



wwPDB EM Validation Summary Report ⓘ

Jul 7, 2024 – 09:10 am BST

PDB ID : 7PT6
EMDB ID : EMD-13619
Title : Structure of MCM2-7 DH complexed with Cdc7-Dbf4 in the presence of ATPgS, state III
Authors : Saleh, A.; Noguchi, Y.; Aramayo, R.; Ivanova, M.E.; Speck, C.
Deposited on : 2021-09-26
Resolution : 3.20 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.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

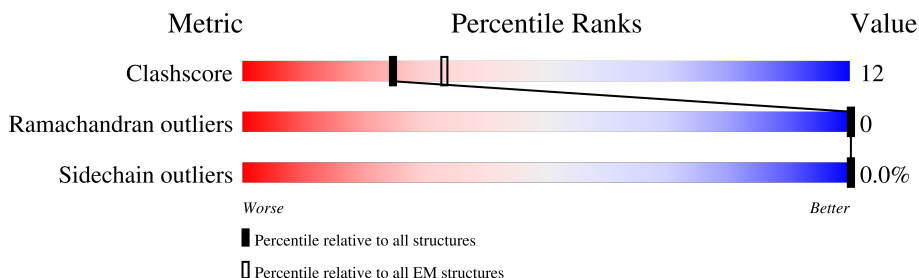
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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





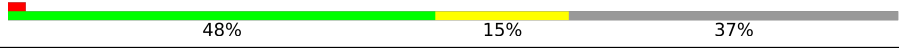





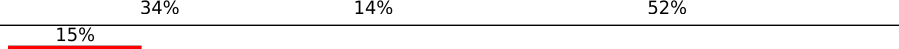
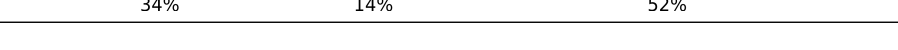
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1	4	<div> <div>25%</div> <div>100%</div> </div>
1	A	4	<div> <div>50%</div> <div>100%</div> </div>
2	2	868	<div> <div>52%</div> <div>20%</div> <div>28%</div> </div>
2	B	868	<div> <div>52%</div> <div>20%</div> <div>28%</div> </div>
3	3	971	<div> <div>54%</div> <div>12%</div> <div>34%</div> </div>
3	C	971	<div> <div>54%</div> <div>12%</div> <div>34%</div> </div>
4	4	933	<div> <div>57%</div> <div>14%</div> <div>28%</div> </div>
4	D	933	<div> <div>57%</div> <div>15%</div> <div>28%</div> </div>

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Mol	Chain	Length	Quality of chain
5	5	775	
5	E	775	
6	6	1017	
6	F	1017	
7	7	845	
7	G	845	
8	8	507	
8	H	507	
9	9	704	
9	I	704	

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
10	AGS	8	1001	-	-	X	-
10	AGS	H	1001	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 74358 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 Undefined Mcm4 flexible N-terminal tail.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	1	4	Total	C	N	O	0	0
			20	12	4	4		
1	A	4	Total	C	N	O	0	0
			20	12	4	4		

- Molecule 2 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	629	Total	C	N	O	S	0	0
			4989	3140	886	944	19		
2	B	629	Total	C	N	O	S	0	0
			4989	3140	886	944	19		

- Molecule 3 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	637	Total	C	N	O	S	0	0
			5000	3164	890	933	13		
3	C	637	Total	C	N	O	S	0	0
			5000	3164	890	933	13		

- Molecule 4 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	668	Total	C	N	O	S	0	0
			5323	3341	920	1033	29		
4	D	668	Total	C	N	O	S	0	0
			5323	3341	920	1033	29		

- Molecule 5 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	644	Total	C	N	O	S	0	0
			5037	3162	864	987	24		
5	E	644	Total	C	N	O	S	0	0
			5037	3162	864	987	24		

- Molecule 6 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	637	Total	C	N	O	S	0	0
			5048	3179	883	961	25		
6	F	637	Total	C	N	O	S	0	0
			5048	3179	883	961	25		

- Molecule 7 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	683	Total	C	N	O	S	0	0
			5370	3382	924	1034	30		
7	G	683	Total	C	N	O	S	0	0
			5370	3382	924	1034	30		

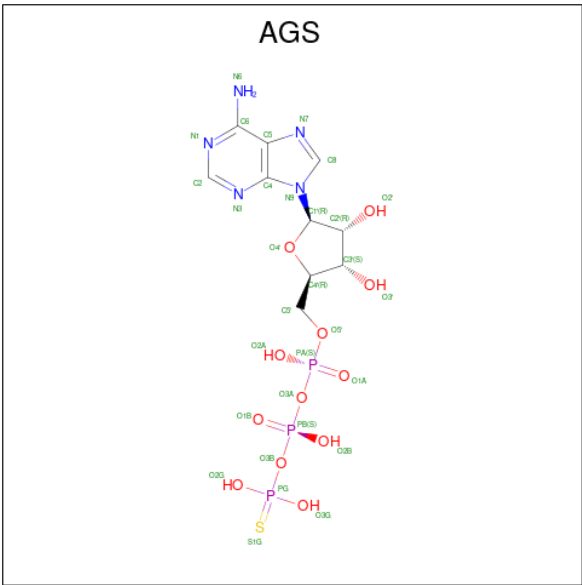
- Molecule 8 is a protein called Cell division control protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	402	Total	C	N	O	S	0	0
			3292	2126	551	599	16		
8	H	402	Total	C	N	O	S	0	0
			3292	2126	551	599	16		

- Molecule 9 is a protein called DDK kinase regulatory subunit DBF4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	341	Total	C	N	O	S	0	0
			2846	1814	499	521	12		
9	I	341	Total	C	N	O	S	0	0
			2846	1814	499	521	12		

- Molecule 10 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
10	2	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
10	4	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
10	5	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
10	6	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
10	6	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
10	8	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
10	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
10	D	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
10	E	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
10	F	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
10	F	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
10	H	1	Total 31	C 10	N 5	O 12	P 3	S 1	0

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Lig- and of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
11	2	2	Total 2	Mg 2	0
11	3	1	Total 1	Mg 1	0
11	6	1	Total 1	Mg 1	0
11	7	2	Total 2	Mg 2	0
11	8	1	Total 1	Mg 1	0
11	B	2	Total 2	Mg 2	0
11	C	1	Total 1	Mg 1	0
11	F	1	Total 1	Mg 1	0
11	G	2	Total 2	Mg 2	0
11	H	1	Total 1	Mg 1	0

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

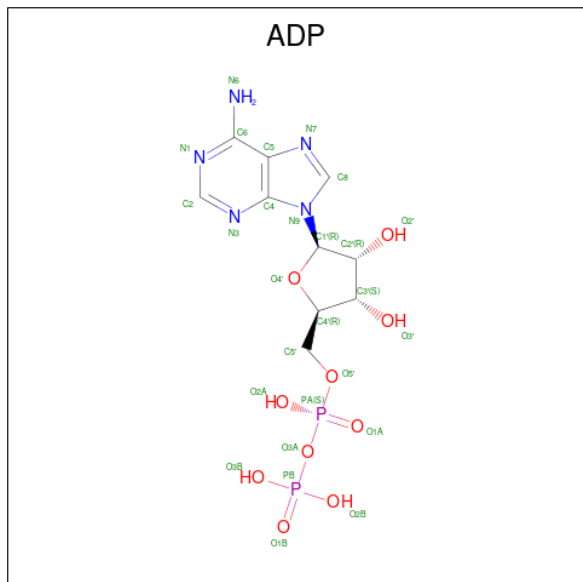
Mol	Chain	Residues	Atoms		AltConf
12	2	1	Total 1	Zn 1	0
12	4	1	Total 1	Zn 1	0
12	5	1	Total 1	Zn 1	0
12	6	1	Total 1	Zn 1	0
12	7	1	Total 1	Zn 1	0
12	8	1	Total 1	Zn 1	0
12	9	1	Total 1	Zn 1	0
12	B	1	Total 1	Zn 1	0
12	D	1	Total 1	Zn 1	0

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Mol	Chain	Residues	Atoms		AltConf
12	E	1	Total	Zn	0
			1	1	
12	F	1	Total	Zn	0
			1	1	
12	G	1	Total	Zn	0
			1	1	
12	H	1	Total	Zn	0
			1	1	
12	I	1	Total	Zn	0
			1	1	

- Molecule 13 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
13	3	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	7	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	G	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots

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

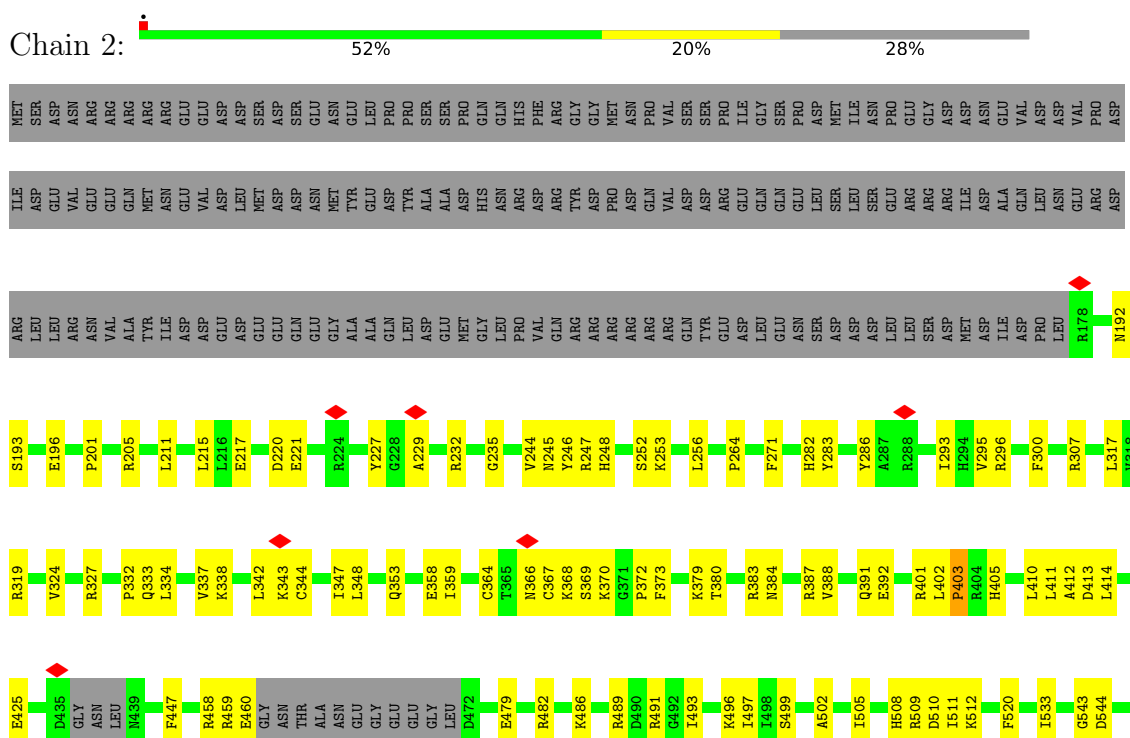
- Molecule 1: Undefined Mcm4 flexible N-terminal tail

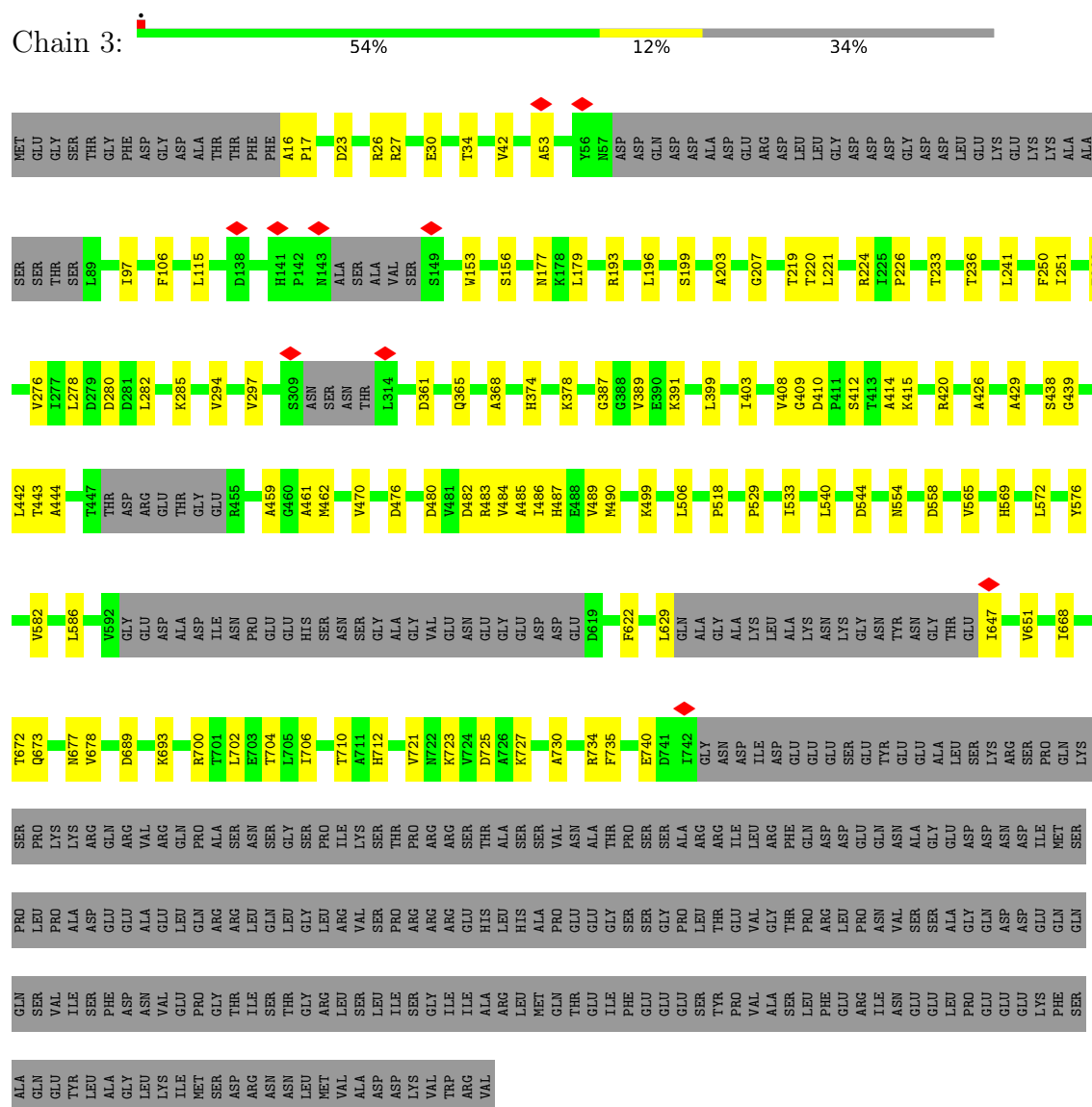


- Molecule 1: Undefined Mcm4 flexible N-terminal tail

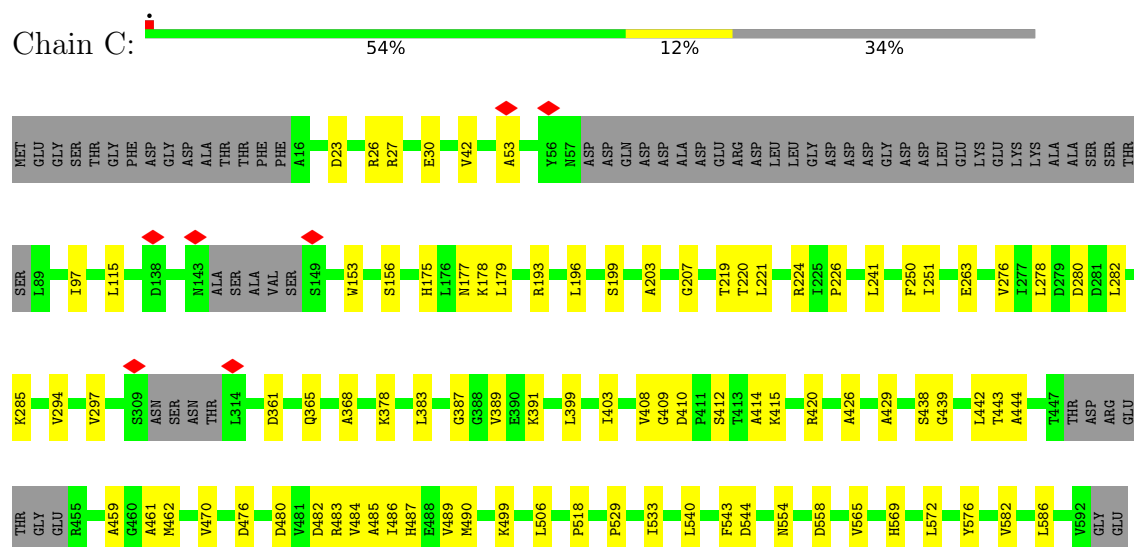


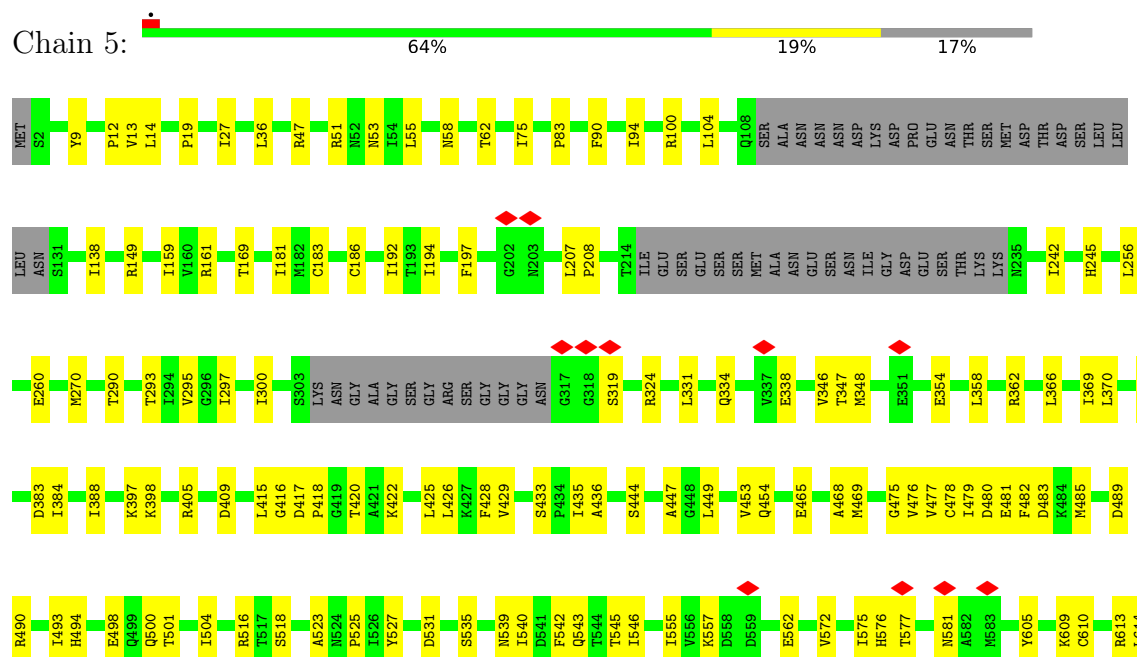
- Molecule 2: DNA replication licensing factor MCM2



