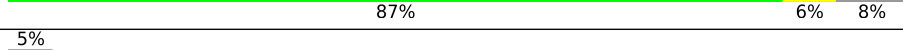
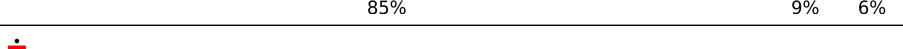
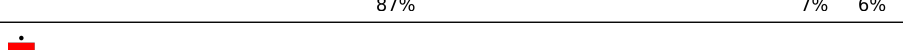
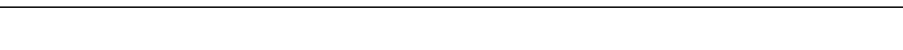
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14599 (2.75 - 3.75)

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	415	 93%
1	B	415	 88% 8%
1	C	415	 89% 7%
1	D	415	 87% 5% 7%

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Mol	Chain	Length	Quality of chain
1	E	415	 90% 7%
1	F	415	 86% 6% 8%
1	G	415	 85% 9% 6%
1	H	415	 87% 6% 7%
1	I	415	 90% 5% 5%
1	J	415	 88% 8%
1	K	415	 89% 7%
1	L	415	 87% 6% 8%
2	M	610	 85% 9% 6%
2	N	610	 87% 7% 6%
2	O	610	 88% 8%
2	P	610	 82% 8% 10%
2	Q	610	 80% 11% 10%
2	R	610	 74% 11% 14%

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
4	AGS	N	701	X	-	-	-
4	AGS	O	701	X	-	-	-
4	AGS	P	701	X	-	-	-
4	AGS	Q	701	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 64624 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 SIR2-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	398	Total	C	N	O	S	0	0
			3185	2048	532	599	6		
1	B	381	Total	C	N	O	S	0	0
			3054	1969	509	570	6		
1	C	398	Total	C	N	O	S	0	0
			3185	2048	532	599	6		
1	D	384	Total	C	N	O	S	0	0
			3071	1978	513	574	6		
1	E	400	Total	C	N	O	S	0	0
			3194	2053	534	601	6		
1	F	383	Total	C	N	O	S	0	0
			3066	1975	512	573	6		
1	G	390	Total	C	N	O	S	0	0
			3119	2006	520	587	6		
1	H	384	Total	C	N	O	S	0	0
			3071	1978	513	574	6		
1	I	394	Total	C	N	O	S	0	0
			3145	2021	525	593	6		
1	J	383	Total	C	N	O	S	0	0
			3067	1976	512	573	6		
1	K	398	Total	C	N	O	S	0	0
			3182	2047	532	597	6		
1	L	383	Total	C	N	O	S	0	0
			3067	1976	512	573	6		

- Molecule 2 is a protein called Nucleoside triphosphate hydrolase.

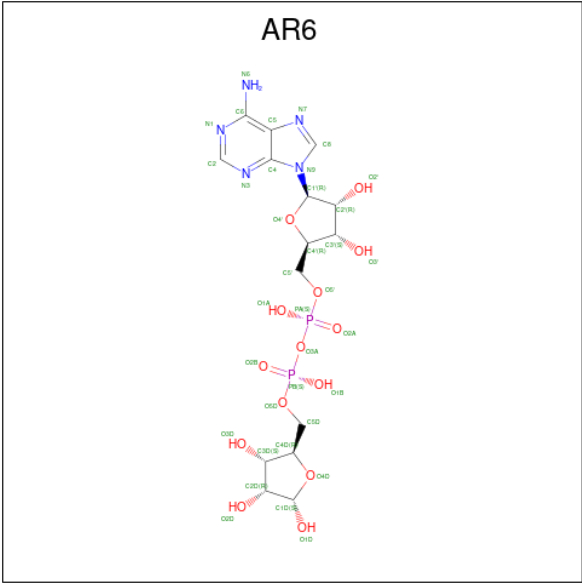
Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	573	Total	C	N	O	S	0	0
			4536	2887	798	838	13		
2	N	574	Total	C	N	O	S	0	0
			4548	2898	799	839	12		
2	O	585	Total	C	N	O	S	0	0
			4637	2951	812	862	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	P	549	Total 4346	2777	752	805	12	0	0
2	Q	552	Total 4389	2806	765	805	13	0	0
2	R	524	Total 4170	2660	728	771	11	0	0

- Molecule 3 is [(2R,3S,4R,5R)-5-(6-AMINOPURIN-9-YL)-3,4-DIHYDROXY-OXOLAN-2-YL]METHYL [HYDROXY-[(2R,3S,4R,5S)-3,4,5-TRIHIDROXYOXOLAN-2-YL]METHOXY]PHOSPHORYL] HYDROGEN PHOSPHATE (CCD ID: AR6) (formula: C₁₅H₂₃N₅O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



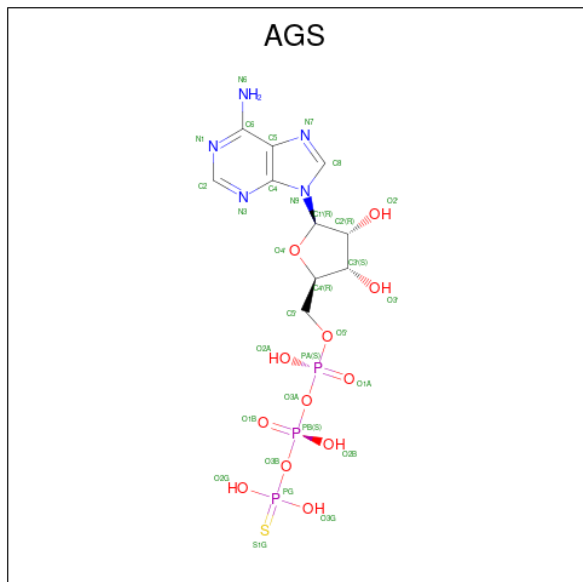
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	Total 36	15	5	14	2	0
3	B	1	Total 36	15	5	14	2	0
3	C	1	Total 36	15	5	14	2	0
3	D	1	Total 36	15	5	14	2	0
3	E	1	Total 36	15	5	14	2	0
3	F	1	Total 36	15	5	14	2	0
3	G	1	Total 36	15	5	14	2	0

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Mol	Chain	Residues	Atoms					AltConf
3	H	1	Total	C	N	O	P	0
			36	15	5	14	2	
3	I	1	Total	C	N	O	P	0
			36	15	5	14	2	
3	J	1	Total	C	N	O	P	0
			36	15	5	14	2	
3	K	1	Total	C	N	O	P	0
			36	15	5	14	2	
3	L	1	Total	C	N	O	P	0
			36	15	5	14	2	

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
4	M	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
4	N	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
4	O	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
4	P	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
4	Q	1	Total 31	C 10	N 5	O 12	P 3	S 1	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of

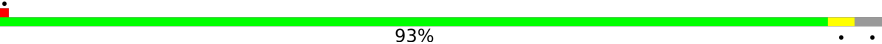
Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	M	1	Total 1	Mg 1	0
5	N	1	Total 1	Mg 1	0
5	O	1	Total 1	Mg 1	0
5	P	1	Total 1	Mg 1	0
5	Q	1	Total 1	Mg 1	0

3 Residue-property plots [i](#)

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

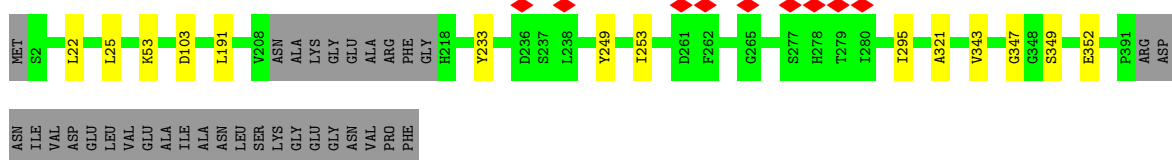
- Molecule 1: SIR2-like domain-containing protein

Chain A:  93%



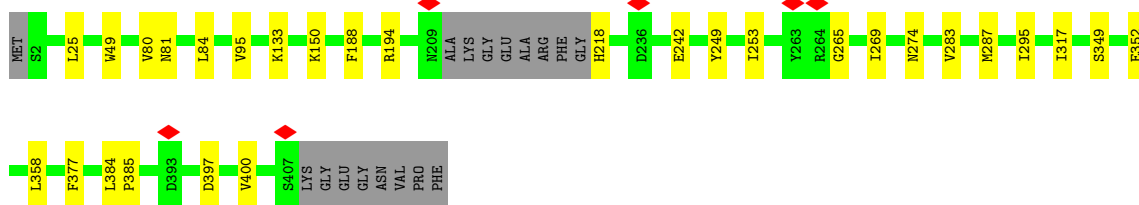
- Molecule 1: SIR2-like domain-containing protein

Chain B:  88% 8%



- Molecule 1: SIR2-like domain-containing protein

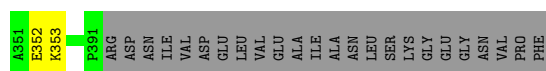
Chain C:  89% 7%



- Molecule 1: SIR2-like domain-containing protein

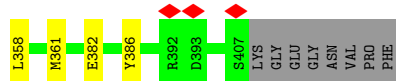
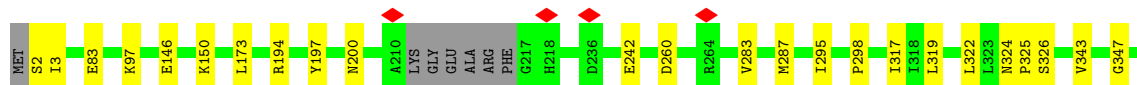
Chain D:  87% 5% 7%





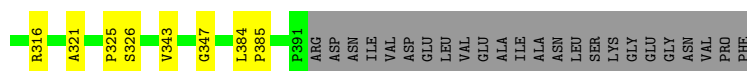
- Molecule 1: SIR2-like domain-containing protein

Chain E: 90% 7%



- Molecule 1: SIR2-like domain-containing protein

Chain F: 86% 6% 8%



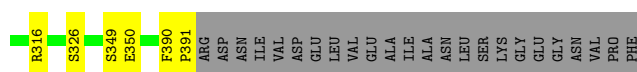
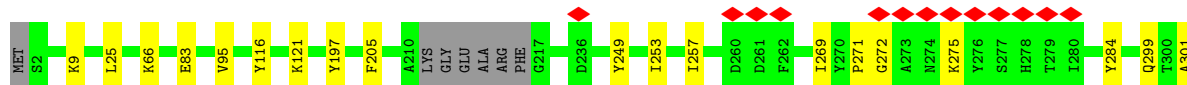
- Molecule 1: SIR2-like domain-containing protein

Chain G: 85% 9% 6%



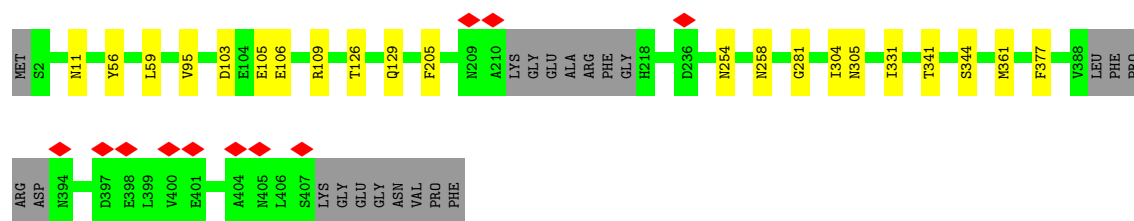
- Molecule 1: SIR2-like domain-containing protein

Chain H: 87% 6% 7%



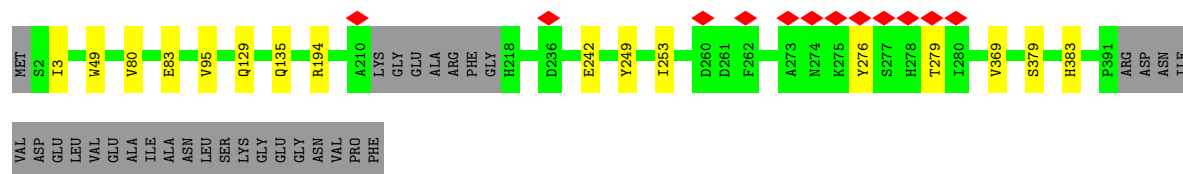
- Molecule 1: SIR2-like domain-containing protein

Chain I: 90% 5% 5%



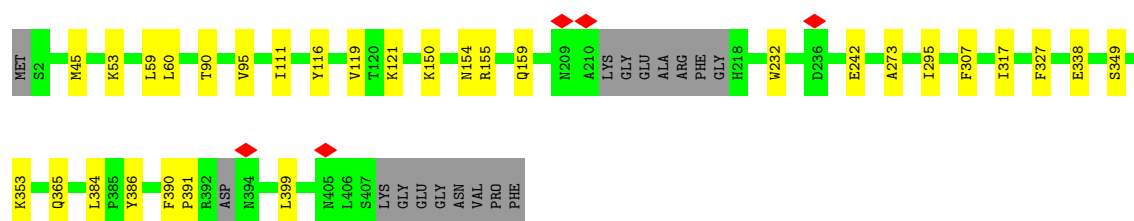
- Molecule 1: SIR2-like domain-containing protein

Chain J: 88% 8%



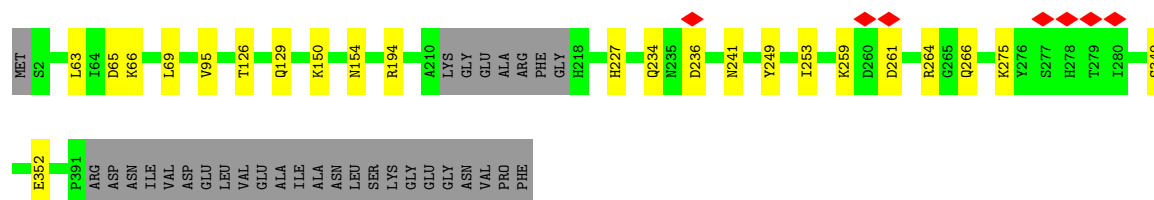
- Molecule 1: SIR2-like domain-containing protein

Chain K: 89% 7%



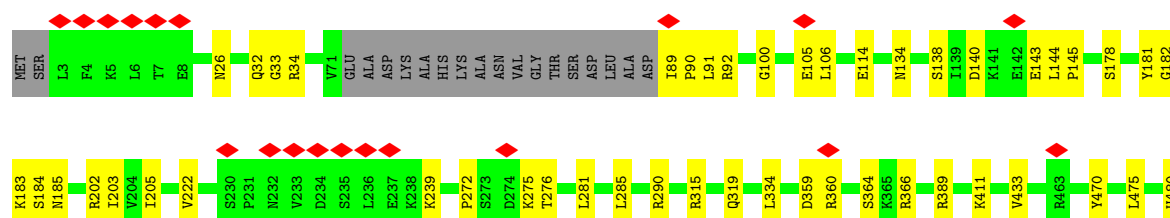
- Molecule 1: SIR2-like domain-containing protein

Chain L: 87% 6% 8%



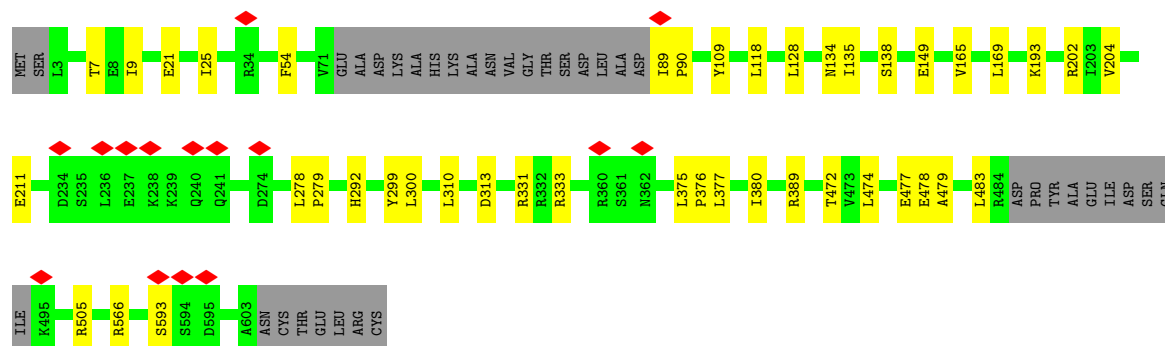
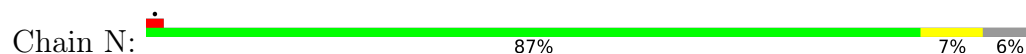
- Molecule 2: Nucleoside triphosphate hydrolase

