



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:51 AM UTC

PDB ID : 7FGG / pdb_00007fgg
EMDB ID : EMD-31580
Title : Cryo-EM Structure of Chikungunya Virus Nonstructural Protein 1 with m7GTP
Authors : Zhang, K.; Law, M.C.Y.; Nguyen, T.M.; Tan, Y.B.; Wirawan, M.; Law, Y.S.; Luo, D.H.
Deposited on : 2021-07-27
Resolution : 2.19 Å(reported)

This is a Full wwPDB EM Validation 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:

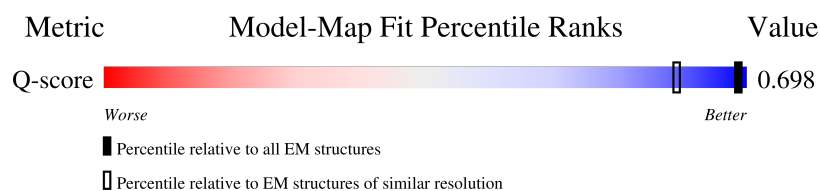
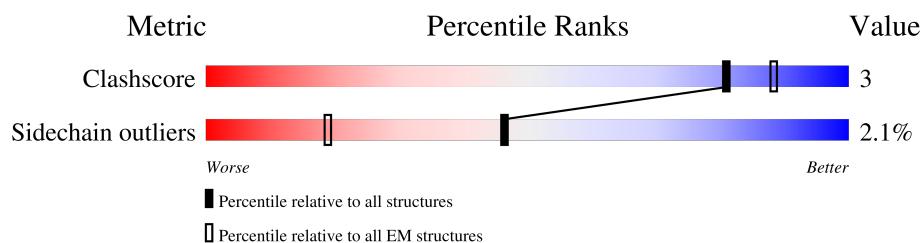
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.19 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.



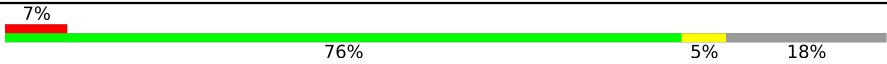
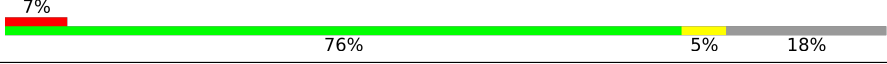
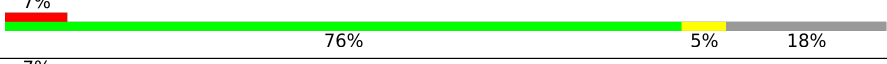
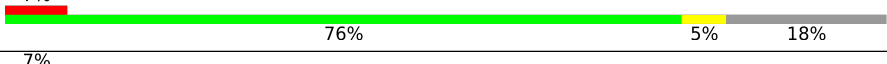
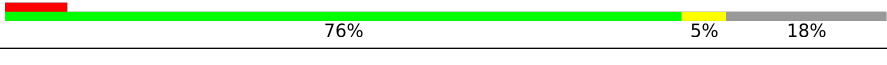
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2745 (1.70 - 2.69)

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	552	
1	B	552	
1	C	552	
1	D	552	
1	E	552	

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Mol	Chain	Length	Quality of chain
1	F	552	
1	G	552	
1	H	552	
1	I	552	
1	J	552	
1	K	552	
1	L	552	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 45132 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 mRNA-capping enzyme nsP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	451	Total	C	N	O	S	2	0
			3553	2244	621	660	28		
1	B	451	Total	C	N	O	S	2	0
			3553	2244	621	660	28		
1	C	451	Total	C	N	O	S	2	0
			3553	2244	621	660	28		
1	D	451	Total	C	N	O	S	2	0
			3553	2244	621	660	28		
1	E	451	Total	C	N	O	S	2	0
			3553	2244	621	660	28		
1	F	451	Total	C	N	O	S	2	0
			3553	2244	621	660	28		
1	G	451	Total	C	N	O	S	2	0
			3553	2244	621	660	28		
1	H	451	Total	C	N	O	S	2	0
			3553	2244	621	660	28		
1	I	451	Total	C	N	O	S	2	0
			3553	2244	621	660	28		
1	J	451	Total	C	N	O	S	2	0
			3553	2244	621	660	28		
1	K	451	Total	C	N	O	S	2	0
			3553	2244	621	660	28		
1	L	451	Total	C	N	O	S	2	0
			3553	2244	621	660	28		

