



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 07:18 AM UTC

PDB ID : 7PT7 / pdb_00007pt7
EMDB ID : EMD-13620
Title : Structure of MCM2-7 DH complexed with Cdc7-Dbf4 in the presence of ADP:BeF₃, state I
Authors : Saleh, A.; Noguchi, Y.; Aramayo, R.; Ivanova, M.E.; Speck, C.
Deposited on : 2021-09-26
Resolution : 3.80 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:

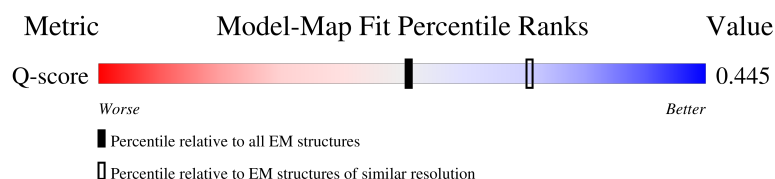
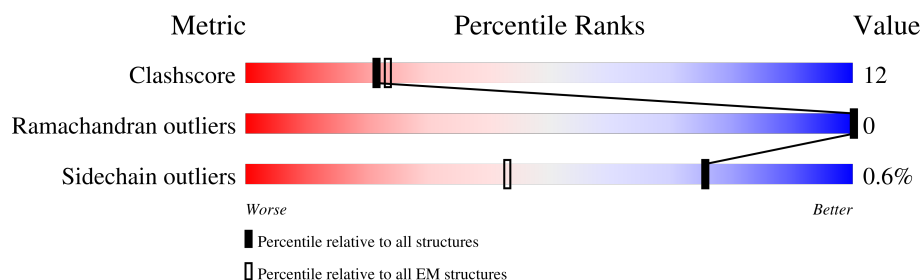
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.80 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.



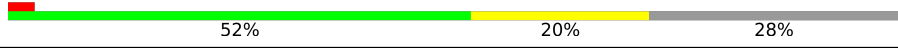
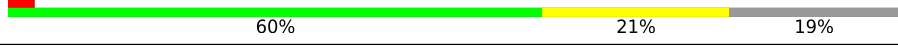
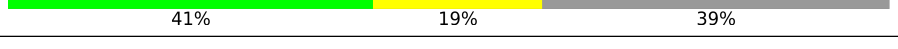
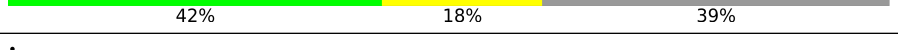
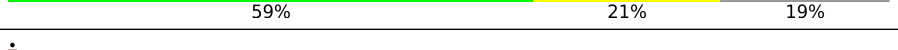
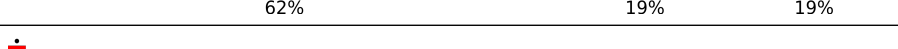
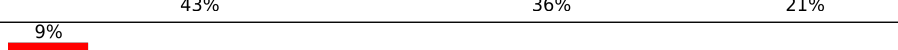
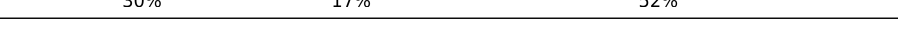
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	100% 100%
2	2	868	7% 51% 21% 28%
2	B	868	8% 51% 21% 28%
3	3	971	50% 16% 35%

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Mol	Chain	Length	Quality of chain
3	C	971	
4	4	933	
4	D	933	
5	5	775	
5	E	775	
6	6	1017	
6	F	1017	
7	7	845	
7	G	845	
8	8	507	
9	9	704	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 67420 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		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	626	Total	C	N	O	S	0	0
			4960	3124	880	937	19		
2	B	626	Total	C	N	O	S	0	0
			4960	3124	880	937	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	635	Total	C	N	O	S	0	0
			4986	3152	885	936	13		
3	C	633	Total	C	N	O	S	0	0
			4966	3141	880	932	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	628	Total	C	N	O	S	0	0
			4927	3098	844	962	23		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	628	Total	C	N	O	S	0	0
			4927	3098	844	962	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	617	Total	C	N	O	S	0	0
			4889	3083	850	931	25		
6	F	617	Total	C	N	O	S	0	0
			4889	3083	850	931	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		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	337	Total	C	N	O	S	0	0
			2813	1793	494	514	12		

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
10	2	1	Total 27	C 10	N 5	O 10	P 2	0
10	3	1	Total 27	C 10	N 5	O 10	P 2	0
10	4	1	Total 27	C 10	N 5	O 10	P 2	0
10	5	1	Total 27	C 10	N 5	O 10	P 2	0
10	6	1	Total 27	C 10	N 5	O 10	P 2	0
10	7	1	Total 27	C 10	N 5	O 10	P 2	0
10	8	1	Total 27	C 10	N 5	O 10	P 2	0
10	B	1	Total 27	C 10	N 5	O 10	P 2	0
10	C	1	Total 27	C 10	N 5	O 10	P 2	0
10	D	1	Total 27	C 10	N 5	O 10	P 2	0
10	E	1	Total 27	C 10	N 5	O 10	P 2	0
10	F	1	Total 27	C 10	N 5	O 10	P 2	0
10	G	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of

Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
11	2	1	Total 1	Mg 1	0
11	3	1	Total 1	Mg 1	0
11	4	1	Total 1	Mg 1	0
11	5	1	Total 1	Mg 1	0
11	6	1	Total 1	Mg 1	0
11	7	1	Total 1	Mg 1	0
11	8	2	Total 2	Mg 2	0
11	B	1	Total 1	Mg 1	0
11	C	1	Total 1	Mg 1	0
11	D	1	Total 1	Mg 1	0
11	E	1	Total 1	Mg 1	0
11	F	1	Total 1	Mg 1	0
11	G	1	Total 1	Mg 1	0

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

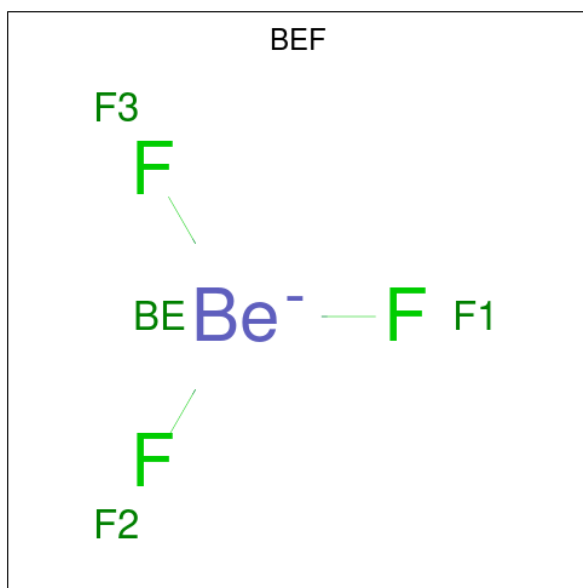
Mol	Chain	Residues	Atoms		AltConf
12	2	1	Total 1	Zn 1	0
12	4	1	Total 1	Zn 1	0
12	5	1	Total 1	Zn 1	0
12	6	1	Total 1	Zn 1	0
12	7	1	Total 1	Zn 1	0

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

- Molecule 13 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
13	3	1	Total 4	Be 1	F 3	0
13	3	1	Total 4	Be 1	F 3	0
13	4	1	Total 4	Be 1	F 3	0
13	8	1	Total 4	Be 1	F 3	0

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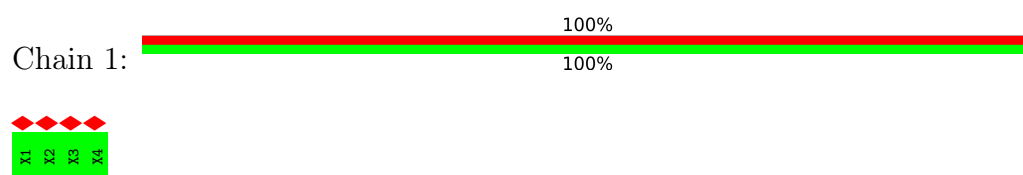
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Mol	Chain	Residues	Atoms			AltConf
13	D	1	Total 4	Be 1	F 3	0
13	E	1	Total 4	Be 1	F 3	0
13	G	1	Total 4	Be 1	F 3	0

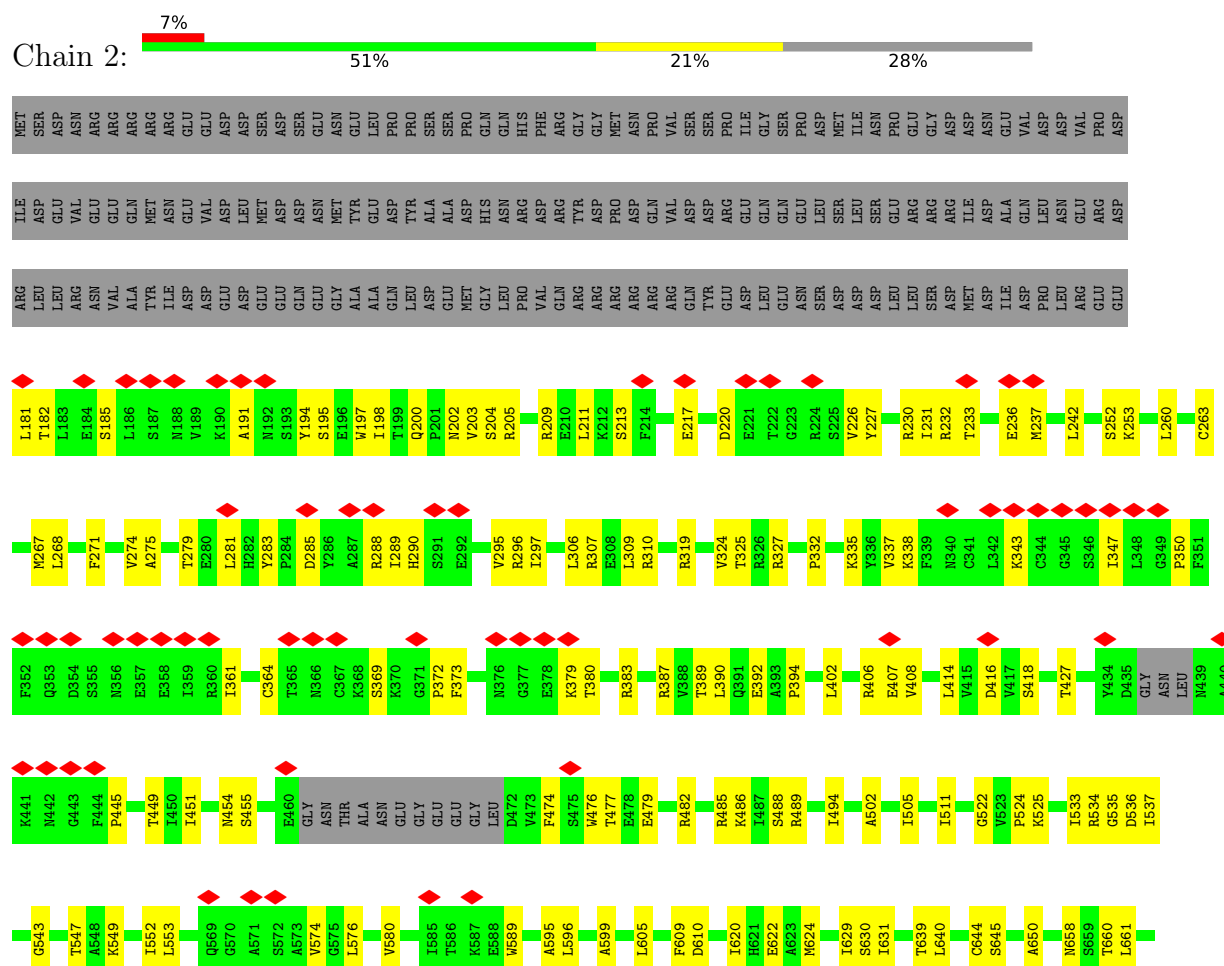
3 Residue-property plots

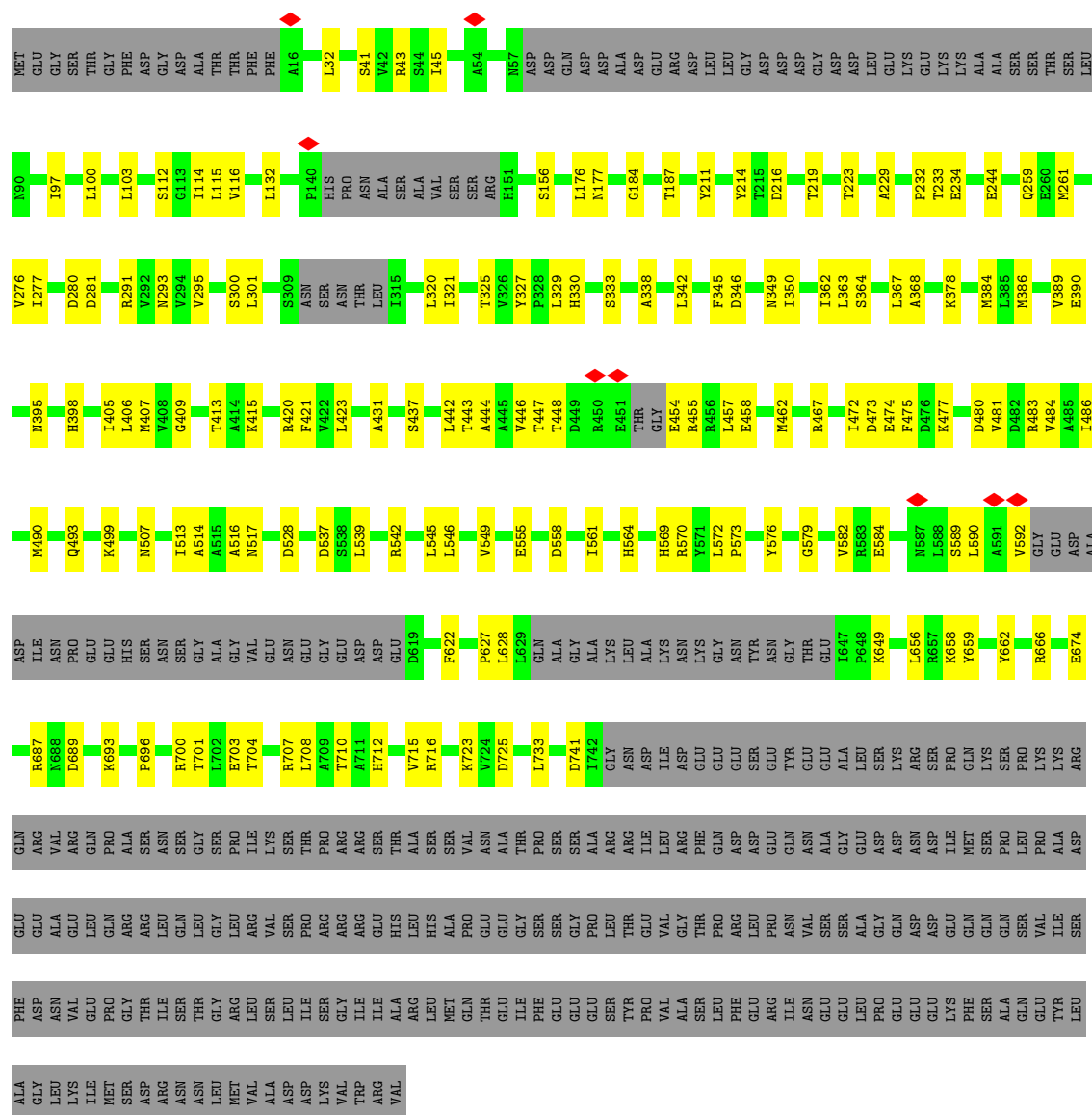
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