Chain M: 5% 85% 9% 6%

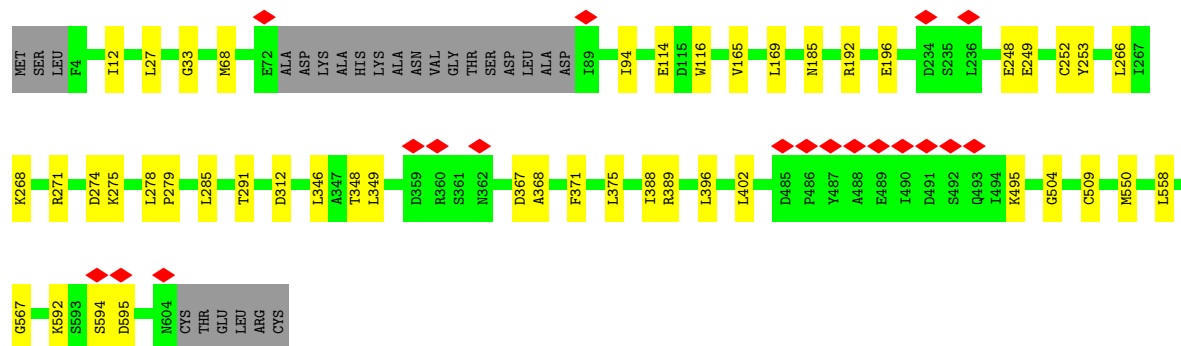
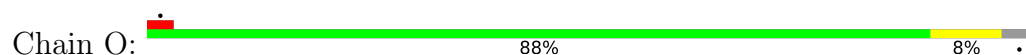




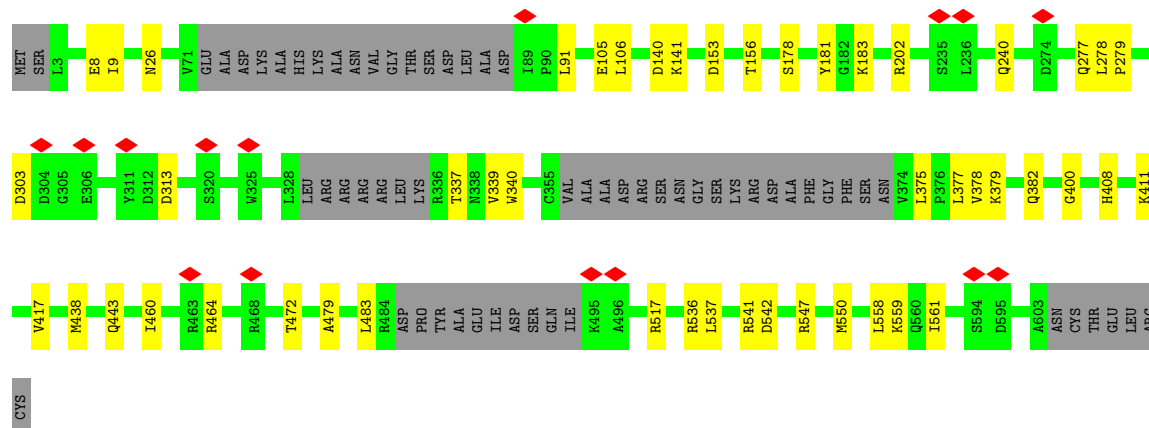
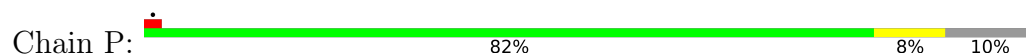
• Molecule 2: Nucleoside triphosphate hydrolase



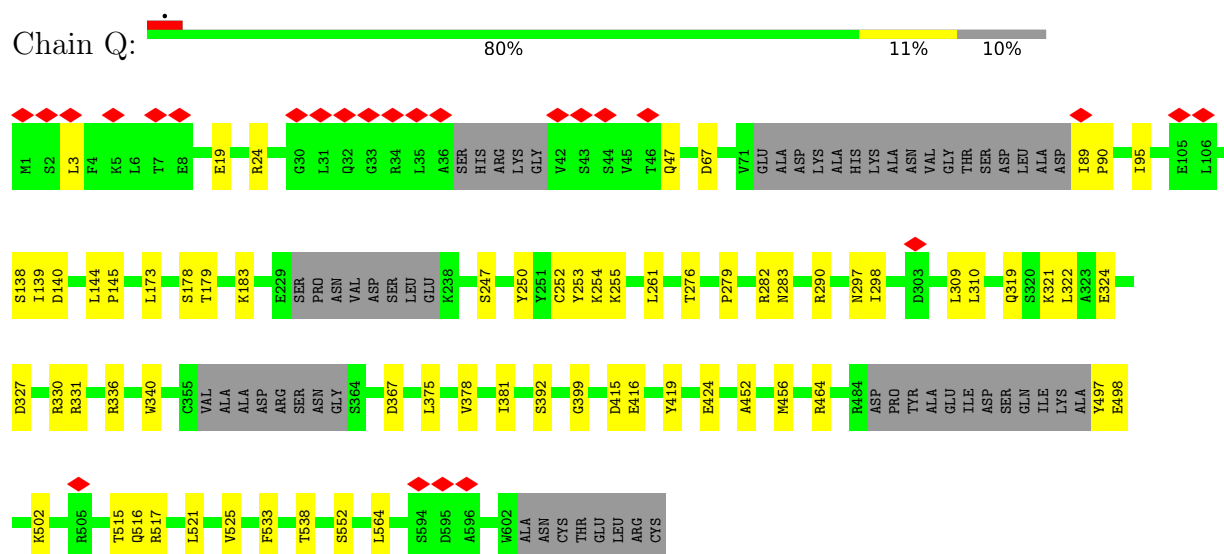
• Molecule 2: Nucleoside triphosphate hydrolase



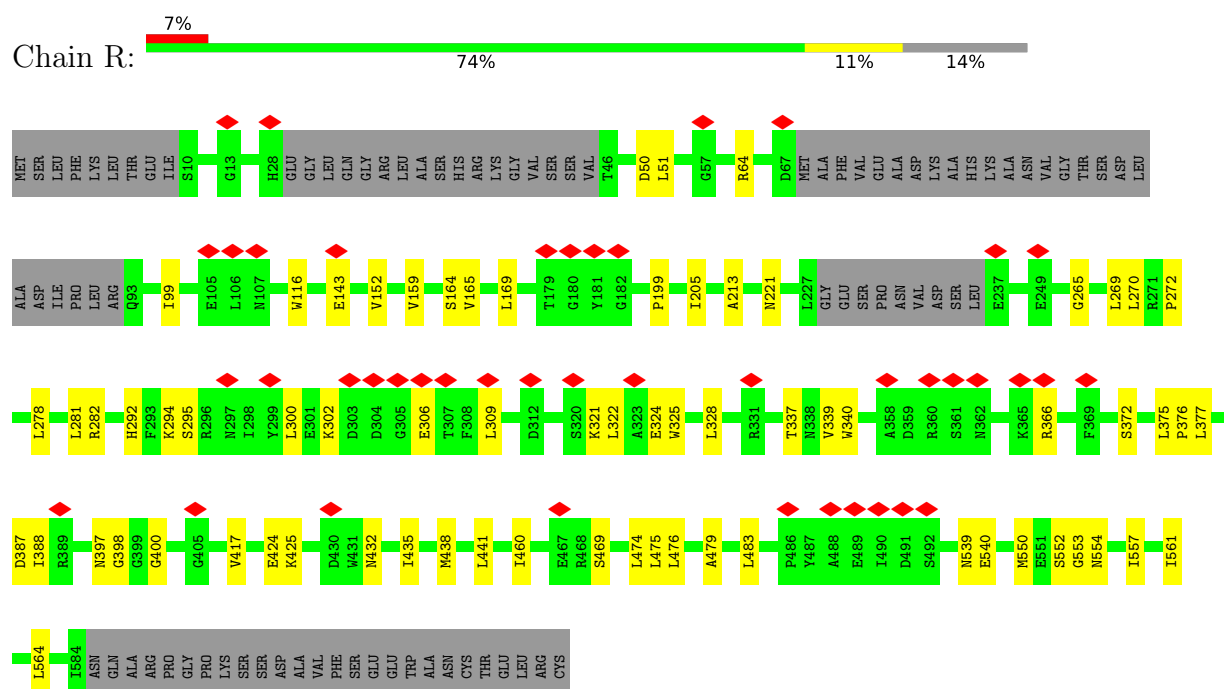
• Molecule 2: Nucleoside triphosphate hydrolase



- Molecule 2: Nucleoside triphosphate hydrolase



- Molecule 2: Nucleoside triphosphate hydrolase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	232183	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.063	Depositor
Minimum map value	-0.028	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.0666	Depositor
Map size ($\text{\AA}$)	355.2, 355.2, 355.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.11, 1.11, 1.11	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AR6, AGS, 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	0.11	0/3259	0.28	0/4406
1	B	0.10	0/3128	0.26	0/4227
1	C	0.11	0/3259	0.32	2/4406 (0.0%)
1	D	0.11	0/3145	0.29	0/4250
1	E	0.11	0/3268	0.28	0/4418
1	F	0.11	0/3140	0.28	0/4243
1	G	0.10	0/3190	0.25	0/4310
1	H	0.11	0/3145	0.28	0/4250
1	I	0.11	0/3216	0.27	0/4346
1	J	0.10	0/3141	0.26	0/4245
1	K	0.11	0/3255	0.29	0/4399
1	L	0.10	0/3141	0.26	0/4245
2	M	0.11	0/4624	0.28	0/6243
2	N	0.11	0/4637	0.29	0/6260
2	O	0.12	0/4729	0.30	0/6388
2	P	0.10	0/4431	0.28	0/5985
2	Q	0.11	0/4473	0.29	0/6033
2	R	0.12	0/4250	0.31	0/5737
All	All	0.11	0/65431	0.28	2/88391 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	385	PRO	CA-C-N	7.97	140.96	122.31
1	C	385	PRO	C-N-CA	7.97	140.96	122.31

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	3185	0	3109	6	0
1	B	3054	0	2981	10	0
1	C	3185	0	3109	19	0
1	D	3071	0	2995	15	0
1	E	3194	0	3117	20	0
1	F	3066	0	2990	14	0
1	G	3119	0	3044	21	0
1	H	3071	0	2995	17	0
1	I	3145	0	3069	13	0
1	J	3067	0	2992	10	0
1	K	3182	0	3109	20	0
1	L	3067	0	2992	13	0
2	M	4536	0	4576	31	0
2	N	4548	0	4591	25	0
2	O	4637	0	4664	27	0
2	P	4346	0	4380	32	0
2	Q	4389	0	4438	43	0
2	R	4170	0	4203	45	0
3	A	36	0	21	0	0
3	B	36	0	21	0	0
3	C	36	0	21	1	0
3	D	36	0	21	1	0
3	E	36	0	21	1	0
3	F	36	0	21	0	0
3	G	36	0	21	0	0
3	H	36	0	21	1	0
3	I	36	0	21	0	0
3	J	36	0	21	1	0
3	K	36	0	21	1	0
3	L	36	0	21	0	0
4	M	31	0	12	4	0
4	N	31	0	12	2	0
4	O	31	0	12	3	0
4	P	31	0	12	0	0
4	Q	31	0	12	0	0
5	M	1	0	0	1	0
5	N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	O	1	0	0	1	0
5	P	1	0	0	0	0
5	Q	1	0	0	0	0
All	All	64624	0	63666	366	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 3.

The worst 5 of 366 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)
4:M:701:AGS:S1G	5:M:702:MG:MG	1.65	0.80
2:R:340:TRP:HB2	2:R:400:GLY:H	1.51	0.75
1:E:197:TYR:O	1:E:200:ASN:ND2	2.23	0.72
2:P:313:ASP:OD2	2:Q:330:ARG:NH1	2.24	0.71
2:M:178:SER:O	2:M:183:LYS:NZ	2.25	0.69

There are no symmetry-related clashes.

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	394/415 (95%)	376 (95%)	18 (5%)	0	100	100
1	B	377/415 (91%)	362 (96%)	15 (4%)	0	100	100
1	C	394/415 (95%)	384 (98%)	10 (2%)	0	100	100
1	D	380/415 (92%)	363 (96%)	17 (4%)	0	100	100
1	E	396/415 (95%)	371 (94%)	25 (6%)	0	100	100
1	F	379/415 (91%)	360 (95%)	19 (5%)	0	100	100
1	G	384/415 (92%)	362 (94%)	22 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	380/415 (92%)	362 (95%)	18 (5%)	0	100	100
1	I	388/415 (94%)	373 (96%)	15 (4%)	0	100	100
1	J	379/415 (91%)	366 (97%)	13 (3%)	0	100	100
1	K	392/415 (94%)	371 (95%)	21 (5%)	0	100	100
1	L	379/415 (91%)	365 (96%)	14 (4%)	0	100	100
2	M	567/610 (93%)	542 (96%)	25 (4%)	0	100	100
2	N	568/610 (93%)	531 (94%)	37 (6%)	0	100	100
2	O	581/610 (95%)	557 (96%)	24 (4%)	0	100	100
2	P	539/610 (88%)	515 (96%)	24 (4%)	0	100	100
2	Q	540/610 (88%)	524 (97%)	16 (3%)	0	100	100
2	R	516/610 (85%)	499 (97%)	17 (3%)	0	100	100
All	All	7933/8640 (92%)	7583 (96%)	350 (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	340/351 (97%)	340 (100%)	0	100	100
1	B	325/351 (93%)	325 (100%)	0	100	100
1	C	340/351 (97%)	340 (100%)	0	100	100
1	D	326/351 (93%)	326 (100%)	0	100	100
1	E	340/351 (97%)	340 (100%)	0	100	100
1	F	326/351 (93%)	326 (100%)	0	100	100
1	G	332/351 (95%)	332 (100%)	0	100	100
1	H	326/351 (93%)	326 (100%)	0	100	100
1	I	335/351 (95%)	335 (100%)	0	100	100
1	J	326/351 (93%)	326 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	339/351 (97%)	338 (100%)	1 (0%)	86	86
1	L	326/351 (93%)	326 (100%)	0	100	100
2	M	489/519 (94%)	489 (100%)	0	100	100
2	N	489/519 (94%)	489 (100%)	0	100	100
2	O	499/519 (96%)	499 (100%)	0	100	100
2	P	469/519 (90%)	469 (100%)	0	100	100
2	Q	473/519 (91%)	473 (100%)	0	100	100
2	R	448/519 (86%)	448 (100%)	0	100	100
All	All	6848/7326 (94%)	6847 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	45	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
2	N	172	HIS
2	Q	556	GLN
2	N	318	ASN
2	O	187	ASN
2	R	283	ASN

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 22 ligands modelled in this entry, 5 are monoatomic - leaving 17 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	AR6	L	501	-	39,39,39	1.27	2 (5%)	56,60,60	0.73	0
3	AR6	I	501	-	39,39,39	1.28	2 (5%)	56,60,60	0.67	0
3	AR6	E	501	-	39,39,39	1.21	2 (5%)	56,60,60	0.71	1 (1%)
4	AGS	N	701	5	32,33,33	3.56	10 (31%)	45,52,52	1.92	12 (26%)
3	AR6	J	501	-	39,39,39	1.30	2 (5%)	56,60,60	0.69	0
3	AR6	K	501	-	39,39,39	1.22	2 (5%)	56,60,60	0.74	0
3	AR6	H	501	-	39,39,39	1.21	2 (5%)	56,60,60	0.71	0
4	AGS	O	701	-	32,33,33	3.58	12 (37%)	45,52,52	1.96	11 (24%)
4	AGS	P	701	5	32,33,33	3.73	12 (37%)	45,52,52	1.91	11 (24%)
4	AGS	Q	701	-	32,33,33	3.77	12 (37%)	45,52,52	1.90	10 (22%)
3	AR6	D	501	-	39,39,39	1.23	2 (5%)	56,60,60	0.72	0
3	AR6	F	501	-	39,39,39	1.27	2 (5%)	56,60,60	0.68	0
3	AR6	G	501	-	39,39,39	1.26	2 (5%)	56,60,60	0.67	0
3	AR6	B	501	-	39,39,39	1.26	2 (5%)	56,60,60	0.73	0
3	AR6	C	501	-	39,39,39	1.22	2 (5%)	56,60,60	0.67	0
4	AGS	M	701	-	32,33,33	3.40	11 (34%)	45,52,52	2.06	12 (26%)
3	AR6	A	501	-	39,39,39	1.26	2 (5%)	56,60,60	0.70	0

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	AR6	L	501	-	-	13/22/54/54	0/4/4/4
4	AGS	N	701	5	1/1/7/7	5/21/38/38	0/3/3/3
4	AGS	O	701	-	3/3/7/7	3/21/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AGS	P	701	5	1/1/7/7	5/21/38/38	0/3/3/3
3	AR6	E	501	-	-	10/22/54/54	0/4/4/4
3	AR6	I	501	-	-	4/22/54/54	0/4/4/4
3	AR6	H	501	-	-	9/22/54/54	0/4/4/4
4	AGS	Q	701	-	1/1/7/7	10/21/38/38	0/3/3/3
3	AR6	J	501	-	-	9/22/54/54	0/4/4/4
3	AR6	K	501	-	-	10/22/54/54	0/4/4/4
3	AR6	D	501	-	-	9/22/54/54	0/4/4/4
3	AR6	F	501	-	-	8/22/54/54	0/4/4/4
3	AR6	G	501	-	-	9/22/54/54	0/4/4/4
3	AR6	B	501	-	-	14/22/54/54	0/4/4/4
3	AR6	C	501	-	-	12/22/54/54	0/4/4/4
4	AGS	M	701	-	-	5/21/38/38	0/3/3/3
3	AR6	A	501	-	-	8/22/54/54	0/4/4/4