There are 432 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	517	GLY	-	expression tag	UNP Q8JUX6
A	518	GLY	-	expression tag	UNP Q8JUX6
A	519	GLY	-	expression tag	UNP Q8JUX6
A	520	GLY	-	expression tag	UNP Q8JUX6
A	521	SER	-	expression tag	UNP Q8JUX6
A	522	TRP	-	expression tag	UNP Q8JUX6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	523	SER	-	expression tag	UNP Q8JUX6
A	524	HIS	-	expression tag	UNP Q8JUX6
A	525	PRO	-	expression tag	UNP Q8JUX6
A	526	GLN	-	expression tag	UNP Q8JUX6
A	527	PHE	-	expression tag	UNP Q8JUX6
A	528	GLU	-	expression tag	UNP Q8JUX6
A	529	LYS	-	expression tag	UNP Q8JUX6
A	530	MET	-	expression tag	UNP Q8JUX6
A	531	ASP	-	expression tag	UNP Q8JUX6
A	532	TYR	-	expression tag	UNP Q8JUX6
A	533	LYS	-	expression tag	UNP Q8JUX6
A	534	ASP	-	expression tag	UNP Q8JUX6
A	535	HIS	-	expression tag	UNP Q8JUX6
A	536	ASP	-	expression tag	UNP Q8JUX6
A	537	GLY	-	expression tag	UNP Q8JUX6
A	538	ASP	-	expression tag	UNP Q8JUX6
A	539	TYR	-	expression tag	UNP Q8JUX6
A	540	LYS	-	expression tag	UNP Q8JUX6
A	541	ASP	-	expression tag	UNP Q8JUX6
A	542	HIS	-	expression tag	UNP Q8JUX6
A	543	ASP	-	expression tag	UNP Q8JUX6
A	544	ILE	-	expression tag	UNP Q8JUX6
A	545	ASP	-	expression tag	UNP Q8JUX6
A	546	TYR	-	expression tag	UNP Q8JUX6
A	547	LYS	-	expression tag	UNP Q8JUX6
A	548	ASP	-	expression tag	UNP Q8JUX6
A	549	ASP	-	expression tag	UNP Q8JUX6
A	550	ASP	-	expression tag	UNP Q8JUX6
A	551	ASP	-	expression tag	UNP Q8JUX6
A	552	LYS	-	expression tag	UNP Q8JUX6
B	517	GLY	-	expression tag	UNP Q8JUX6
B	518	GLY	-	expression tag	UNP Q8JUX6
B	519	GLY	-	expression tag	UNP Q8JUX6
B	520	GLY	-	expression tag	UNP Q8JUX6
B	521	SER	-	expression tag	UNP Q8JUX6
B	522	TRP	-	expression tag	UNP Q8JUX6
B	523	SER	-	expression tag	UNP Q8JUX6
B	524	HIS	-	expression tag	UNP Q8JUX6
B	525	PRO	-	expression tag	UNP Q8JUX6
B	526	GLN	-	expression tag	UNP Q8JUX6
B	527	PHE	-	expression tag	UNP Q8JUX6
B	528	GLU	-	expression tag	UNP Q8JUX6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	529	LYS	-	expression tag	UNP Q8JUX6
B	530	MET	-	expression tag	UNP Q8JUX6
B	531	ASP	-	expression tag	UNP Q8JUX6
B	532	TYR	-	expression tag	UNP Q8JUX6
B	533	LYS	-	expression tag	UNP Q8JUX6
B	534	ASP	-	expression tag	UNP Q8JUX6
B	535	HIS	-	expression tag	UNP Q8JUX6
B	536	ASP	-	expression tag	UNP Q8JUX6
B	537	GLY	-	expression tag	UNP Q8JUX6
B	538	ASP	-	expression tag	UNP Q8JUX6
B	539	TYR	-	expression tag	UNP Q8JUX6
B	540	LYS	-	expression tag	UNP Q8JUX6
B	541	ASP	-	expression tag	UNP Q8JUX6
B	542	HIS	-	expression tag	UNP Q8JUX6
B	543	ASP	-	expression tag	UNP Q8JUX6
B	544	ILE	-	expression tag	UNP Q8JUX6
B	545	ASP	-	expression tag	UNP Q8JUX6
B	546	TYR	-	expression tag	UNP Q8JUX6
B	547	LYS	-	expression tag	UNP Q8JUX6
B	548	ASP	-	expression tag	UNP Q8JUX6
B	549	ASP	-	expression tag	UNP Q8JUX6
B	550	ASP	-	expression tag	UNP Q8JUX6
B	551	ASP	-	expression tag	UNP Q8JUX6
B	552	LYS	-	expression tag	UNP Q8JUX6
C	517	GLY	-	expression tag	UNP Q8JUX6
C	518	GLY	-	expression tag	UNP Q8JUX6
C	519	GLY	-	expression tag	UNP Q8JUX6
C	520	GLY	-	expression tag	UNP Q8JUX6
C	521	SER	-	expression tag	UNP Q8JUX6
C	522	TRP	-	expression tag	UNP Q8JUX6
C	523	SER	-	expression tag	UNP Q8JUX6
C	524	HIS	-	expression tag	UNP Q8JUX6
C	525	PRO	-	expression tag	UNP Q8JUX6
C	526	GLN	-	expression tag	UNP Q8JUX6
C	527	PHE	-	expression tag	UNP Q8JUX6
C	528	GLU	-	expression tag	UNP Q8JUX6
C	529	LYS	-	expression tag	UNP Q8JUX6
C	530	MET	-	expression tag	UNP Q8JUX6
C	531	ASP	-	expression tag	UNP Q8JUX6
C	532	TYR	-	expression tag	UNP Q8JUX6
C	533	LYS	-	expression tag	UNP Q8JUX6
C	534	ASP	-	expression tag	UNP Q8JUX6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	535	HIS	-	expression tag	UNP Q8JUX6
C	536	ASP	-	expression tag	UNP Q8JUX6
C	537	GLY	-	expression tag	UNP Q8JUX6
C	538	ASP	-	expression tag	UNP Q8JUX6
C	539	TYR	-	expression tag	UNP Q8JUX6
C	540	LYS	-	expression tag	UNP Q8JUX6
C	541	ASP	-	expression tag	UNP Q8JUX6
C	542	HIS	-	expression tag	UNP Q8JUX6
C	543	ASP	-	expression tag	UNP Q8JUX6
C	544	ILE	-	expression tag	UNP Q8JUX6
C	545	ASP	-	expression tag	UNP Q8JUX6
C	546	TYR	-	expression tag	UNP Q8JUX6
C	547	LYS	-	expression tag	UNP Q8JUX6
C	548	ASP	-	expression tag	UNP Q8JUX6
C	549	ASP	-	expression tag	UNP Q8JUX6
C	550	ASP	-	expression tag	UNP Q8JUX6
C	551	ASP	-	expression tag	UNP Q8JUX6
C	552	LYS	-	expression tag	UNP Q8JUX6
D	517	GLY	-	expression tag	UNP Q8JUX6
D	518	GLY	-	expression tag	UNP Q8JUX6
D	519	GLY	-	expression tag	UNP Q8JUX6
D	520	GLY	-	expression tag	UNP Q8JUX6
D	521	SER	-	expression tag	UNP Q8JUX6
D	522	TRP	-	expression tag	UNP Q8JUX6
D	523	SER	-	expression tag	UNP Q8JUX6
D	524	HIS	-	expression tag	UNP Q8JUX6
D	525	PRO	-	expression tag	UNP Q8JUX6
D	526	GLN	-	expression tag	UNP Q8JUX6
D	527	PHE	-	expression tag	UNP Q8JUX6
D	528	GLU	-	expression tag	UNP Q8JUX6
D	529	LYS	-	expression tag	UNP Q8JUX6
D	530	MET	-	expression tag	UNP Q8JUX6
D	531	ASP	-	expression tag	UNP Q8JUX6
D	532	TYR	-	expression tag	UNP Q8JUX6
D	533	LYS	-	expression tag	UNP Q8JUX6
D	534	ASP	-	expression tag	UNP Q8JUX6
D	535	HIS	-	expression tag	UNP Q8JUX6
D	536	ASP	-	expression tag	UNP Q8JUX6
D	537	GLY	-	expression tag	UNP Q8JUX6
D	538	ASP	-	expression tag	UNP Q8JUX6
D	539	TYR	-	expression tag	UNP Q8JUX6
D	540	LYS	-	expression tag	UNP Q8JUX6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	541	ASP	-	expression tag	UNP Q8JUX6
D	542	HIS	-	expression tag	UNP Q8JUX6
D	543	ASP	-	expression tag	UNP Q8JUX6
D	544	ILE	-	expression tag	UNP Q8JUX6
D	545	ASP	-	expression tag	UNP Q8JUX6
D	546	TYR	-	expression tag	UNP Q8JUX6
D	547	LYS	-	expression tag	UNP Q8JUX6
D	548	ASP	-	expression tag	UNP Q8JUX6
D	549	ASP	-	expression tag	UNP Q8JUX6
D	550	ASP	-	expression tag	UNP Q8JUX6
D	551	ASP	-	expression tag	UNP Q8JUX6
D	552	LYS	-	expression tag	UNP Q8JUX6
E	517	GLY	-	expression tag	UNP Q8JUX6
E	518	GLY	-	expression tag	UNP Q8JUX6
E	519	GLY	-	expression tag	UNP Q8JUX6
E	520	GLY	-	expression tag	UNP Q8JUX6
E	521	SER	-	expression tag	UNP Q8JUX6
E	522	TRP	-	expression tag	UNP Q8JUX6
E	523	SER	-	expression tag	UNP Q8JUX6
E	524	HIS	-	expression tag	UNP Q8JUX6
E	525	PRO	-	expression tag	UNP Q8JUX6
E	526	GLN	-	expression tag	UNP Q8JUX6
E	527	PHE	-	expression tag	UNP Q8JUX6
E	528	GLU	-	expression tag	UNP Q8JUX6
E	529	LYS	-	expression tag	UNP Q8JUX6
E	530	MET	-	expression tag	UNP Q8JUX6
E	531	ASP	-	expression tag	UNP Q8JUX6
E	532	TYR	-	expression tag	UNP Q8JUX6
E	533	LYS	-	expression tag	UNP Q8JUX6
E	534	ASP	-	expression tag	UNP Q8JUX6
E	535	HIS	-	expression tag	UNP Q8JUX6
E	536	ASP	-	expression tag	UNP Q8JUX6
E	537	GLY	-	expression tag	UNP Q8JUX6
E	538	ASP	-	expression tag	UNP Q8JUX6
E	539	TYR	-	expression tag	UNP Q8JUX6
E	540	LYS	-	expression tag	UNP Q8JUX6
E	541	ASP	-	expression tag	UNP Q8JUX6
E	542	HIS	-	expression tag	UNP Q8JUX6
E	543	ASP	-	expression tag	UNP Q8JUX6
E	544	ILE	-	expression tag	UNP Q8JUX6
E	545	ASP	-	expression tag	UNP Q8JUX6
E	546	TYR	-	expression tag	UNP Q8JUX6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	547	LYS	-	expression tag	UNP Q8JUX6
E	548	ASP	-	expression tag	UNP Q8JUX6
E	549	ASP	-	expression tag	UNP Q8JUX6
E	550	ASP	-	expression tag	UNP Q8JUX6
E	551	ASP	-	expression tag	UNP Q8JUX6
E	552	LYS	-	expression tag	UNP Q8JUX6
F	517	GLY	-	expression tag	UNP Q8JUX6
F	518	GLY	-	expression tag	UNP Q8JUX6
F	519	GLY	-	expression tag	UNP Q8JUX6
F	520	GLY	-	expression tag	UNP Q8JUX6
F	521	SER	-	expression tag	UNP Q8JUX6
F	522	TRP	-	expression tag	UNP Q8JUX6
F	523	SER	-	expression tag	UNP Q8JUX6
F	524	HIS	-	expression tag	UNP Q8JUX6
F	525	PRO	-	expression tag	UNP Q8JUX6
F	526	GLN	-	expression tag	UNP Q8JUX6
F	527	PHE	-	expression tag	UNP Q8JUX6
F	528	GLU	-	expression tag	UNP Q8JUX6
F	529	LYS	-	expression tag	UNP Q8JUX6
F	530	MET	-	expression tag	UNP Q8JUX6
F	531	ASP	-	expression tag	UNP Q8JUX6
F	532	TYR	-	expression tag	UNP Q8JUX6
F	533	LYS	-	expression tag	UNP Q8JUX6
F	534	ASP	-	expression tag	UNP Q8JUX6
F	535	HIS	-	expression tag	UNP Q8JUX6
F	536	ASP	-	expression tag	UNP Q8JUX6
F	537	GLY	-	expression tag	UNP Q8JUX6
F	538	ASP	-	expression tag	UNP Q8JUX6
F	539	TYR	-	expression tag	UNP Q8JUX6
F	540	LYS	-	expression tag	UNP Q8JUX6
F	541	ASP	-	expression tag	UNP Q8JUX6
F	542	HIS	-	expression tag	UNP Q8JUX6
F	543	ASP	-	expression tag	UNP Q8JUX6
F	544	ILE	-	expression tag	UNP Q8JUX6
F	545	ASP	-	expression tag	UNP Q8JUX6
F	546	TYR	-	expression tag	UNP Q8JUX6
F	547	LYS	-	expression tag	UNP Q8JUX6
F	548	ASP	-	expression tag	UNP Q8JUX6
F	549	ASP	-	expression tag	UNP Q8JUX6
F	550	ASP	-	expression tag	UNP Q8JUX6
F	551	ASP	-	expression tag	UNP Q8JUX6
F	552	LYS	-	expression tag	UNP Q8JUX6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	517	GLY	-	expression tag	UNP Q8JUX6
G	518	GLY	-	expression tag	UNP Q8JUX6
G	519	GLY	-	expression tag	UNP Q8JUX6
G	520	GLY	-	expression tag	UNP Q8JUX6
G	521	SER	-	expression tag	UNP Q8JUX6
G	522	TRP	-	expression tag	UNP Q8JUX6
G	523	SER	-	expression tag	UNP Q8JUX6
G	524	HIS	-	expression tag	UNP Q8JUX6
G	525	PRO	-	expression tag	UNP Q8JUX6
G	526	GLN	-	expression tag	UNP Q8JUX6
G	527	PHE	-	expression tag	UNP Q8JUX6
G	528	GLU	-	expression tag	UNP Q8JUX6
G	529	LYS	-	expression tag	UNP Q8JUX6
G	530	MET	-	expression tag	UNP Q8JUX6
G	531	ASP	-	expression tag	UNP Q8JUX6
G	532	TYR	-	expression tag	UNP Q8JUX6
G	533	LYS	-	expression tag	UNP Q8JUX6
G	534	ASP	-	expression tag	UNP Q8JUX6
G	535	HIS	-	expression tag	UNP Q8JUX6
G	536	ASP	-	expression tag	UNP Q8JUX6
G	537	GLY	-	expression tag	UNP Q8JUX6
G	538	ASP	-	expression tag	UNP Q8JUX6
G	539	TYR	-	expression tag	UNP Q8JUX6
G	540	LYS	-	expression tag	UNP Q8JUX6
G	541	ASP	-	expression tag	UNP Q8JUX6
G	542	HIS	-	expression tag	UNP Q8JUX6
G	543	ASP	-	expression tag	UNP Q8JUX6
G	544	ILE	-	expression tag	UNP Q8JUX6
G	545	ASP	-	expression tag	UNP Q8JUX6
G	546	TYR	-	expression tag	UNP Q8JUX6
G	547	LYS	-	expression tag	UNP Q8JUX6
G	548	ASP	-	expression tag	UNP Q8JUX6
G	549	ASP	-	expression tag	UNP Q8JUX6
G	550	ASP	-	expression tag	UNP Q8JUX6
G	551	ASP	-	expression tag	UNP Q8JUX6
G	552	LYS	-	expression tag	UNP Q8JUX6
H	517	GLY	-	expression tag	UNP Q8JUX6
H	518	GLY	-	expression tag	UNP Q8JUX6
H	519	GLY	-	expression tag	UNP Q8JUX6
H	520	GLY	-	expression tag	UNP Q8JUX6
H	521	SER	-	expression tag	UNP Q8JUX6
H	522	TRP	-	expression tag	UNP Q8JUX6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	523	SER	-	expression tag	UNP Q8JUX6
H	524	HIS	-	expression tag	UNP Q8JUX6
H	525	PRO	-	expression tag	UNP Q8JUX6
H	526	GLN	-	expression tag	UNP Q8JUX6
H	527	PHE	-	expression tag	UNP Q8JUX6
H	528	GLU	-	expression tag	UNP Q8JUX6
H	529	LYS	-	expression tag	UNP Q8JUX6
H	530	MET	-	expression tag	UNP Q8JUX6
H	531	ASP	-	expression tag	UNP Q8JUX6
H	532	TYR	-	expression tag	UNP Q8JUX6
H	533	LYS	-	expression tag	UNP Q8JUX6
H	534	ASP	-	expression tag	UNP Q8JUX6
H	535	HIS	-	expression tag	UNP Q8JUX6
H	536	ASP	-	expression tag	UNP Q8JUX6
H	537	GLY	-	expression tag	UNP Q8JUX6
H	538	ASP	-	expression tag	UNP Q8JUX6
H	539	TYR	-	expression tag	UNP Q8JUX6
H	540	LYS	-	expression tag	UNP Q8JUX6
H	541	ASP	-	expression tag	UNP Q8JUX6
H	542	HIS	-	expression tag	UNP Q8JUX6
H	543	ASP	-	expression tag	UNP Q8JUX6
H	544	ILE	-	expression tag	UNP Q8JUX6
H	545	ASP	-	expression tag	UNP Q8JUX6
H	546	TYR	-	expression tag	UNP Q8JUX6
H	547	LYS	-	expression tag	UNP Q8JUX6
H	548	ASP	-	expression tag	UNP Q8JUX6
H	549	ASP	-	expression tag	UNP Q8JUX6
H	550	ASP	-	expression tag	UNP Q8JUX6
H	551	ASP	-	expression tag	UNP Q8JUX6
H	552	LYS	-	expression tag	UNP Q8JUX6
I	517	GLY	-	expression tag	UNP Q8JUX6
I	518	GLY	-	expression tag	UNP Q8JUX6
I	519	GLY	-	expression tag	UNP Q8JUX6
I	520	GLY	-	expression tag	UNP Q8JUX6
I	521	SER	-	expression tag	UNP Q8JUX6
I	522	TRP	-	expression tag	UNP Q8JUX6
I	523	SER	-	expression tag	UNP Q8JUX6
I	524	HIS	-	expression tag	UNP Q8JUX6
I	525	PRO	-	expression tag	UNP Q8JUX6
I	526	GLN	-	expression tag	UNP Q8JUX6
I	527	PHE	-	expression tag	UNP Q8JUX6
I	528	GLU	-	expression tag	UNP Q8JUX6