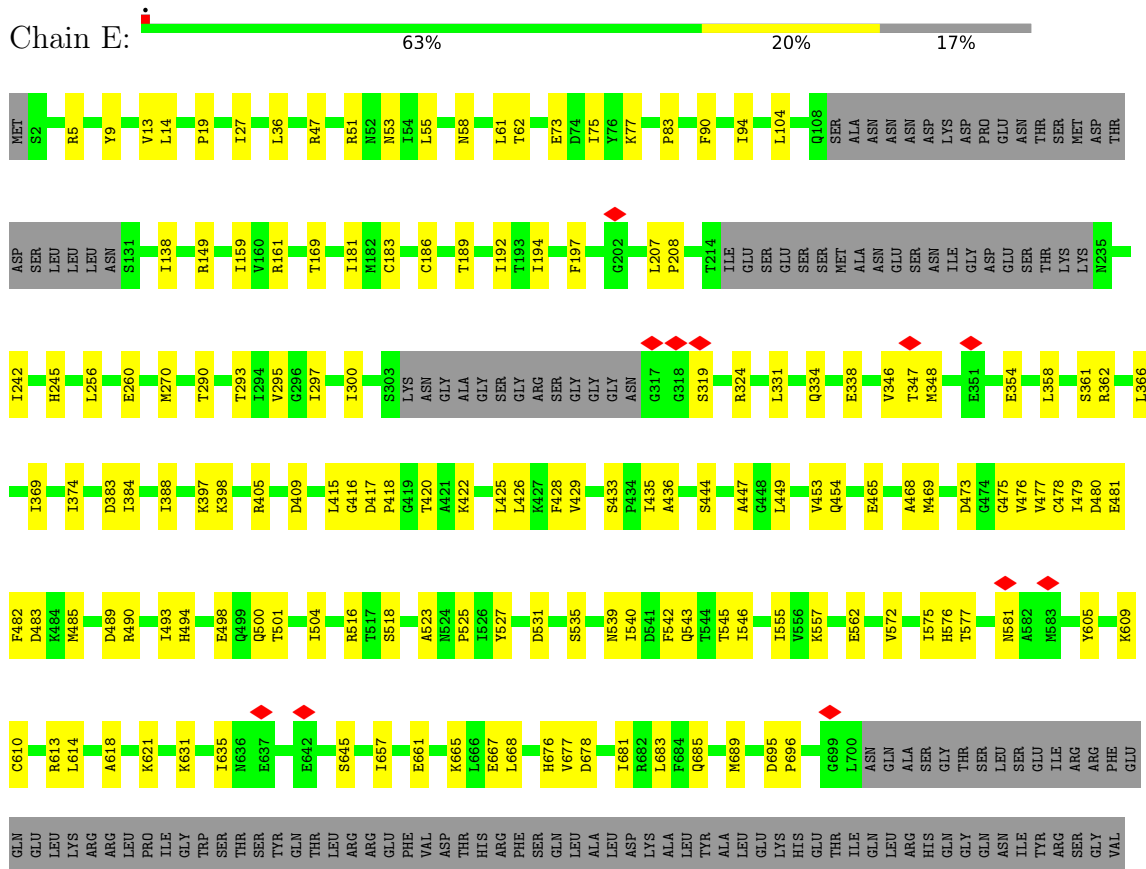


- Molecule 3: DNA replication licensing factor MCM3

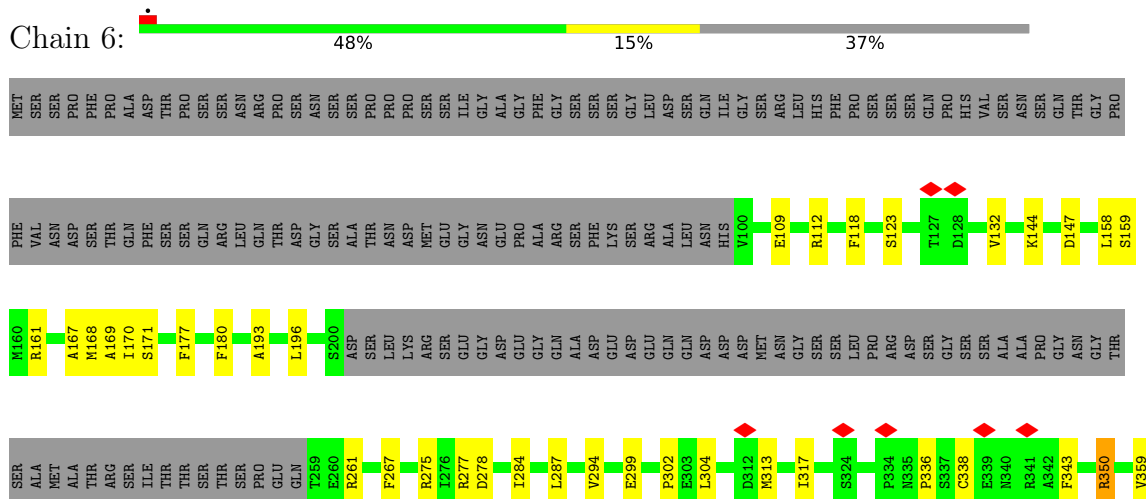


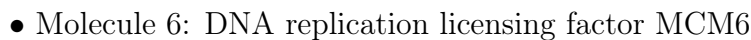


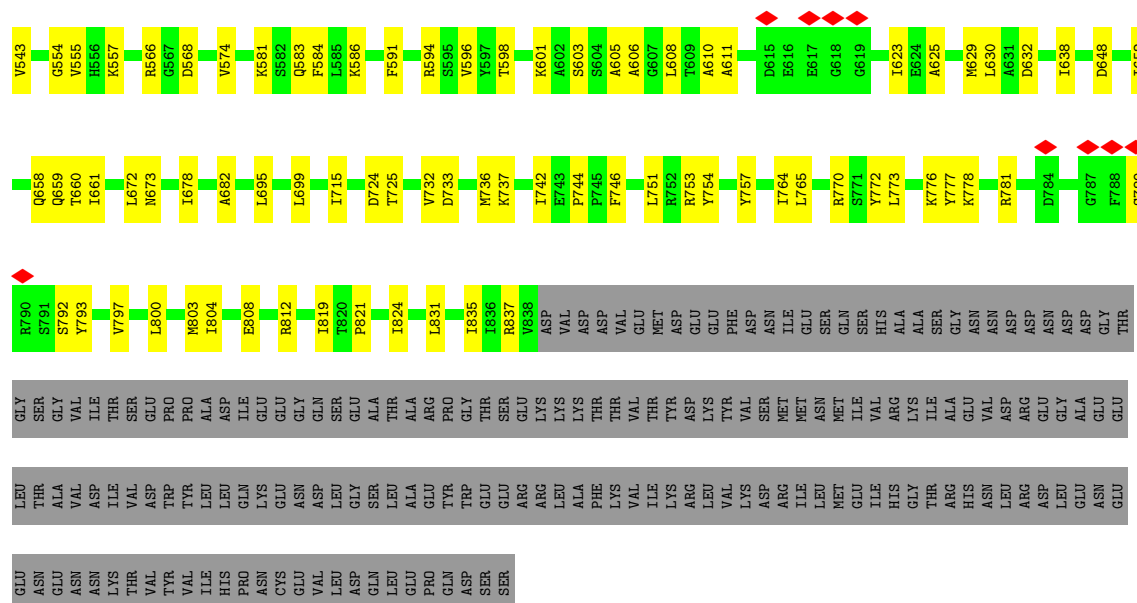
- Molecule 5: Minichromosome maintenance protein 5



- Molecule 6: DNA replication licensing factor MCM6

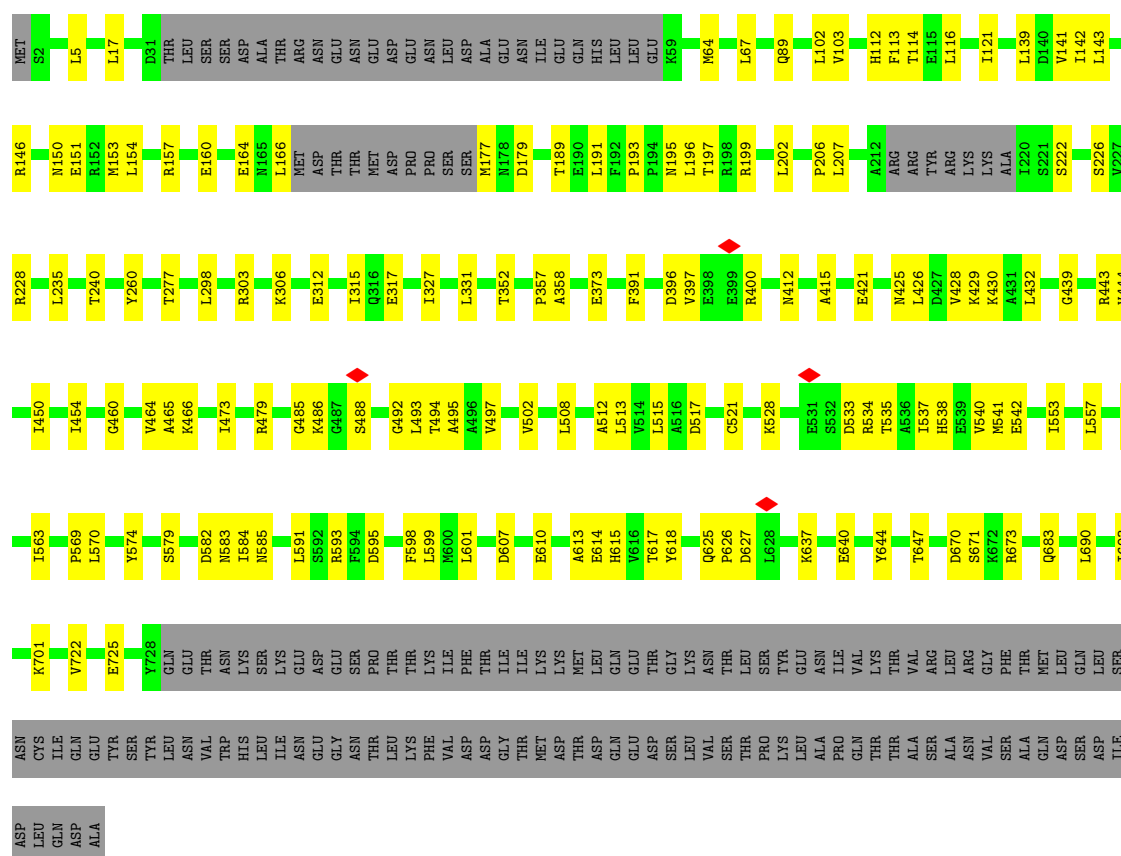






• Molecule 7: DNA replication licensing factor MCM7

Chain 7: 64% 17% 19%



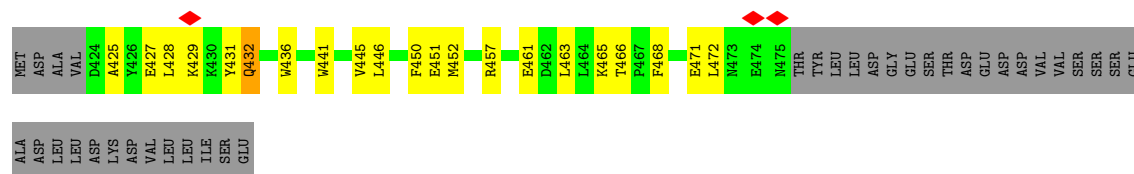
• Molecule 7: DNA replication licensing factor MCM7