The worst 5 of 81 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	701	AGS	PA-O3A	10.48	1.70	1.59
4	P	701	AGS	PA-O3A	10.19	1.70	1.59
4	Q	701	AGS	PB-O3A	10.09	1.70	1.59
4	P	701	AGS	PB-O3A	9.99	1.70	1.59
4	O	701	AGS	PA-O3A	9.65	1.69	1.59

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	701	AGS	C5-C4-N3	-5.53	119.10	126.72
4	Q	701	AGS	C5-C4-N3	-5.47	119.18	126.72
4	P	701	AGS	C5-C4-N3	-5.41	119.26	126.72
4	O	701	AGS	C5-C4-N3	-5.31	119.40	126.72
4	M	701	AGS	C5-C4-N3	-5.27	119.45	126.72

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	N	701	AGS	C2'
4	O	701	AGS	C3'
4	O	701	AGS	C2'

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Mol	Chain	Res	Type	Atom
4	O	701	AGS	C4'
4	P	701	AGS	C4'

5 of 143 torsion outliers are listed below:

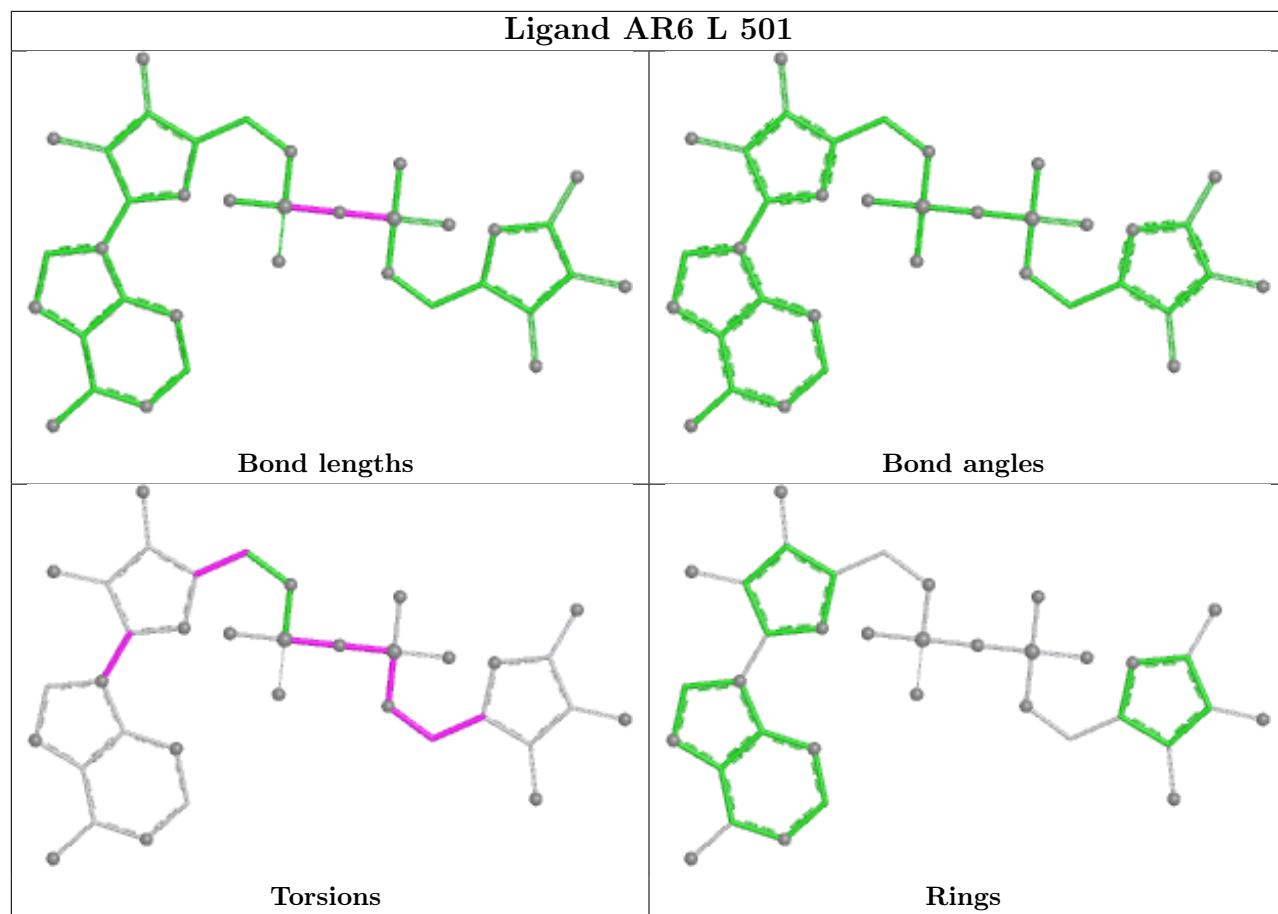
Mol	Chain	Res	Type	Atoms
3	A	501	AR6	C5D-O5D-PB-O1B
3	A	501	AR6	C5D-O5D-PB-O3A
3	B	501	AR6	C5'-O5'-PA-O1A
3	B	501	AR6	C5'-O5'-PA-O3A
3	B	501	AR6	C5D-O5D-PB-O2B

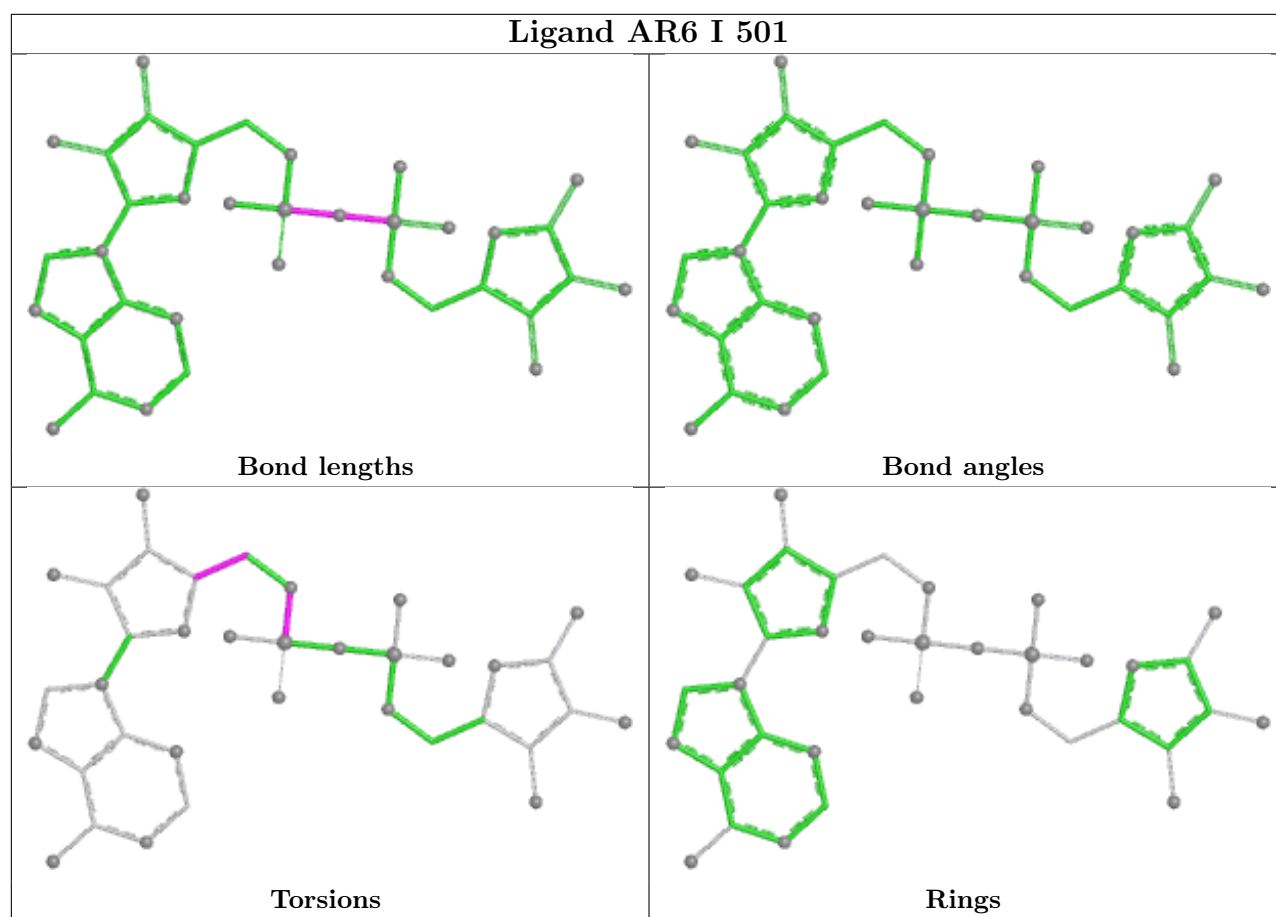
There are no ring outliers.

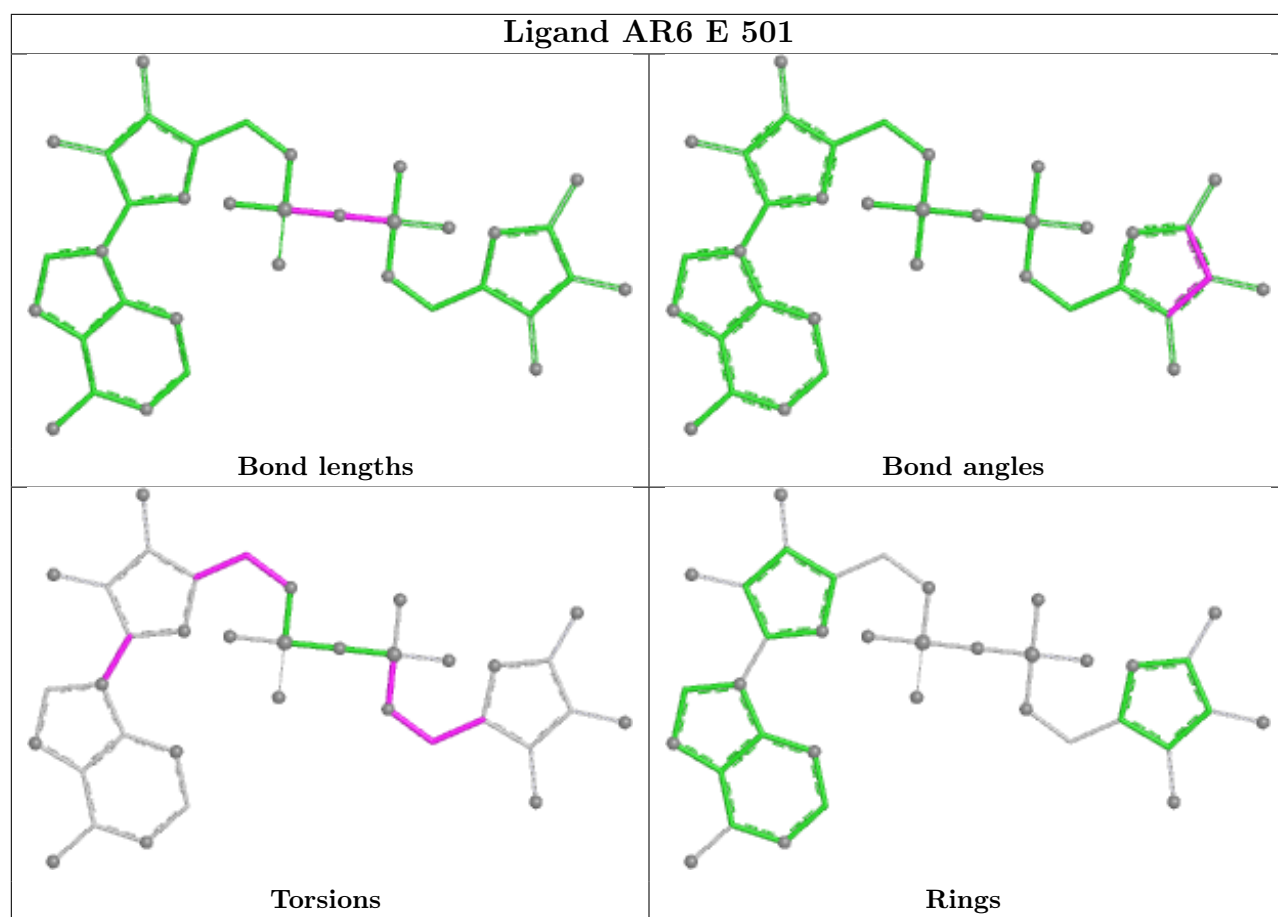
9 monomers are involved in 15 short contacts:

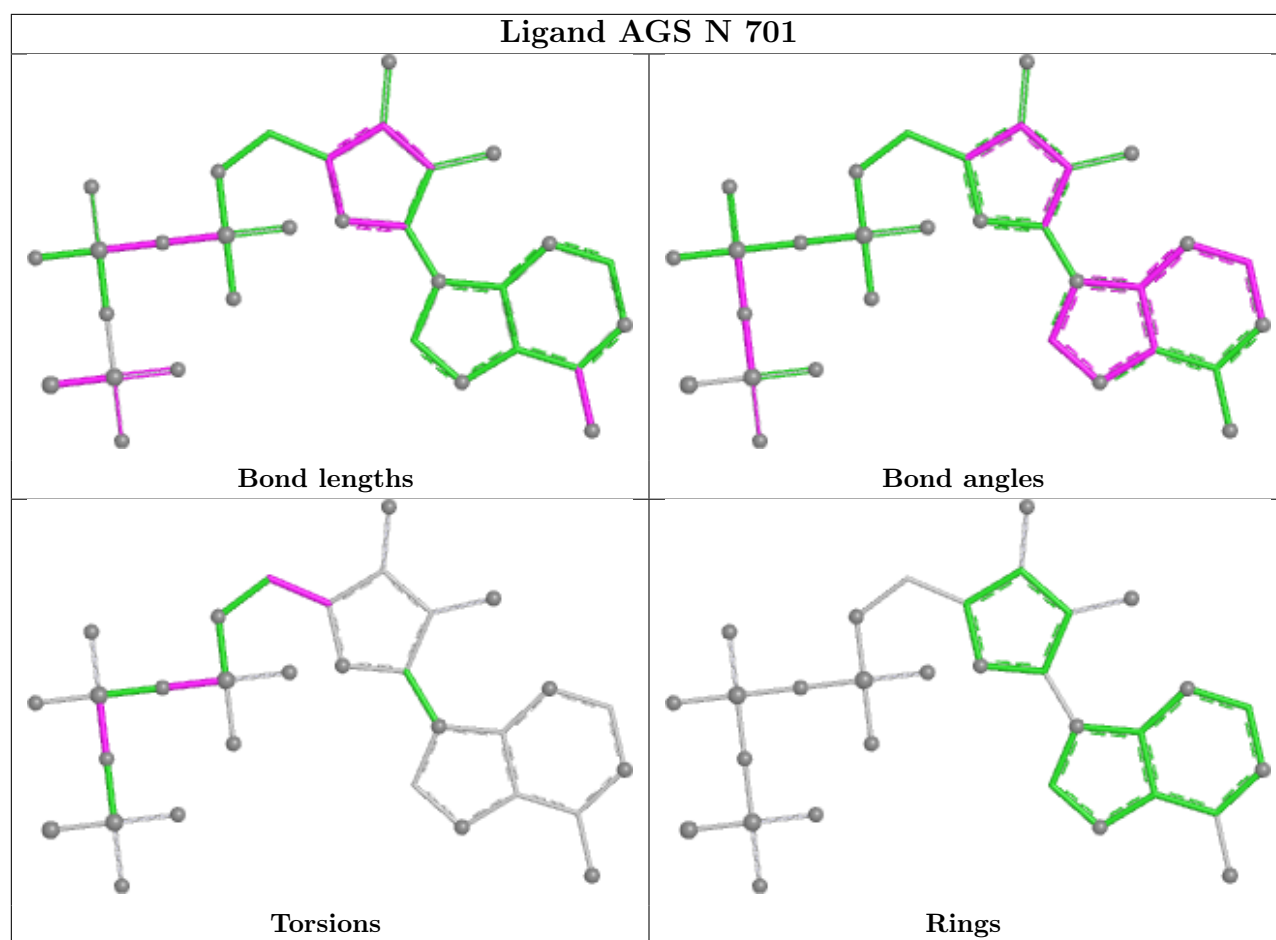
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	501	AR6	1	0
4	N	701	AGS	2	0
3	J	501	AR6	1	0
3	K	501	AR6	1	0
3	H	501	AR6	1	0
4	O	701	AGS	3	0
3	D	501	AR6	1	0
3	C	501	AR6	1	0
4	M	701	AGS	4	0