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Chain	Residue	Modelled	Actual	Comment	Reference
I	529	LYS	-	expression tag	UNP Q8JUX6
I	530	MET	-	expression tag	UNP Q8JUX6
I	531	ASP	-	expression tag	UNP Q8JUX6
I	532	TYR	-	expression tag	UNP Q8JUX6
I	533	LYS	-	expression tag	UNP Q8JUX6
I	534	ASP	-	expression tag	UNP Q8JUX6
I	535	HIS	-	expression tag	UNP Q8JUX6
I	536	ASP	-	expression tag	UNP Q8JUX6
I	537	GLY	-	expression tag	UNP Q8JUX6
I	538	ASP	-	expression tag	UNP Q8JUX6
I	539	TYR	-	expression tag	UNP Q8JUX6
I	540	LYS	-	expression tag	UNP Q8JUX6
I	541	ASP	-	expression tag	UNP Q8JUX6
I	542	HIS	-	expression tag	UNP Q8JUX6
I	543	ASP	-	expression tag	UNP Q8JUX6
I	544	ILE	-	expression tag	UNP Q8JUX6
I	545	ASP	-	expression tag	UNP Q8JUX6
I	546	TYR	-	expression tag	UNP Q8JUX6
I	547	LYS	-	expression tag	UNP Q8JUX6
I	548	ASP	-	expression tag	UNP Q8JUX6
I	549	ASP	-	expression tag	UNP Q8JUX6
I	550	ASP	-	expression tag	UNP Q8JUX6
I	551	ASP	-	expression tag	UNP Q8JUX6
I	552	LYS	-	expression tag	UNP Q8JUX6
J	517	GLY	-	expression tag	UNP Q8JUX6
J	518	GLY	-	expression tag	UNP Q8JUX6
J	519	GLY	-	expression tag	UNP Q8JUX6
J	520	GLY	-	expression tag	UNP Q8JUX6
J	521	SER	-	expression tag	UNP Q8JUX6
J	522	TRP	-	expression tag	UNP Q8JUX6
J	523	SER	-	expression tag	UNP Q8JUX6
J	524	HIS	-	expression tag	UNP Q8JUX6
J	525	PRO	-	expression tag	UNP Q8JUX6
J	526	GLN	-	expression tag	UNP Q8JUX6
J	527	PHE	-	expression tag	UNP Q8JUX6
J	528	GLU	-	expression tag	UNP Q8JUX6
J	529	LYS	-	expression tag	UNP Q8JUX6
J	530	MET	-	expression tag	UNP Q8JUX6
J	531	ASP	-	expression tag	UNP Q8JUX6
J	532	TYR	-	expression tag	UNP Q8JUX6
J	533	LYS	-	expression tag	UNP Q8JUX6
J	534	ASP	-	expression tag	UNP Q8JUX6