Response	Percentage
Yes	63%
No	18%
Don't know	19%

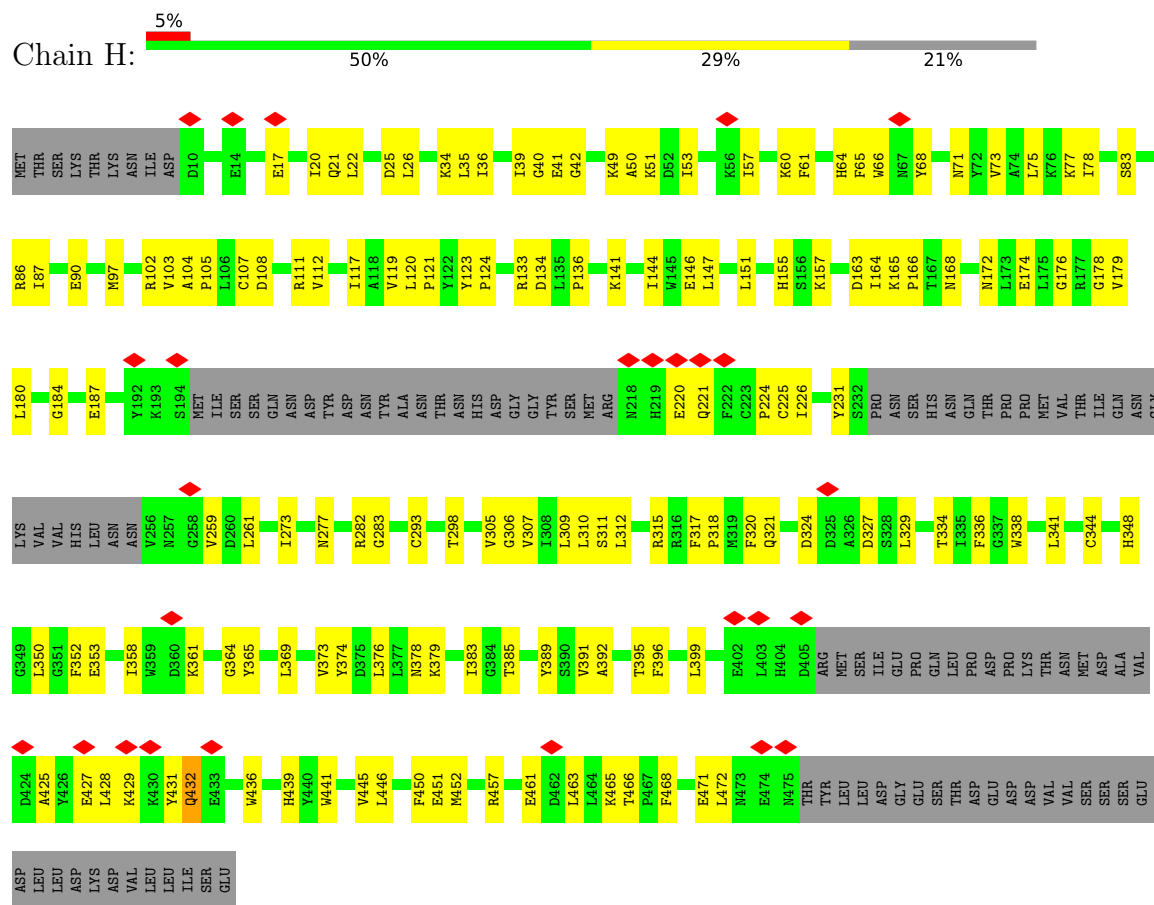


Frequency	Percentage
Daily	50%
Weekly	29%
Monthly	21%

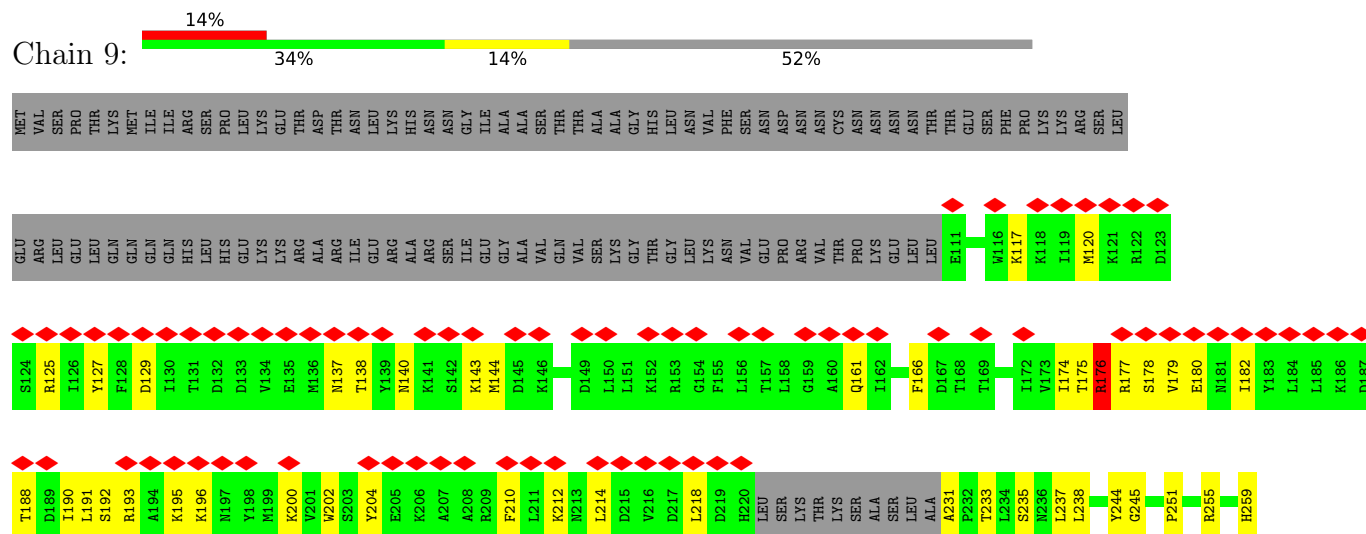


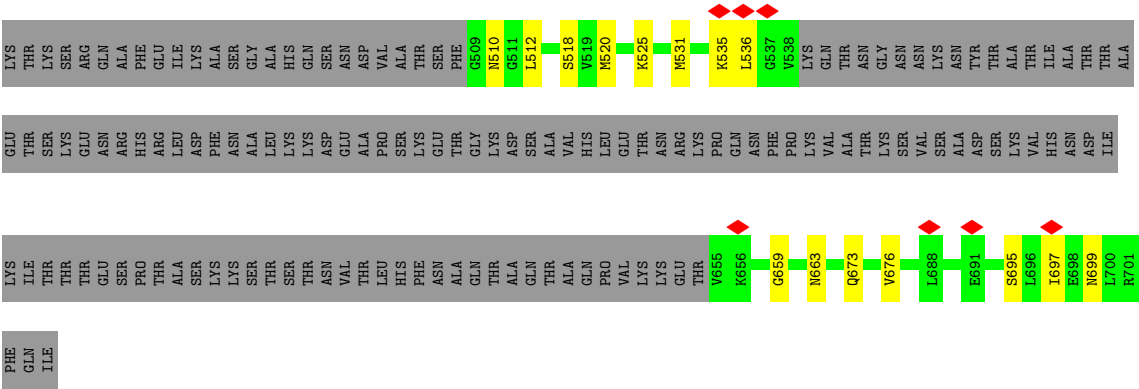


• Molecule 8: Cell division control protein 7



• Molecule 9: DDK kinase regulatory subunit DBF4





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	73093	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.252	Depositor
Minimum map value	-0.172	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.019	Depositor
Map size (\AA)	381.59998, 381.59998, 381.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
2	2	0.36	1/5075 (0.0%)	0.64	0/6855
2	B	0.36	1/5075 (0.0%)	0.64	0/6855
3	3	0.31	0/5089	0.57	1/6901 (0.0%)
3	C	0.31	0/5089	0.57	1/6901 (0.0%)
4	4	0.33	0/5401	0.57	1/7302 (0.0%)
4	D	0.33	0/5401	0.57	1/7302 (0.0%)
5	5	0.34	2/5111 (0.0%)	0.59	2/6915 (0.0%)
5	E	0.34	2/5111 (0.0%)	0.59	2/6915 (0.0%)
6	6	0.38	2/5129 (0.0%)	0.65	6/6919 (0.1%)
6	F	0.38	2/5129 (0.0%)	0.65	6/6919 (0.1%)
7	7	0.33	0/5451	0.60	1/7368 (0.0%)
7	G	0.33	0/5451	0.60	1/7368 (0.0%)
8	8	0.37	0/3373	0.66	2/4549 (0.0%)
8	H	0.37	0/3373	0.66	2/4549 (0.0%)
9	9	0.32	0/2906	0.65	2/3911 (0.1%)
9	I	0.32	0/2906	0.65	2/3911 (0.1%)
All	All	0.34	10/75070 (0.0%)	0.61	30/101440 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	2	0	1
2	B	0	1
3	3	0	1
3	C	0	1
6	6	0	1
6	F	0	1
9	9	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
9	I	0	2
All	All	0	10

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	336	PRO	N-CD	-9.99	1.33	1.47
6	6	336	PRO	N-CD	-9.98	1.33	1.47
5	5	418	PRO	N-CD	7.38	1.58	1.47
5	E	418	PRO	N-CD	7.38	1.58	1.47
6	F	374	PRO	N-CD	-5.70	1.39	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	224	PRO	N-CA-C	-8.35	90.39	112.10
8	8	224	PRO	N-CA-C	-8.33	90.43	112.10
6	6	350	ARG	CG-CD-NE	6.86	126.21	111.80
6	F	350	ARG	CG-CD-NE	6.86	126.20	111.80
6	6	336	PRO	CA-N-CD	6.85	121.29	111.70

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	247	ARG	Sidechain
3	3	224	ARG	Sidechain
6	6	350	ARG	Sidechain
9	9	176	ARG	Sidechain
9	9	324	VAL	Mainchain

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	1	20	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	20	0	7	0	0
2	2	4989	0	5026	156	0
2	B	4989	0	5026	157	0
3	3	5000	0	5077	76	0
3	C	5000	0	5077	73	0
4	4	5323	0	5387	100	0
4	D	5323	0	5387	105	0
5	5	5037	0	5085	101	0
5	E	5037	0	5085	103	0
6	6	5048	0	5083	139	0
6	F	5048	0	5083	138	0
7	7	5370	0	5426	123	0
7	G	5370	0	5426	124	0
8	8	3292	0	3248	180	0
8	H	3292	0	3248	181	0
9	9	2846	0	2846	102	0
9	I	2846	0	2846	102	0
10	2	31	0	12	2	0
10	4	31	0	12	0	0
10	5	31	0	12	1	0
10	6	62	0	24	2	0
10	8	31	0	12	10	0
10	B	31	0	12	2	0
10	D	31	0	12	0	0
10	E	31	0	12	0	0
10	F	62	0	24	2	0
10	H	31	0	12	11	0
11	2	2	0	0	0	0
11	3	1	0	0	0	0
11	6	1	0	0	0	0
11	7	2	0	0	0	0
11	8	1	0	0	0	0
11	B	2	0	0	0	0
11	C	1	0	0	0	0
11	F	1	0	0	0	0
11	G	2	0	0	0	0
11	H	1	0	0	0	0
12	2	1	0	0	0	0
12	4	1	0	0	0	0
12	5	1	0	0	0	0
12	6	1	0	0	0	0
12	7	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	8	1	0	0	1	0
12	9	1	0	0	0	0
12	B	1	0	0	0	0
12	D	1	0	0	0	0
12	E	1	0	0	0	0
12	F	1	0	0	0	0
12	G	1	0	0	0	0
12	H	1	0	0	1	0
12	I	1	0	0	0	0
13	3	27	0	12	3	0
13	7	27	0	12	1	0
13	C	27	0	12	3	0
13	G	27	0	12	1	0
All	All	74358	0	74562	1737	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 12.

The worst 5 of 1737 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)
8:H:75:LEU:CD2	8:H:119:VAL:HG22	1.31	1.61
8:8:75:LEU:CD2	8:8:119:VAL:HG22	1.31	1.58
8:8:432:GLN:NE2	8:8:436:TRP:CZ2	1.72	1.54
8:H:432:GLN:NE2	8:H:436:TRP:CZ2	1.72	1.53
7:7:542:GLU:HB2	7:7:593:ARG:NH1	1.23	1.49

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	
2	2	621/868 (72%)	603 (97%)	18 (3%)	0	100	100
2	B	621/868 (72%)	603 (97%)	18 (3%)	0	100	100
3	3	623/971 (64%)	609 (98%)	14 (2%)	0	100	100
3	C	623/971 (64%)	608 (98%)	15 (2%)	0	100	100
4	4	664/933 (71%)	643 (97%)	21 (3%)	0	100	100
4	D	664/933 (71%)	643 (97%)	21 (3%)	0	100	100
5	5	636/775 (82%)	614 (96%)	22 (4%)	0	100	100
5	E	636/775 (82%)	614 (96%)	22 (4%)	0	100	100
6	6	629/1017 (62%)	611 (97%)	18 (3%)	0	100	100
6	F	629/1017 (62%)	611 (97%)	18 (3%)	0	100	100
7	7	675/845 (80%)	654 (97%)	21 (3%)	0	100	100
7	G	675/845 (80%)	654 (97%)	21 (3%)	0	100	100
8	8	394/507 (78%)	375 (95%)	19 (5%)	0	100	100
8	H	394/507 (78%)	375 (95%)	19 (5%)	0	100	100
9	9	331/704 (47%)	319 (96%)	12 (4%)	0	100	100
9	I	331/704 (47%)	318 (96%)	13 (4%)	0	100	100
All	All	9146/13240 (69%)	8854 (97%)	292 (3%)	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	
2	2	554/770 (72%)	553 (100%)	1 (0%)	93	98
2	B	554/770 (72%)	554 (100%)	0	100	100
3	3	552/835 (66%)	552 (100%)	0	100	100
3	C	552/835 (66%)	552 (100%)	0	100	100
4	4	607/848 (72%)	607 (100%)	0	100	100

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	607/848 (72%)	607 (100%)	0	100	100
5	5	575/688 (84%)	575 (100%)	0	100	100
5	E	575/688 (84%)	575 (100%)	0	100	100
6	6	559/886 (63%)	559 (100%)	0	100	100
6	F	559/886 (63%)	559 (100%)	0	100	100
7	7	603/753 (80%)	603 (100%)	0	100	100
7	G	603/753 (80%)	603 (100%)	0	100	100
8	8	356/454 (78%)	356 (100%)	0	100	100
8	H	356/454 (78%)	356 (100%)	0	100	100
9	9	316/639 (50%)	316 (100%)	0	100	100
9	I	316/639 (50%)	316 (100%)	0	100	100
All	All	8244/11746 (70%)	8243 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
2	2	694	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	493	GLN
5	E	576	HIS
4	D	410	GLN
5	E	499	GLN
5	E	694	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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 44 ligands modelled in this entry, 28 are monoatomic - leaving 16 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
10	AGS	6	1101	-	26,33,33	0.80	0	26,52,52	0.76	1 (3%)
10	AGS	B	1001	11	26,33,33	0.82	0	26,52,52	0.73	1 (3%)
13	ADP	3	1001	11	24,29,29	0.77	1 (4%)	29,45,45	0.78	1 (3%)
10	AGS	F	1101	-	26,33,33	0.80	0	26,52,52	0.77	1 (3%)
10	AGS	4	1001	11	26,33,33	0.80	0	26,52,52	0.96	2 (7%)
10	AGS	E	1001	11	26,33,33	0.86	1 (3%)	26,52,52	0.84	1 (3%)
10	AGS	6	1102	11	26,33,33	0.82	0	26,52,52	0.82	1 (3%)
13	ADP	7	902	11	24,29,29	0.81	1 (4%)	29,45,45	0.85	1 (3%)
13	ADP	C	1001	11	24,29,29	0.77	1 (4%)	29,45,45	0.78	1 (3%)
10	AGS	H	1001	11	26,33,33	0.83	1 (3%)	26,52,52	0.85	1 (3%)
13	ADP	G	902	11	24,29,29	0.81	0	29,45,45	0.85	1 (3%)
10	AGS	2	1001	11	26,33,33	0.82	0	26,52,52	0.73	1 (3%)
10	AGS	5	1001	11	26,33,33	0.86	1 (3%)	26,52,52	0.84	1 (3%)
10	AGS	F	1102	11	26,33,33	0.82	0	26,52,52	0.83	1 (3%)
10	AGS	D	1001	11	26,33,33	0.80	0	26,52,52	0.96	2 (7%)
10	AGS	8	1001	11	26,33,33	0.83	1 (3%)	26,52,52	0.85	1 (3%)

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
10	AGS	6	1101	-	-	7/17/38/38	0/3/3/3
10	AGS	B	1001	11	-	6/17/38/38	0/3/3/3
13	ADP	3	1001	11	-	3/12/32/32	0/3/3/3
10	AGS	F	1101	-	-	7/17/38/38	0/3/3/3
10	AGS	4	1001	11	-	3/17/38/38	0/3/3/3
10	AGS	E	1001	11	-	3/17/38/38	0/3/3/3
10	AGS	6	1102	11	-	3/17/38/38	0/3/3/3
13	ADP	7	902	11	-	3/12/32/32	0/3/3/3
13	ADP	C	1001	11	-	3/12/32/32	0/3/3/3
10	AGS	H	1001	11	-	7/17/38/38	0/3/3/3
13	ADP	G	902	11	-	3/12/32/32	0/3/3/3
10	AGS	2	1001	11	-	6/17/38/38	0/3/3/3
10	AGS	5	1001	11	-	3/17/38/38	0/3/3/3
10	AGS	F	1102	11	-	3/17/38/38	0/3/3/3
10	AGS	D	1001	11	-	3/17/38/38	0/3/3/3
10	AGS	8	1001	11	-	7/17/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	H	1001	AGS	C8-N7	-2.06	1.31	1.34
13	C	1001	ADP	C8-N7	-2.05	1.31	1.34
13	7	902	ADP	C8-N7	-2.03	1.31	1.34
10	E	1001	AGS	C8-N7	-2.03	1.31	1.34
13	3	1001	ADP	C8-N7	-2.03	1.31	1.34

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	4	1001	AGS	C3'-C2'-C1'	2.50	104.74	100.98
10	D	1001	AGS	C3'-C2'-C1'	2.49	104.73	100.98
10	4	1001	AGS	C5-C6-N6	2.44	124.06	120.35
10	D	1001	AGS	C5-C6-N6	2.43	124.05	120.35
10	F	1102	AGS	C5-C6-N6	2.33	123.89	120.35