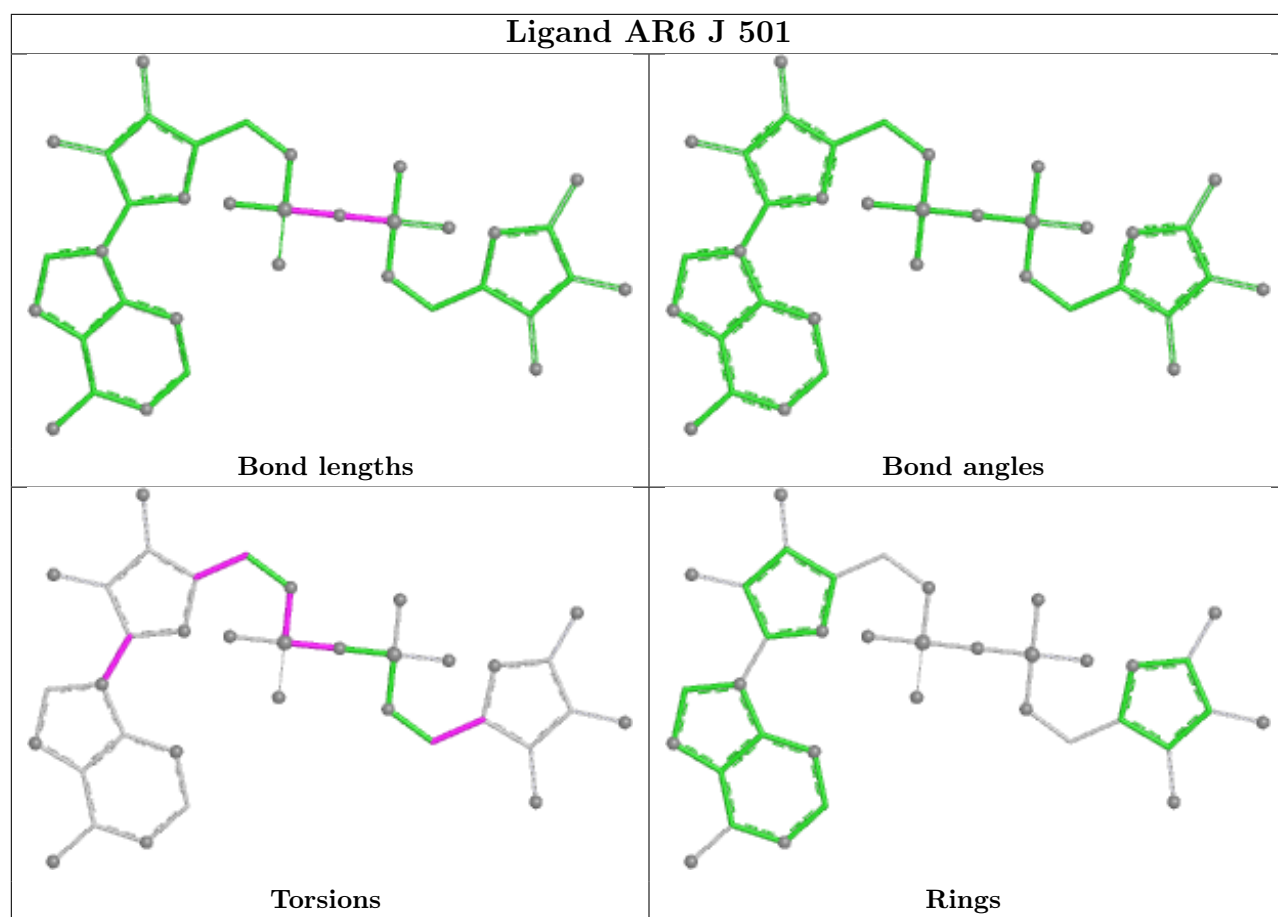
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