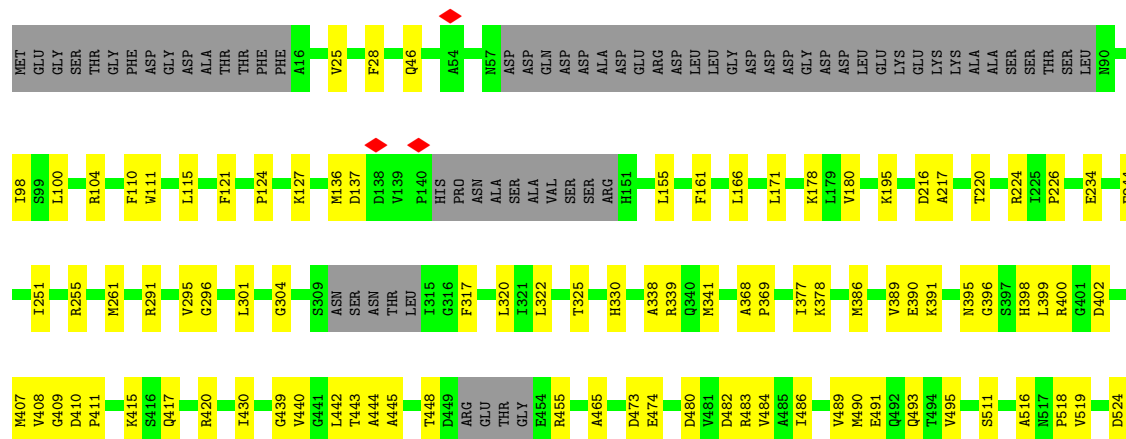


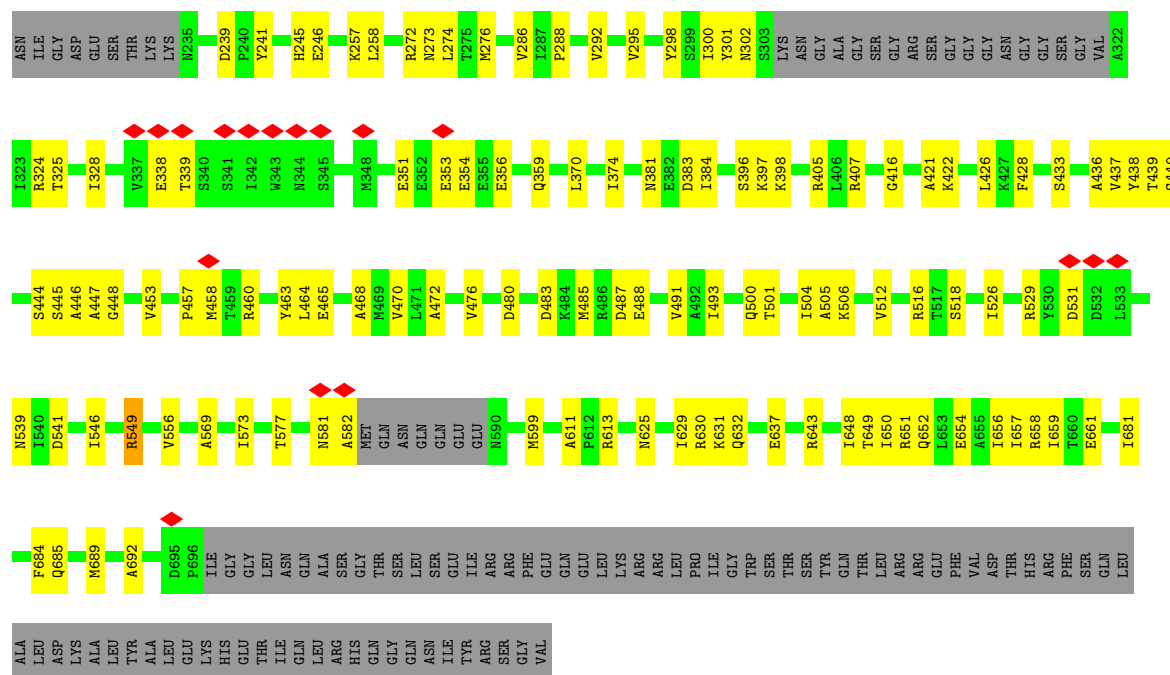
- Molecule 2: DNA replication licensing factor MCM2



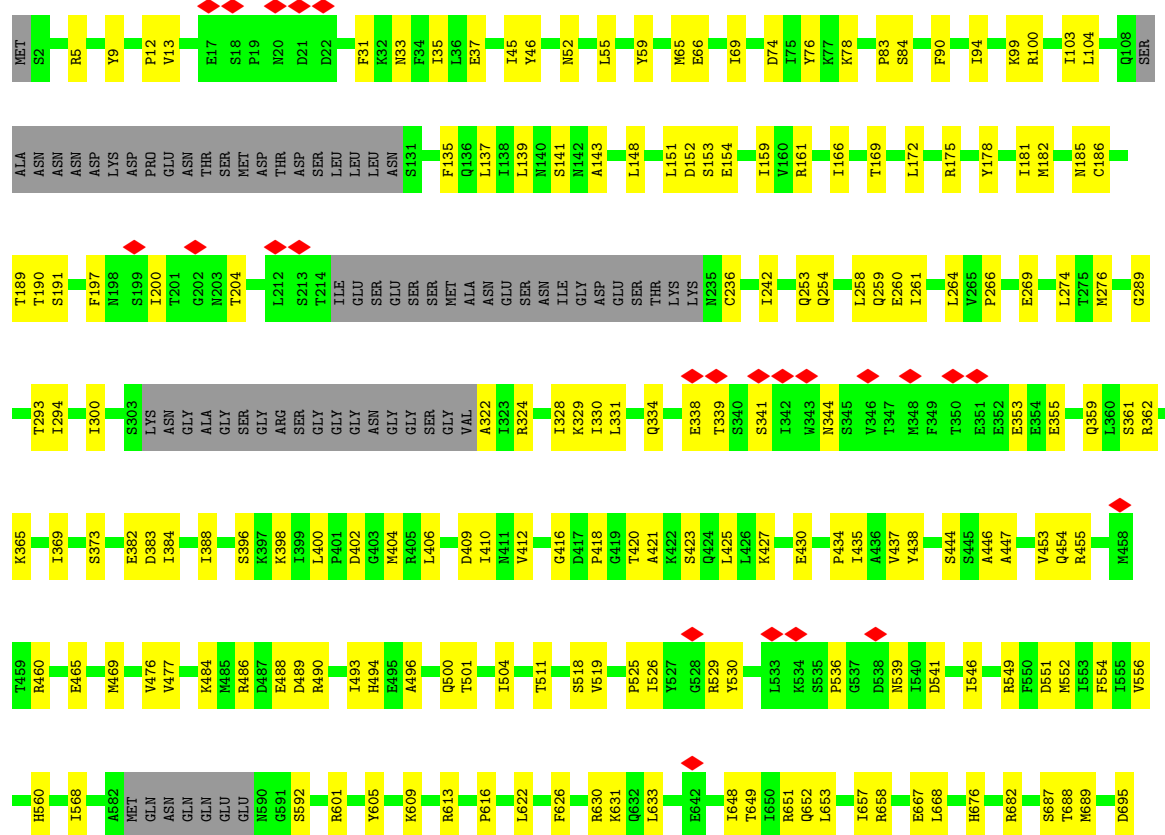


● Molecule 3: DNA replication licensing factor MCM3



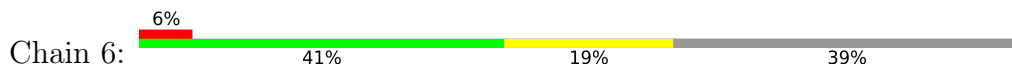


• Molecule 5: Minichromosome maintenance protein 5



GLU	LYS	HIS	GLU	THR	ILE	GLN	LEU	ARG	SER	GLY	GLN	THR	SER	GLN	LEU	ASP	ASP	THR	HIS	ARG	PHE	SER	GLN	LEU	ALA	LEU	ASP	LYS	ALA	LEU	TYR	ALA	LEU																					
P696	ILE	GLY	LEU	ASN	GLN	ALA	SER	GLY	THR	SER	LEU	SER	GLU	ILE	ARG	ARG	PHE	GLY	GLN	GLU	ARG	LEU	PRO	ILE	GLY	THR	SER	THR	TYR	GLN	THR	LEU	ARG	ARG	GLU	PHE	VAL	ASP	THR	HIS	ARG	PHE	SER	GLN	LEU	ALA	LEU	ASP	LYS	ALA	LEU	TYR	ALA	LEU

- Molecule 6: DNA replication licensing factor MCM6



NET	SER	SER	SER	PHE	PRO	ALA	ASP	THR	PRO	SER	SER	SER	ASN	ARG	PRO	PRO	ASN	SER	SER	SER	PRO	PRO	PRO	SER	SER	ILE	GLY	ALA	ALA	PHE	GLY	SER	SER	SER	GLY	LEU	ASP	SER	SER	GLN	ILE	GLY	SER	ARG	LEU	HIS	PHE	PRO	PRO	SER	SER	SER	GLN	PRO	PRO	VAL	SER	GLN	THR	GLY	PRO
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PHE	VAL	ASN	ASP	SER	THR	GLN	PHE	SER	SER	SER	GLN	ARG	LEU	THR	GLN	THR	ASP	GLY	SER	ALA	THR	ASN	ASP	MET	GLU	GLY	ASN	GLU	PRO	ALA	ARG	PHE	LYS	SER	SER	ARG	ALA	LEU	ASN	HIS	VAL	LYS	LYS	VAL	D104	D105	E108	K110	V111	R112	E113	A114	F115	E116	L119	E120	D121	F122	I123
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V124	Q125	S126	L127	D128	T129	G130	E131	E133	K134	V135	R137	A138	Q139	I140	E141	F142	M143	K144	I145	V146	D147	L148	M149	M150	M153	M158	A159	I170	F177	F180	L181	R186	R187	V188	V189	K191	V192	A193	P194	E195	L196	L197	N198	T199	S200	ASP	SER	LEU	LVS	TRC
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SER	GLU	GLY	ASP	GLU	GLN	ALA	ASP	GLU	ASP	GLU	GLN	ASP	ASP	ASP	MET	ASN	GLY	SER	SER	LEU	PRO	ARG	ASP	SER	SER	SER	ALA	ALA	PRO	GLY	ASN	GLY	THR	SER	ALA	MET	MET	ALA	THR	ARG	SER	ILE	THR	THR	THR	SER	SER	PRO	GLU	GLN	T259	E260	R261	V262	F263	I264
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R275	R276	R277	R278	R279	R280		R284		V294		E303	L304	Y385	K306	A307	S308	F309	T310	C311	D312	M313	C314	R315	A316	L317	V318	D319	N320	V321	E322	Q323	S324	F325	K326	Y327	T328	E329	P330	T331	F332	C333	P334		C338	E339	N340	R341	A342	F343	U344	T345	L346		R350	S351	R352		U356	R357
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Protein	Score	Category
E363	0.000000	Protein
N364	0.000000	Protein
E367	0.000000	Protein
I368	0.000000	Protein
G371	0.000000	Protein
P374	0.000000	Protein
V379	0.000000	Protein
E387	0.000000	Protein
R388	0.000000	Protein
A399	0.000000	Protein
K390	0.000000	Protein
D393	0.000000	Protein
E401	0.000000	Protein
D406	0.000000	Protein
V407	0.000000	Protein
T408	0.000000	Protein
Q409	0.000000	Protein
L410	0.000000	Protein
G411	0.000000	Protein
L412	0.000000	Protein
P413	0.000000	Protein
P417	0.000000	Protein
S418	0.000000	Protein
S419	0.000000	Protein
T420	0.000000	Protein
L421	0.000000	Protein
ASP	0.000000	Protein
THR	0.000000	Protein
ARG	0.000000	Protein
GLY	0.000000	Protein
ILE	0.000000	Protein
SER	0.000000	Protein
LYS	0.000000	Protein
THR	0.000000	Protein
THR	0.000000	Protein
GLU	0.000000	Protein
GLY	0.000000	Protein
LEU	0.000000	Protein
ASN	0.000000	Protein
SER	0.000000	Protein
GLY	0.000000	Protein
VAL	0.000000	Protein
THR	0.000000	Protein
GLY	0.000000	Protein
GLY	0.000000	Protein
ARG	0.000000	Protein
S442	0.000000	Protein
L443	0.000000	Protein
G444	0.000000	Protein
L445	0.000000	Protein

Category	Count
L516	100
K517	95
V520	90
K521	85
Y526	80
D527	75
K528	70
R531	65
V537	60
H540	55
K544	50
V555	45
H556	40
K557	35
E561	30
R566	25
D568	20
I571	15
S580	10
K581	5
F584	5
L585	5
V589	5
Y597	5
G600	5
K601	5
A605	5
L608	5
A611	5
G612	5
V613	5
R614	5
D615	5
E616	5
G617	5
G618	5
G619	5
D620	5
Y621	5
T622	5
T623	5

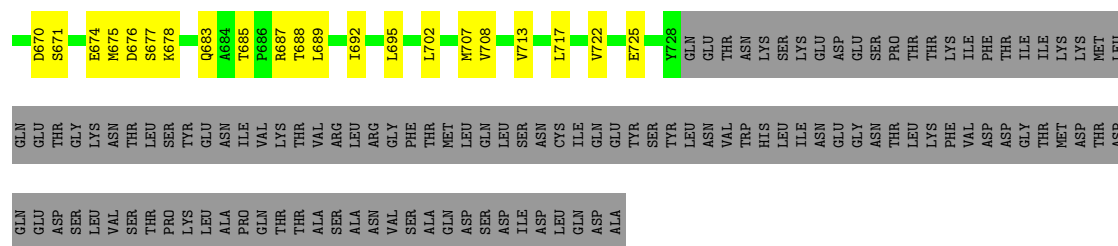
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A627	1
L628	1
M629	1
D632	1
G637	2
L638	2
D639	2
E640	2
M644	1
D648	1
L652	2
H653	2
E654	2
A655	3
M656	3
E657	3
Q658	2
Q659	2
T660	1
L672	2
N673	2
A674	2
R675	2
L695	2
R696	2
L699	2
N700	4
M701	1
I705	2
M706	2
D710	1
L711	1
F712	2
N720	1
I723	1
D724	2
T725	1
M736	1
R759	1
R770	1
V774	1

K76		R781		R782	D783	D784	A785	Q786	GLY	PHE	SER	R790	S791	S792		T796	R797	Q799	L800	E801		L806		N814	C815	V816		F823		Y828	D829	B832		R837	V838	ASP	VAL	ASP	ASP	VAL	GLU	GLU	GLU	PHE	ASP	ASN	TLE	GLU	SER	GLN	SER	HIS	ALA	ALA
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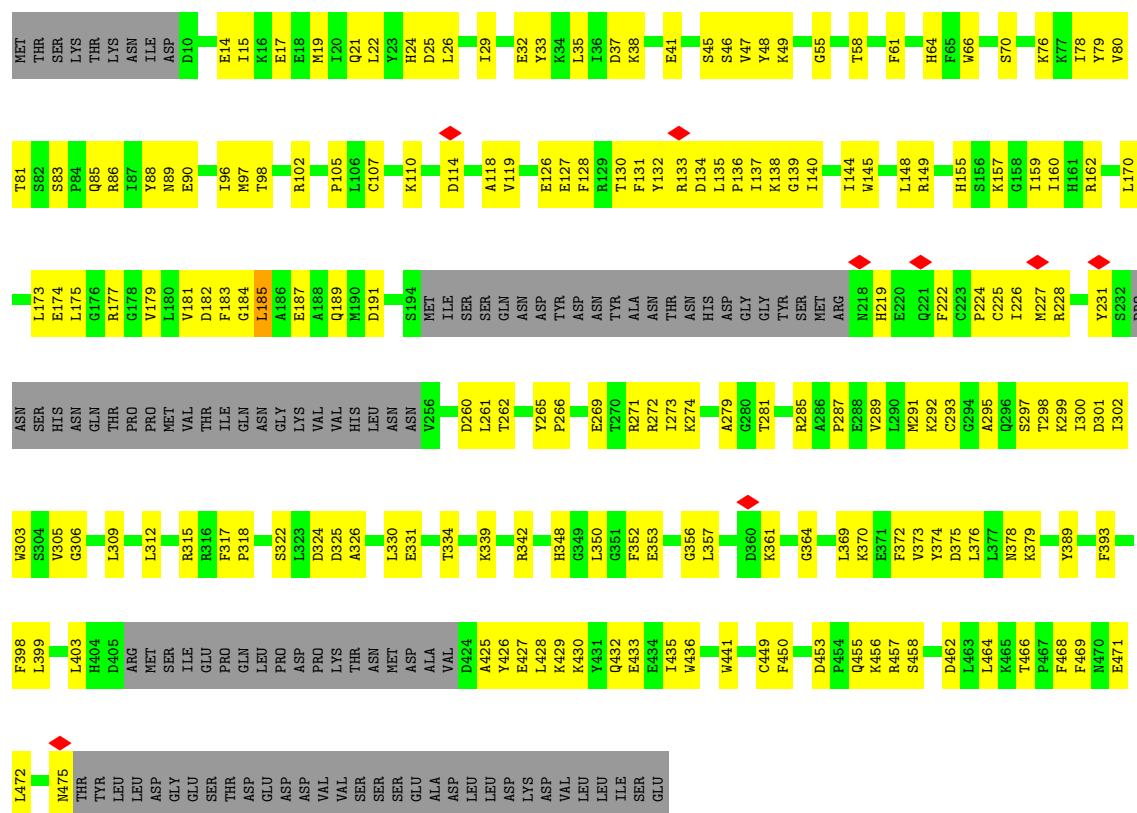
SER.	GLY	ASN	ASN	ASP	ASN	ASP	ASP	GLY	THR	THR	SER.	SER.	GLU	ALA	ALA	ALA	ARG	PRO	PRO	GLY	THR	THR	GLU	LYS	LYS	THR	THR	VAL	THR	THR	Tyr	ASP	LYS	Tyr	VAL	THR	VAL	ILE	VAL	ILE	ALA	ARG	LYS
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[illegible]

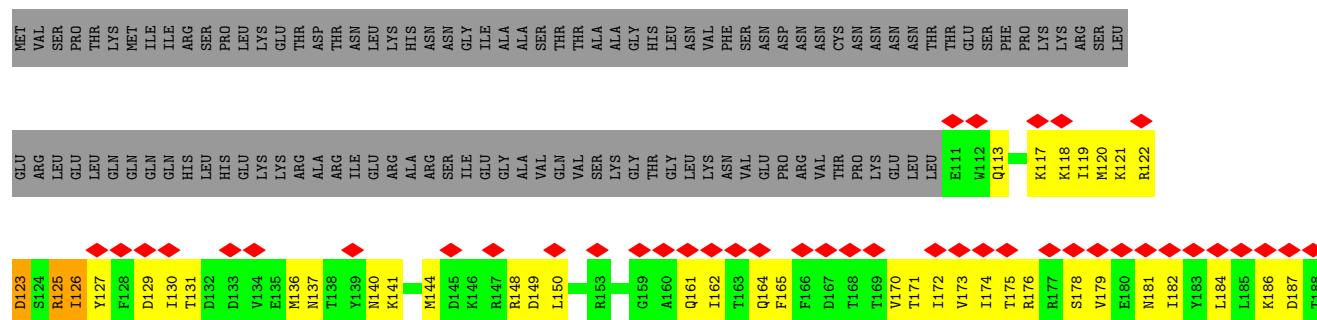
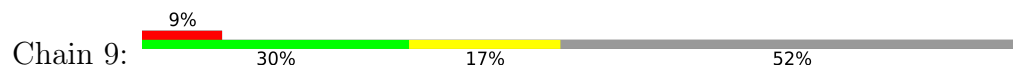
THR	ARG	HIS	ASN	LEU	ARG	ASP	LEU	GLU	ASN	GLU	ASN	GLU	ASN	ASN	LYS	THR	VAL	TYR	VAL	ILE	HIS	PRO	ASN	CYS	GLU	VAL	LEU	ASP	GLN	LEU	GLU	PRO	GLN	ASP	SER	SER
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