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

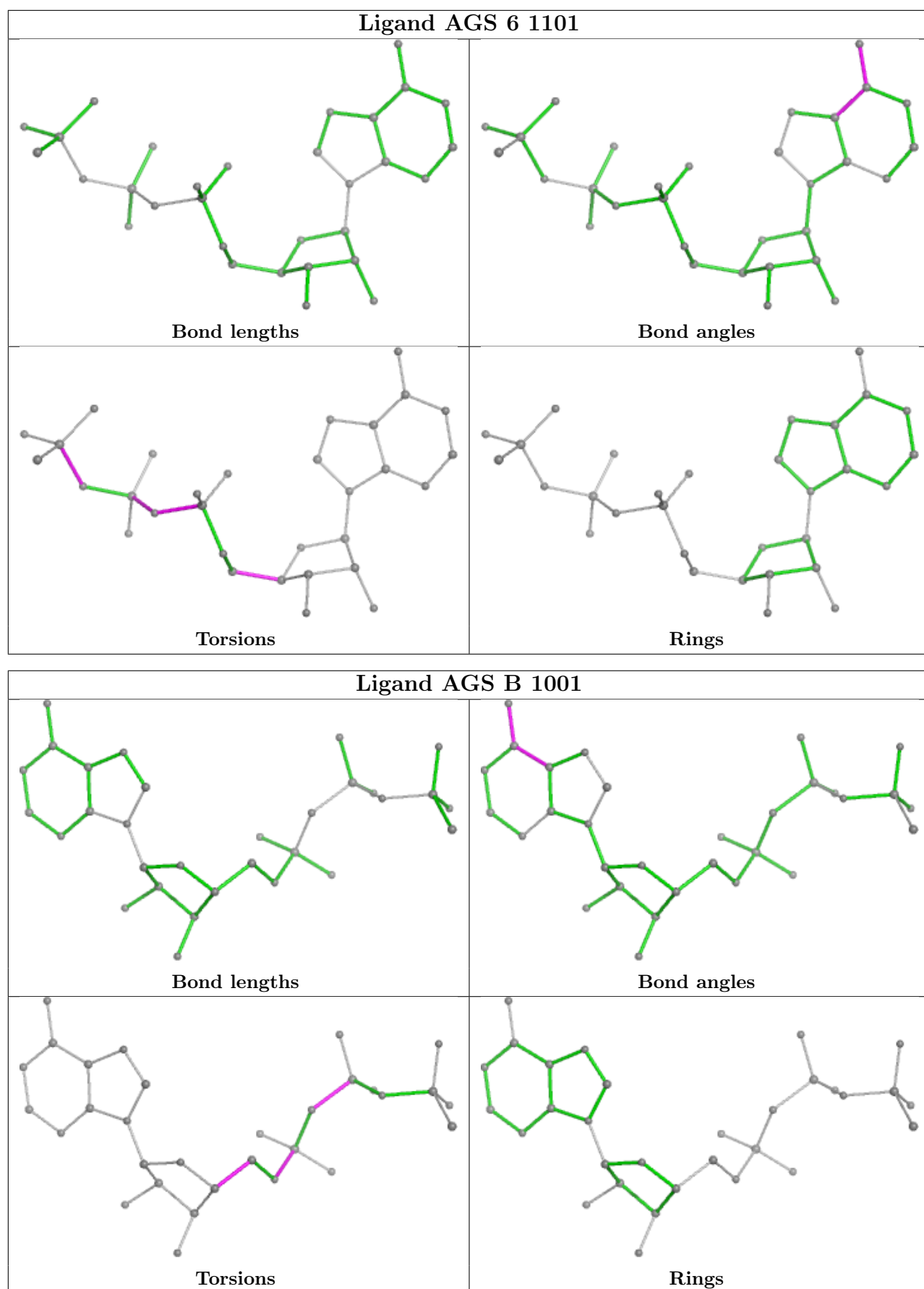
Mol	Chain	Res	Type	Atoms
10	2	1001	AGS	C5'-O5'-PA-O1A
10	2	1001	AGS	O4'-C4'-C5'-O5'
10	5	1001	AGS	C5'-O5'-PA-O1A
10	5	1001	AGS	C5'-O5'-PA-O2A
10	6	1101	AGS	PB-O3B-PG-O2G

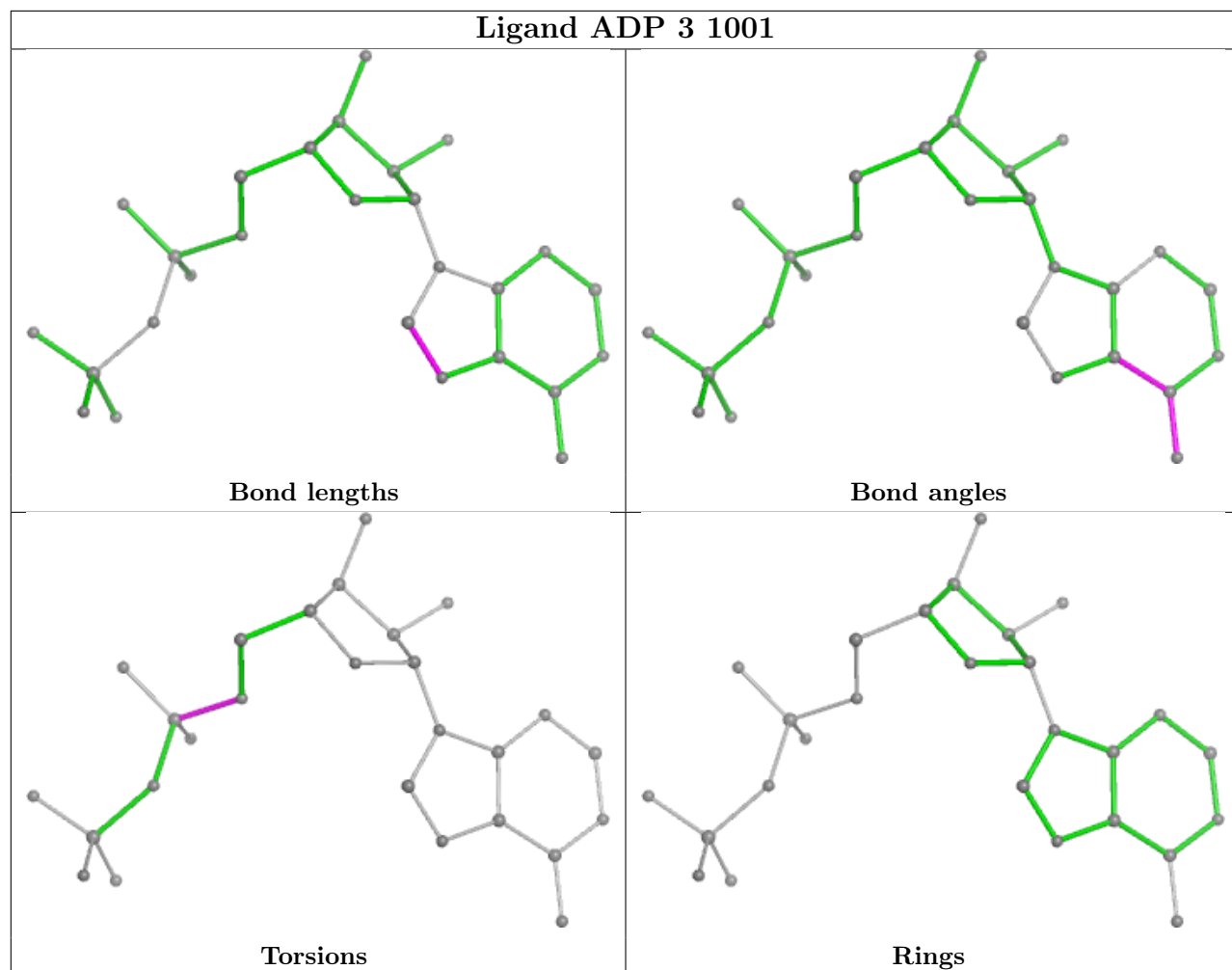
There are no ring outliers.

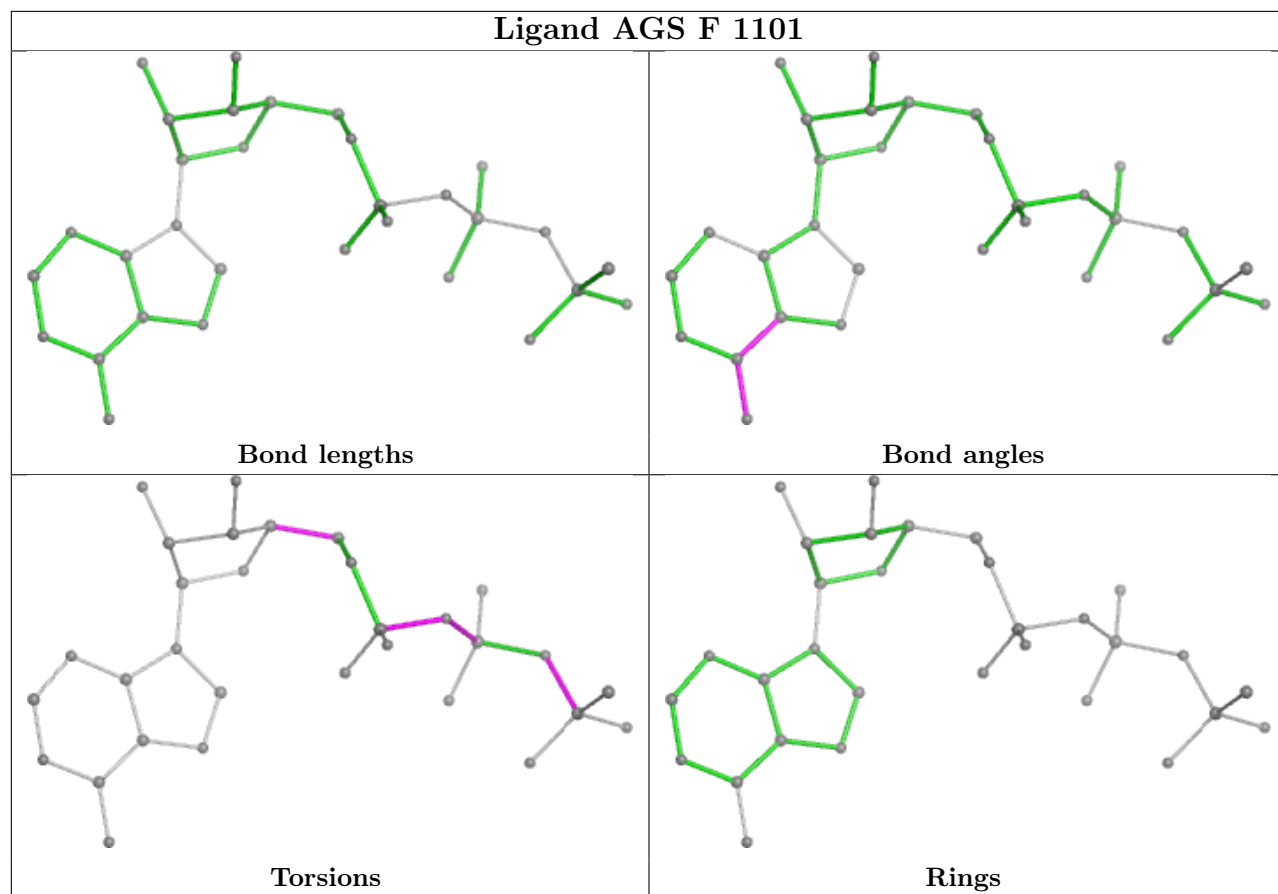
13 monomers are involved in 38 short contacts:

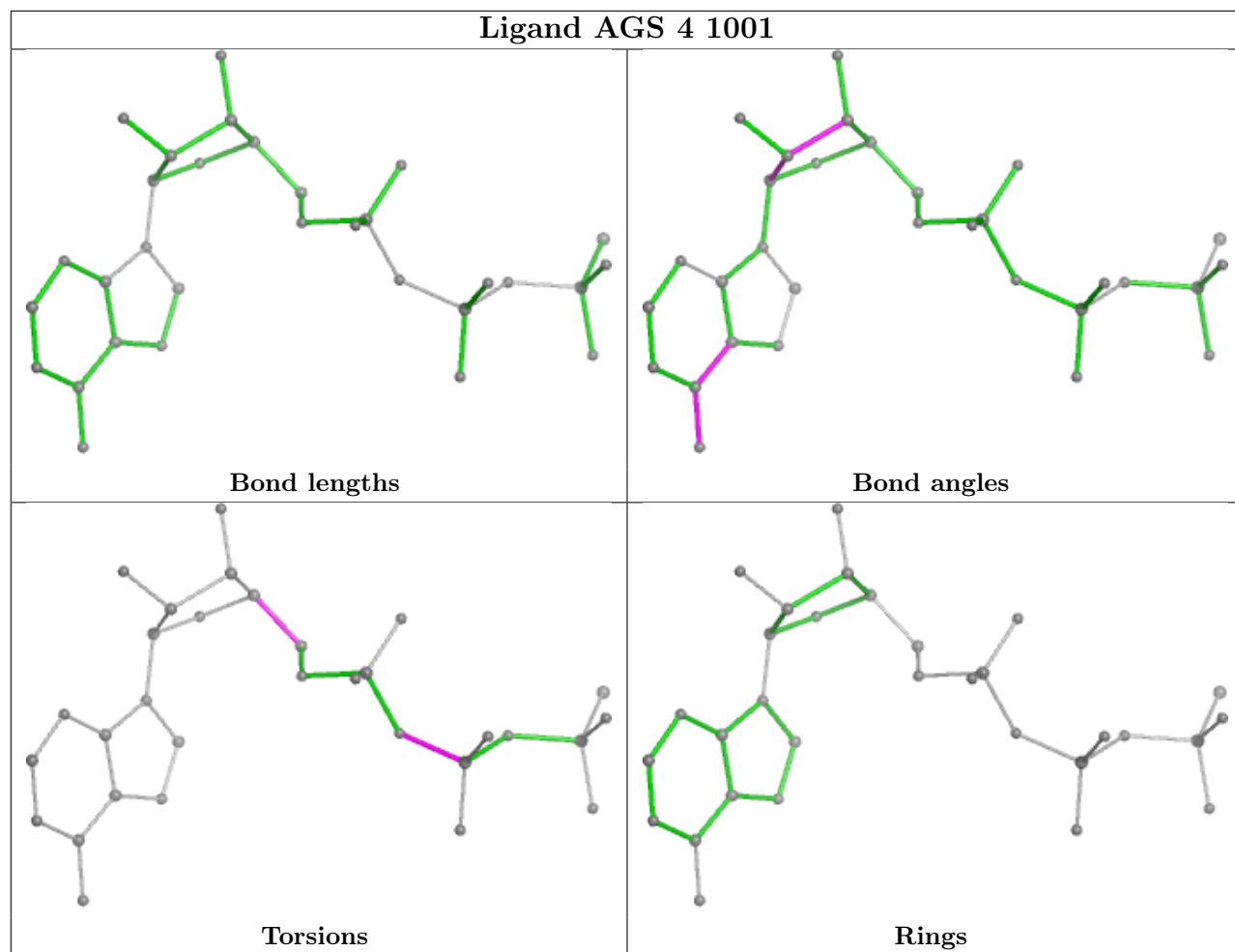
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	6	1101	AGS	1	0
10	B	1001	AGS	2	0
13	3	1001	ADP	3	0
10	F	1101	AGS	1	0
10	6	1102	AGS	1	0
13	7	902	ADP	1	0
13	C	1001	ADP	3	0
10	H	1001	AGS	11	0
13	G	902	ADP	1	0
10	2	1001	AGS	2	0
10	5	1001	AGS	1	0
10	F	1102	AGS	1	0
10	8	1001	AGS	10	0

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.