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Chain	Residue	Modelled	Actual	Comment	Reference
J	535	HIS	-	expression tag	UNP Q8JUX6
J	536	ASP	-	expression tag	UNP Q8JUX6
J	537	GLY	-	expression tag	UNP Q8JUX6
J	538	ASP	-	expression tag	UNP Q8JUX6
J	539	TYR	-	expression tag	UNP Q8JUX6
J	540	LYS	-	expression tag	UNP Q8JUX6
J	541	ASP	-	expression tag	UNP Q8JUX6
J	542	HIS	-	expression tag	UNP Q8JUX6
J	543	ASP	-	expression tag	UNP Q8JUX6
J	544	ILE	-	expression tag	UNP Q8JUX6
J	545	ASP	-	expression tag	UNP Q8JUX6
J	546	TYR	-	expression tag	UNP Q8JUX6
J	547	LYS	-	expression tag	UNP Q8JUX6
J	548	ASP	-	expression tag	UNP Q8JUX6
J	549	ASP	-	expression tag	UNP Q8JUX6
J	550	ASP	-	expression tag	UNP Q8JUX6
J	551	ASP	-	expression tag	UNP Q8JUX6
J	552	LYS	-	expression tag	UNP Q8JUX6
K	517	GLY	-	expression tag	UNP Q8JUX6
K	518	GLY	-	expression tag	UNP Q8JUX6
K	519	GLY	-	expression tag	UNP Q8JUX6
K	520	GLY	-	expression tag	UNP Q8JUX6
K	521	SER	-	expression tag	UNP Q8JUX6
K	522	TRP	-	expression tag	UNP Q8JUX6
K	523	SER	-	expression tag	UNP Q8JUX6
K	524	HIS	-	expression tag	UNP Q8JUX6
K	525	PRO	-	expression tag	UNP Q8JUX6
K	526	GLN	-	expression tag	UNP Q8JUX6
K	527	PHE	-	expression tag	UNP Q8JUX6
K	528	GLU	-	expression tag	UNP Q8JUX6
K	529	LYS	-	expression tag	UNP Q8JUX6
K	530	MET	-	expression tag	UNP Q8JUX6
K	531	ASP	-	expression tag	UNP Q8JUX6
K	532	TYR	-	expression tag	UNP Q8JUX6
K	533	LYS	-	expression tag	UNP Q8JUX6
K	534	ASP	-	expression tag	UNP Q8JUX6
K	535	HIS	-	expression tag	UNP Q8JUX6
K	536	ASP	-	expression tag	UNP Q8JUX6
K	537	GLY	-	expression tag	UNP Q8JUX6
K	538	ASP	-	expression tag	UNP Q8JUX6
K	539	TYR	-	expression tag	UNP Q8JUX6
K	540	LYS	-	expression tag	UNP Q8JUX6