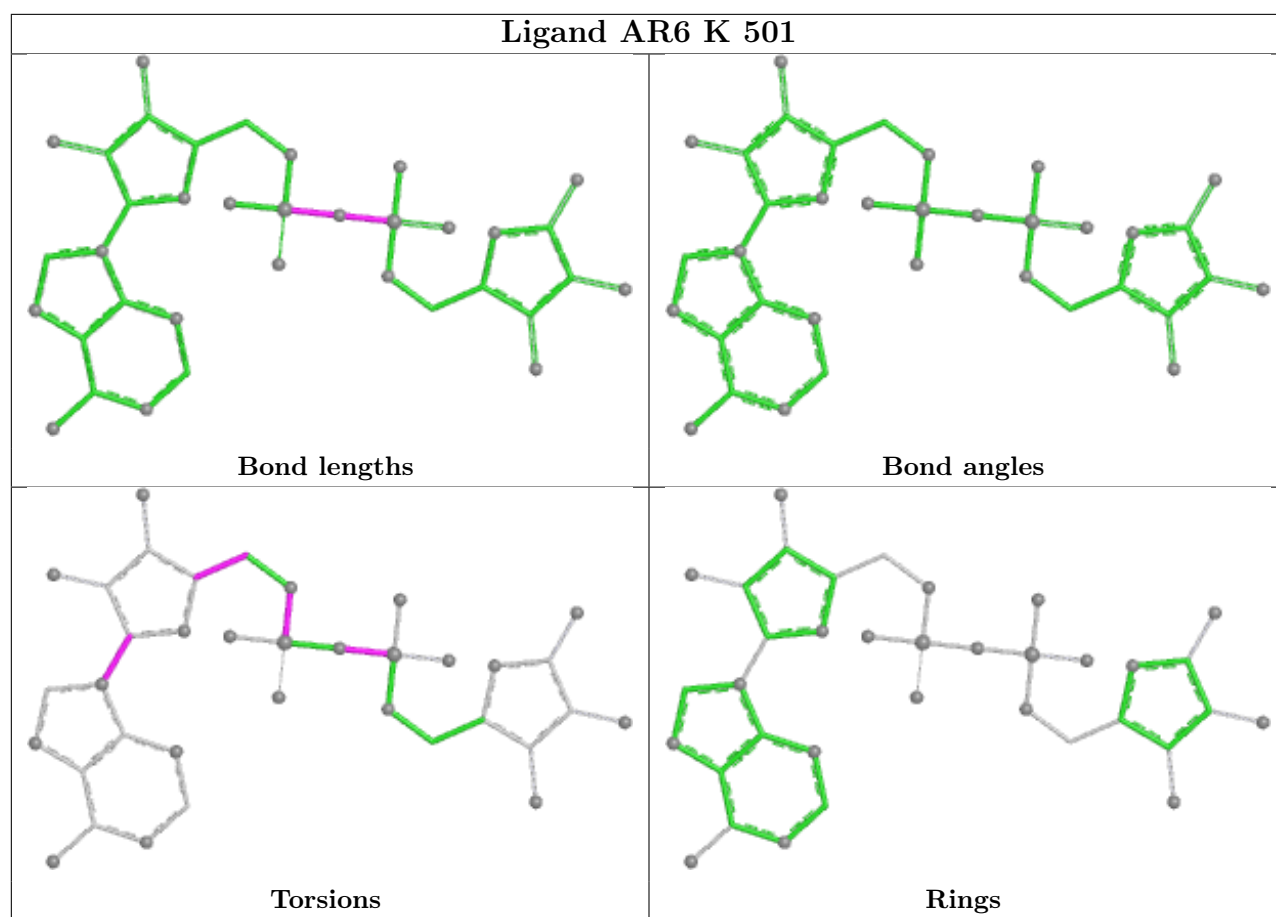


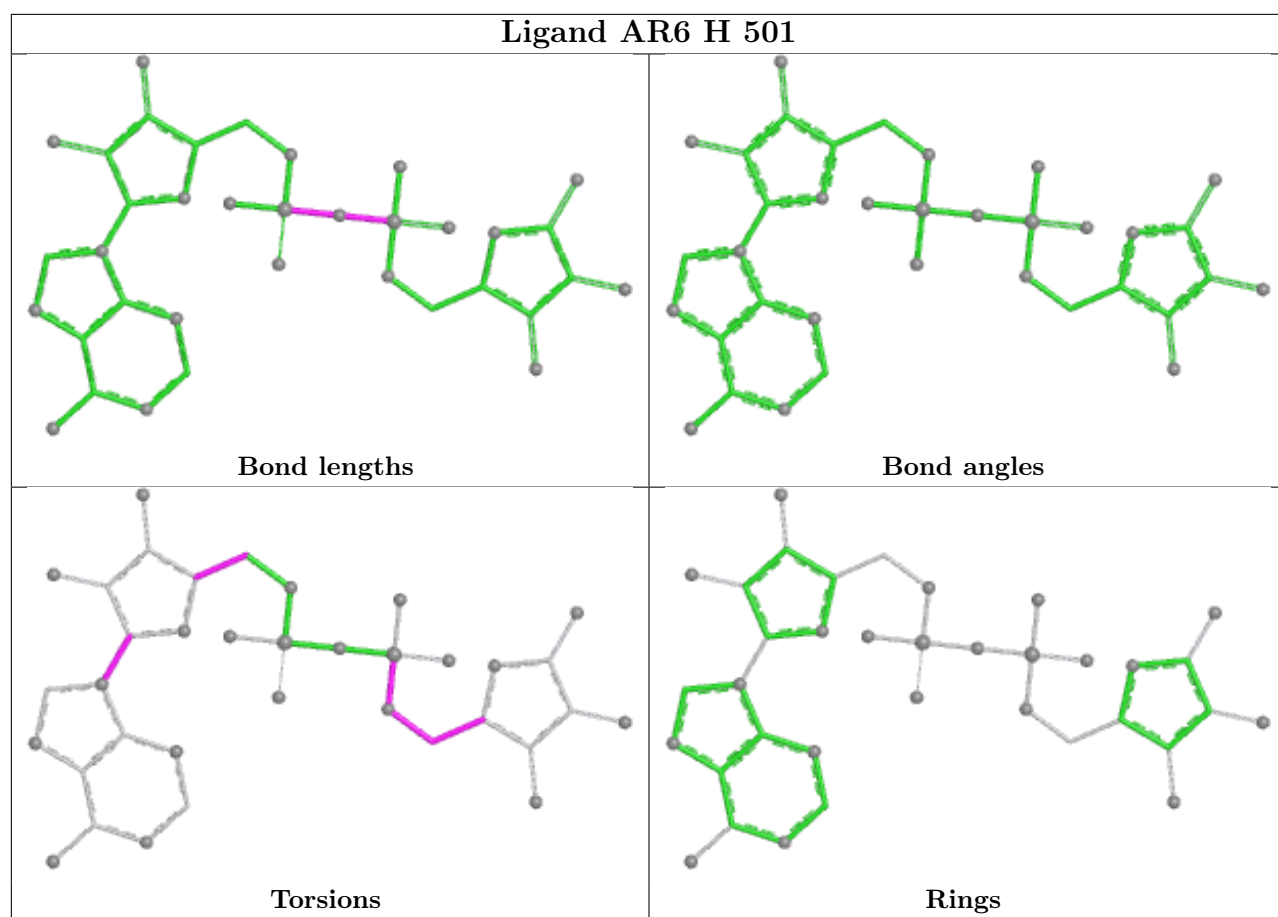


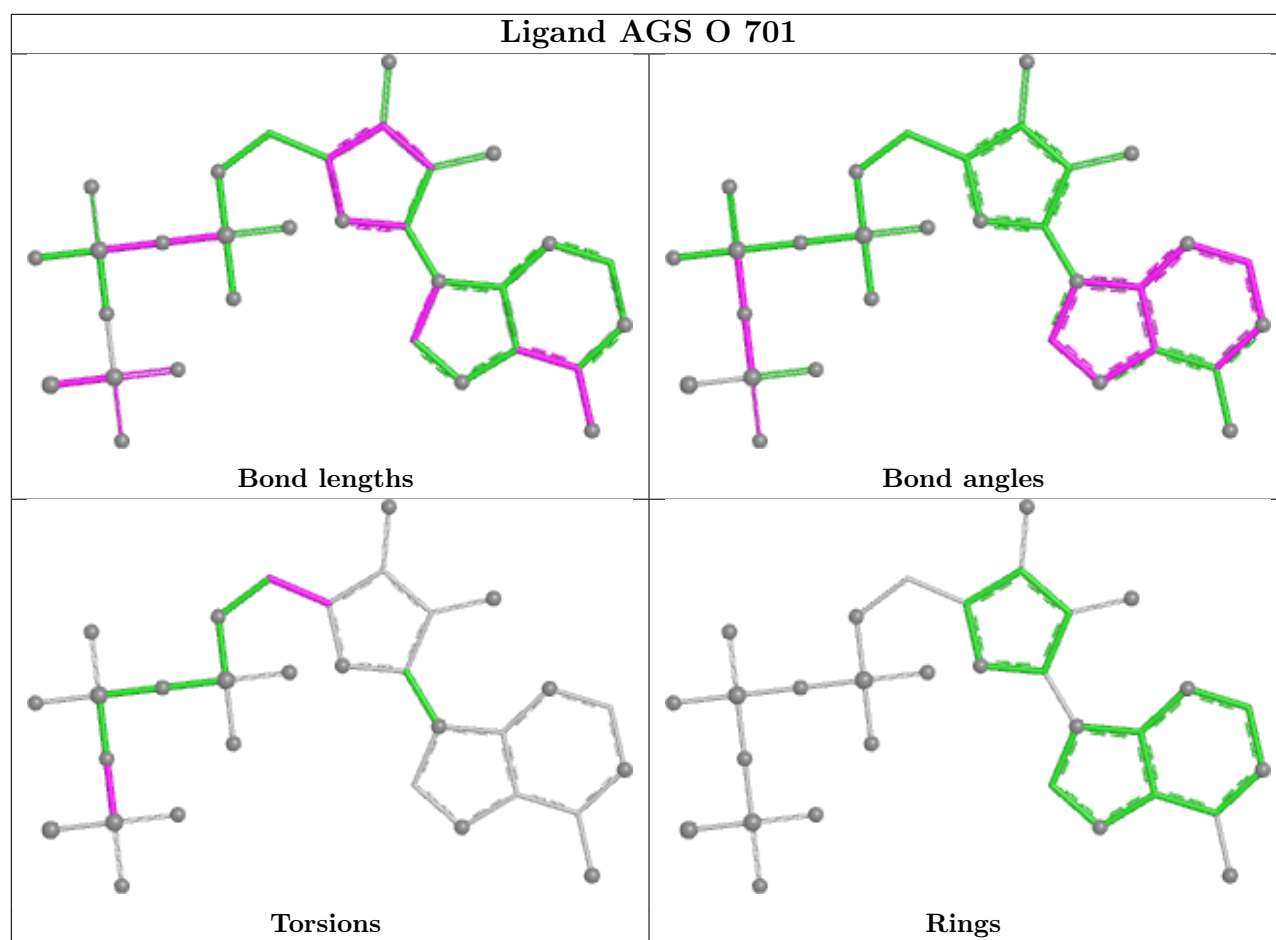


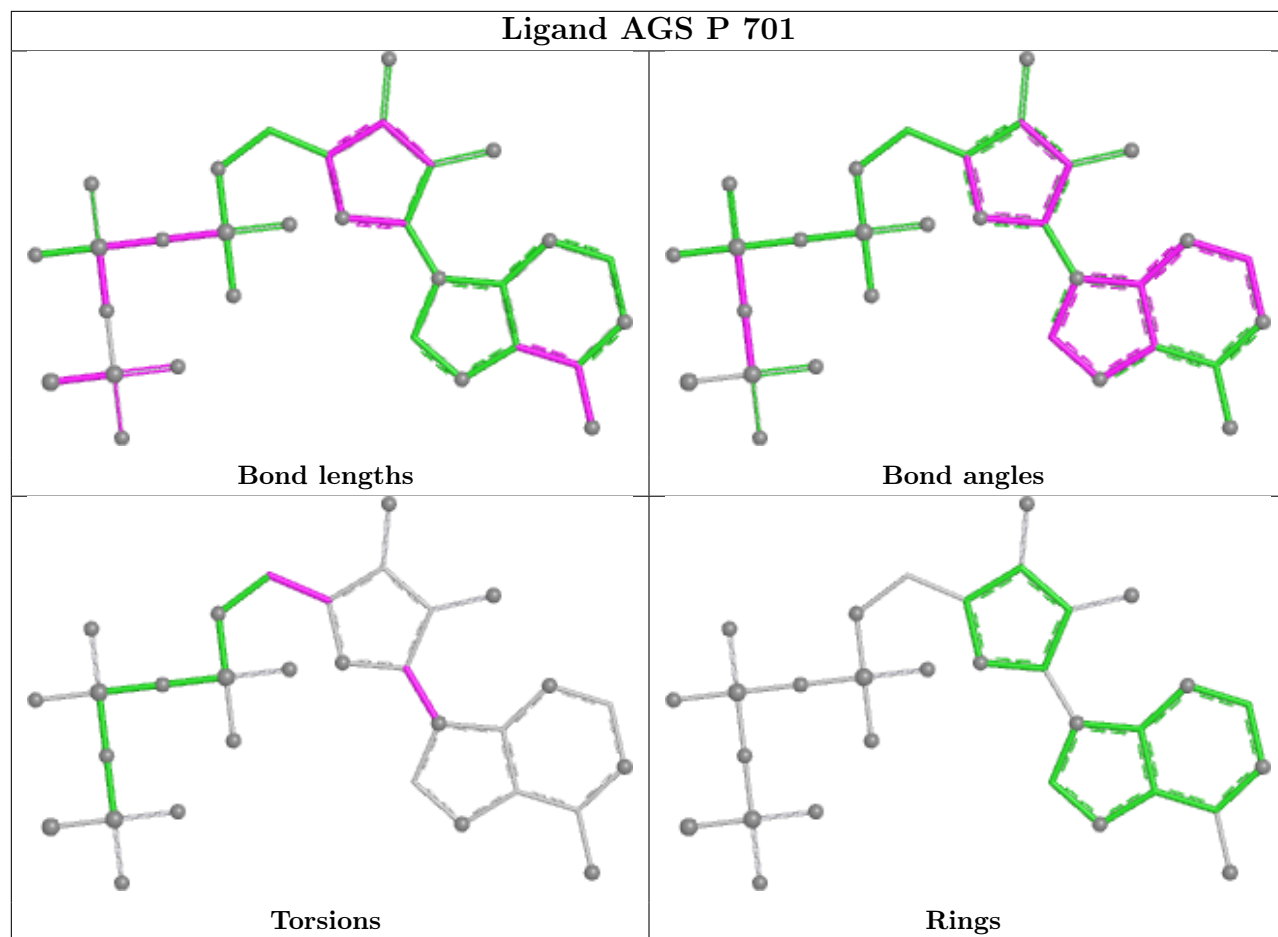


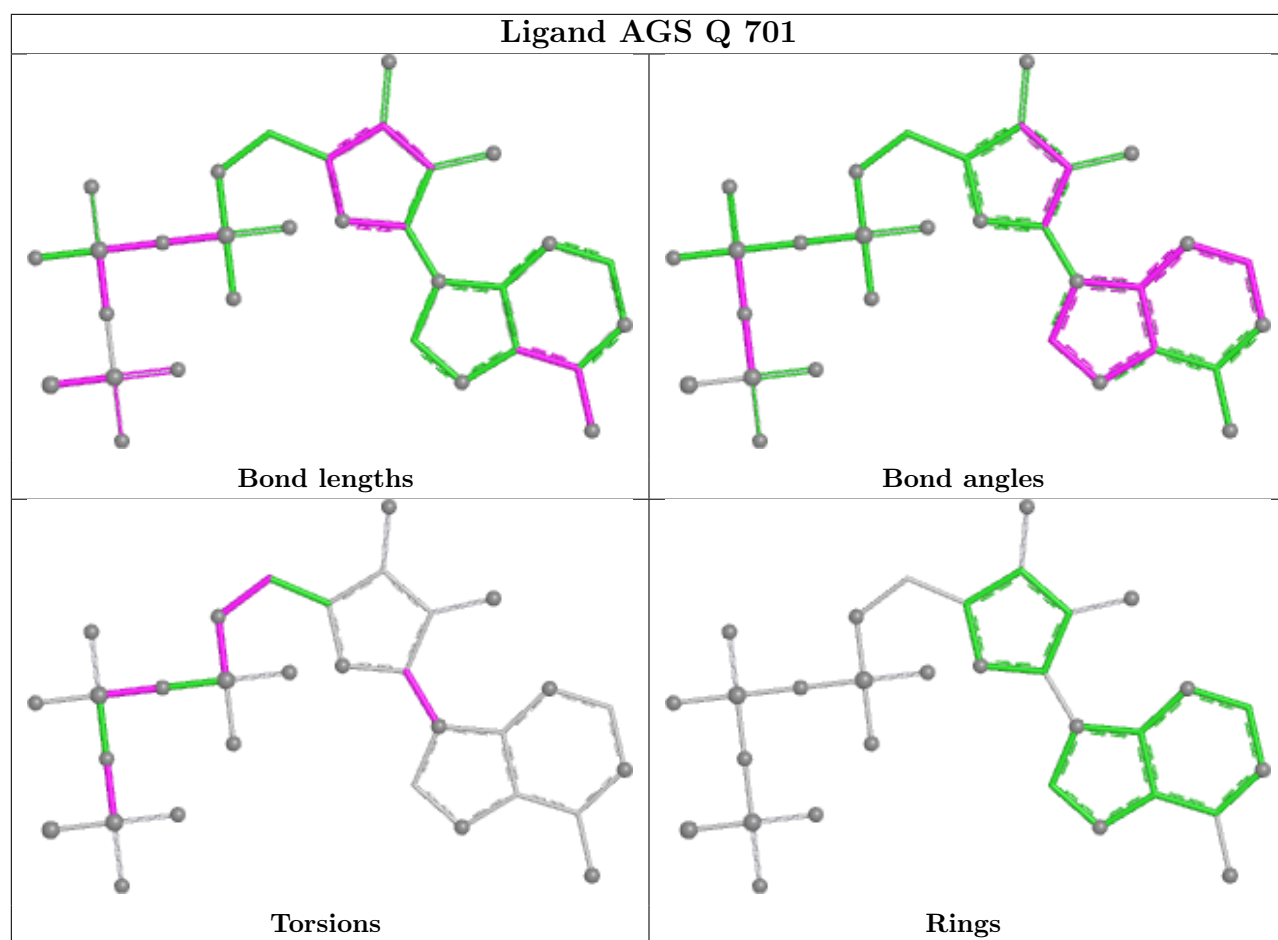


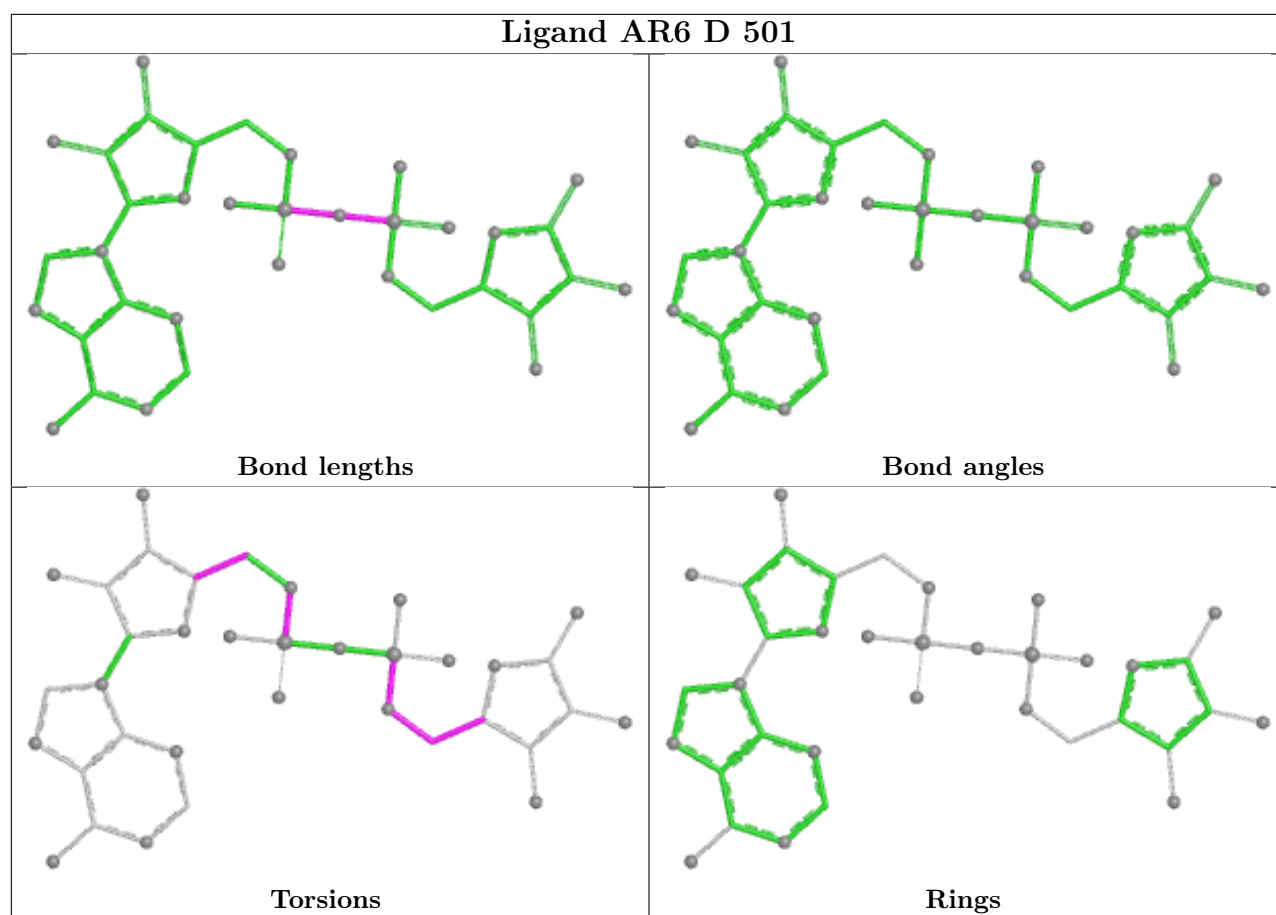


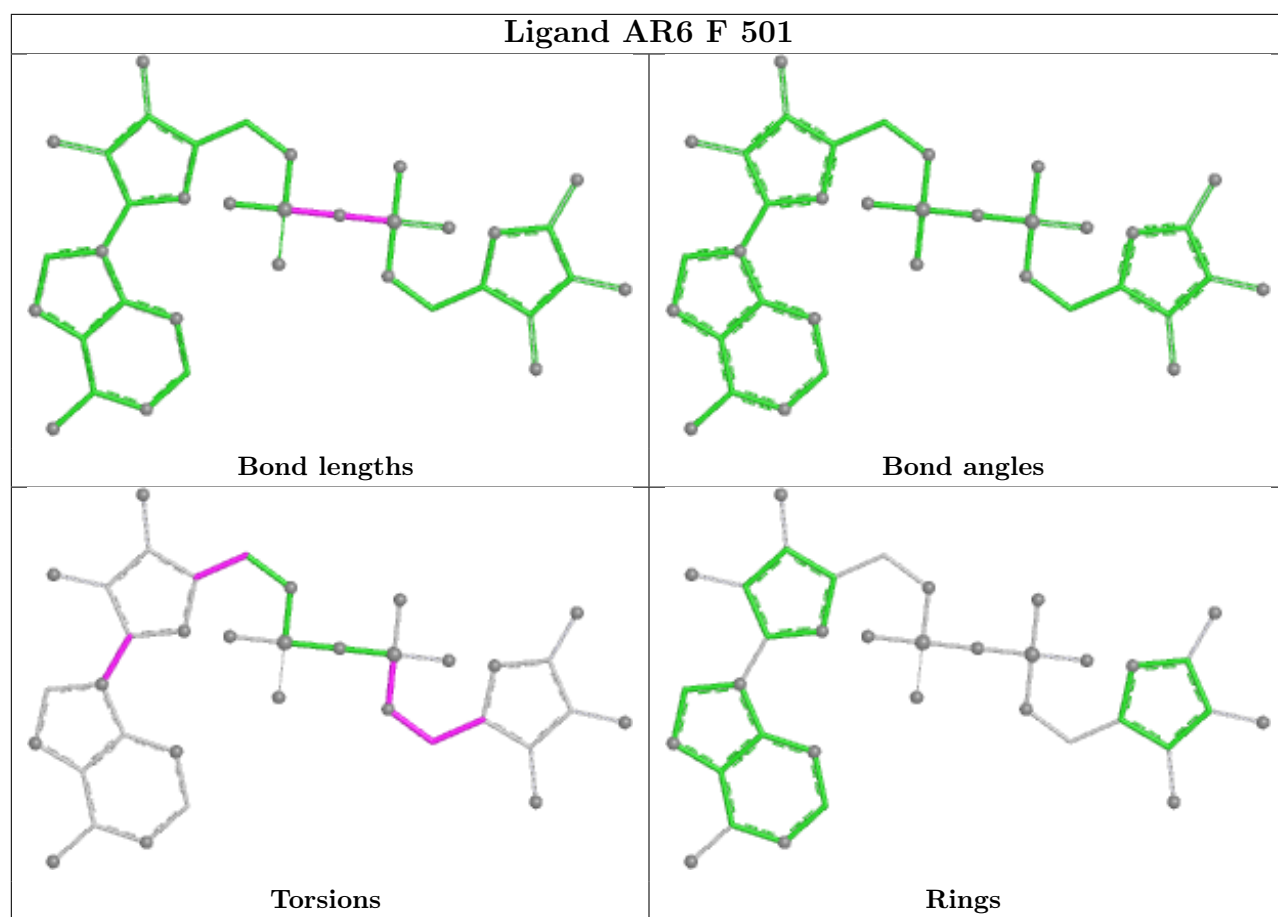


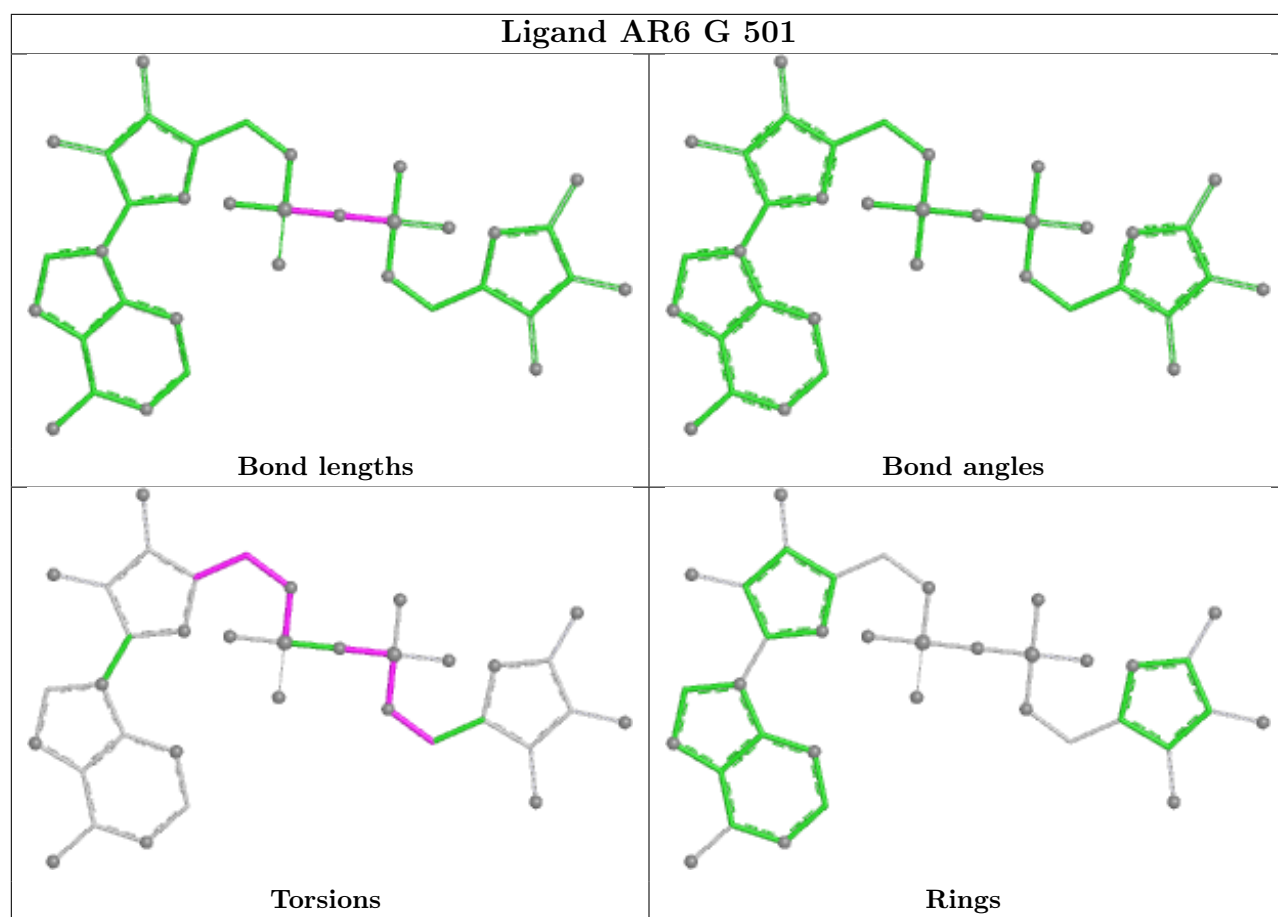


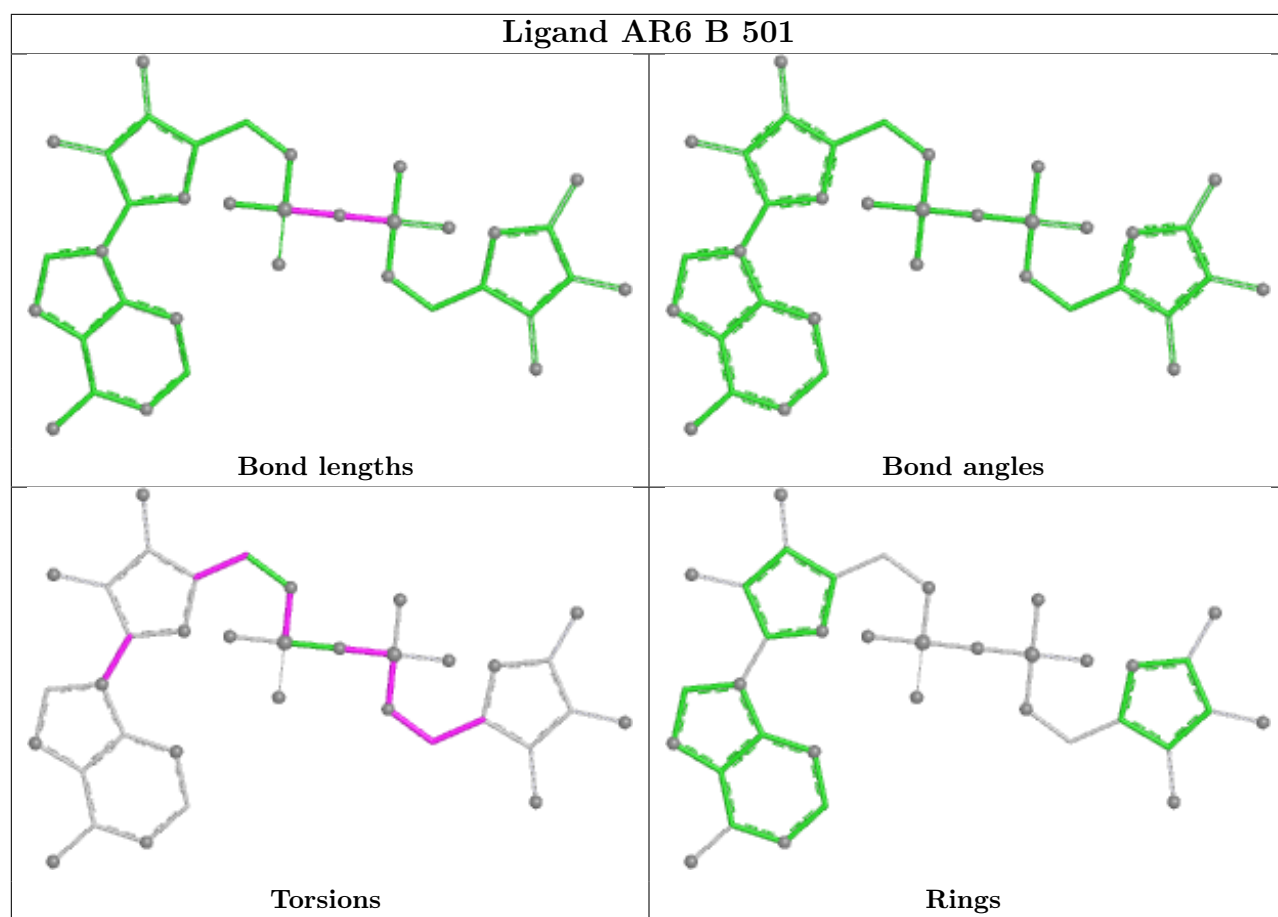