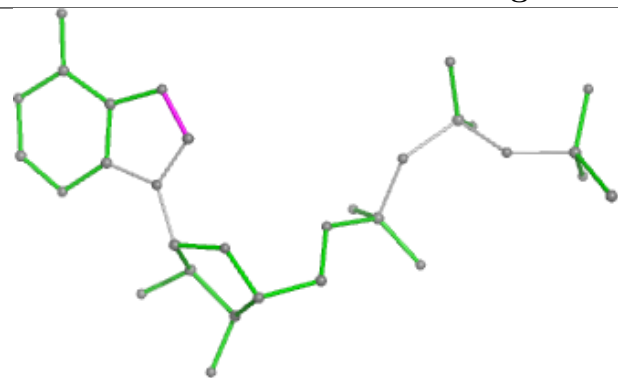




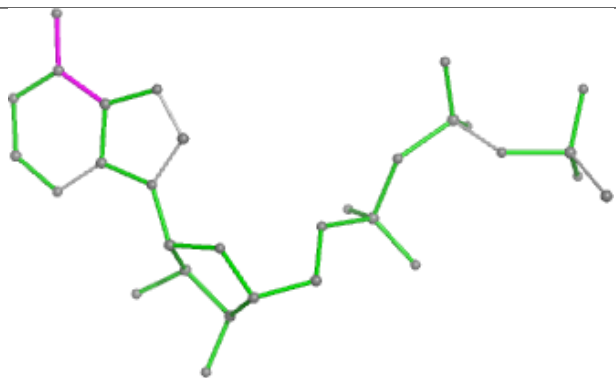




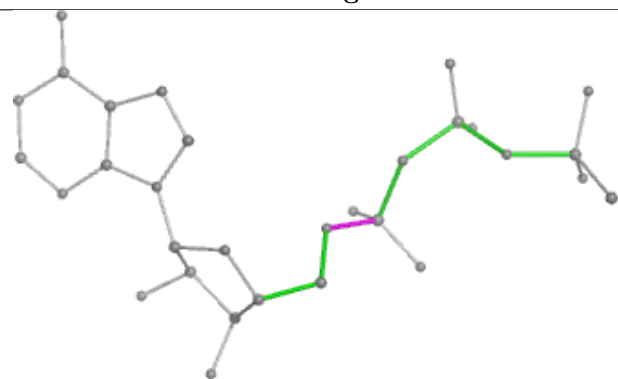
Ligand AGS E 1001



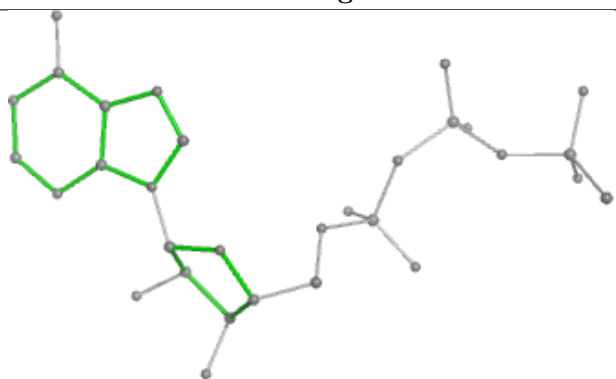
Bond lengths



Bond angles

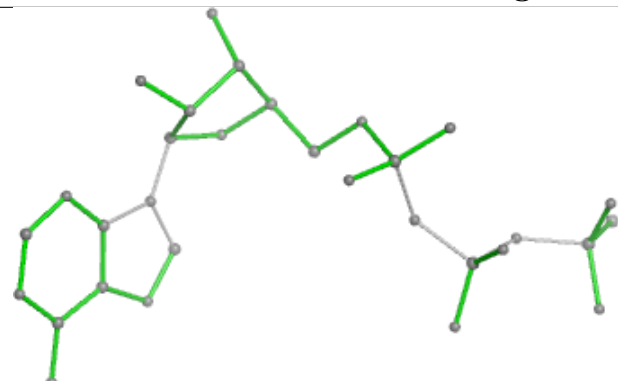


Torsions

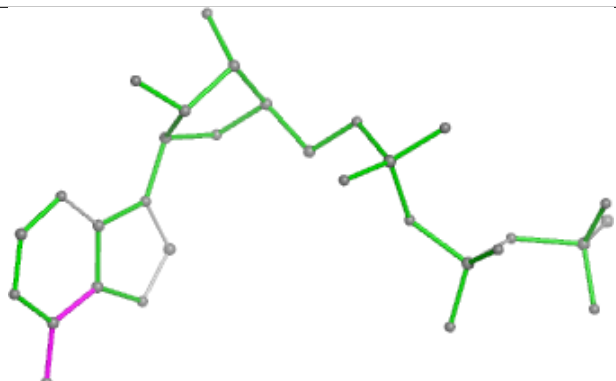


Rings

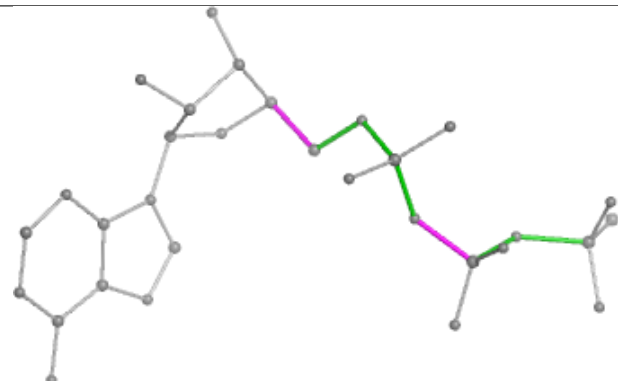
Ligand AGS 6 1102



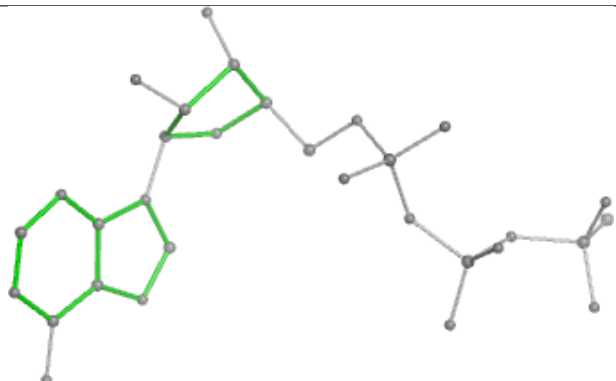
Bond lengths



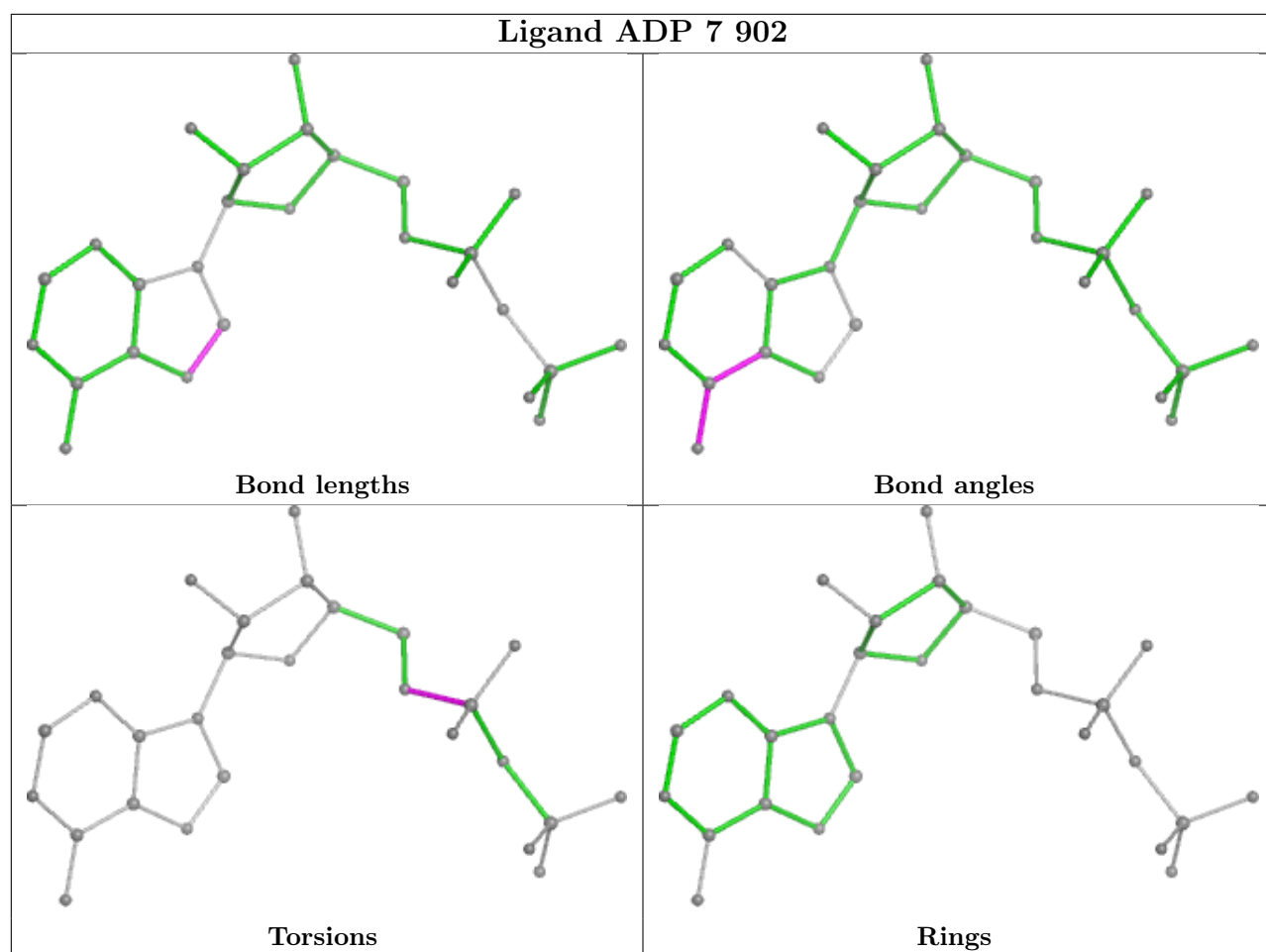
Bond angles

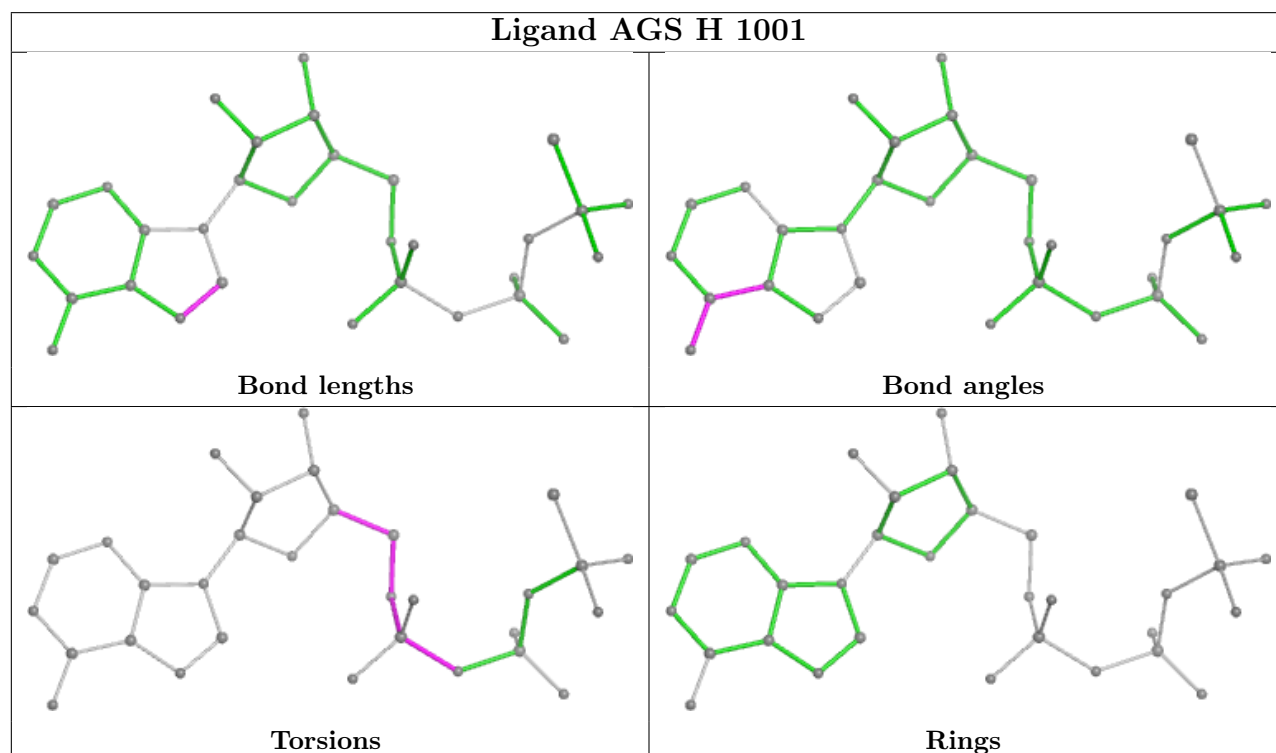
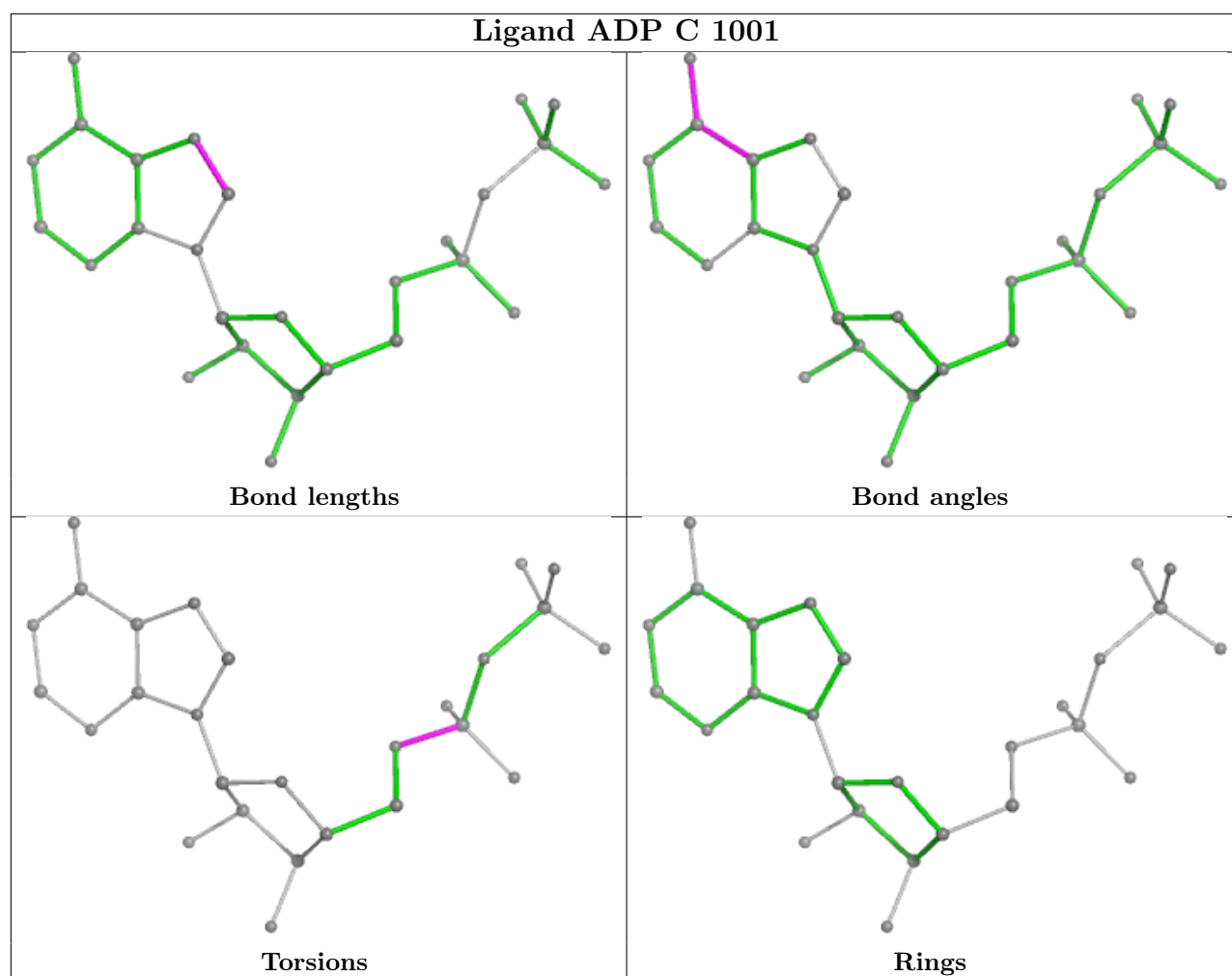