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Chain	Residue	Modelled	Actual	Comment	Reference
K	541	ASP	-	expression tag	UNP Q8JUX6
K	542	HIS	-	expression tag	UNP Q8JUX6
K	543	ASP	-	expression tag	UNP Q8JUX6
K	544	ILE	-	expression tag	UNP Q8JUX6
K	545	ASP	-	expression tag	UNP Q8JUX6
K	546	TYR	-	expression tag	UNP Q8JUX6
K	547	LYS	-	expression tag	UNP Q8JUX6
K	548	ASP	-	expression tag	UNP Q8JUX6
K	549	ASP	-	expression tag	UNP Q8JUX6
K	550	ASP	-	expression tag	UNP Q8JUX6
K	551	ASP	-	expression tag	UNP Q8JUX6
K	552	LYS	-	expression tag	UNP Q8JUX6
L	517	GLY	-	expression tag	UNP Q8JUX6
L	518	GLY	-	expression tag	UNP Q8JUX6
L	519	GLY	-	expression tag	UNP Q8JUX6
L	520	GLY	-	expression tag	UNP Q8JUX6
L	521	SER	-	expression tag	UNP Q8JUX6
L	522	TRP	-	expression tag	UNP Q8JUX6
L	523	SER	-	expression tag	UNP Q8JUX6
L	524	HIS	-	expression tag	UNP Q8JUX6
L	525	PRO	-	expression tag	UNP Q8JUX6
L	526	GLN	-	expression tag	UNP Q8JUX6
L	527	PHE	-	expression tag	UNP Q8JUX6
L	528	GLU	-	expression tag	UNP Q8JUX6
L	529	LYS	-	expression tag	UNP Q8JUX6
L	530	MET	-	expression tag	UNP Q8JUX6
L	531	ASP	-	expression tag	UNP Q8JUX6
L	532	TYR	-	expression tag	UNP Q8JUX6
L	533	LYS	-	expression tag	UNP Q8JUX6
L	534	ASP	-	expression tag	UNP Q8JUX6
L	535	HIS	-	expression tag	UNP Q8JUX6
L	536	ASP	-	expression tag	UNP Q8JUX6
L	537	GLY	-	expression tag	UNP Q8JUX6
L	538	ASP	-	expression tag	UNP Q8JUX6
L	539	TYR	-	expression tag	UNP Q8JUX6
L	540	LYS	-	expression tag	UNP Q8JUX6
L	541	ASP	-	expression tag	UNP Q8JUX6
L	542	HIS	-	expression tag	UNP Q8JUX6
L	543	ASP	-	expression tag	UNP Q8JUX6
L	544	ILE	-	expression tag	UNP Q8JUX6
L	545	ASP	-	expression tag	UNP Q8JUX6
L	546	TYR	-	expression tag	UNP Q8JUX6