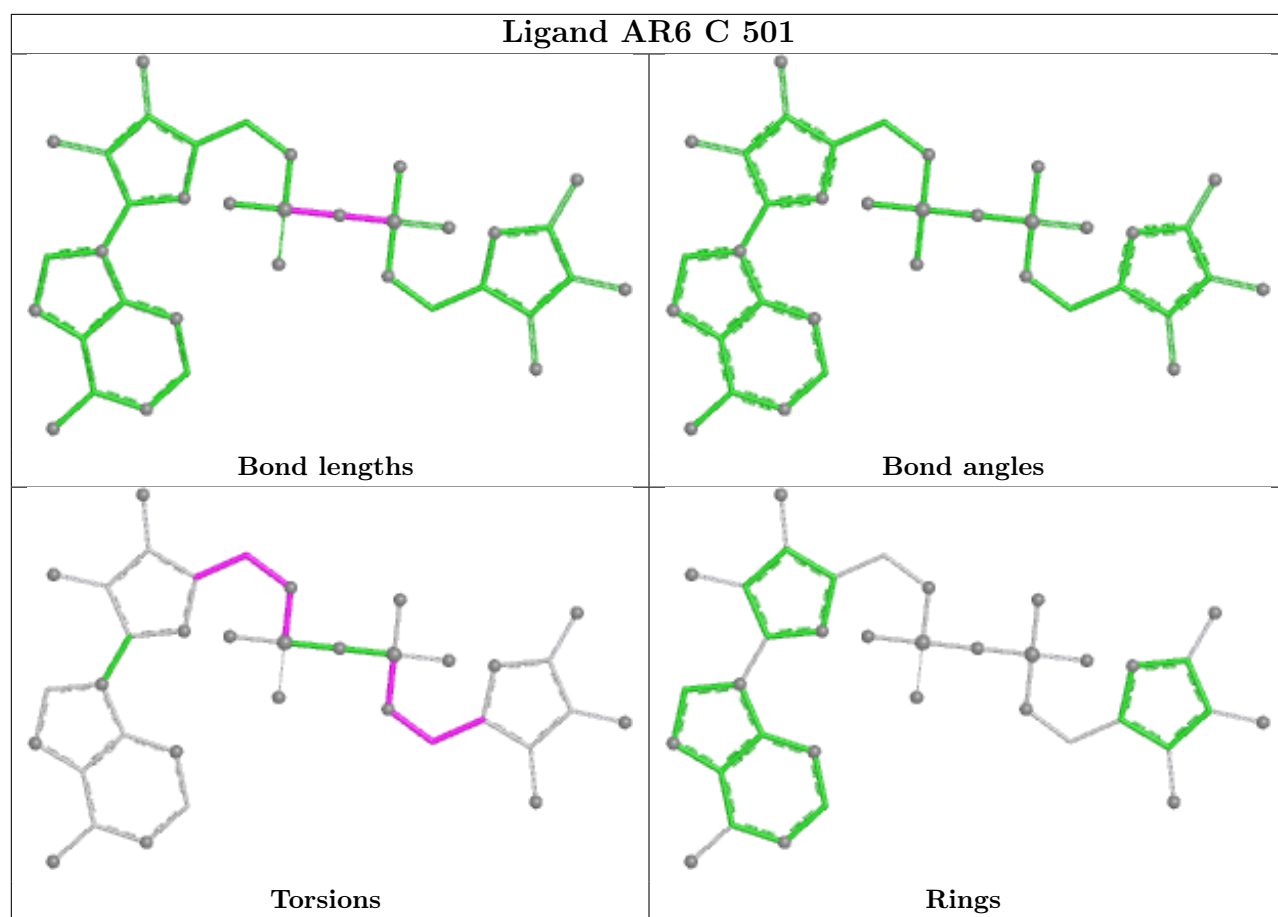


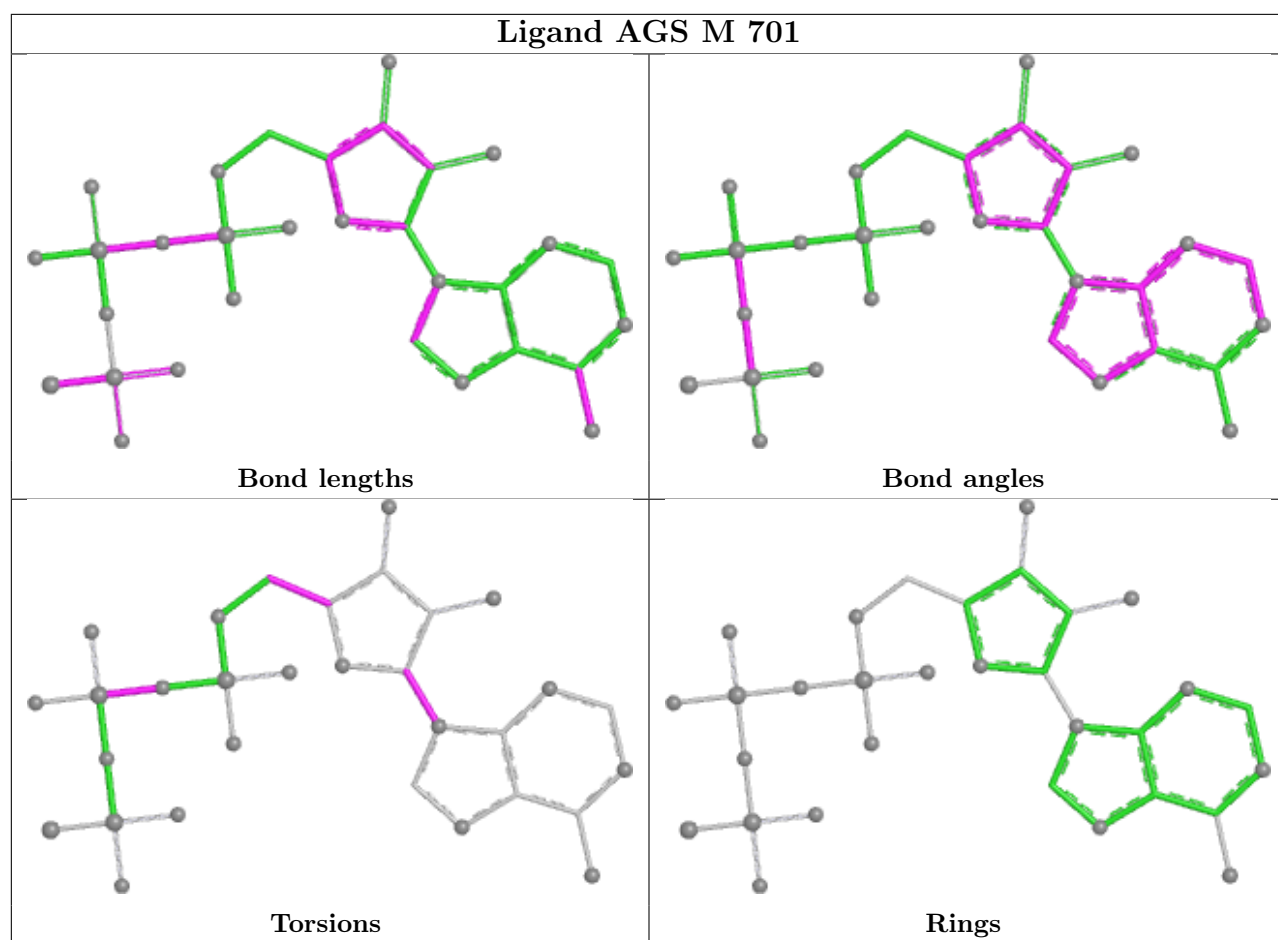


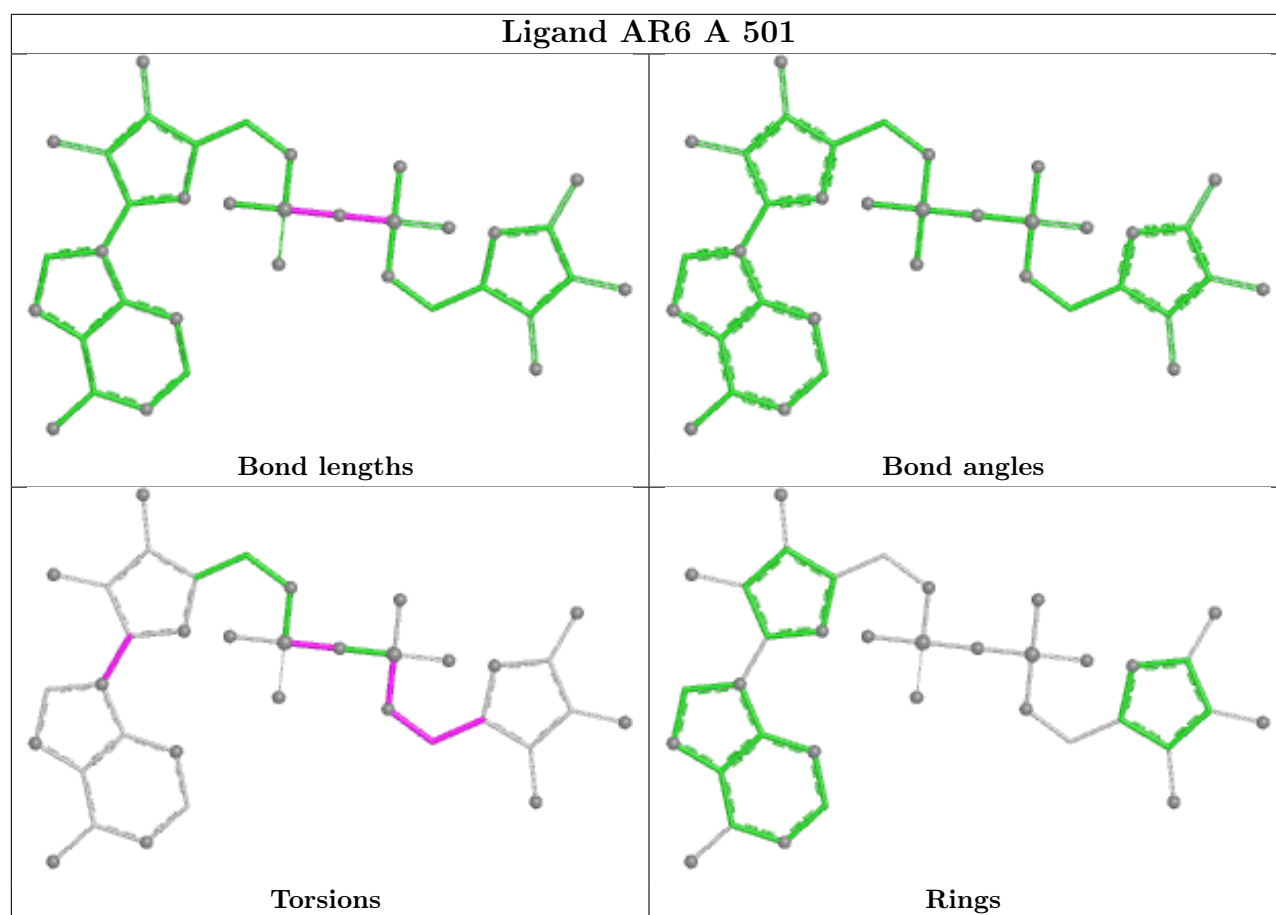












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

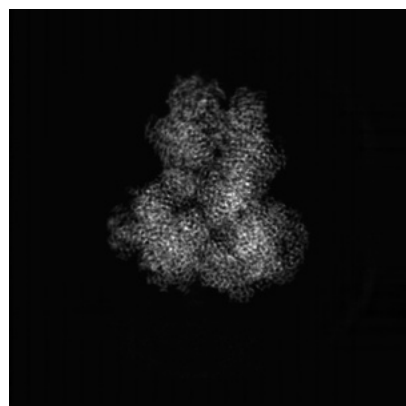
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42061. These allow visual inspection of the internal detail of the map and identification of artifacts.