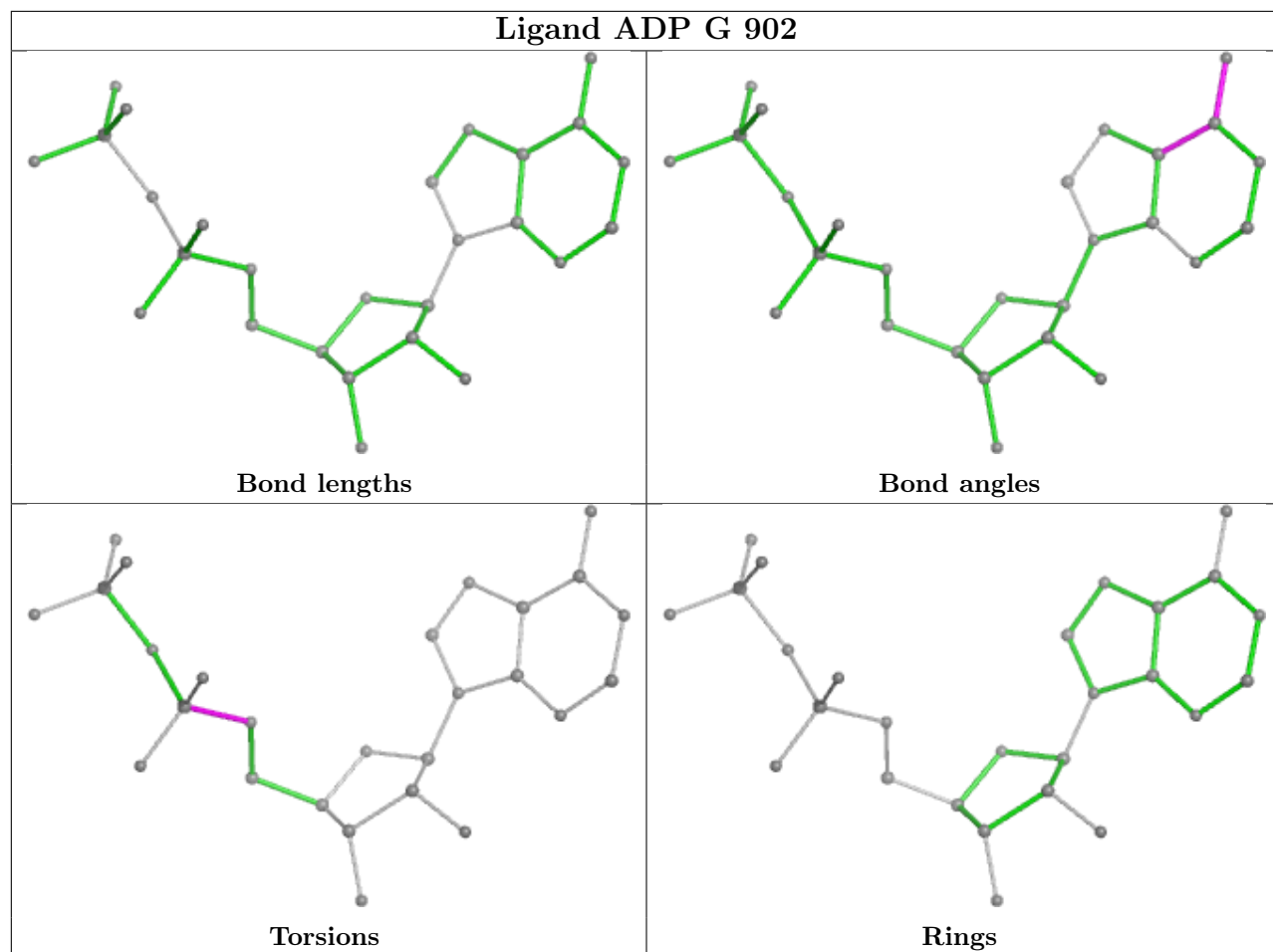
Torsions

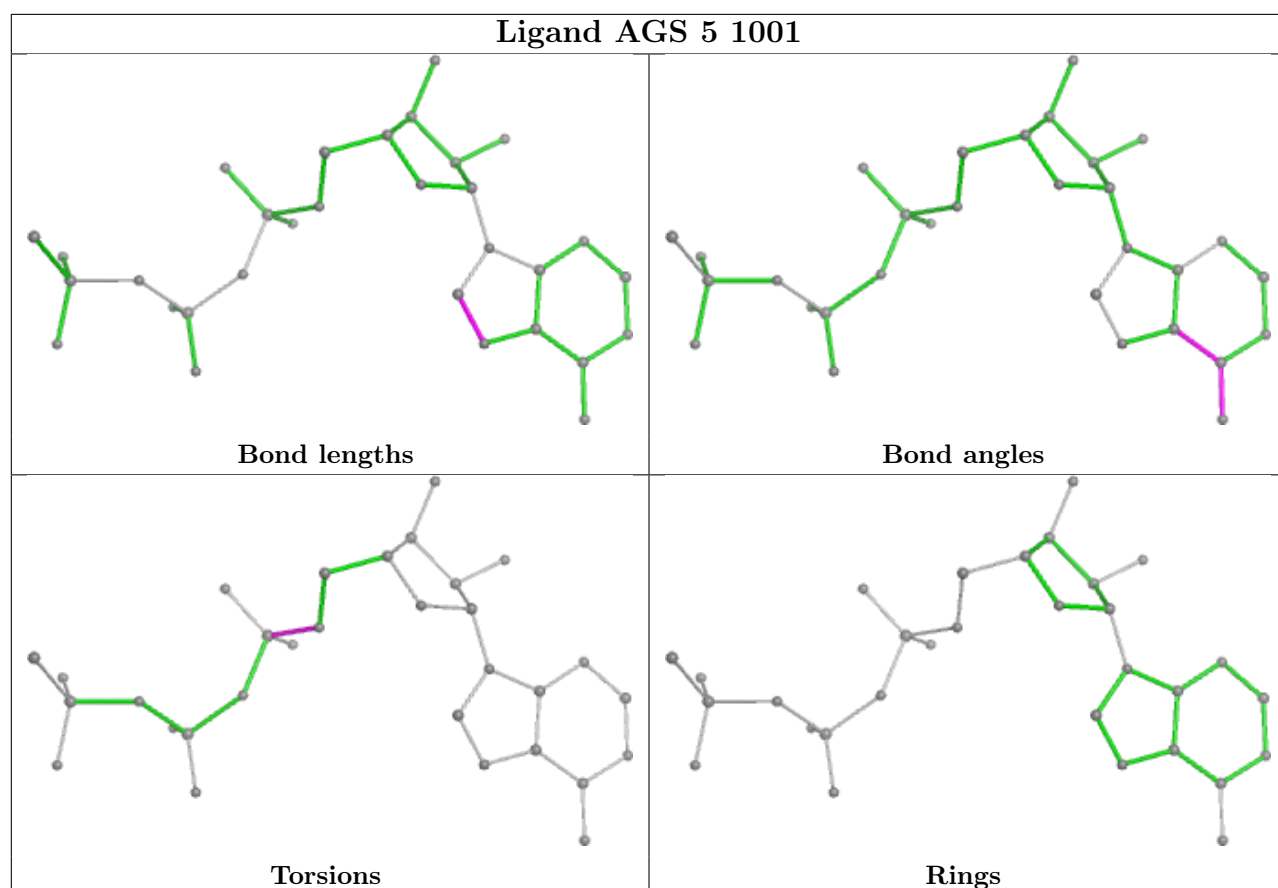
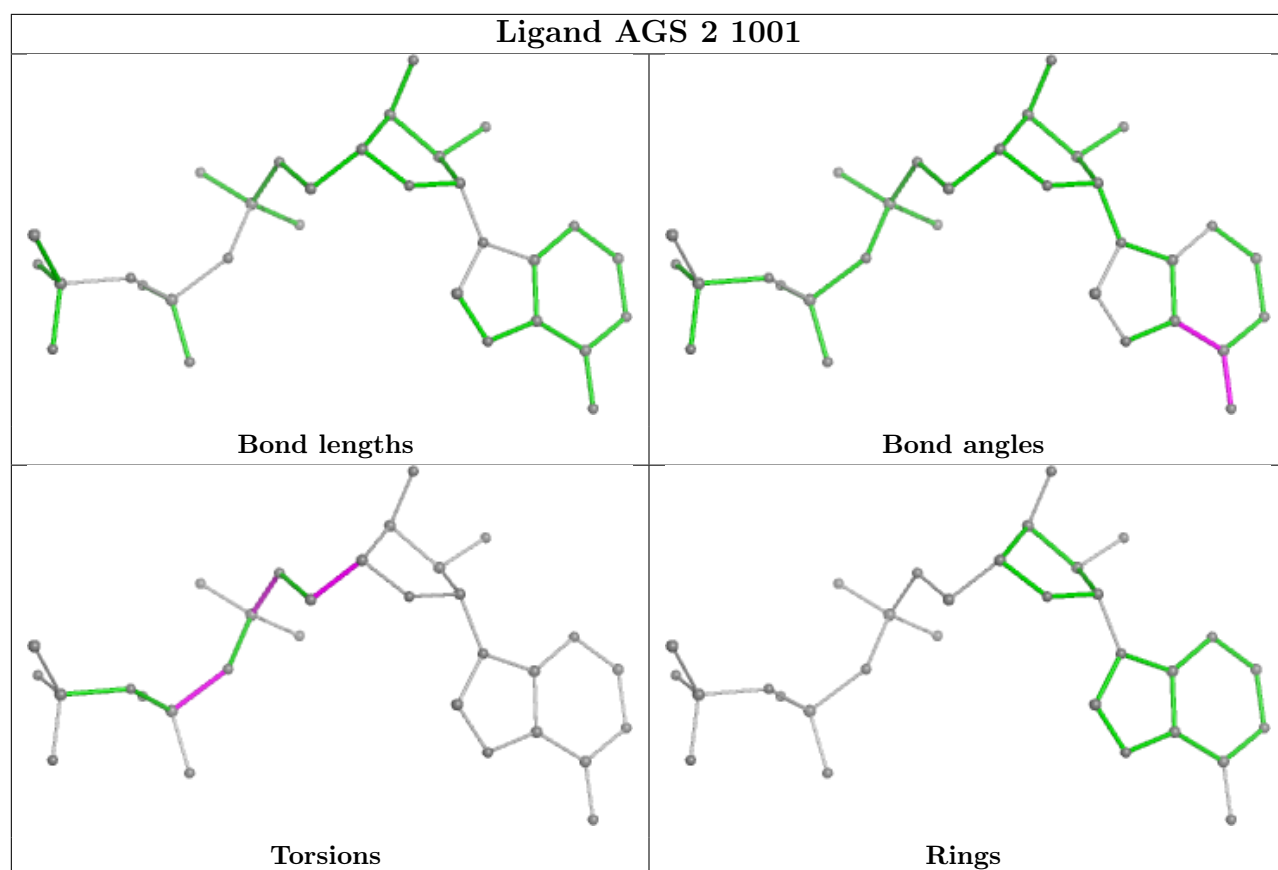


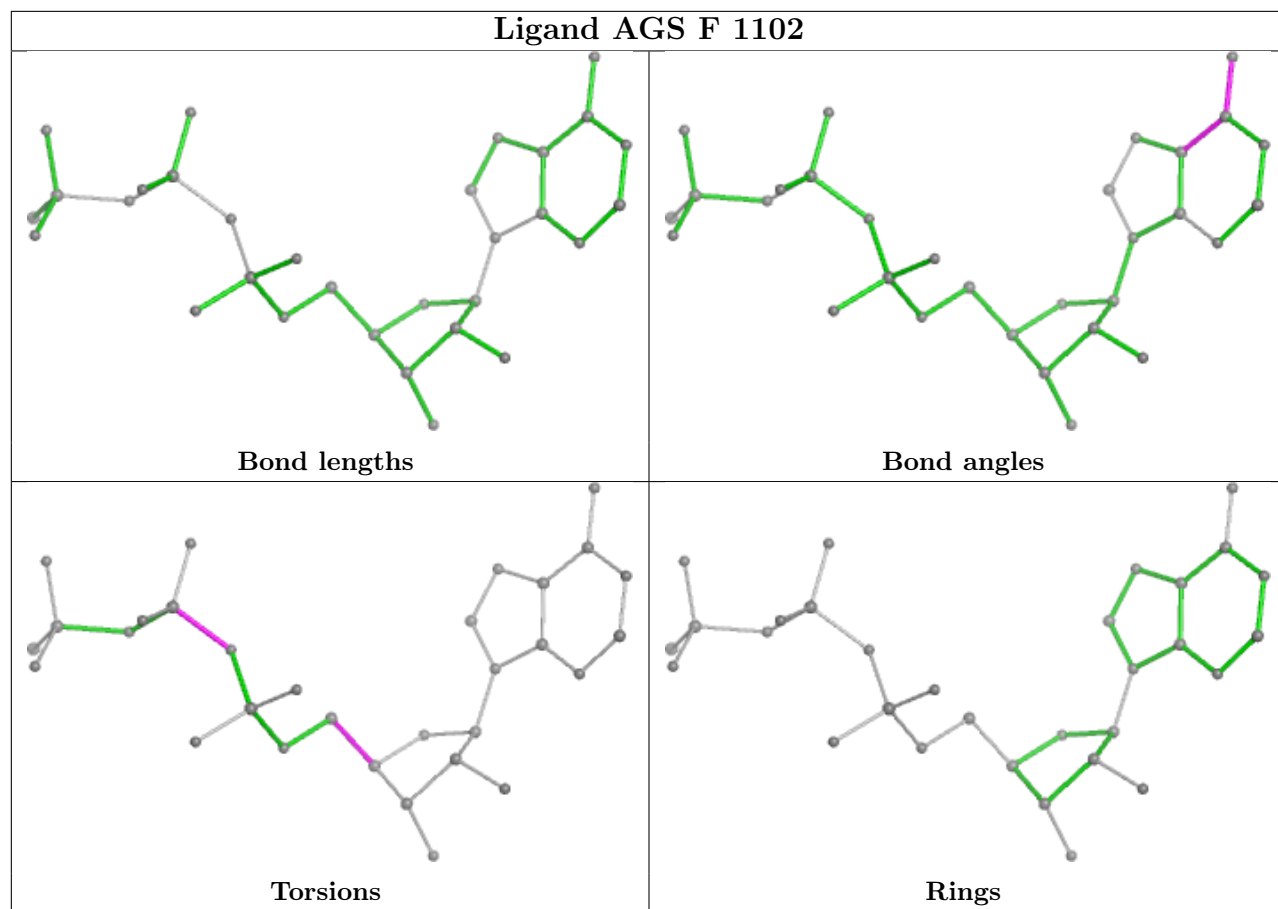
Rings

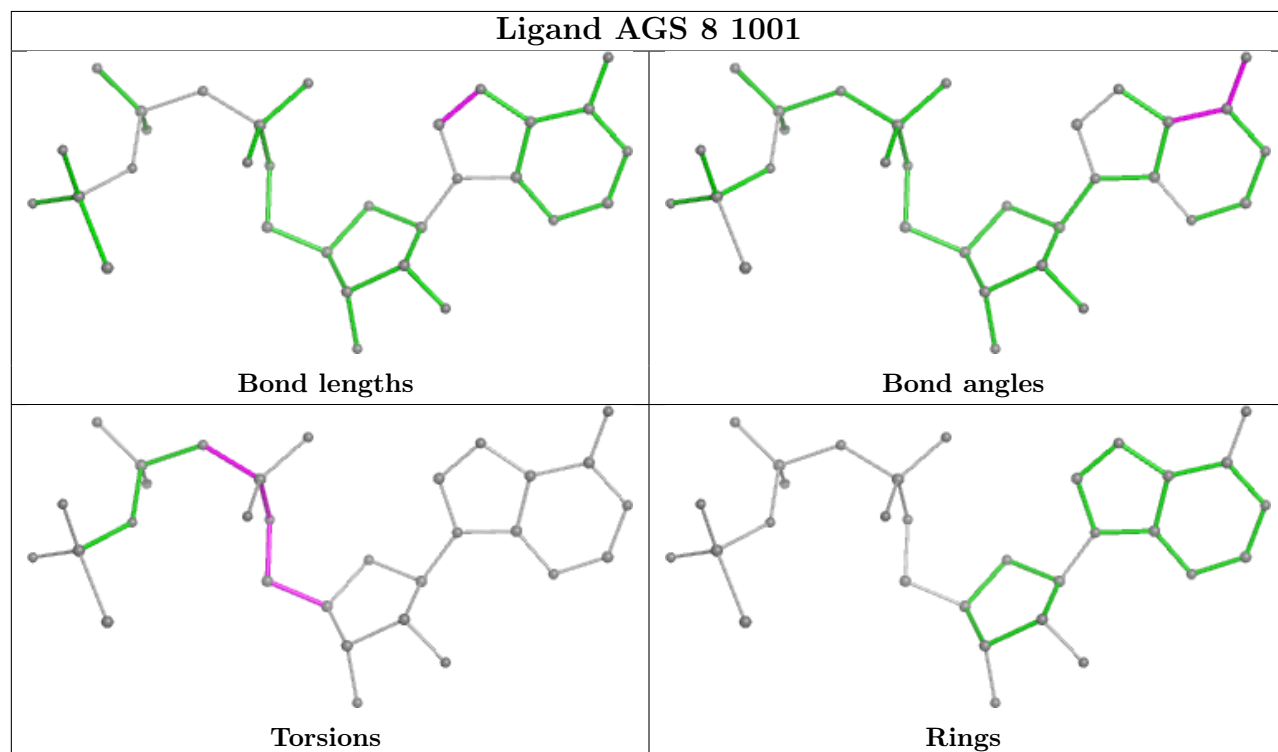
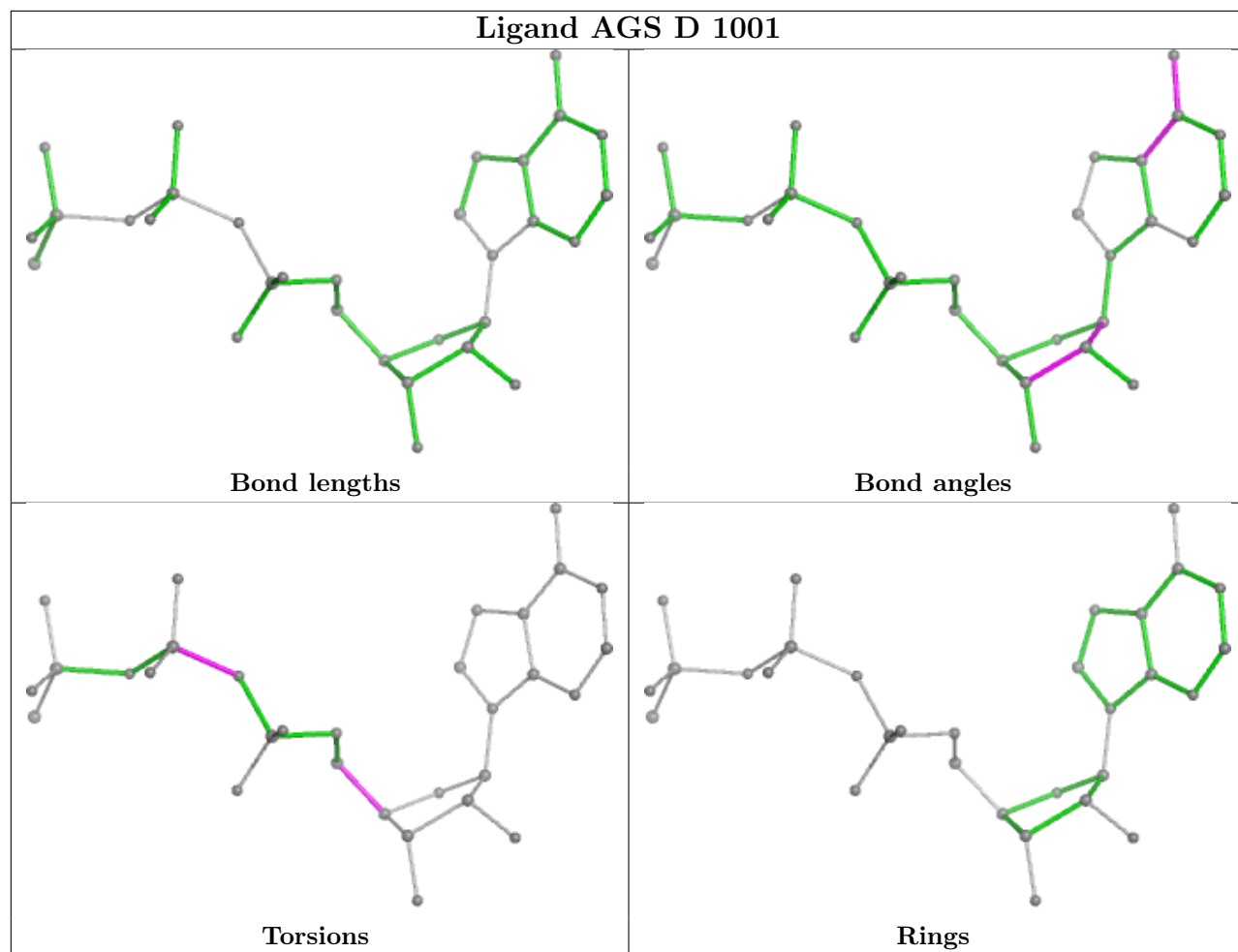












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

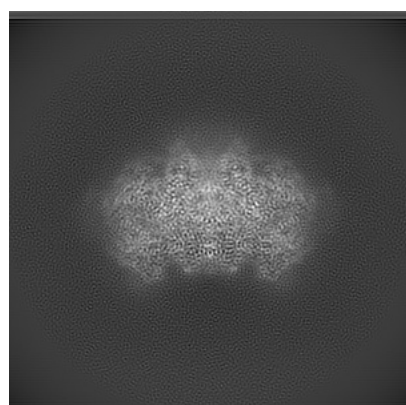
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13619. These allow visual inspection of the internal detail of the map and identification of artifacts.