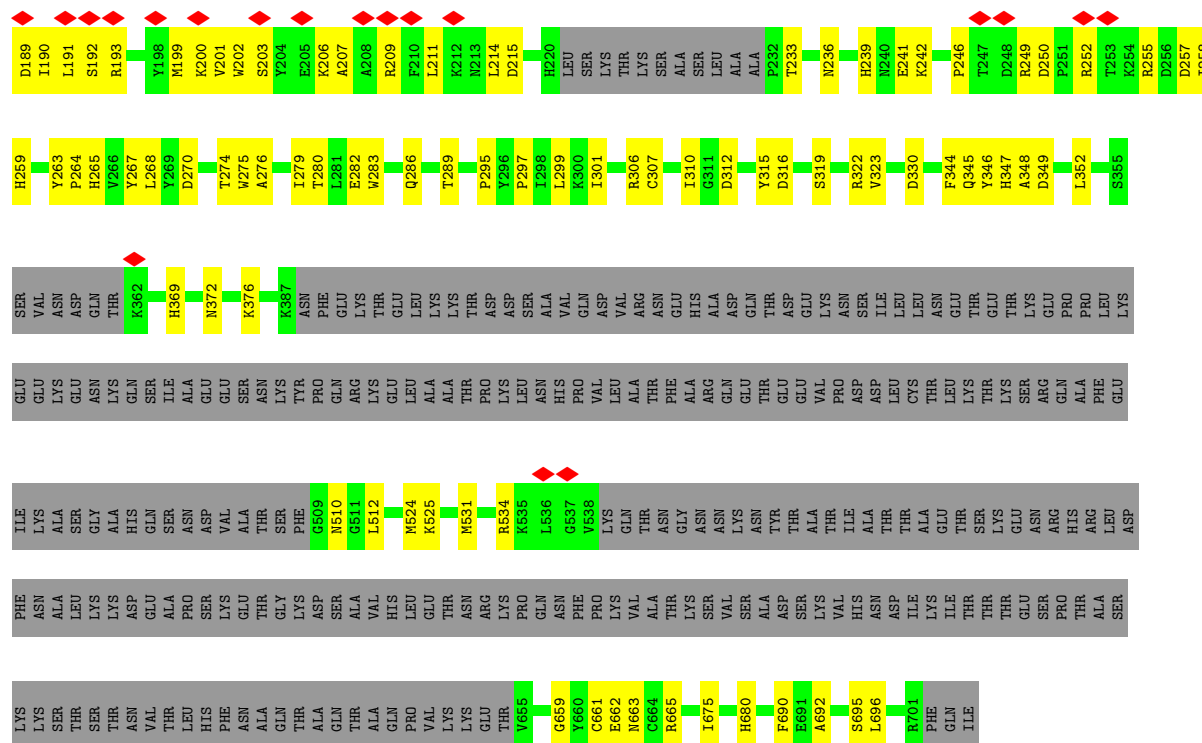


• Molecule 8: Cell division control protein 7



• Molecule 9: DDK kinase regulatory subunit DBF4





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	30807	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 ($e^-/\text{\AA}^2$)	48.4	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	0.086	Depositor
Minimum map value	-0.033	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.014	Depositor
Map size ($\text{\AA}$)	385.92, 385.92, 385.92	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.072, 1.072, 1.072	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BEF, ZN, MG, 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	0.18	0/5046	0.38	1/6817 (0.0%)
2	B	0.17	0/5046	0.35	0/6817
3	3	0.21	0/5073	0.33	1/6878 (0.0%)
3	C	0.28	0/5053	0.39	0/6852
4	4	0.25	0/5401	0.43	1/7302 (0.0%)
4	D	0.21	0/5401	0.35	1/7302 (0.0%)
5	5	0.19	0/5000	0.33	0/6766
5	E	0.19	0/5000	0.34	0/6766
6	6	0.31	0/4968	0.55	3/6704 (0.0%)
6	F	0.26	0/4968	0.49	1/6704 (0.0%)
7	7	0.28	0/5451	0.47	1/7368 (0.0%)
7	G	0.21	0/5451	0.29	0/7368
8	8	0.22	0/3373	0.47	1/4549 (0.0%)
9	9	0.20	0/2872	0.40	0/3864
All	All	0.23	0/68103	0.40	10/92057 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	280	ASP	CB-CA-C	-8.12	107.22	116.63
4	D	601	LEU	N-CA-C	-6.91	101.62	110.53
6	6	515	GLU	N-CA-C	-6.73	103.04	111.11
8	8	183	PHE	N-CA-C	-6.73	103.15	112.30
6	F	752	ARG	N-CA-C	-5.83	104.89	112.23

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	1	20	0	6	0	0
2	2	4960	0	5001	121	0
2	B	4960	0	5002	141	0
3	3	4986	0	5053	111	0
3	C	4966	0	5034	98	0
4	4	5323	0	5387	128	0
4	D	5323	0	5387	130	0
5	5	4927	0	4982	122	0
5	E	4927	0	4982	146	0
6	6	4889	0	4913	134	0
6	F	4889	0	4913	137	0
7	7	5370	0	5426	140	0
7	G	5370	0	5426	101	0
8	8	3292	0	3249	150	0
9	9	2813	0	2821	109	0
10	2	27	0	12	0	0
10	3	27	0	12	3	0
10	4	27	0	12	1	0
10	5	27	0	12	3	0
10	6	27	0	12	2	0
10	7	27	0	12	1	0
10	8	27	0	12	6	0
10	B	27	0	12	3	0
10	C	27	0	12	1	0
10	D	27	0	12	2	0
10	E	27	0	12	2	0
10	F	27	0	12	2	0
10	G	27	0	12	0	0
11	2	1	0	0	0	0
11	3	1	0	0	0	0
11	4	1	0	0	0	0
11	5	1	0	0	0	0
11	6	1	0	0	0	0
11	7	1	0	0	0	0
11	8	2	0	0	0	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	D	1	0	0	0	0
11	E	1	0	0	0	0
11	F	1	0	0	0	0
11	G	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
12	8	1	0	0	0	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
13	3	8	0	0	1	0
13	4	4	0	0	0	0
13	8	4	0	0	0	0
13	D	4	0	0	1	0
13	E	4	0	0	1	0
13	G	4	0	0	0	0
All	All	67420	0	67738	1583	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 1583 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)
3:C:519:VAL:HG21	3:C:534:ALA:CB	1.72	1.16
3:C:519:VAL:HG21	3:C:534:ALA:HB2	1.34	1.09
4:4:519:TYR:CD1	4:4:811:MET:HE1	1.88	1.07
4:4:519:TYR:HD1	4:4:811:MET:HE1	1.14	1.06
4:4:609:VAL:CG1	7:7:506:MET:HG2	1.88	1.03

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	618/868 (71%)	596 (96%)	22 (4%)	0	100	100
2	B	618/868 (71%)	594 (96%)	24 (4%)	0	100	100
3	3	621/971 (64%)	601 (97%)	20 (3%)	0	100	100
3	C	619/971 (64%)	595 (96%)	24 (4%)	0	100	100
4	4	664/933 (71%)	639 (96%)	25 (4%)	0	100	100
4	D	664/933 (71%)	645 (97%)	19 (3%)	0	100	100
5	5	618/775 (80%)	604 (98%)	14 (2%)	0	100	100
5	E	618/775 (80%)	598 (97%)	20 (3%)	0	100	100
6	6	607/1017 (60%)	589 (97%)	18 (3%)	0	100	100
6	F	607/1017 (60%)	588 (97%)	19 (3%)	0	100	100
7	7	675/845 (80%)	655 (97%)	20 (3%)	0	100	100
7	G	675/845 (80%)	652 (97%)	23 (3%)	0	100	100
8	8	394/507 (78%)	381 (97%)	13 (3%)	0	100	100
9	9	327/704 (46%)	312 (95%)	15 (5%)	0	100	100
All	All	8325/12029 (69%)	8049 (97%)	276 (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	551/770 (72%)	550 (100%)	1 (0%)	87	87
2	B	551/770 (72%)	550 (100%)	1 (0%)	87	87
3	3	550/835 (66%)	548 (100%)	2 (0%)	84	83
3	C	548/835 (66%)	548 (100%)	0	100	100
4	4	607/848 (72%)	602 (99%)	5 (1%)	73	76
4	D	607/848 (72%)	607 (100%)	0	100	100
5	5	564/688 (82%)	562 (100%)	2 (0%)	84	83
5	E	564/688 (82%)	564 (100%)	0	100	100
6	6	541/886 (61%)	528 (98%)	13 (2%)	43	62
6	F	541/886 (61%)	532 (98%)	9 (2%)	53	67
7	7	603/753 (80%)	595 (99%)	8 (1%)	61	71
7	G	603/753 (80%)	603 (100%)	0	100	100
8	8	356/454 (78%)	353 (99%)	3 (1%)	73	76
9	9	313/639 (49%)	309 (99%)	4 (1%)	61	71
All	All	7499/10653 (70%)	7451 (99%)	48 (1%)	76	79

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	7	686	PRO
9	9	123	ASP
7	7	689	LEU
8	8	174	GLU
9	9	126	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	499	GLN
5	E	561	ASN
6	F	700	ASN
6	6	540	HIS
6	6	514	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 46 ligands modelled in this entry, 26 are monoatomic - leaving 20 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	$\# Z > 2$
13	BEF	E	801	10	0,3,3	-	-	-		
13	BEF	G	1103	10	0,3,3	-	-	-		
13	BEF	3	1002	10	0,3,3	-	-	-		
10	ADP	4	1102	11,13	28,29,29	0.49	0	43,45,45	0.50	0
10	ADP	3	1001	11,13	28,29,29	0.53	0	43,45,45	0.47	0
10	ADP	F	1101	11	28,29,29	3.22	16 (57%)	43,45,45	2.24	11 (25%)
13	BEF	4	1103	10	0,3,3	-	-	-		
13	BEF	3	1004	10	0,3,3	-	-	-		
13	BEF	D	1103	10	0,3,3	-	-	-		
10	ADP	5	801	11	28,29,29	0.53	0	43,45,45	0.42	0
10	ADP	D	1102	11,13	28,29,29	0.49	0	43,45,45	0.50	0
10	ADP	7	1102	11,13	28,29,29	0.49	0	43,45,45	0.48	0
10	ADP	C	1001	11,13	28,29,29	0.54	0	43,45,45	0.47	0
13	BEF	8	1003	10	0,3,3	-	-	-		
10	ADP	8	1001	11,13	28,29,29	0.49	0	43,45,45	0.48	0
10	ADP	6	1101	11	28,29,29	3.22	16 (57%)	43,45,45	2.25	11 (25%)
10	ADP	2	901	11	28,29,29	0.49	0	43,45,45	0.51	0
10	ADP	G	1102	11,13	28,29,29	0.50	0	43,45,45	0.48	0
10	ADP	E	802	11	28,29,29	0.49	0	43,45,45	0.53	0
10	ADP	B	901	11	28,29,29	0.52	0	43,45,45	0.46	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
10	ADP	7	1102	11,13	-	8/16/32/32	0/3/3/3
10	ADP	C	1001	11,13	-	4/16/32/32	0/3/3/3
10	ADP	G	1102	11,13	-	8/16/32/32	0/3/3/3
10	ADP	8	1001	11,13	-	1/16/32/32	0/3/3/3
10	ADP	4	1102	11,13	-	2/16/32/32	0/3/3/3
10	ADP	3	1001	11,13	-	4/16/32/32	0/3/3/3
10	ADP	E	802	11	-	3/16/32/32	0/3/3/3
10	ADP	5	801	11	-	4/16/32/32	0/3/3/3
10	ADP	6	1101	11	-	4/16/32/32	0/3/3/3
10	ADP	B	901	11	-	6/16/32/32	0/3/3/3
10	ADP	F	1101	11	-	4/16/32/32	0/3/3/3
10	ADP	2	901	11	-	4/16/32/32	0/3/3/3
10	ADP	D	1102	11,13	-	2/16/32/32	0/3/3/3

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	6	1101	ADP	C2'-C3'	-10.04	1.26	1.53
10	F	1101	ADP	C2'-C3'	-10.02	1.26	1.53
10	F	1101	ADP	C6-N6	6.37	1.50	1.34
10	6	1101	ADP	C6-N6	6.36	1.50	1.34
10	F	1101	ADP	C5'-C4'	-4.67	1.37	1.51

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	6	1101	ADP	N3-C2-N1	-5.66	120.02	128.58
10	F	1101	ADP	N3-C2-N1	-5.64	120.05	128.58
10	6	1101	ADP	N9-C8-N7	-5.25	106.48	113.94
10	F	1101	ADP	N9-C8-N7	-5.24	106.50	113.94
10	F	1101	ADP	N6-C6-N1	-5.21	106.78	118.38

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

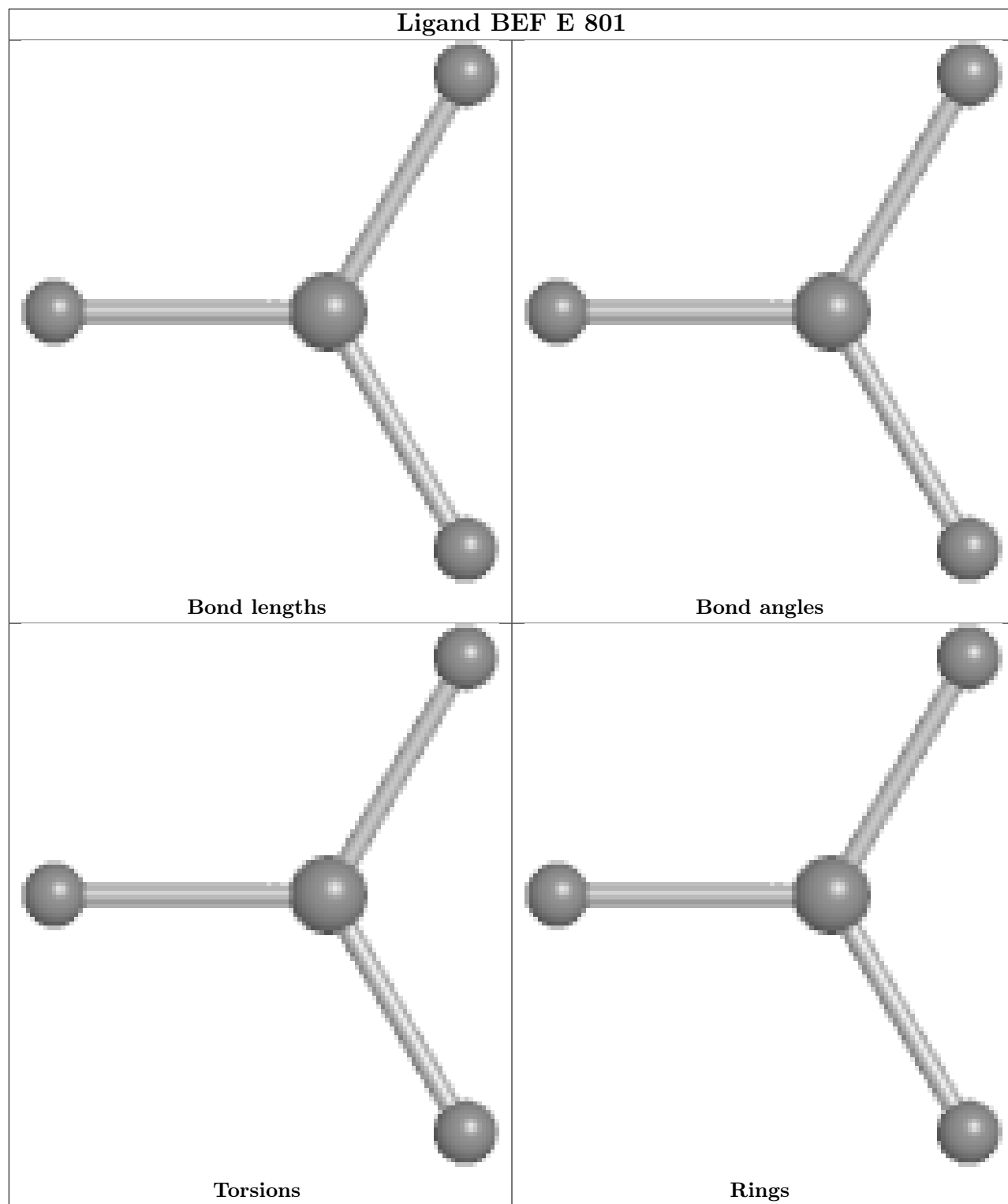
Mol	Chain	Res	Type	Atoms
10	2	901	ADP	PA-O3A-PB-O2B
10	2	901	ADP	PA-O3A-PB-O3B
10	2	901	ADP	C5'-O5'-PA-O2A
10	2	901	ADP	C5'-O5'-PA-O3A
10	3	1001	ADP	PA-O3A-PB-O2B