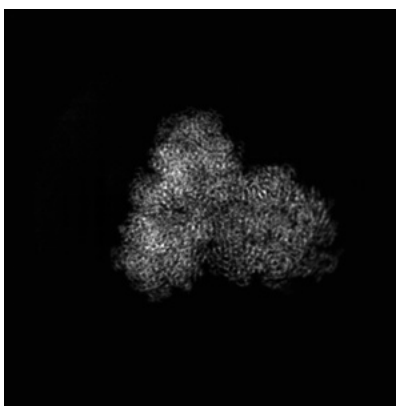
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

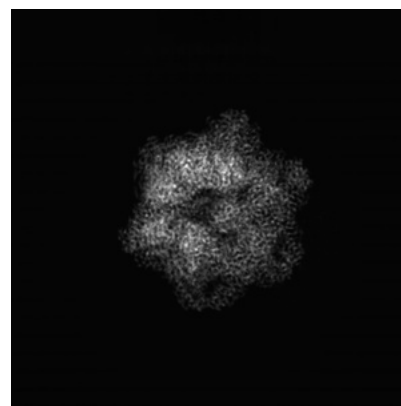
6.1.1 Primary map



X

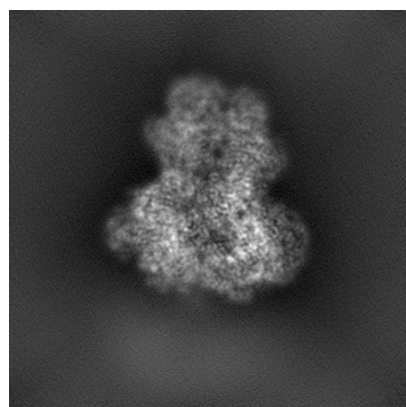


Y

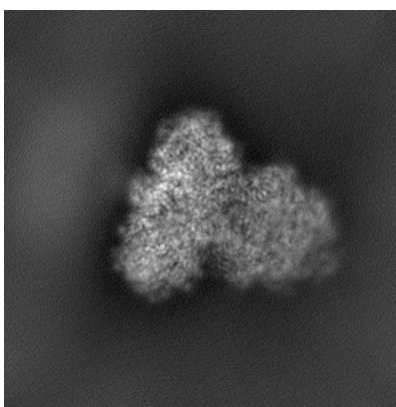


Z

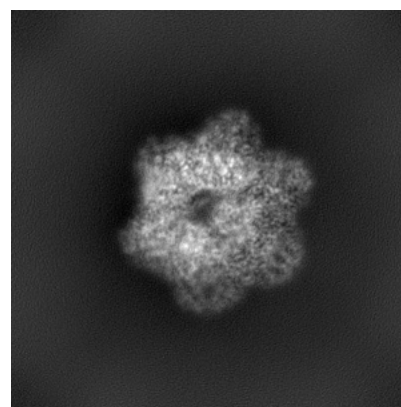
6.1.2 Raw map



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: 160

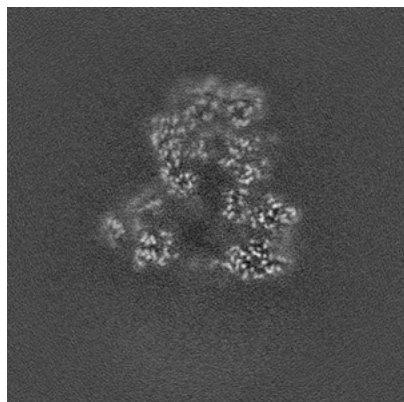


Y Index: 160

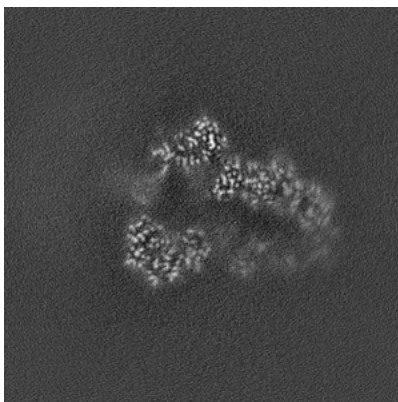


Z Index: 160

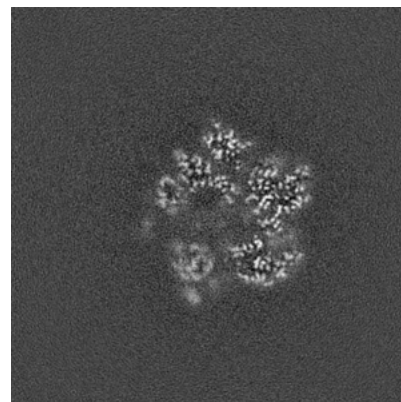
6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

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: 142

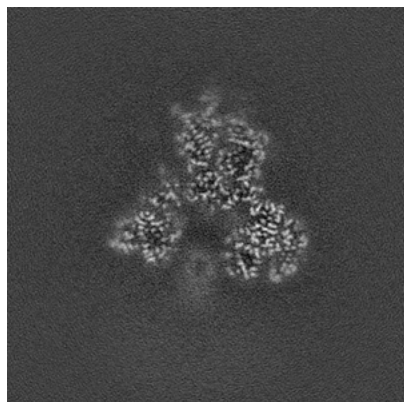


Y Index: 187

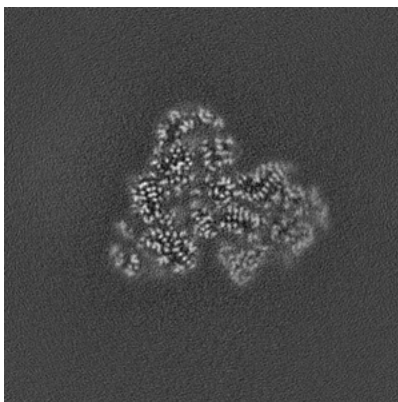


Z Index: 137

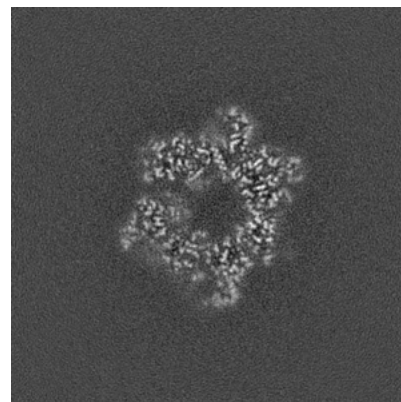
6.3.2 Raw map



X Index: 177



Y Index: 189

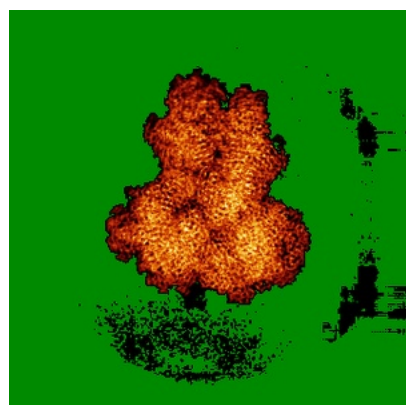


Z Index: 129

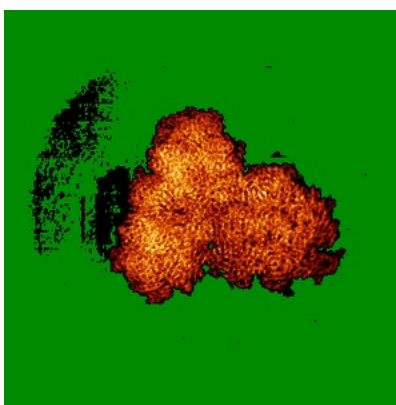
The images above show the largest variance slices of the map in three orthogonal directions.

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

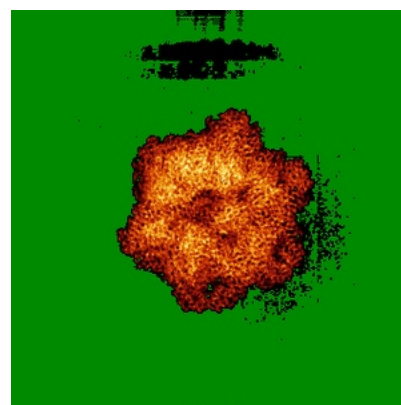
6.4.1 Primary map



X

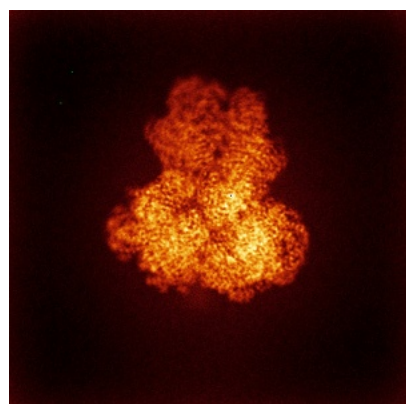


Y

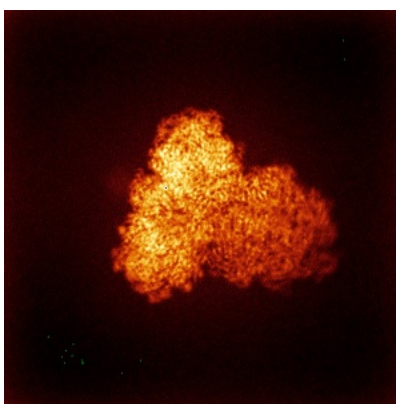


Z

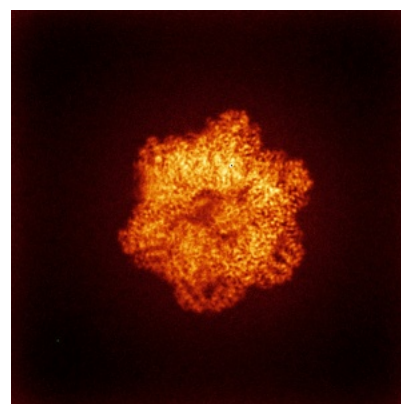
6.4.2 Raw map



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](#)

This section was not generated.

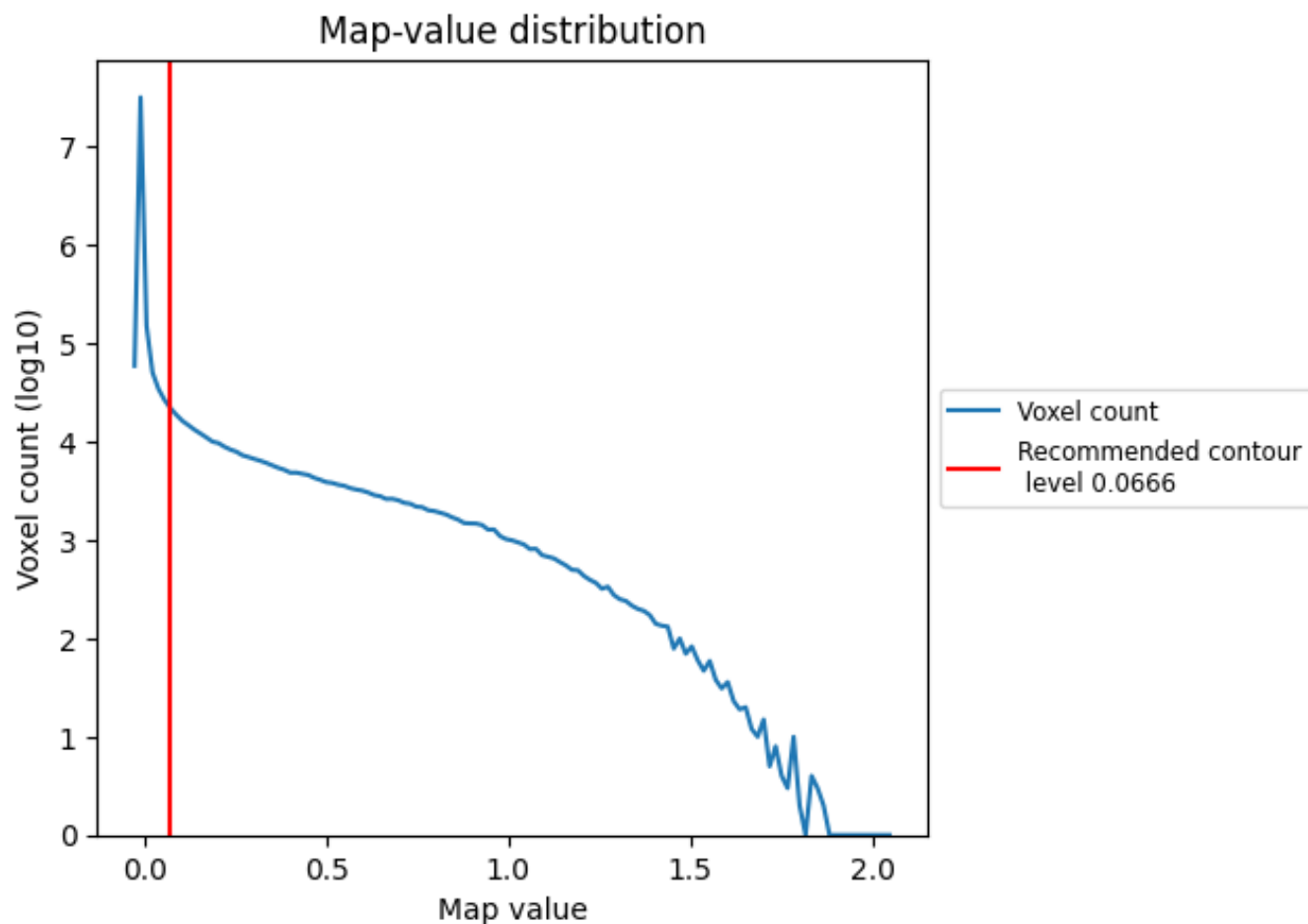
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

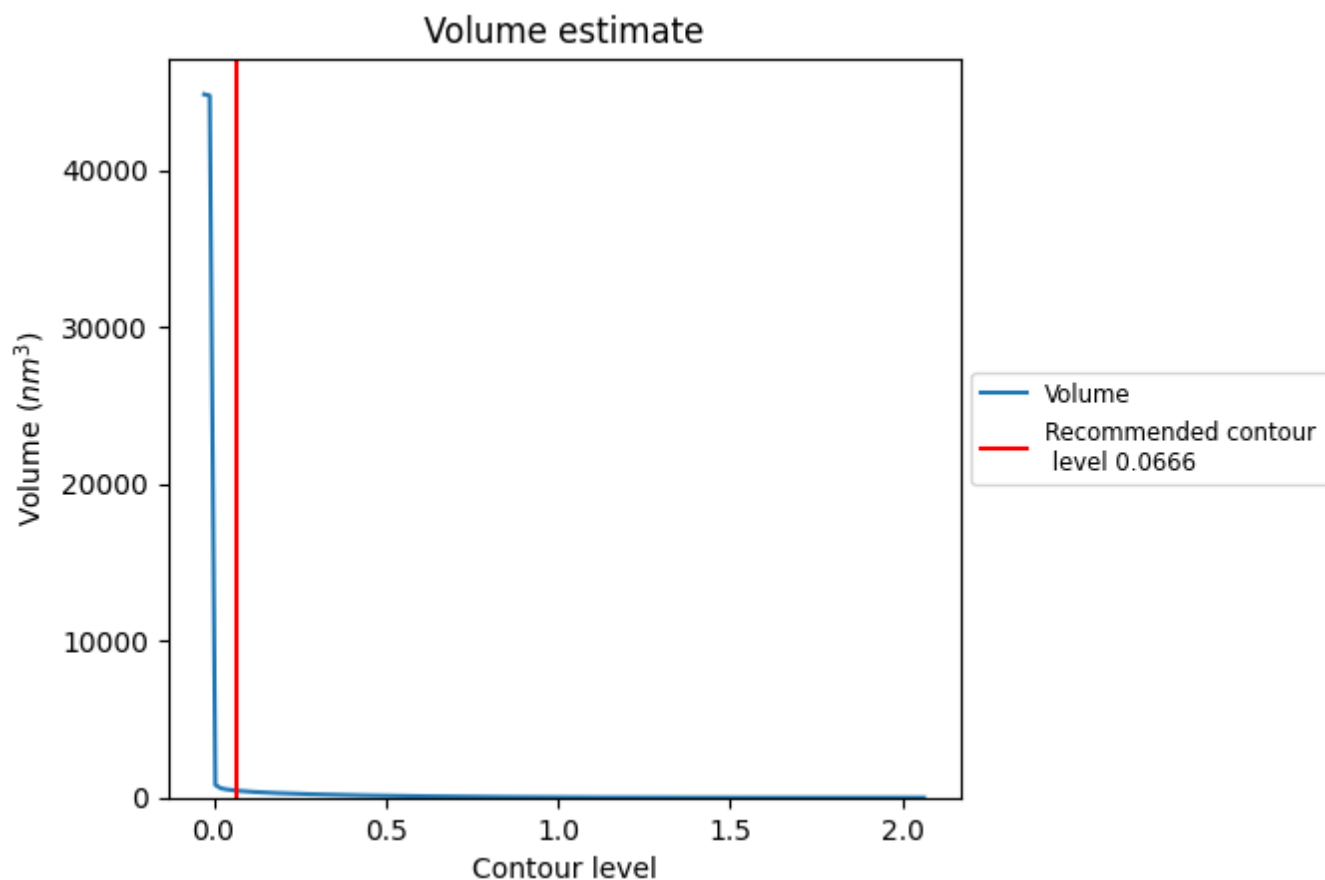
This section contains the results of statistical analysis of the map.

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.