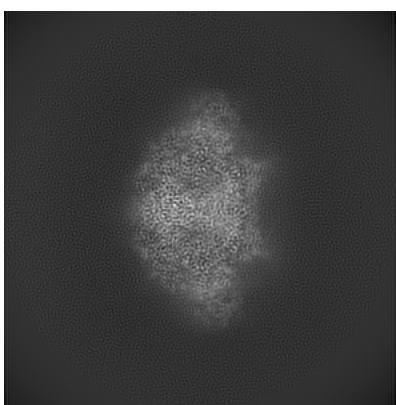
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

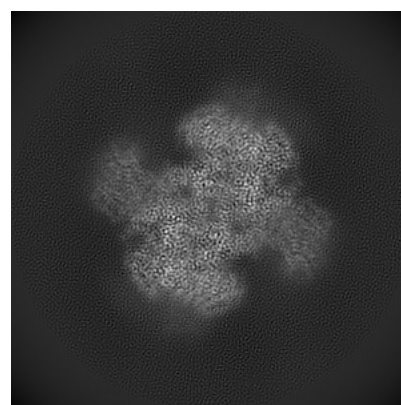
6.1.1 Primary map



X



Y

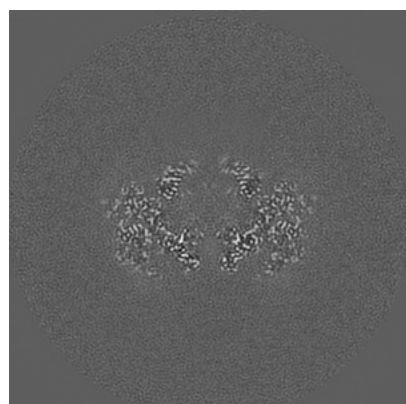


Z

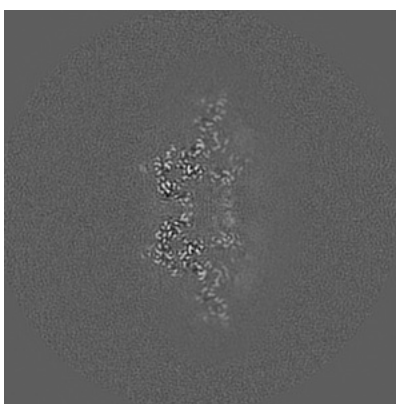
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

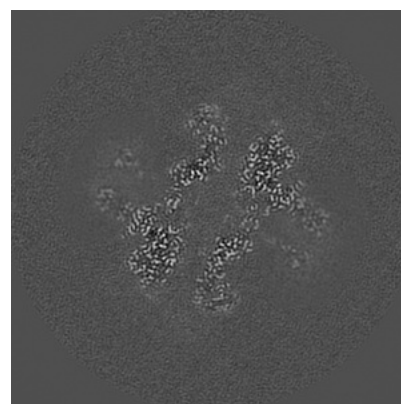
6.2.1 Primary map



X Index: 180



Y Index: 180

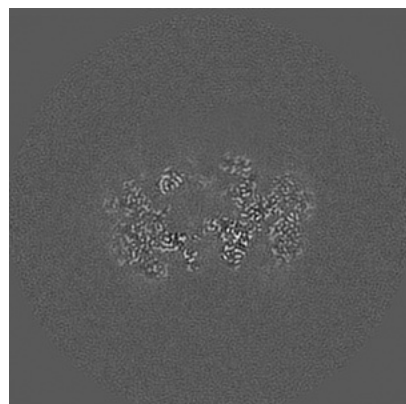


Z Index: 180

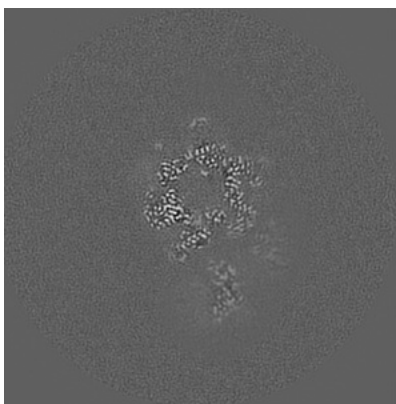
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

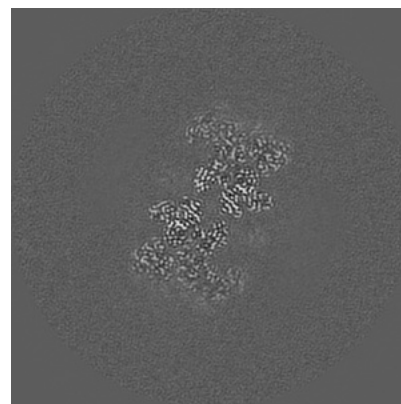
6.3.1 Primary map



X Index: 175



Y Index: 205

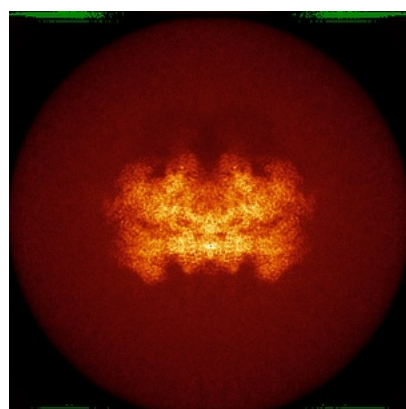


Z Index: 148

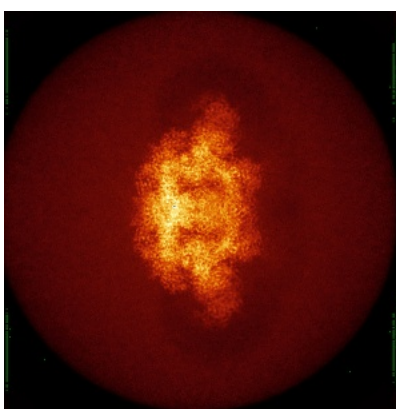
The images above show the largest variance slices of the map in three orthogonal directions.

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

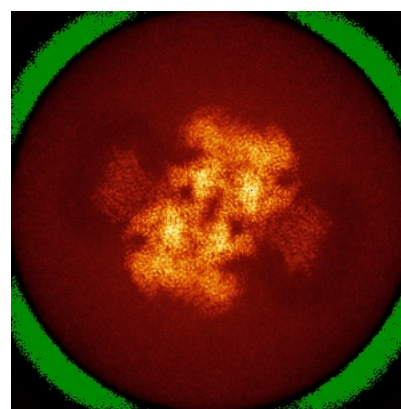
6.4.1 Primary map



X



Y

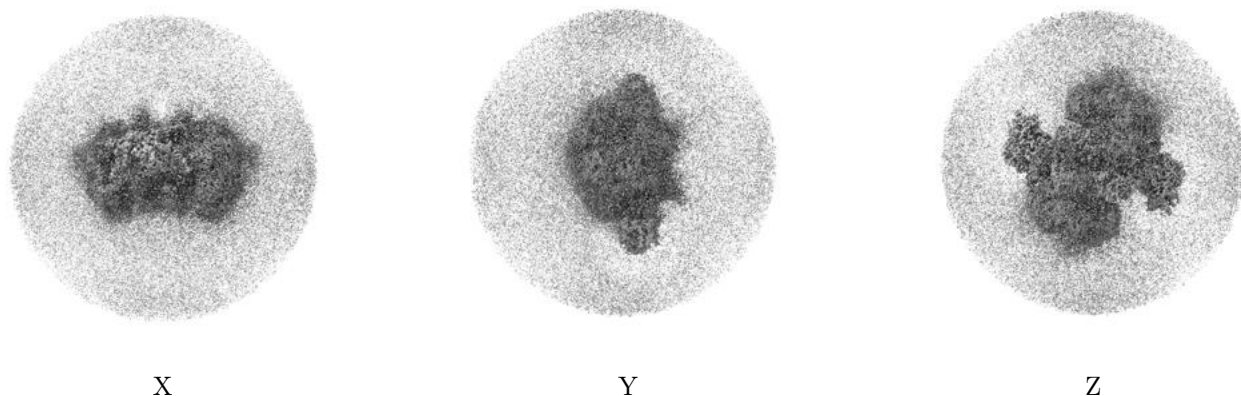


Z

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 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

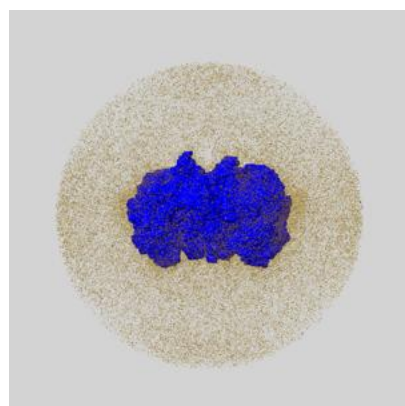
6.6 Mask visualisation [i](#)

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

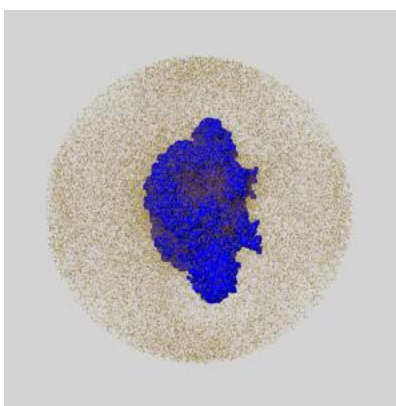
A mask typically either:

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

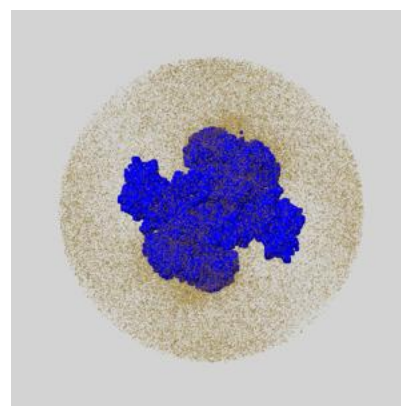
6.6.1 emd_13619_msk_1.map [i](#)