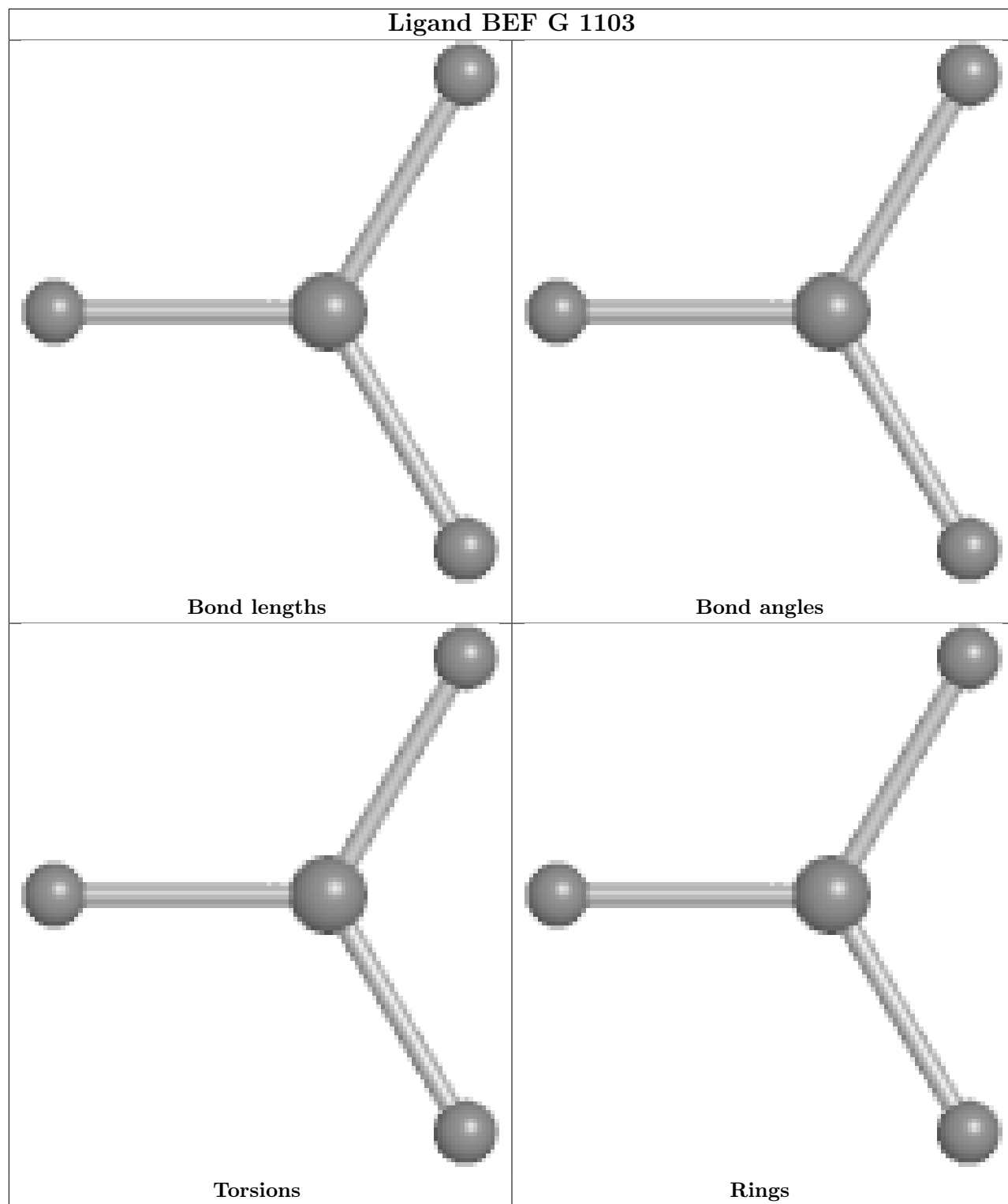
There are no ring outliers.

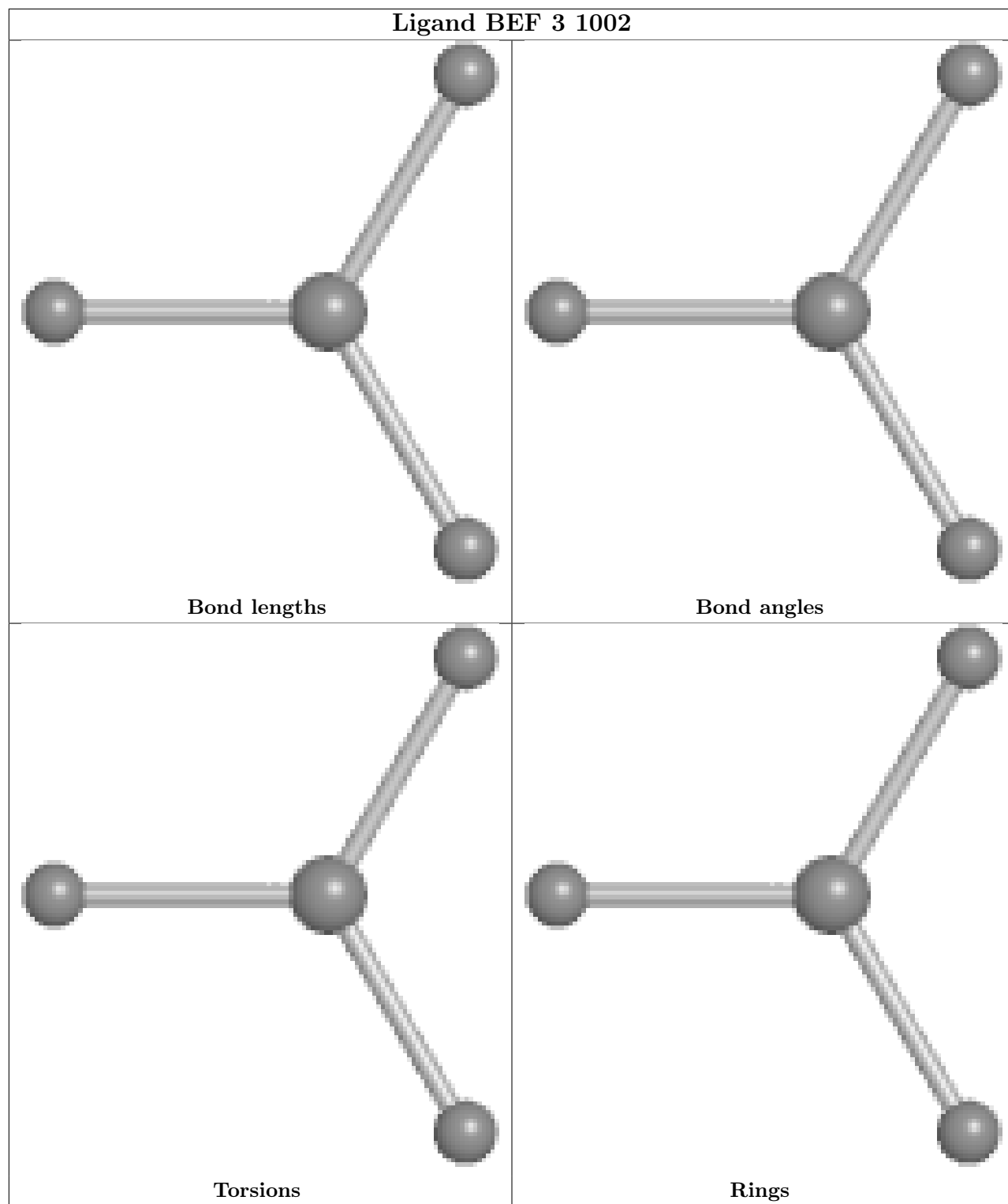
14 monomers are involved in 29 short contacts:

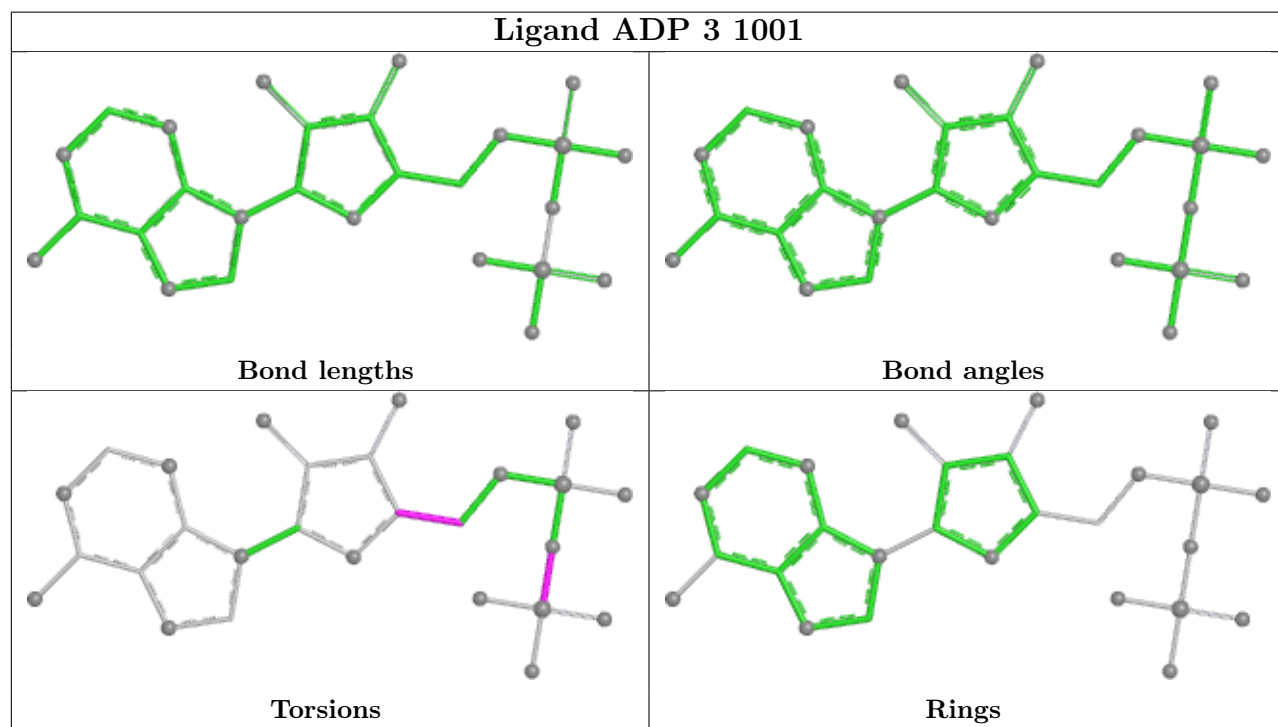
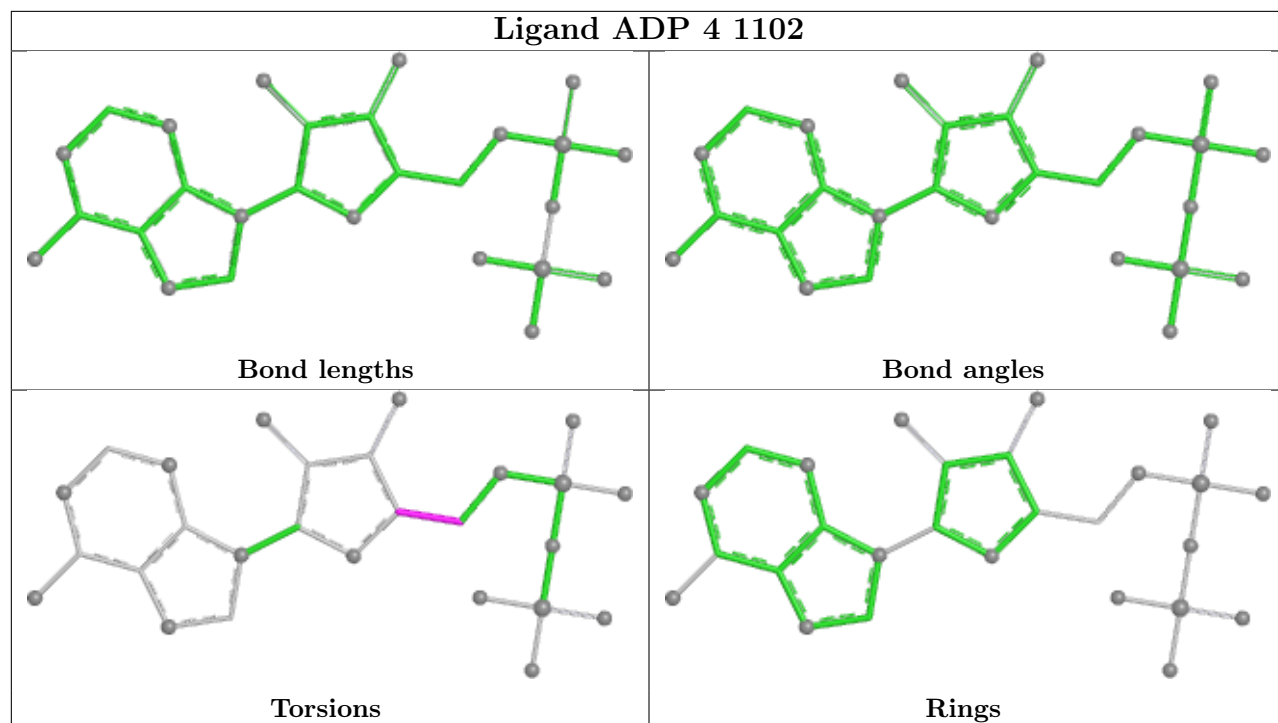
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	E	801	BEF	1	0
13	3	1002	BEF	1	0
10	4	1102	ADP	1	0
10	3	1001	ADP	3	0
10	F	1101	ADP	2	0
13	D	1103	BEF	1	0
10	5	801	ADP	3	0
10	D	1102	ADP	2	0
10	7	1102	ADP	1	0
10	C	1001	ADP	1	0
10	8	1001	ADP	6	0
10	6	1101	ADP	2	0
10	E	802	ADP	2	0
10	B	901	ADP	3	0

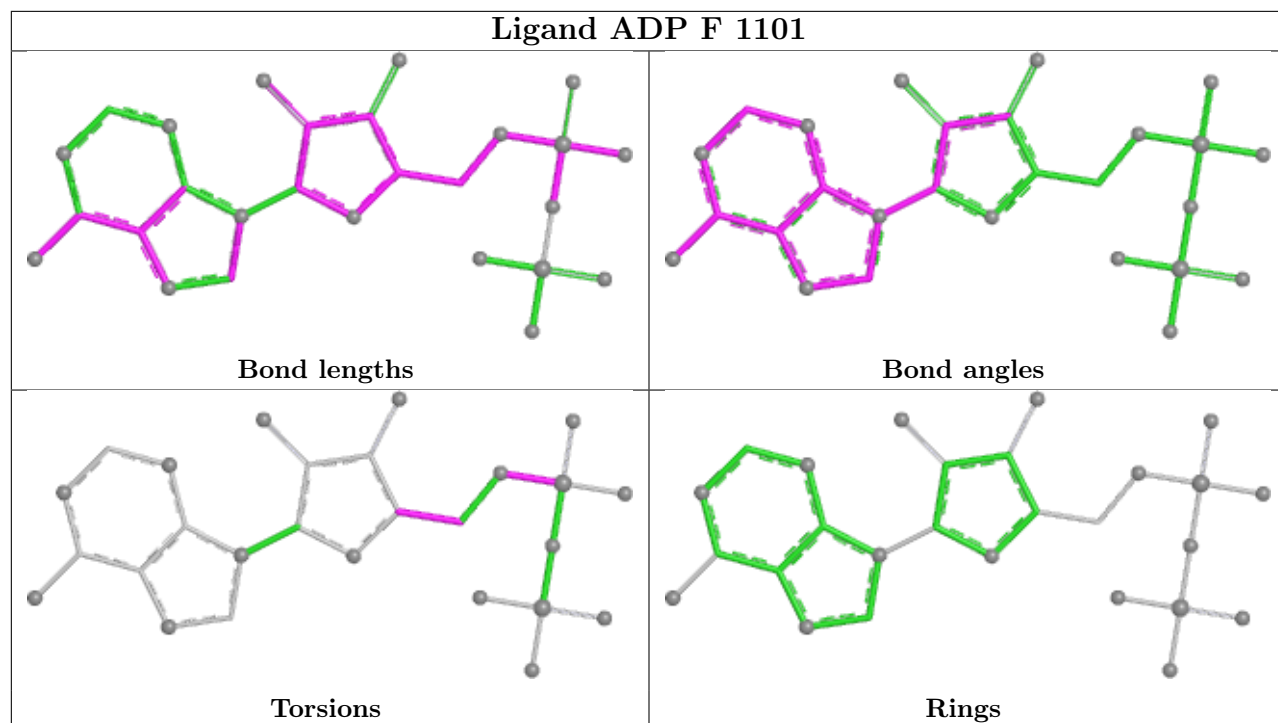
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