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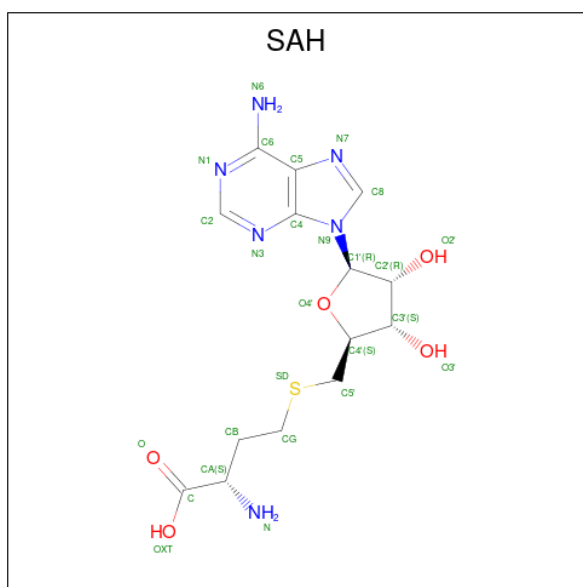
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Chain	Residue	Modelled	Actual	Comment	Reference
L	547	LYS	-	expression tag	UNP Q8JUX6
L	548	ASP	-	expression tag	UNP Q8JUX6
L	549	ASP	-	expression tag	UNP Q8JUX6
L	550	ASP	-	expression tag	UNP Q8JUX6
L	551	ASP	-	expression tag	UNP Q8JUX6
L	552	LYS	-	expression tag	UNP Q8JUX6

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

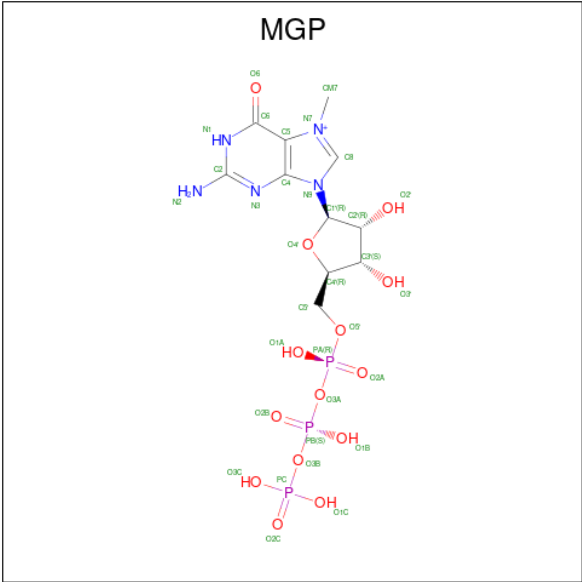
Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total Zn 1 1	0
2	B	1	Total Zn 1 1	0
2	C	1	Total Zn 1 1	0
2	D	1	Total Zn 1 1	0
2	E	1	Total Zn 1 1	0
2	F	1	Total Zn 1 1	0
2	G	1	Total Zn 1 1	0
2	H	1	Total Zn 1 1	0
2	I	1	Total Zn 1 1	0
2	J	1	Total Zn 1 1	0
2	K	1	Total Zn 1 1	0
2	L	1	Total Zn 1 1	0

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	S	0
			26	14	6	5	1	
3	B	1	Total	C	N	O	S	0
			26	14	6	5	1	
3	C	1	Total	C	N	O	S	0
			26	14	6	5	1	
3	D	1	Total	C	N	O	S	0
			26	14	6	5	1	
3	E	1	Total	C	N	O	S	0
			26	14	6	5	1	
3	F	1	Total	C	N	O	S	0
			26	14	6	5	1	
3	G	1	Total	C	N	O	S	0
			26	14	6	5	1	
3	H	1	Total	C	N	O	S	0
			26	14	6	5	1	
3	I	1	Total	C	N	O	S	0
			26	14	6	5	1	
3	J	1	Total	C	N	O	S	0
			26	14	6	5	1	
3	K	1	Total	C	N	O	S	0
			26	14	6	5	1	
3	L	1	Total	C	N	O	S	0
			26	14	6	5	1	

- Molecule 4 is 7-METHYL-GUANOSINE-5'-TRIPHOSPHATE (CCD ID: MGP) (formula: $C_{11}H_{19}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			33	11	5	14	3	
4	B	1	Total	C	N	O	P	0
			33	11	5	14	3	
4	C	1	Total	C	N	O	P	0
			33	11	5	14	3	
4	D	1	Total	C	N	O	P	0
			33	11	5	14	3	
4	E	1	Total	C	N	O	P	0
			33	11	5	14	3	
4	F	1	Total	C	N	O	P	0
			33	11	5	14	3	
4	G	1	Total	C	N	O	P	0
			33	11	5	14	3	
4	H	1	Total	C	N	O	P	0
			33	11	5	14	3	
4	I	1	Total	C	N	O	P	0
			33	11	5	14	3	
4	J	1	Total	C	N	O	P	0
			33	11	5	14	3	
4	K	1	Total	C	N	O	P	0
			33	11	5	14	3	
4	L	1	Total	C	N	O	P	0
			33	11	5	14	3	