X



Y

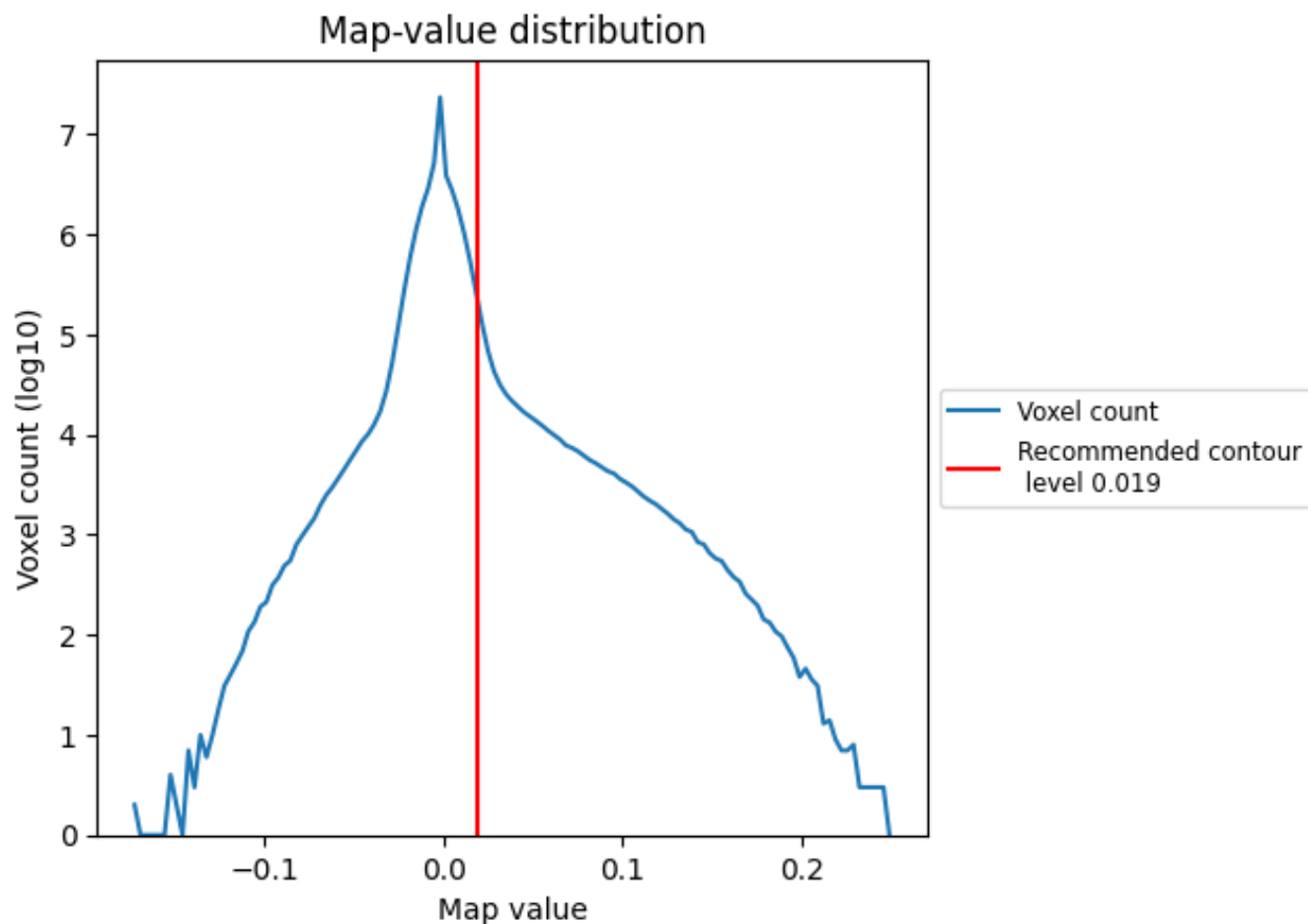


Z

7 Map analysis [i](#)

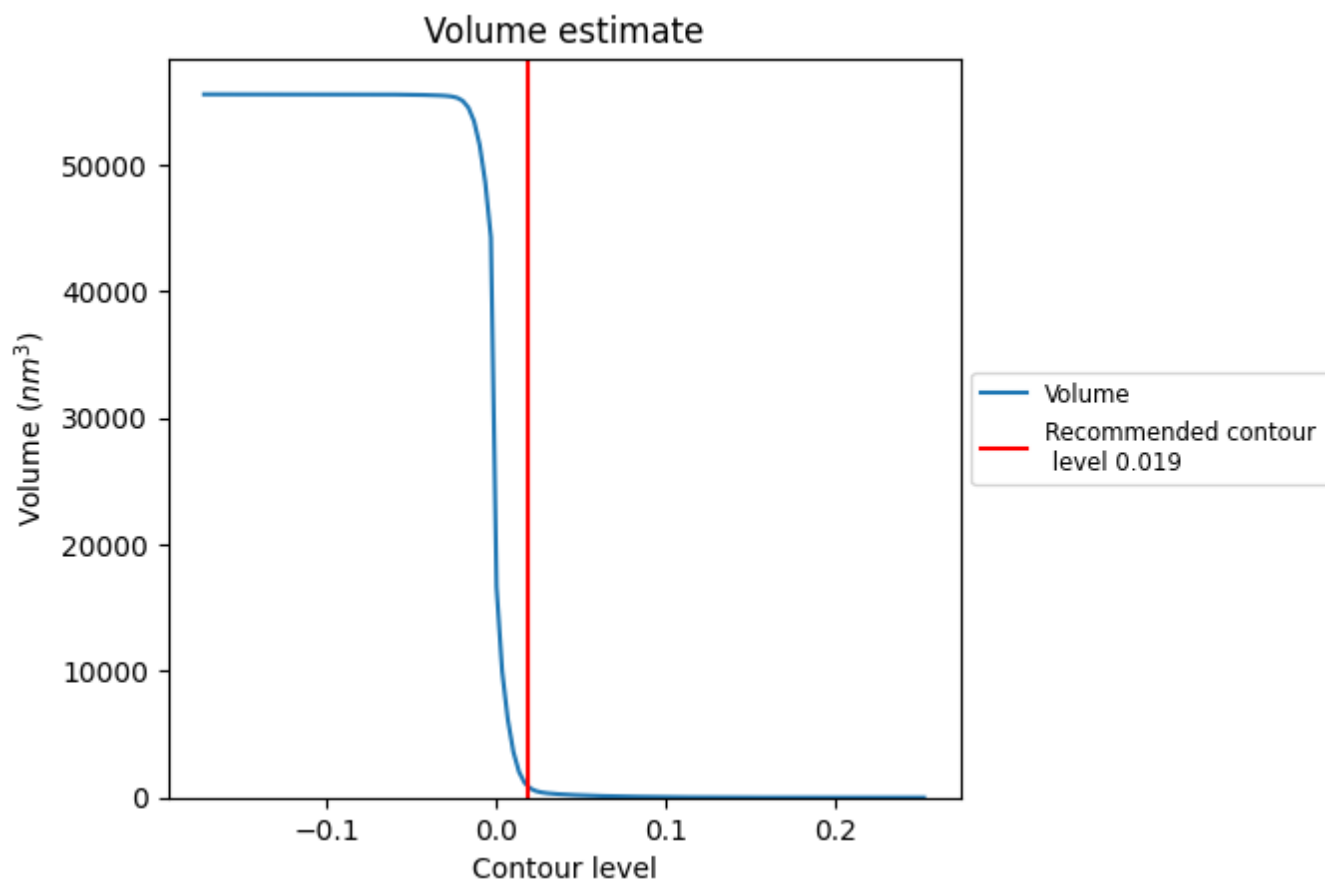
This section contains the results of statistical analysis of the map.

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.

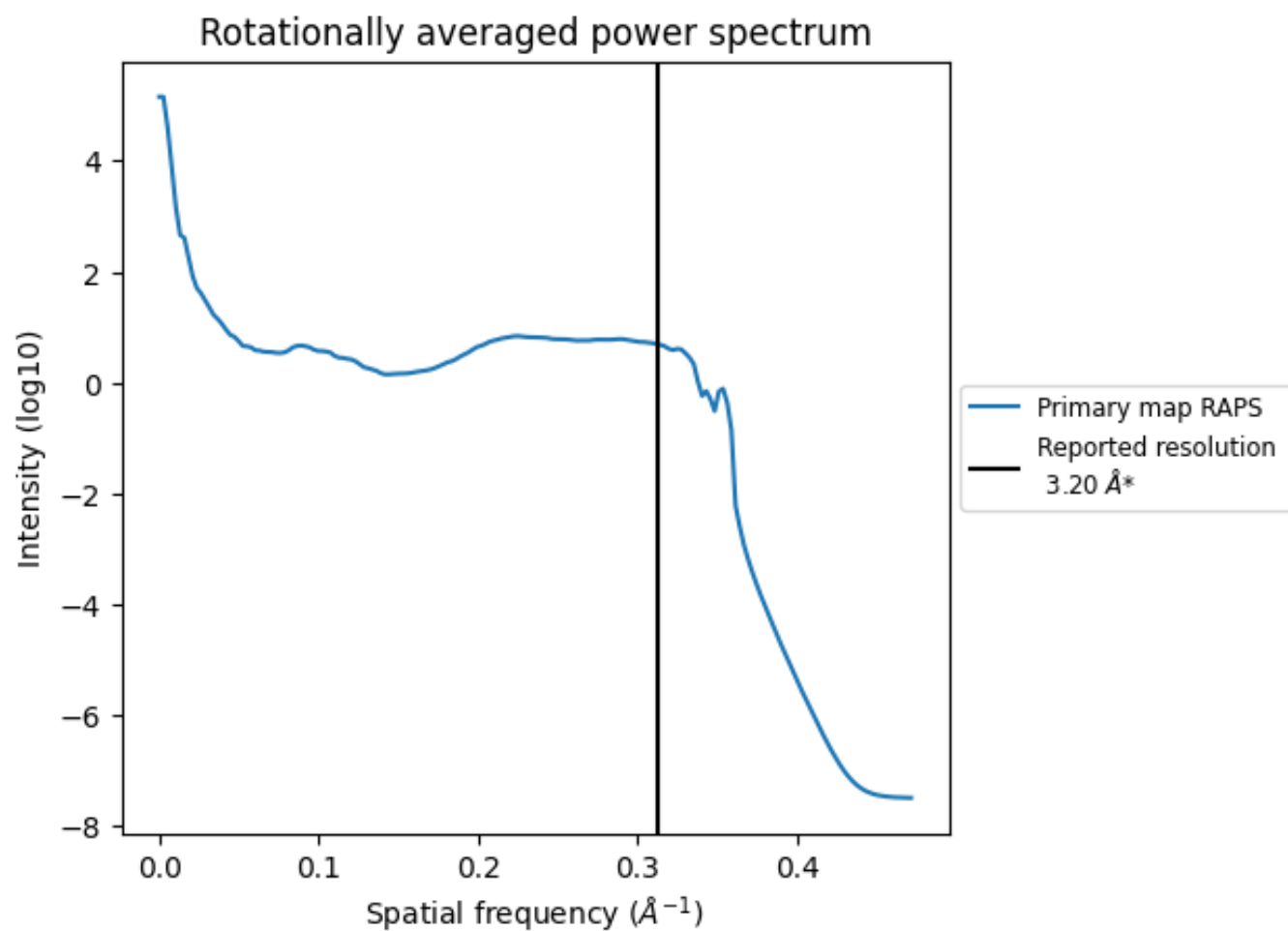
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 866 nm³; this corresponds to an approximate mass of 783 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 0.312 Å⁻¹

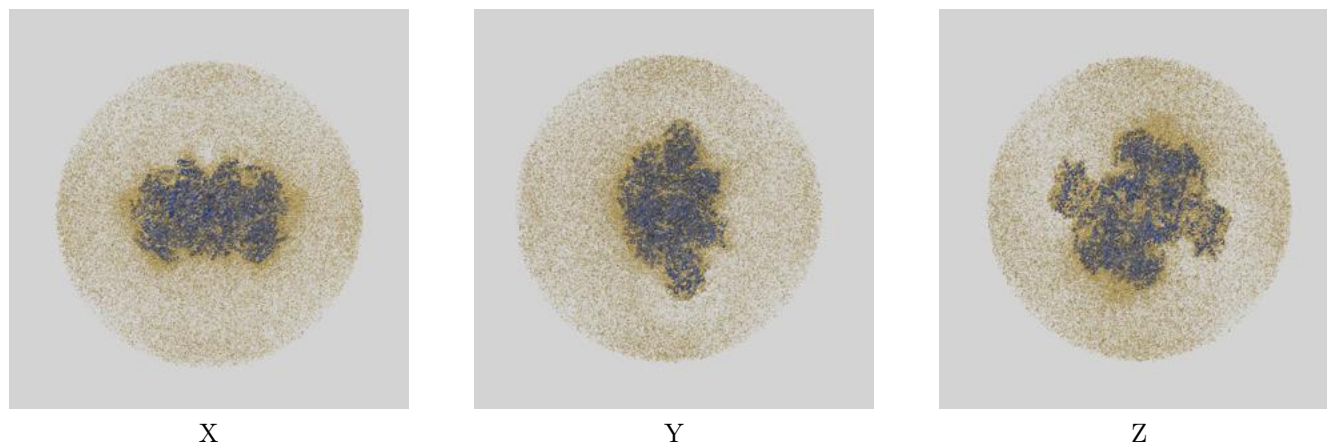
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

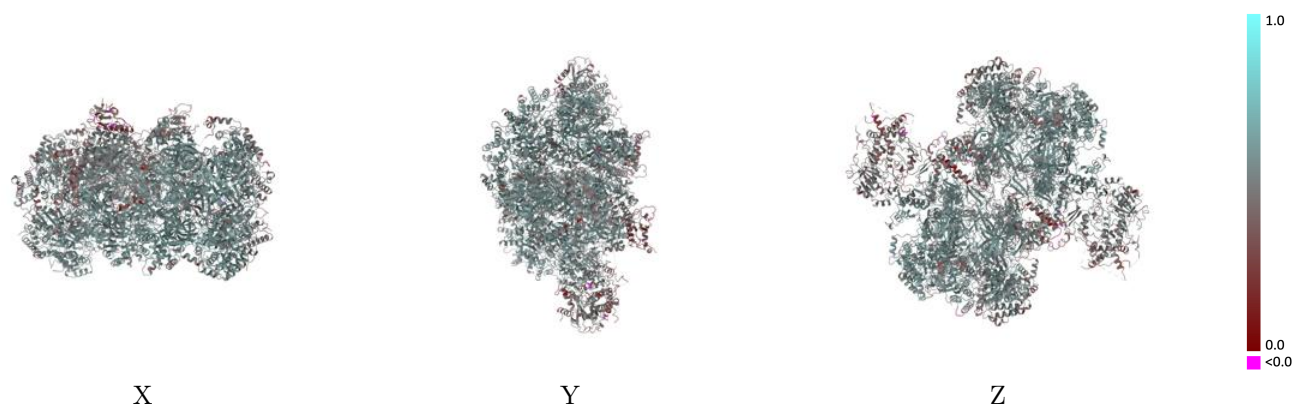
This section contains information regarding the fit between EMDB map EMD-13619 and PDB model 7PT6. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



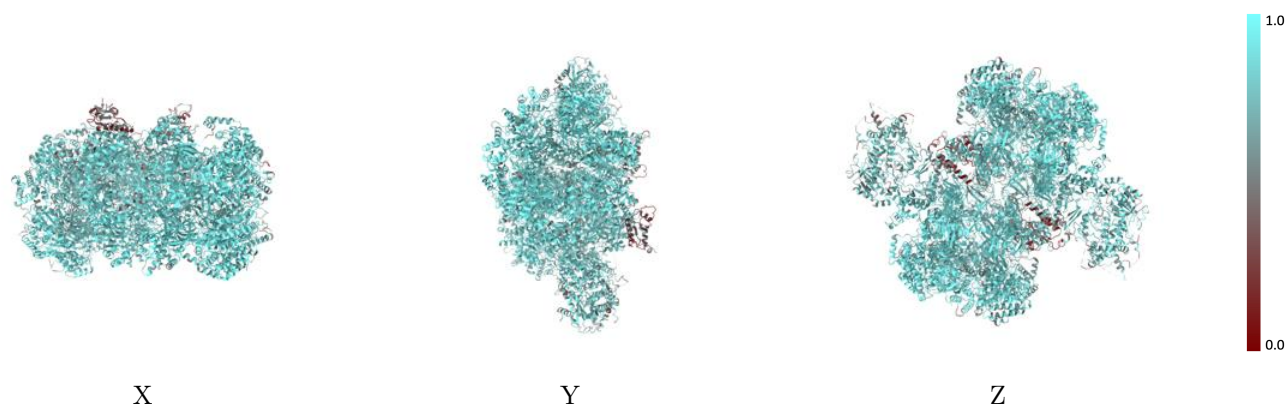
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



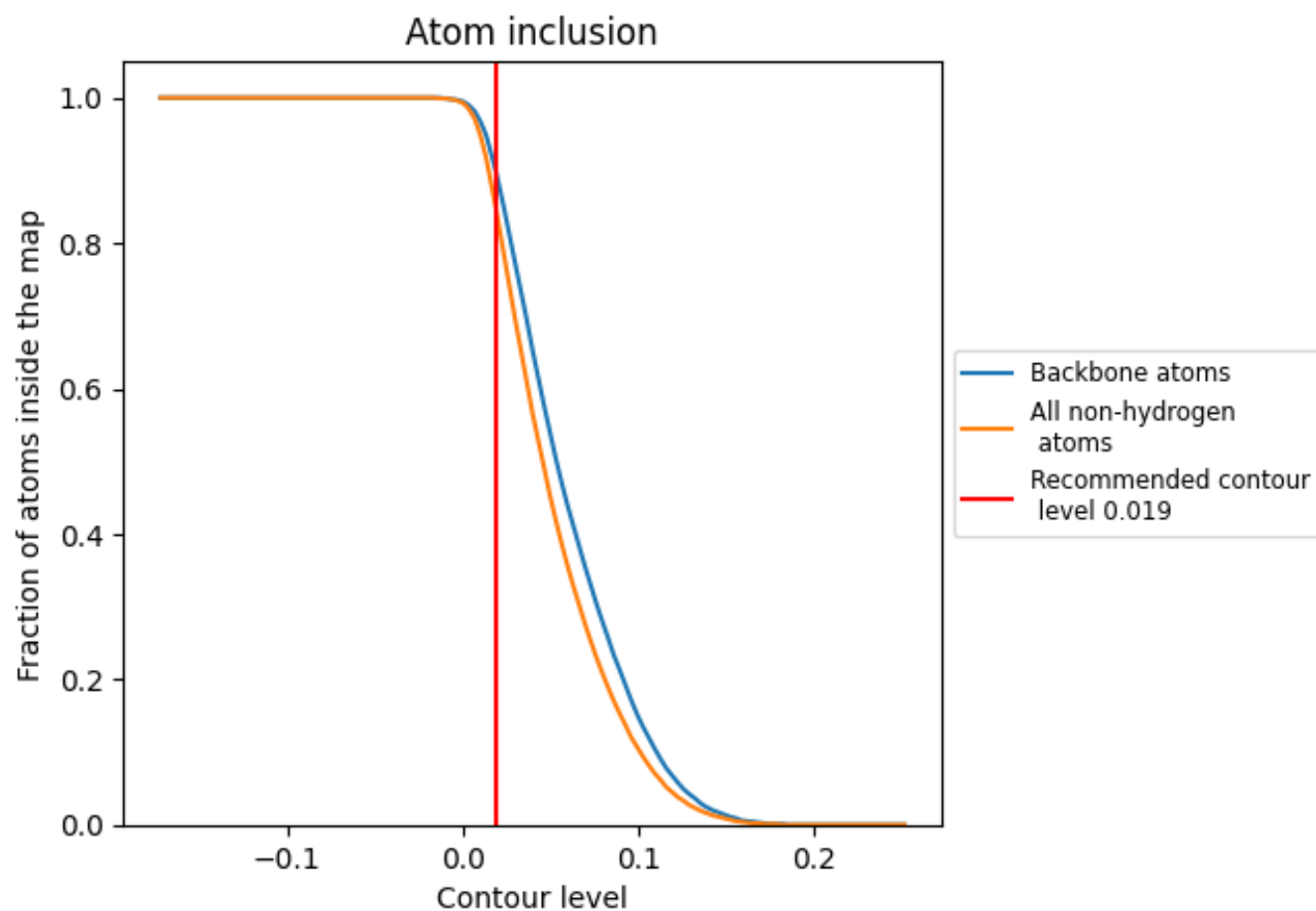
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.019).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 85% 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 (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8490	<div></div> 0.5250
1	<div></div> 0.5500	<div></div> 0.5350
2	<div></div> 0.8550	<div></div> 0.5200
3	<div></div> 0.9090	<div></div> 0.5660
4	<div></div> 0.9110	<div></div> 0.5680
5	<div></div> 0.8810	<div></div> 0.5430
6	<div></div> 0.8660	<div></div> 0.5340
7	<div></div> 0.9050	<div></div> 0.5670
8	<div></div> 0.7660	<div></div> 0.4630
9	<div></div> 0.5770	<div></div> 0.3810
A	<div></div> 0.5500	<div></div> 0.5010
B	<div></div> 0.8490	<div></div> 0.5140
C	<div></div> 0.9040	<div></div> 0.5590
D	<div></div> 0.9040	<div></div> 0.5620
E	<div></div> 0.8770	<div></div> 0.5350
F	<div></div> 0.8620	<div></div> 0.5280
G	<div></div> 0.9010	<div></div> 0.5590
H	<div></div> 0.7220	<div></div> 0.4220
I	<div></div> 0.5720	<div></div> 0.3900

1.0

0.0

<0.0