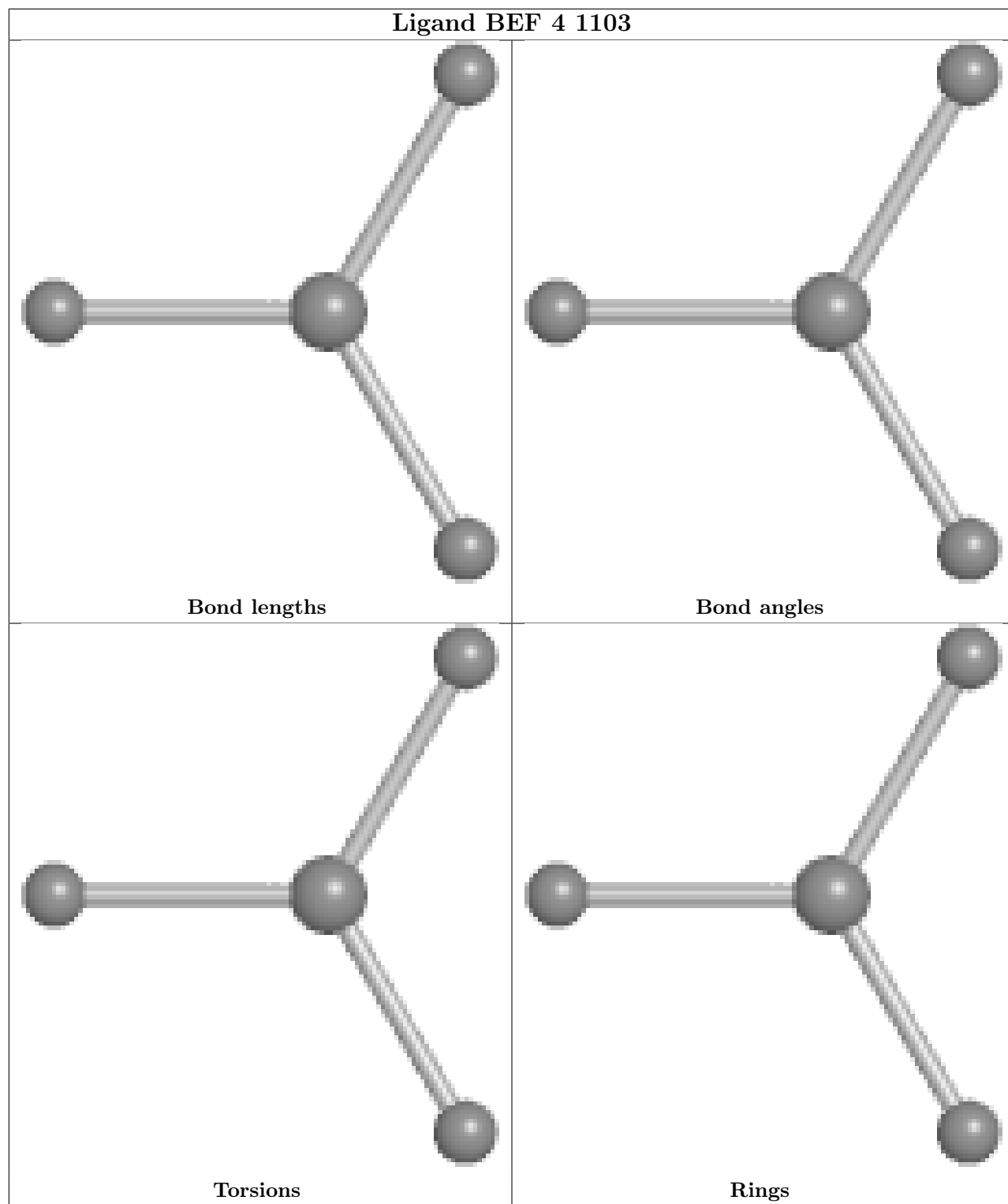


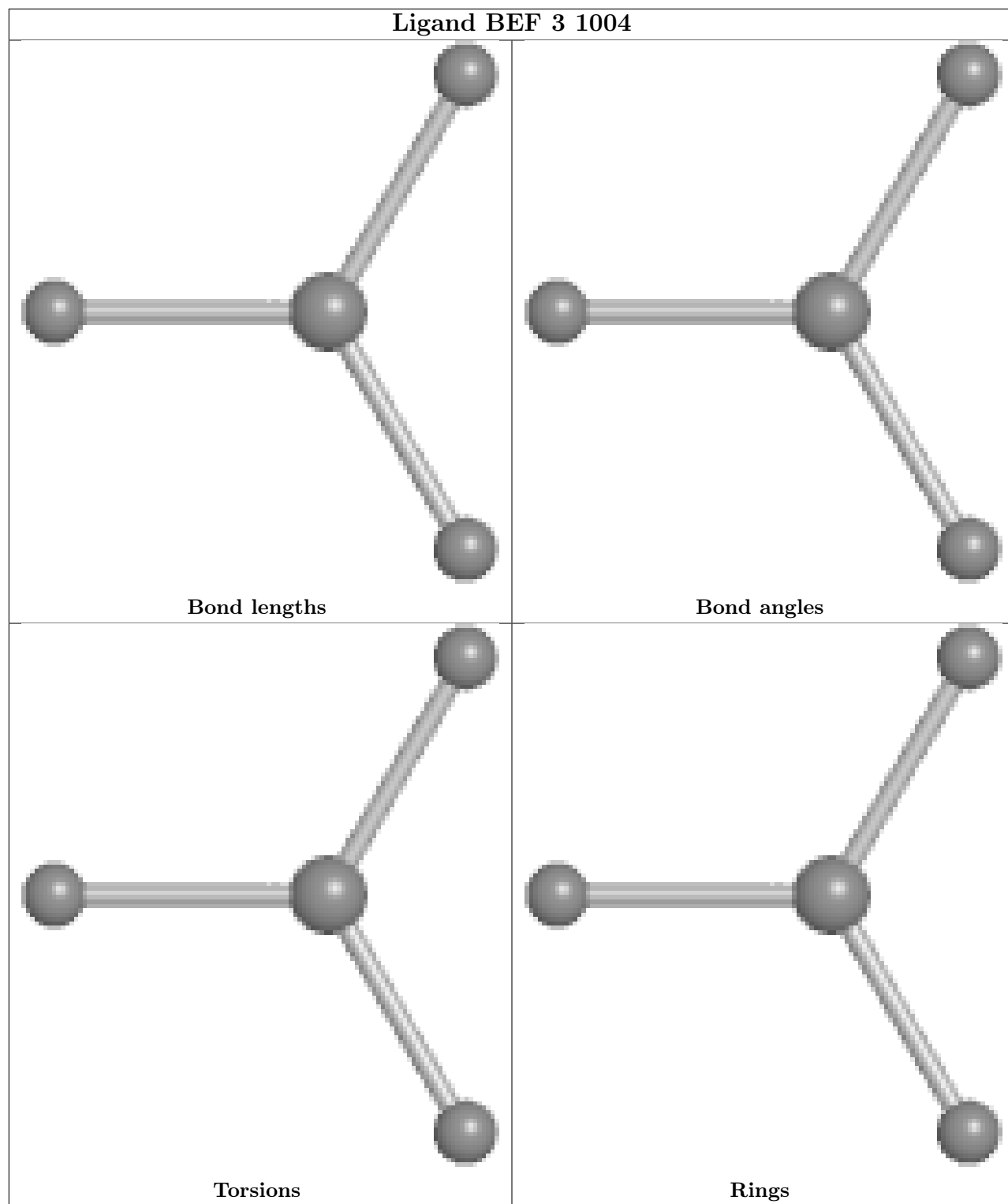


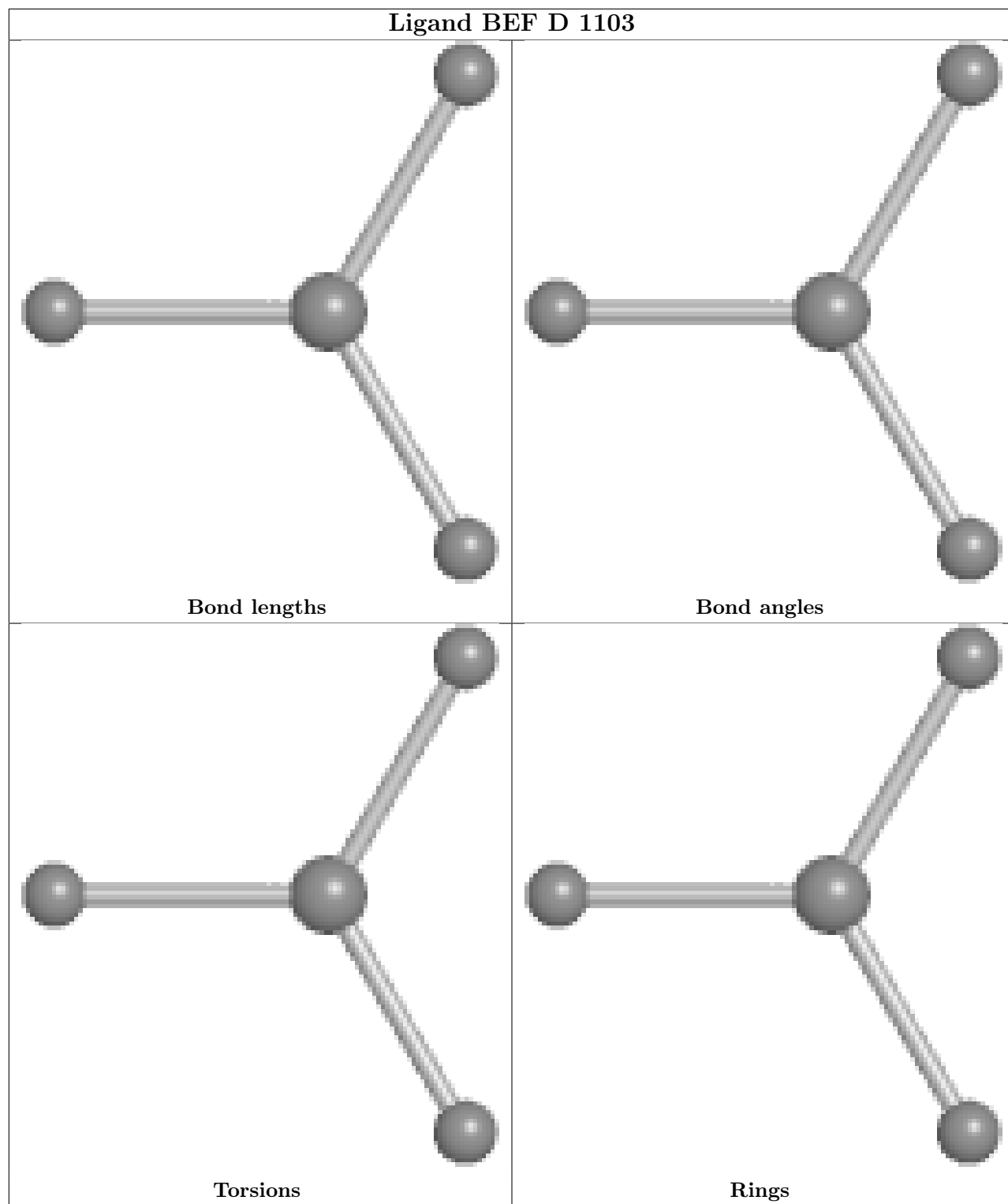


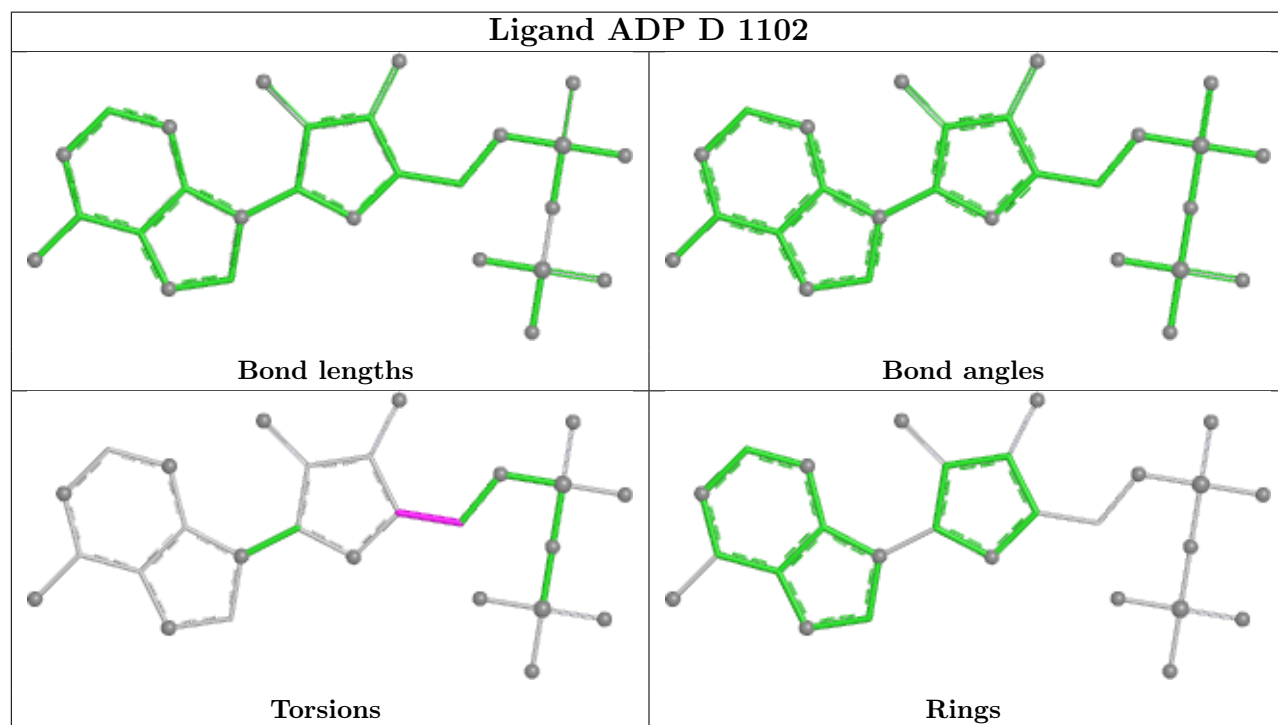
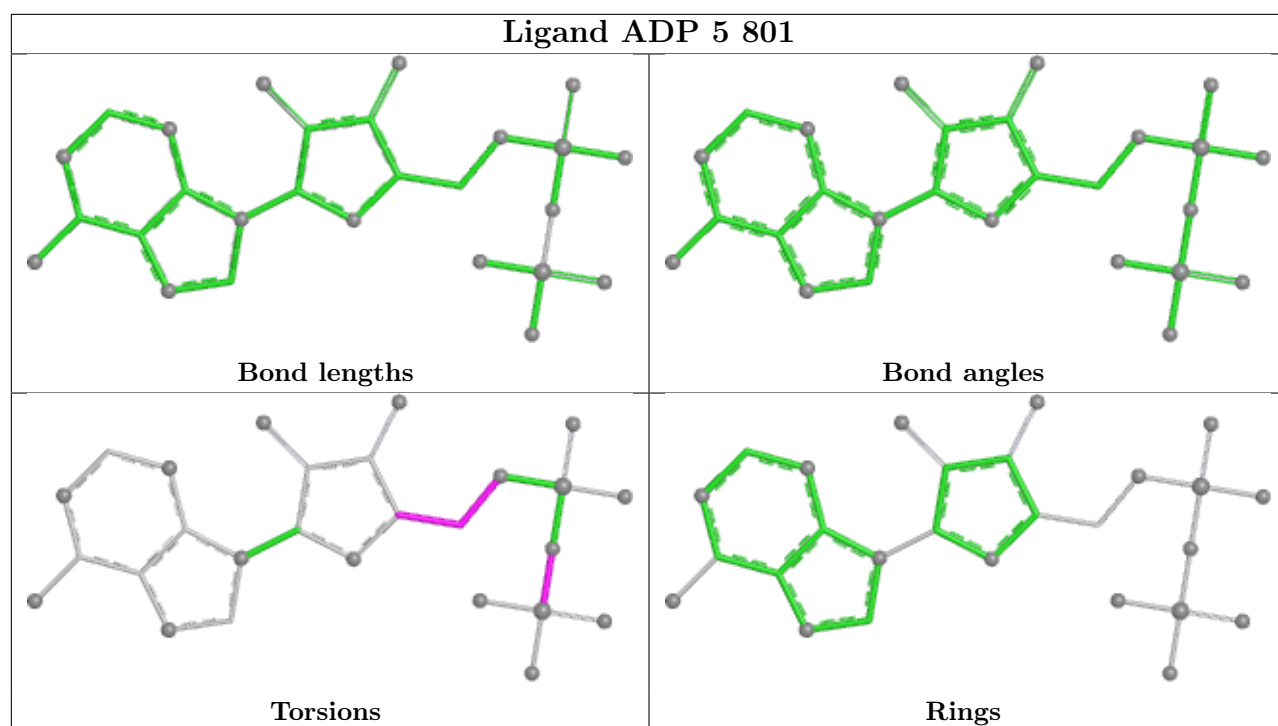