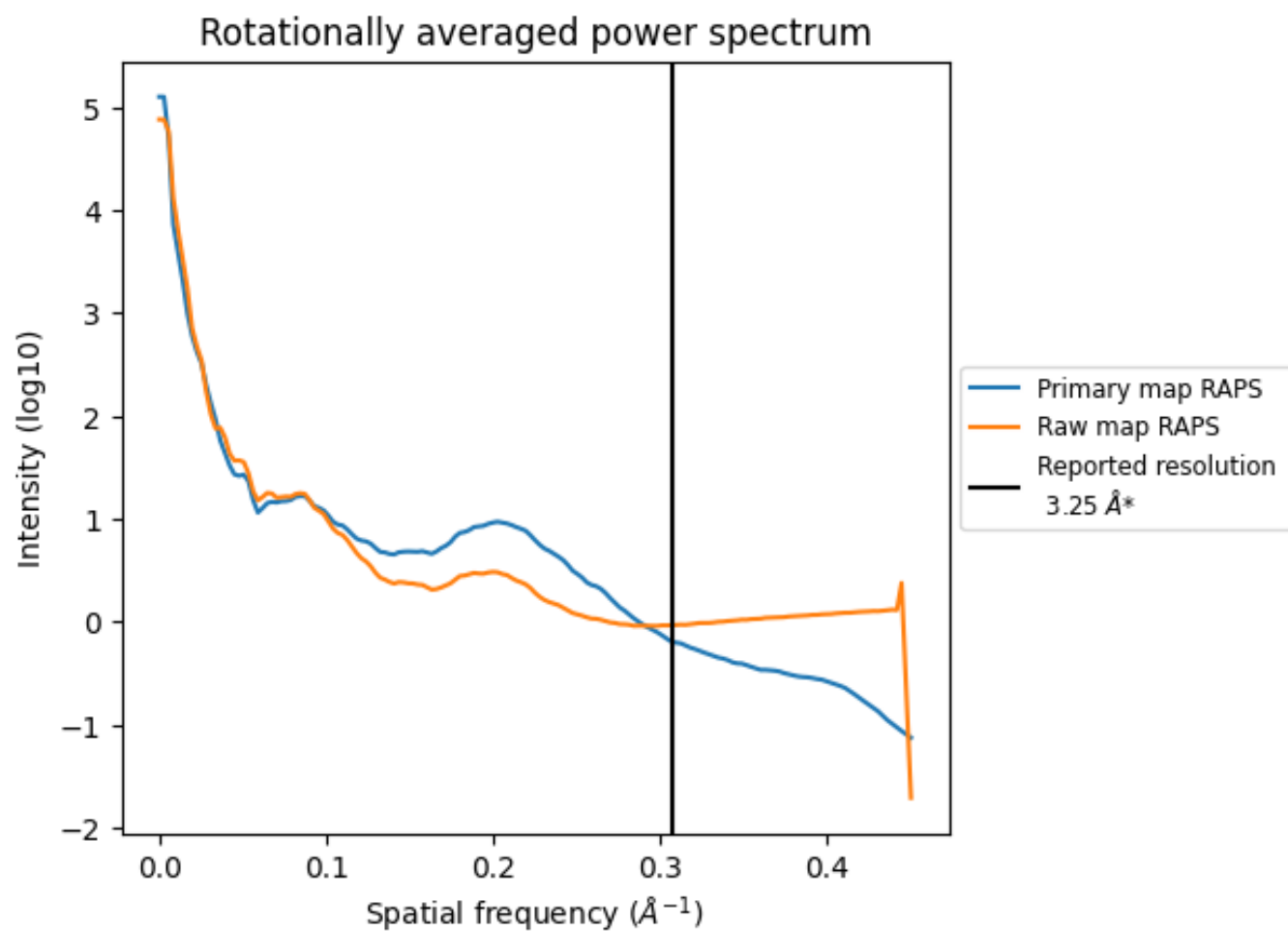
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 443 nm³; this corresponds to an approximate mass of 400 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 ⓘ

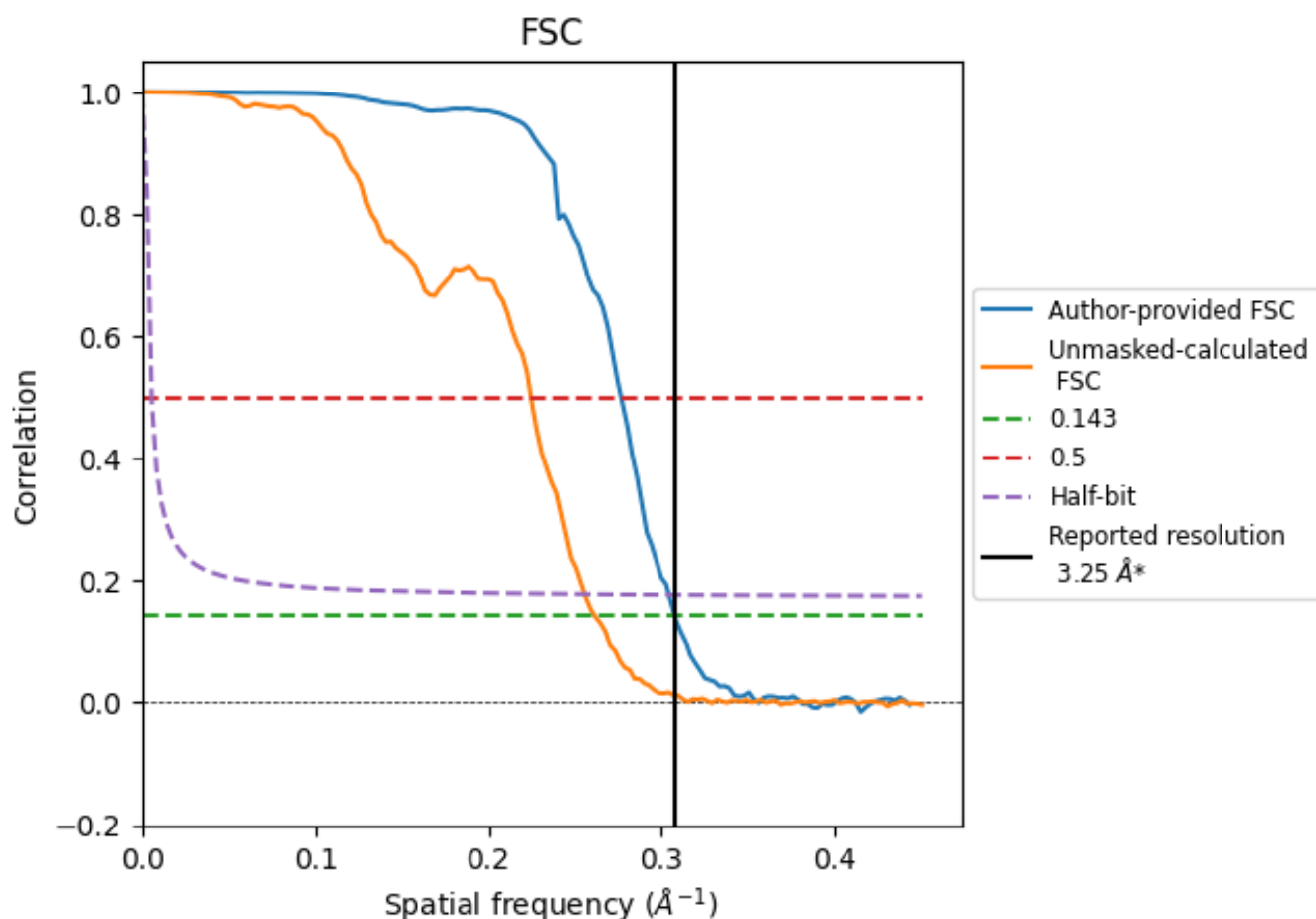


*Reported resolution corresponds to spatial frequency of $0.308 \text{ \AA}^{-1}$

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 $0.308 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

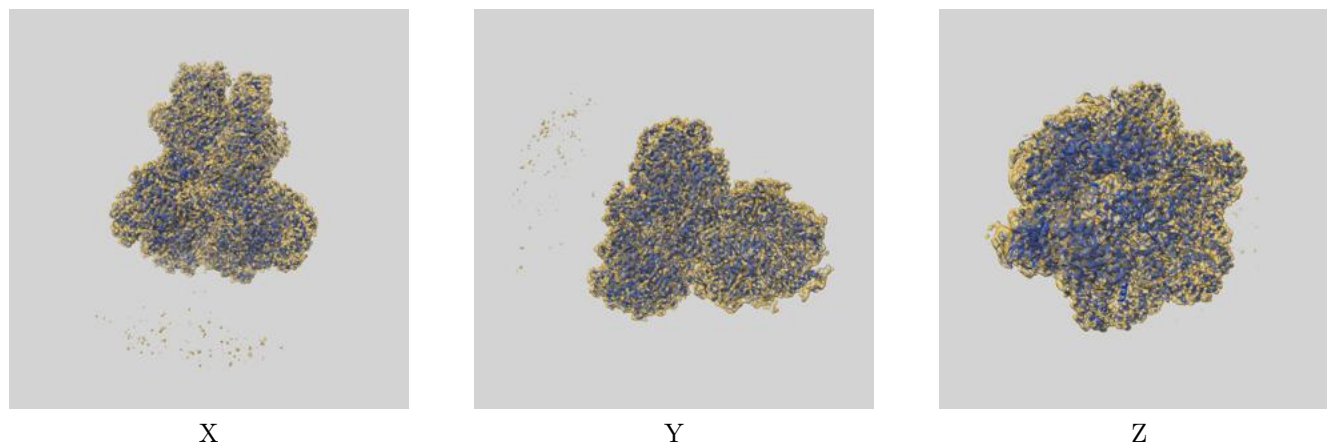
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.25	-	-
Author-provided FSC curve	3.25	3.62	3.29
Unmasked-calculated*	3.83	4.45	3.91

*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 3.83 differs from the reported value 3.25 by more than 10 %

9 Map-model fit [i](#)

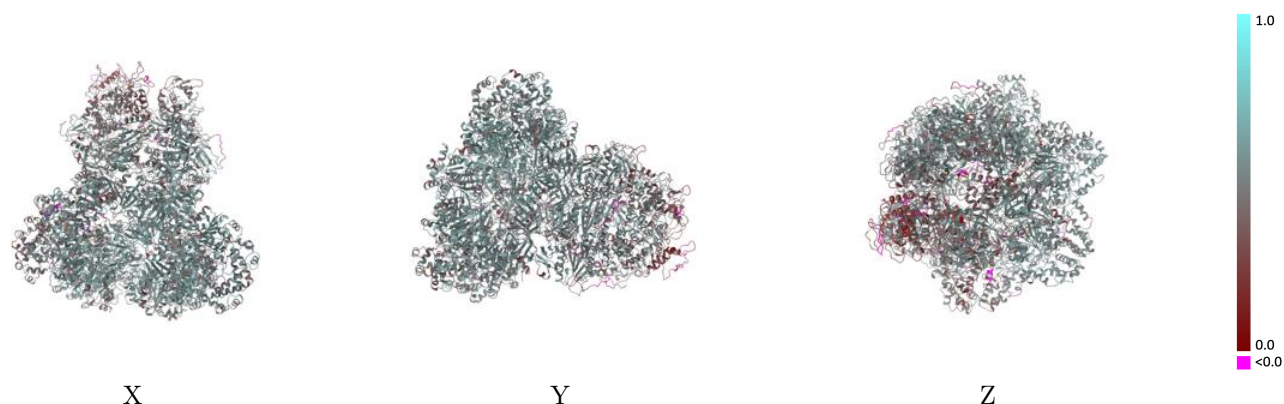
This section contains information regarding the fit between EMDB map EMD-42061 and PDB model 8UAE. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



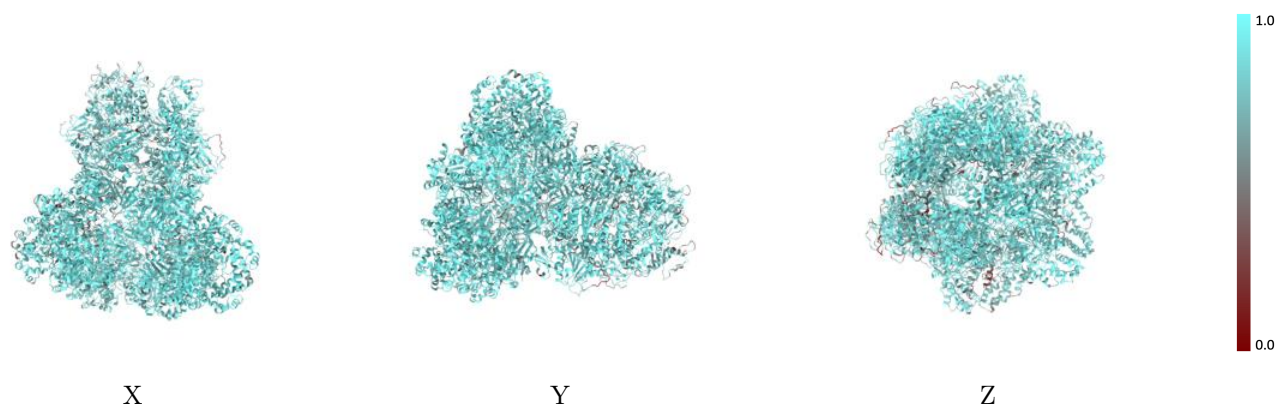
The images above show the 3D surface view of the map at the recommended contour level 0.0666 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



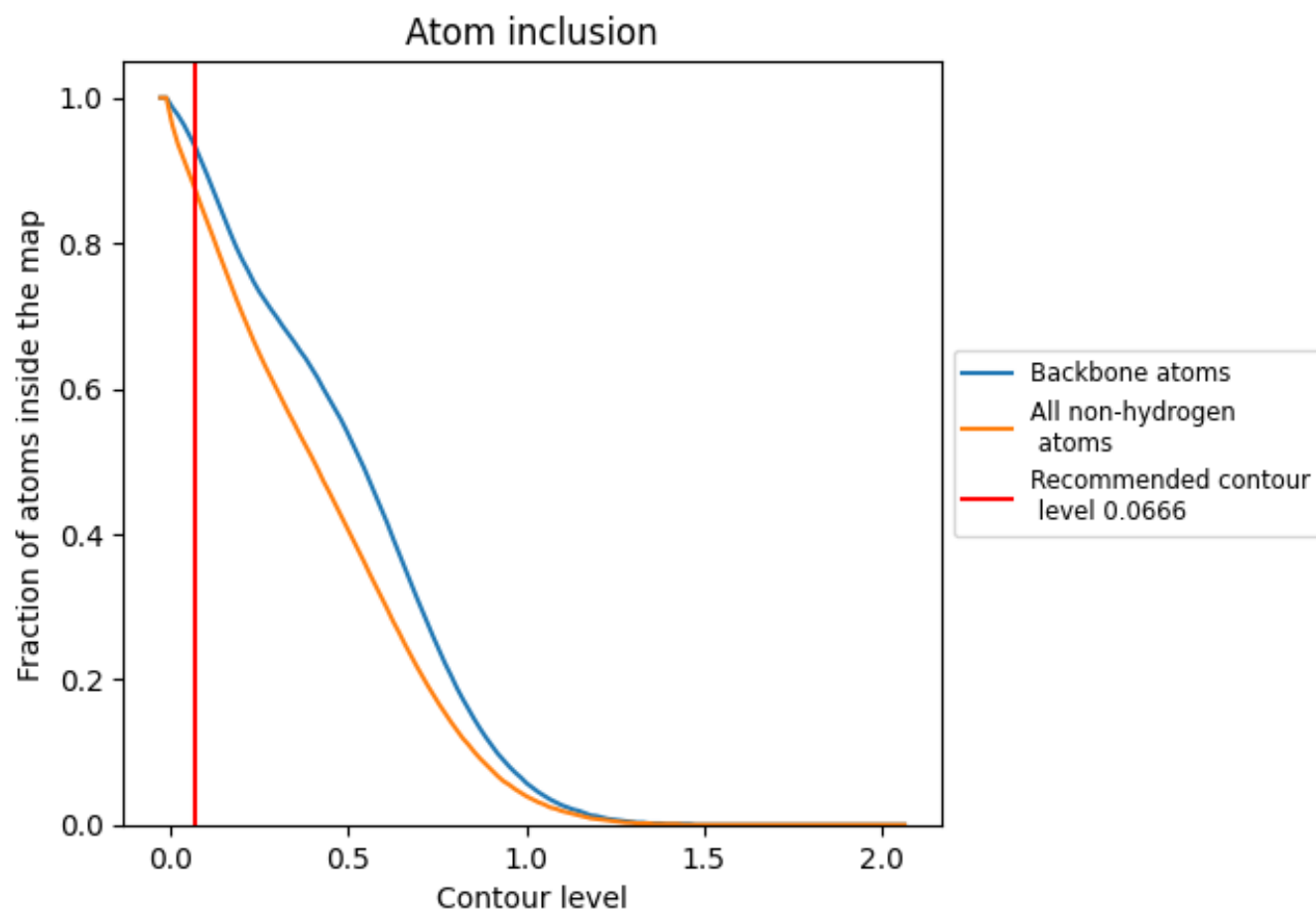
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0666).

9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 88% 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 (0.0666) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8780	0.4920
A	0.9280	0.5440
B	0.9080	0.5390
C	0.9110	0.5280
D	0.8900	0.5150
E	0.8940	0.5090
F	0.8770	0.5110
G	0.8440	0.4450
H	0.8830	0.5070
I	0.8960	0.5240
J	0.9060	0.5340
K	0.9160	0.5430
L	0.9050	0.5420
M	0.8510	0.4610
N	0.8940	0.5080
O	0.8760	0.4860
P	0.8670	0.4610
Q	0.8560	0.4470
R	0.7620	0.3430

1.0

0.0

<0.0