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

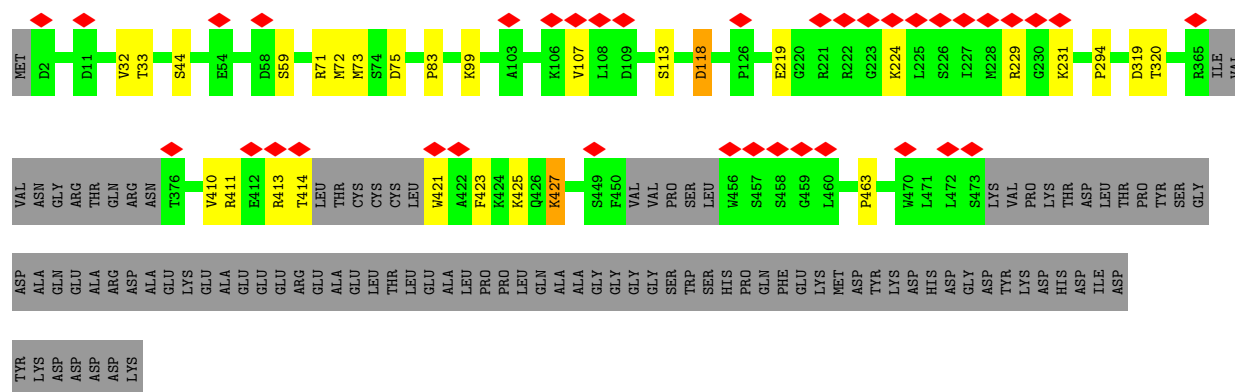
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	AltConf
6	A	147	Total O 147 147	0
6	B	147	Total O 147 147	0
6	C	147	Total O 147 147	0
6	D	147	Total O 147 147	0
6	E	147	Total O 147 147	0
6	F	147	Total O 147 147	0
6	G	147	Total O 147 147	0
6	H	147	Total O 147 147	0

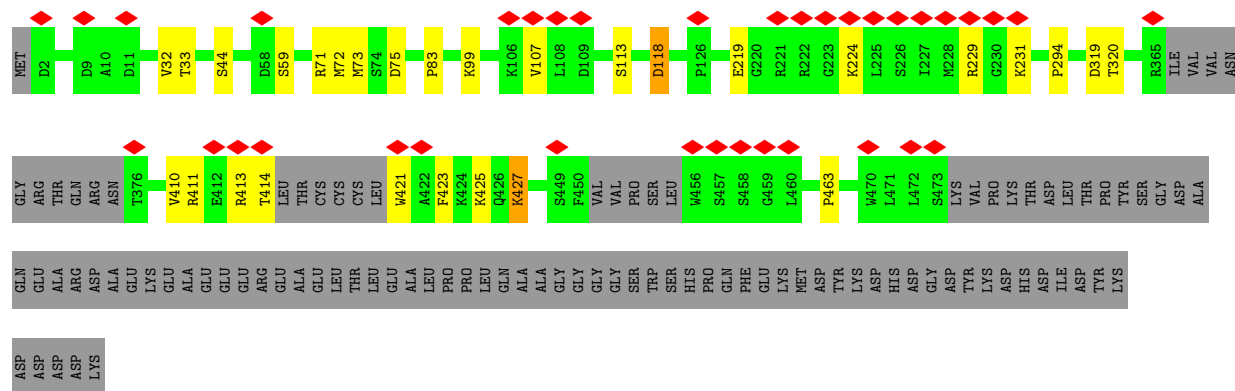
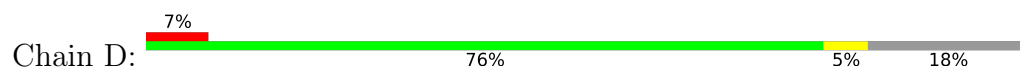
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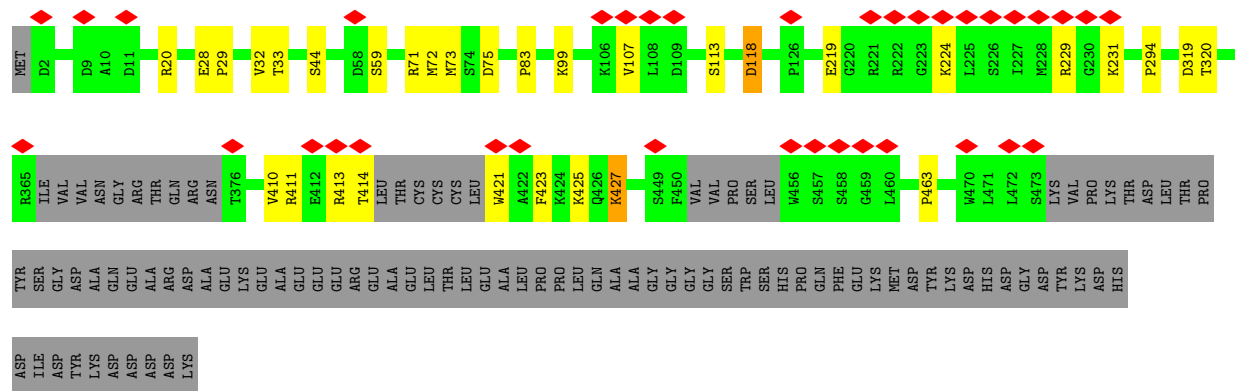
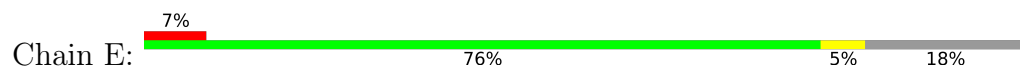
Mol	Chain	Residues	Atoms		AltConf
6	I	147	Total 147	O 147	0
6	J	147	Total 147	O 147	0
6	K	147	Total 147	O 147	0
6	L	147	Total 147	O 147	0