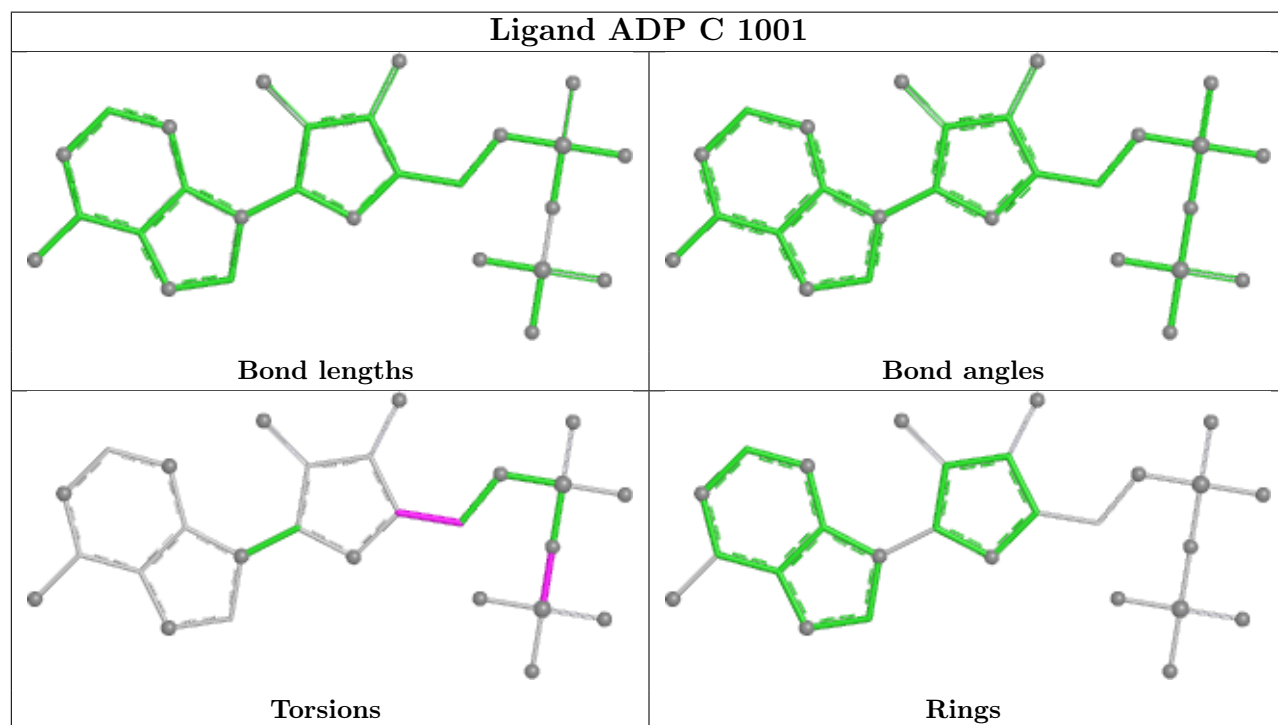
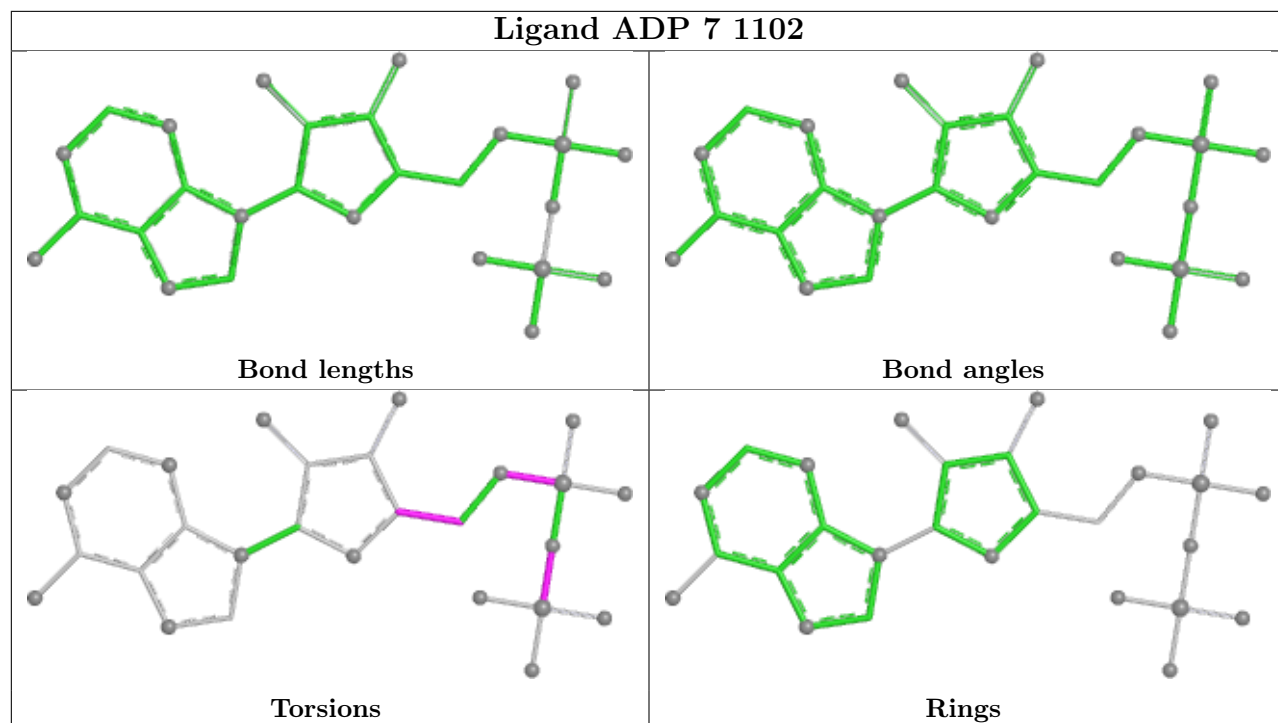


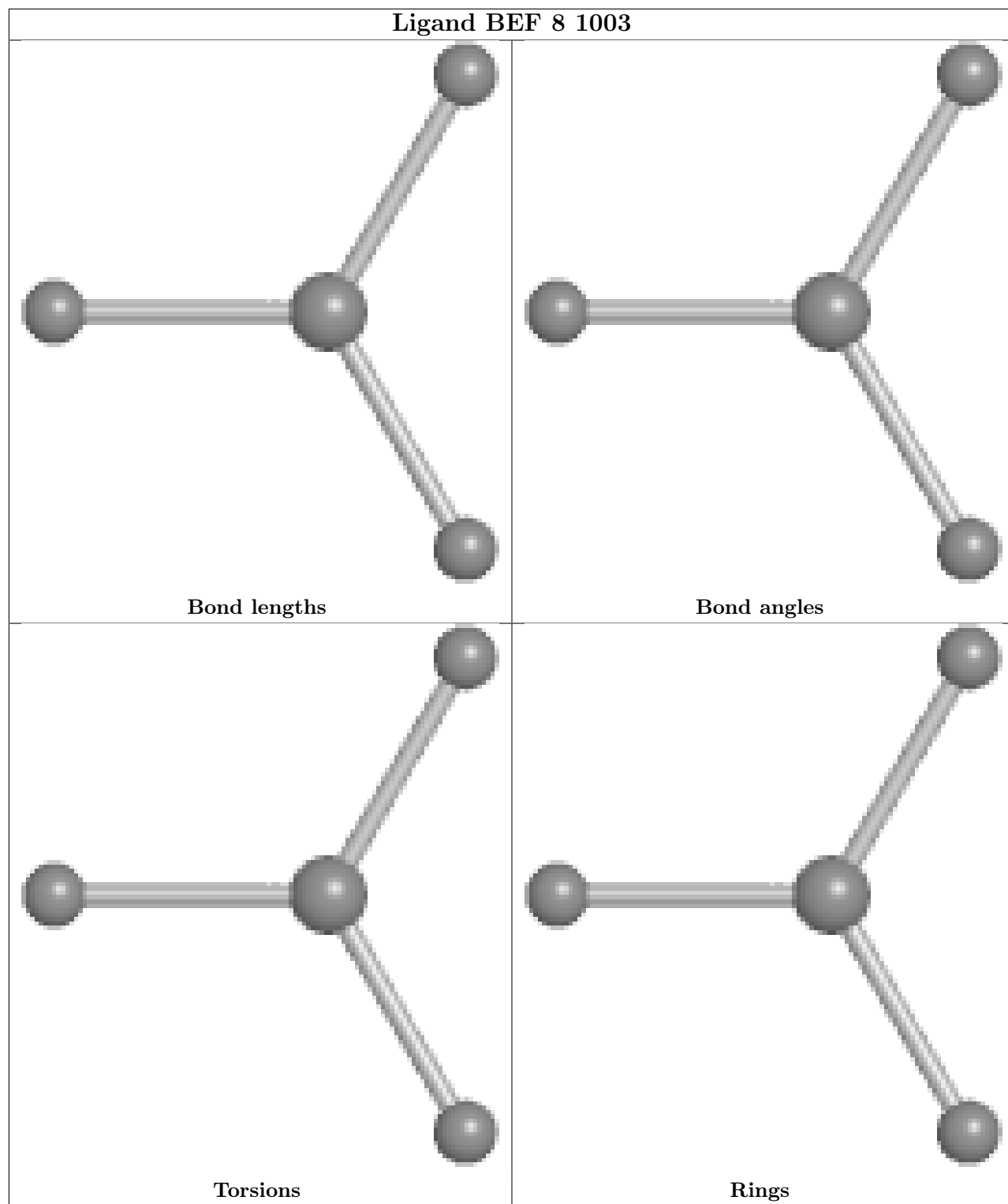


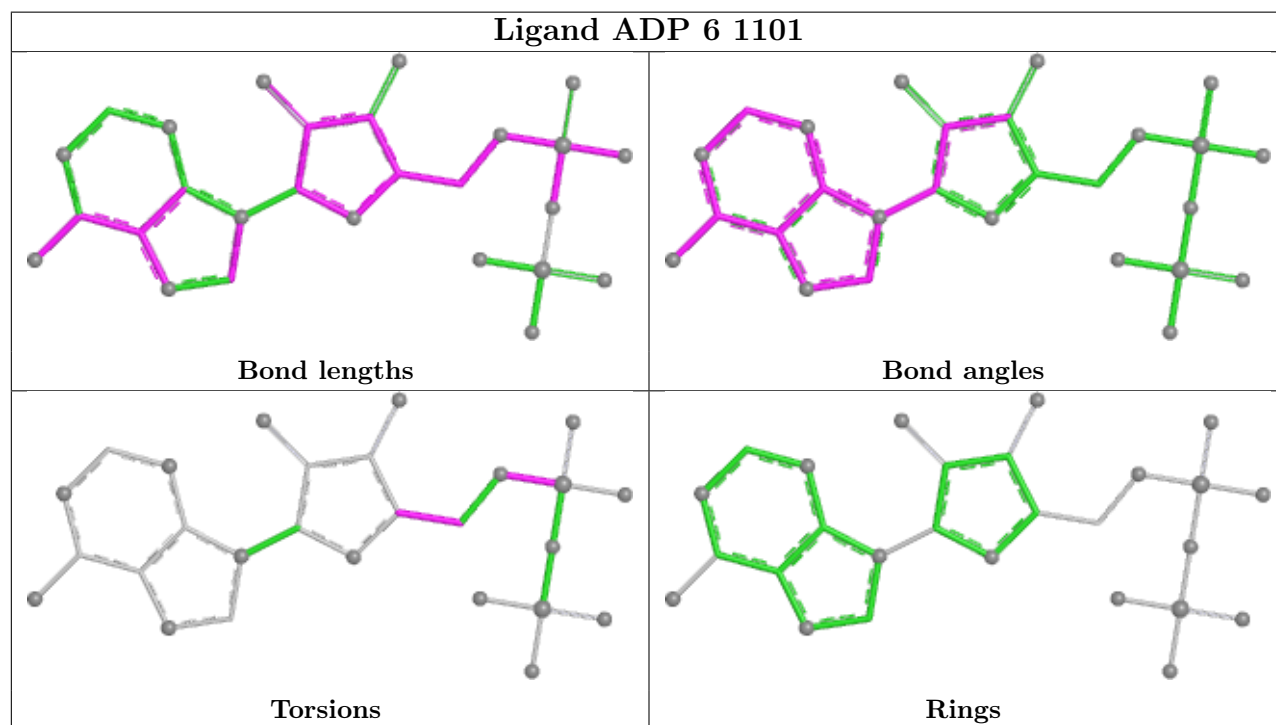
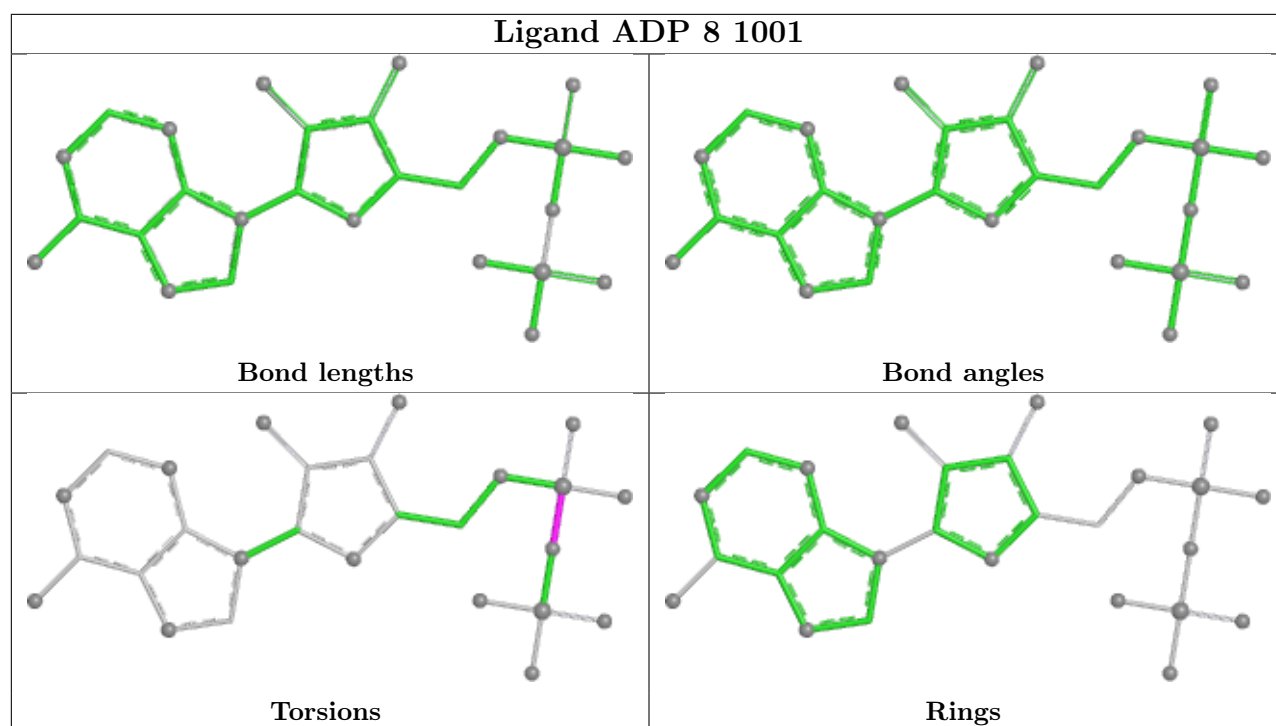


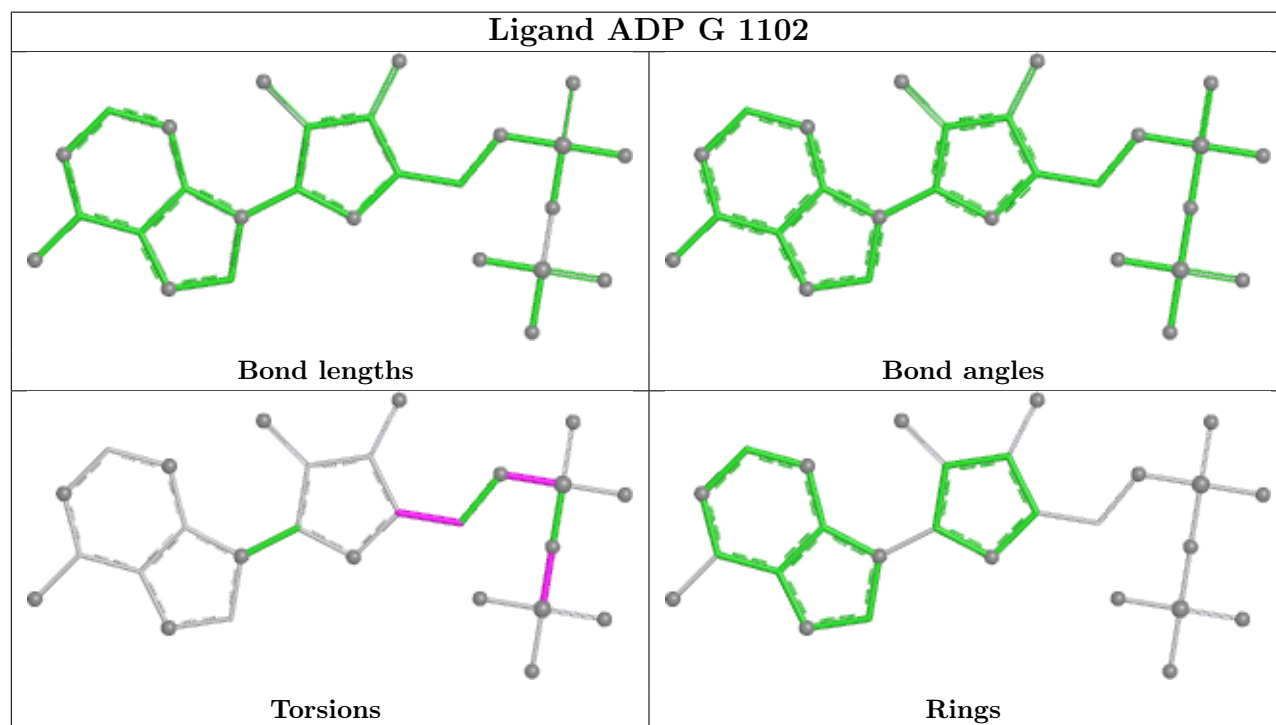
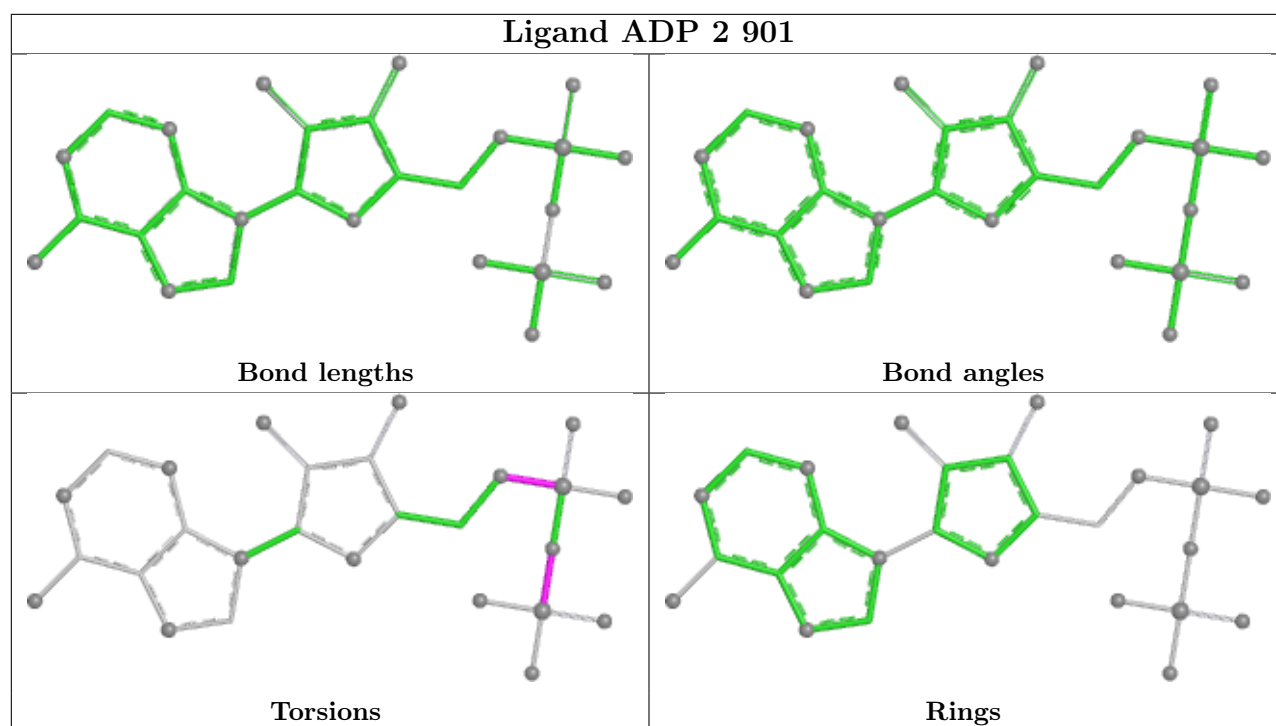


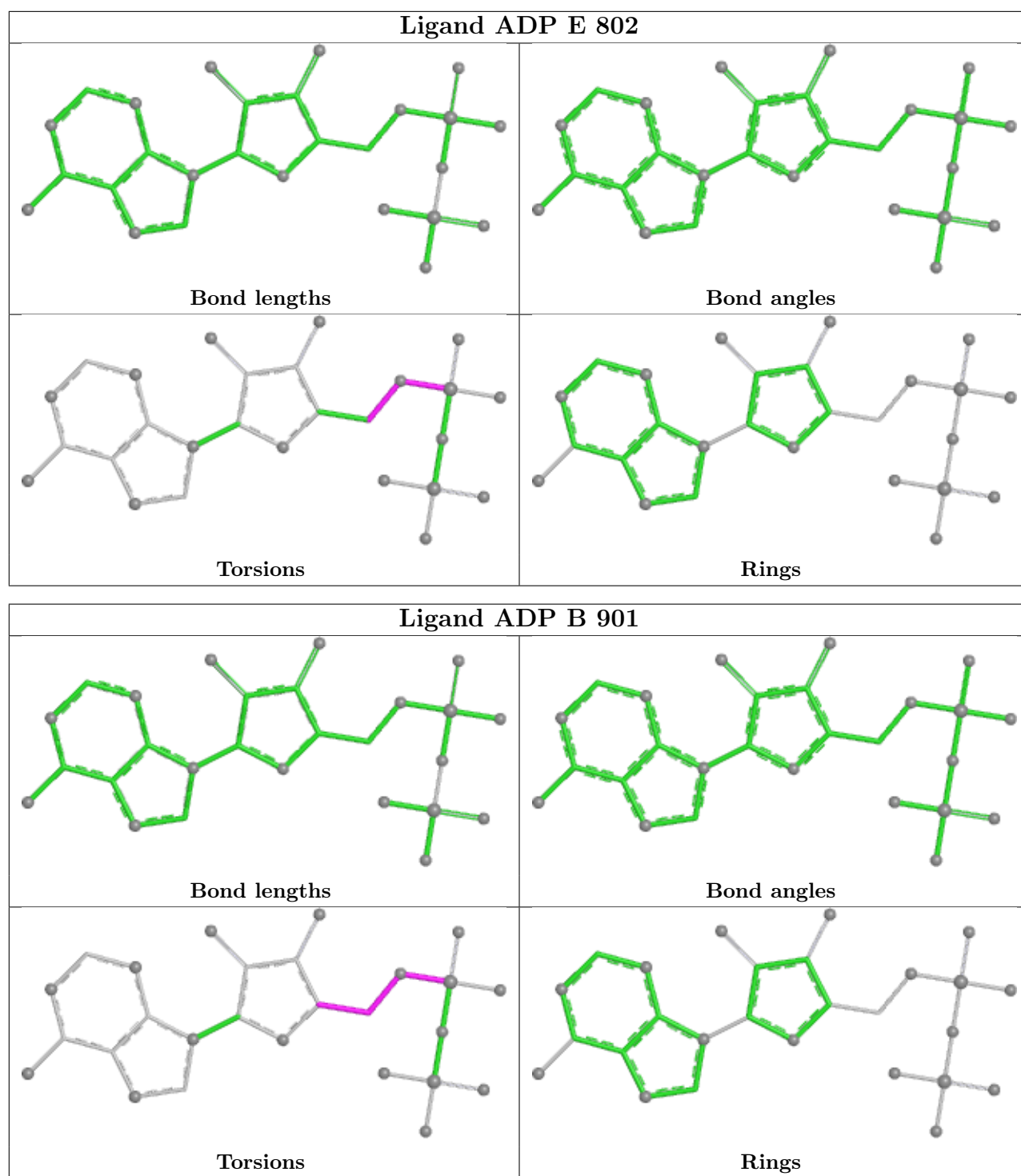












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

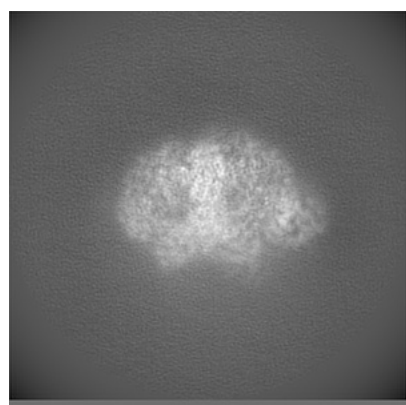
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13620. These allow visual inspection of the internal detail of the map and identification of artifacts.

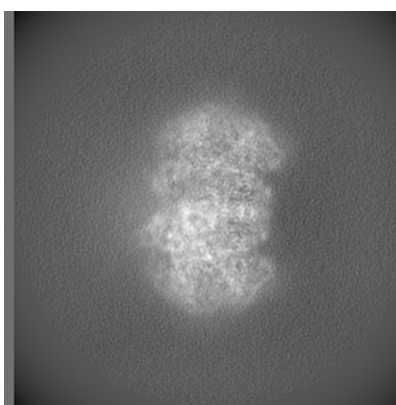
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

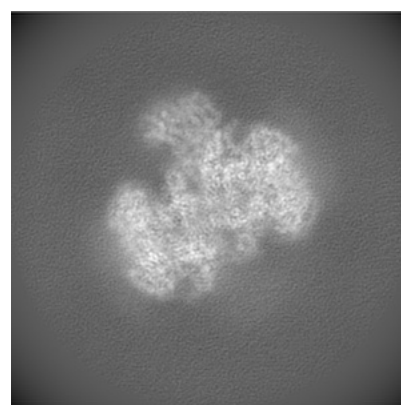
6.1.1 Primary map



X



Y

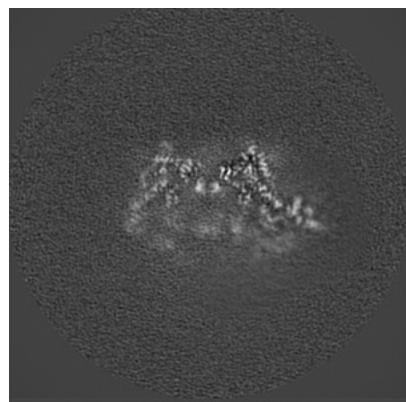


Z

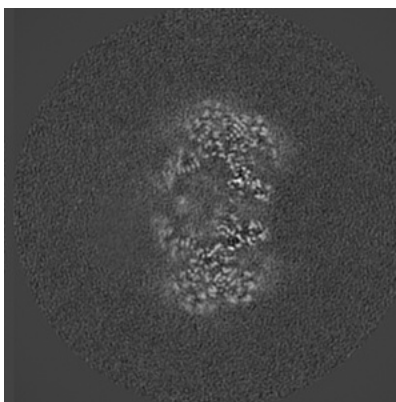
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

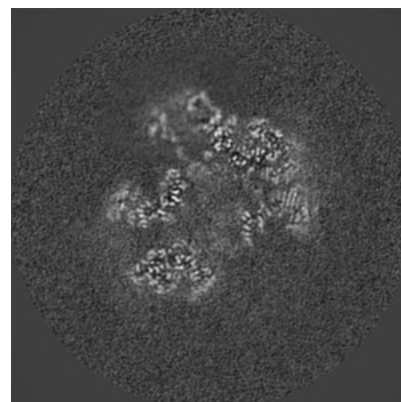
6.2.1 Primary map



X Index: 180



Y Index: 180

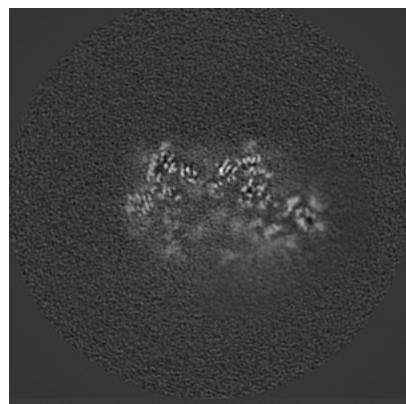


Z Index: 180

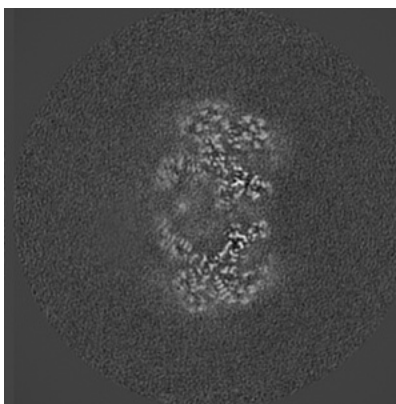
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

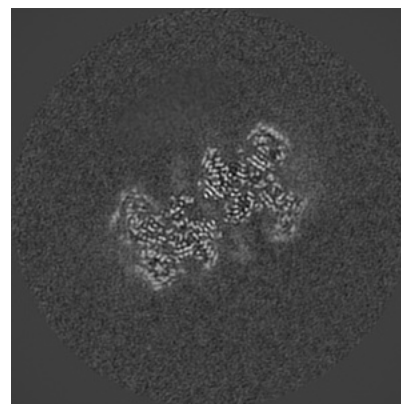
6.3.1 Primary map



X Index: 175



Y Index: 176

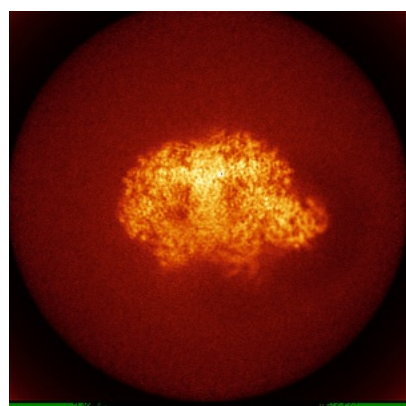


Z Index: 214

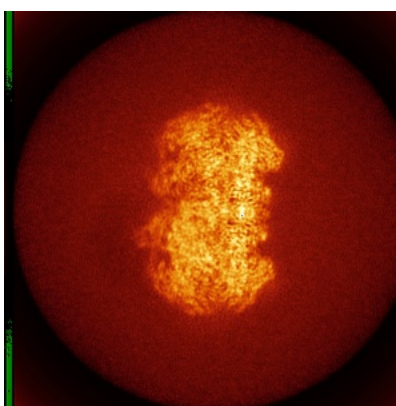
The images above show the largest variance slices of the map in three orthogonal directions.

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

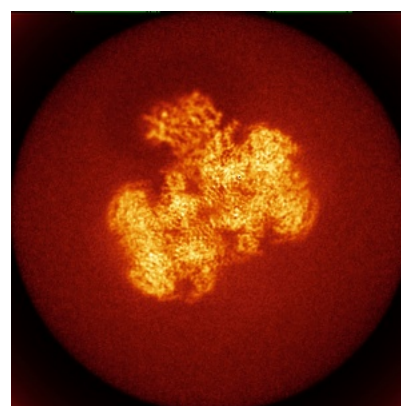
6.4.1 Primary map



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

This section was not generated.

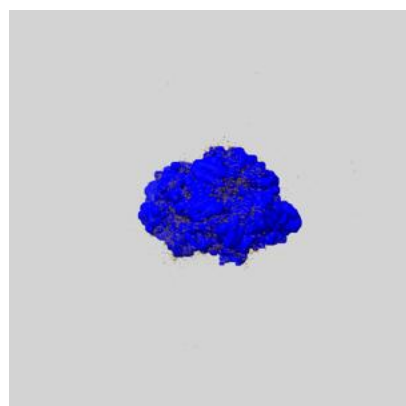
6.6 Mask visualisation [i](#)

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

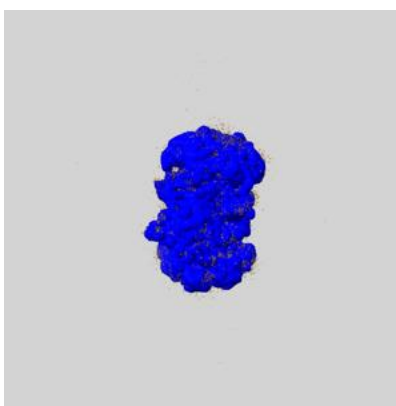
A mask typically either:

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

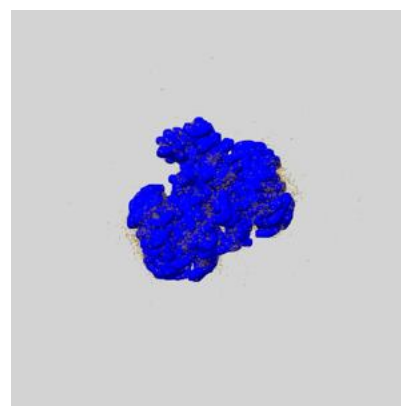
6.6.1 emd_13620_msk_1.map [i](#)



X



Y

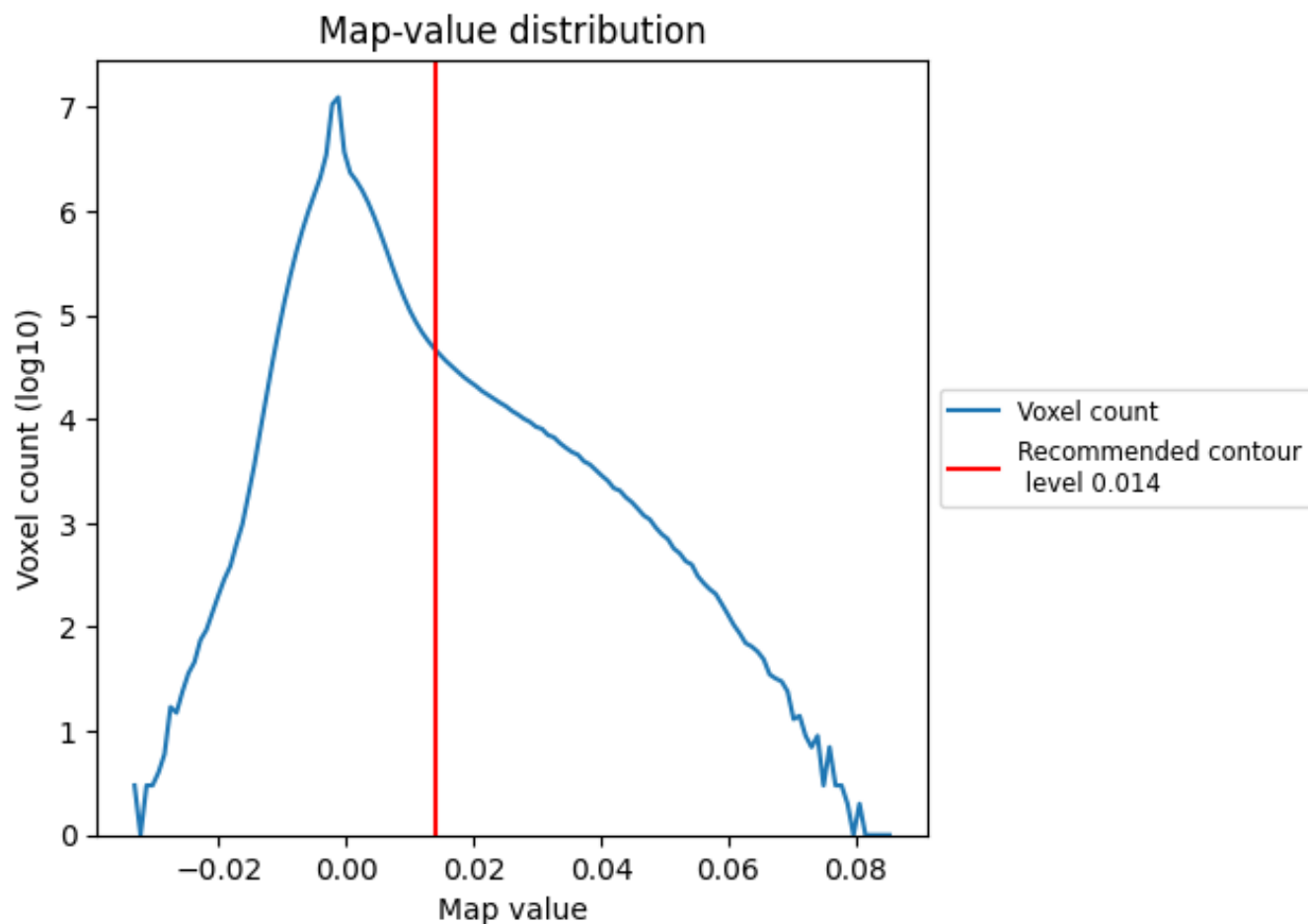


Z

7 Map analysis [i](#)

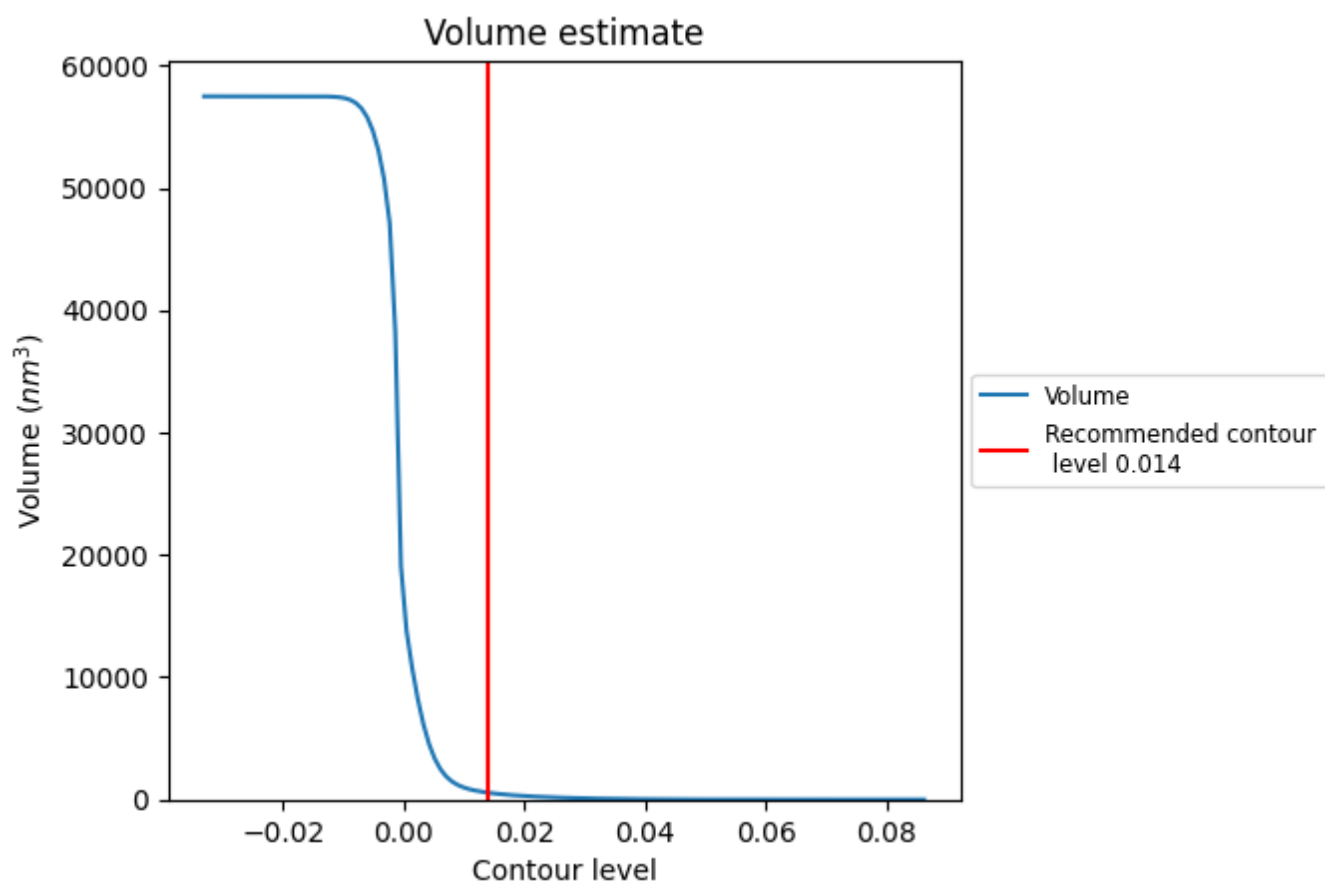
This section contains the results of statistical analysis of the map.

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.

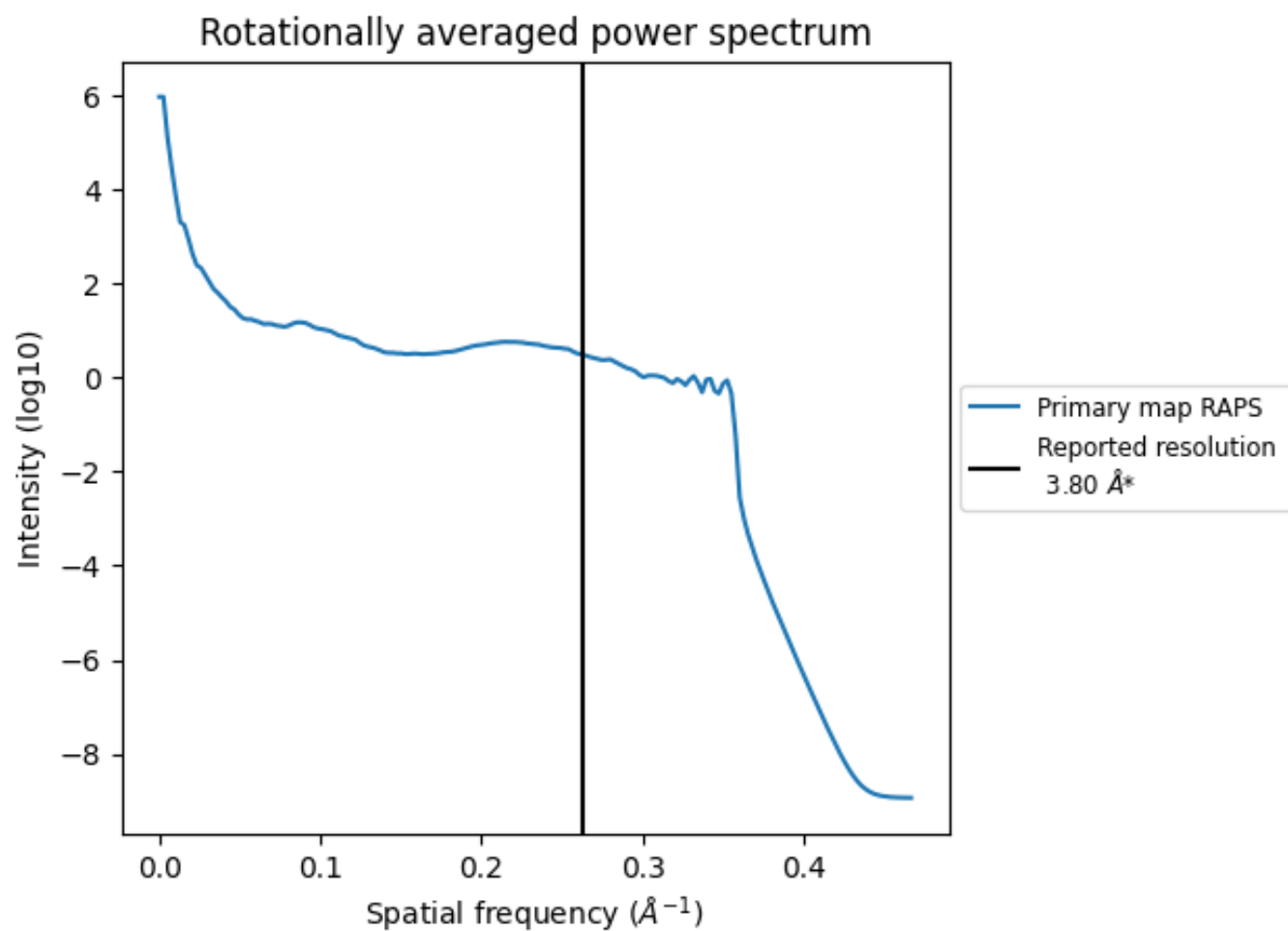
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 557 nm³; this corresponds to an approximate mass of 504 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 0.263 Å⁻¹

8 Fourier-Shell correlation

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

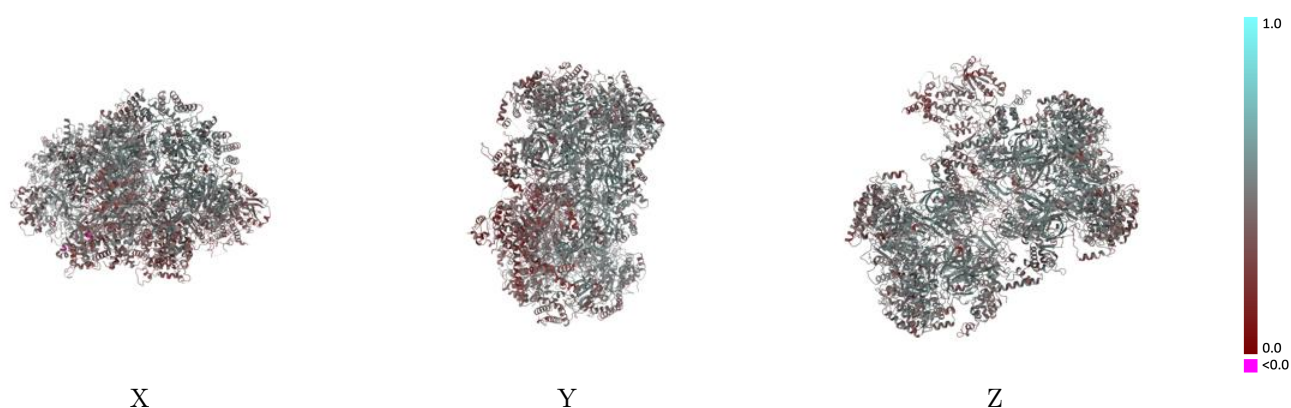
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13620 and PDB model 7PT7. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)

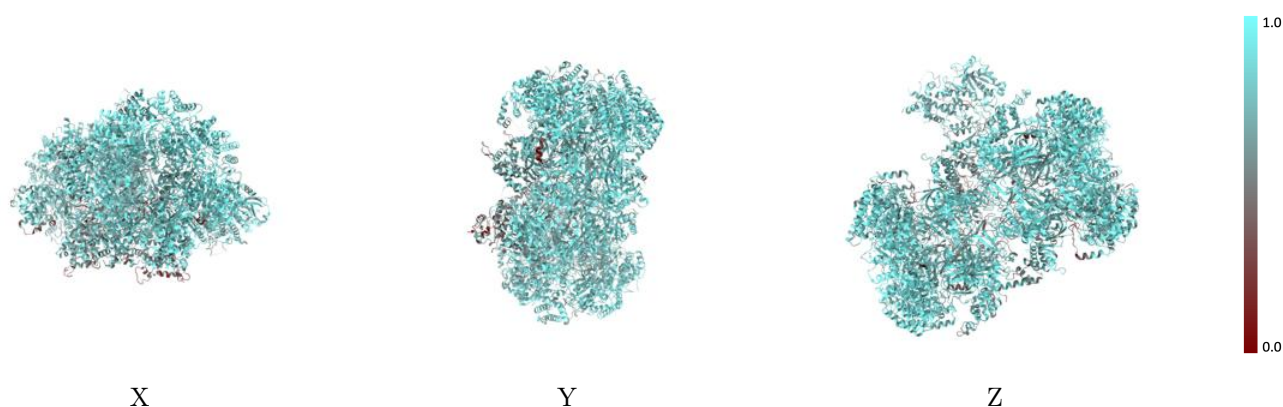
This section was not generated.

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



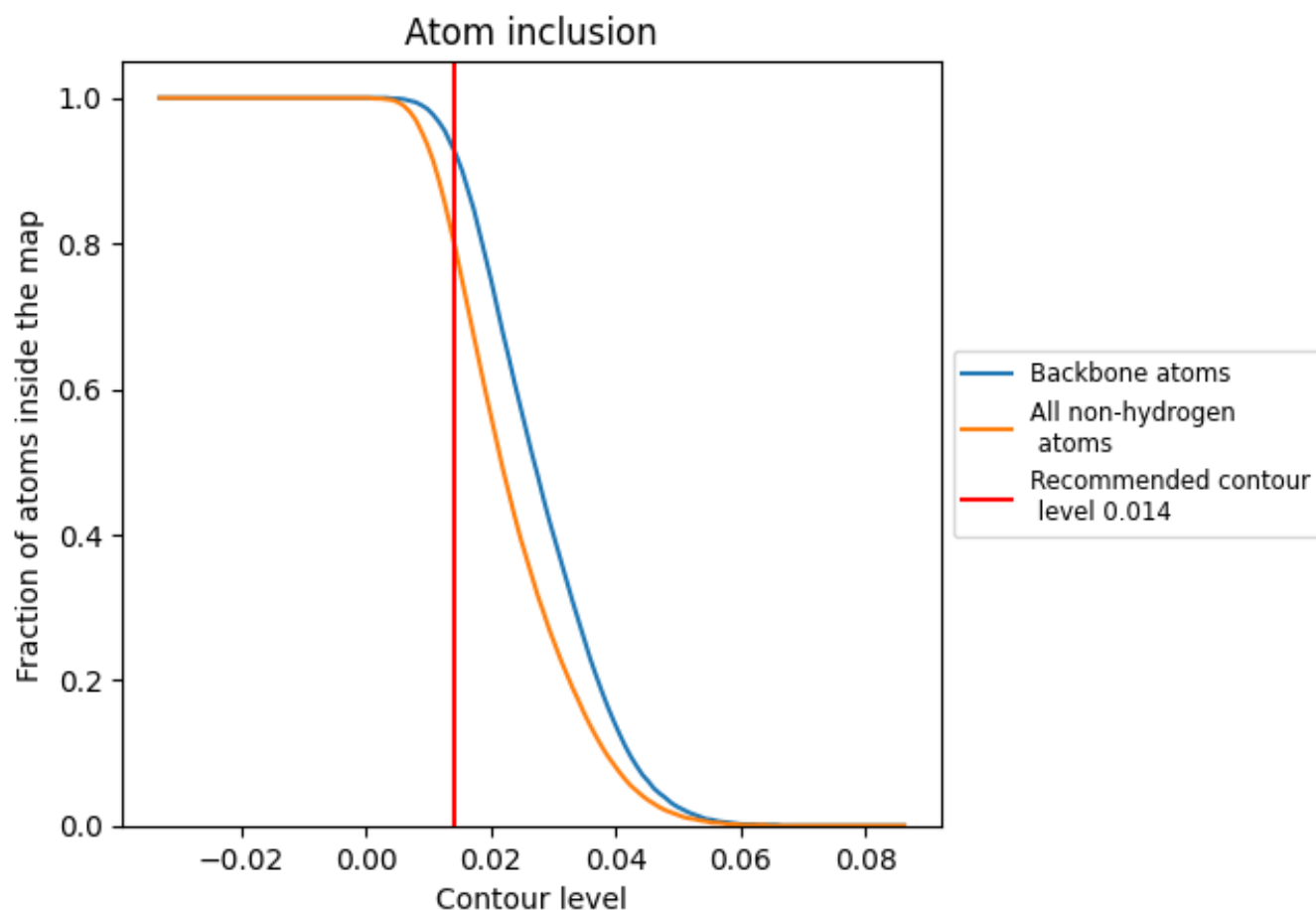
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 80% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8030	0.4450
1	0.0000	0.4240
2	0.7350	0.4080
3	0.8750	0.5000
4	0.8010	0.4490
5	0.8200	0.4650
6	0.7330	0.3940
7	0.8590	0.4870
8	0.7880	0.3500
9	0.6570	0.3090
B	0.7230	0.4050
C	0.8800	0.5050
D	0.8350	0.4750
E	0.8180	0.4590
F	0.7640	0.4160
G	0.8730	0.5010