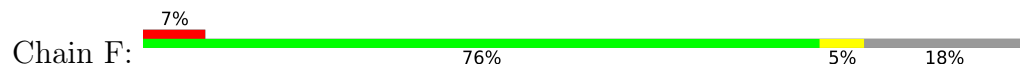
• Molecule 1: mRNA-capping enzyme nsP1

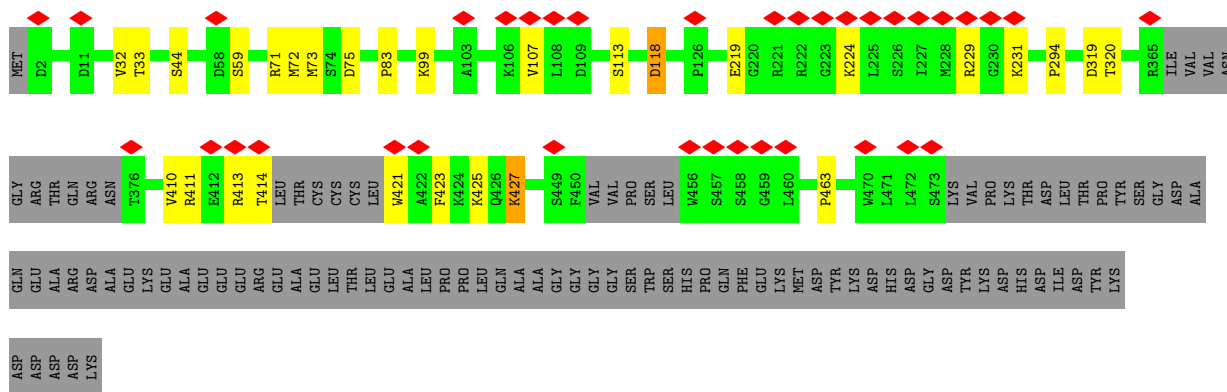


• Molecule 1: mRNA-capping enzyme nsP1

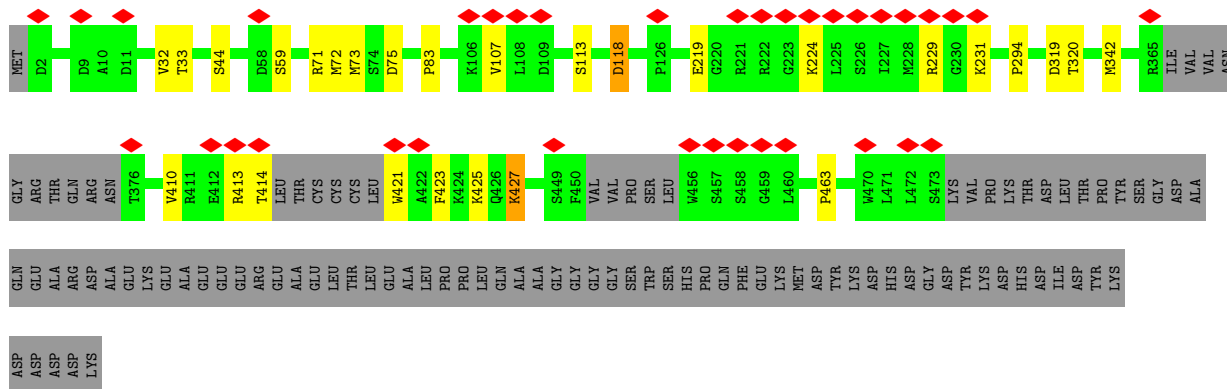
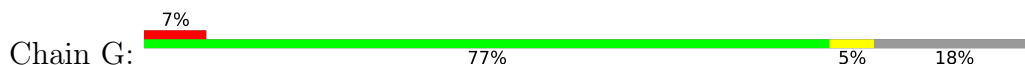


• Molecule 1: mRNA-capping enzyme nsP1

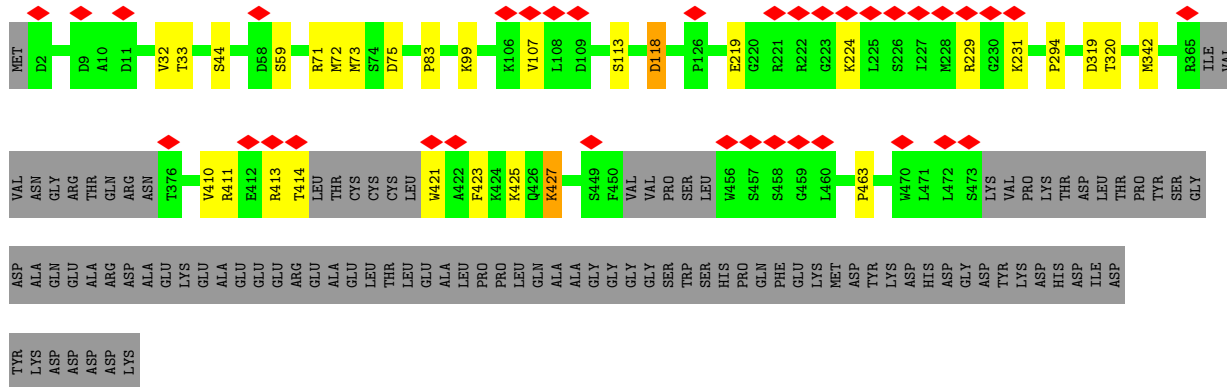
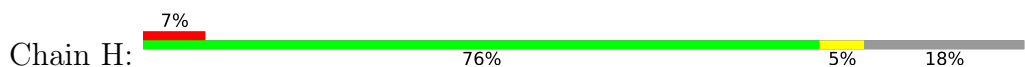




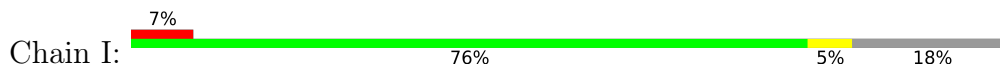
- Molecule 1: mRNA-capping enzyme nsP1

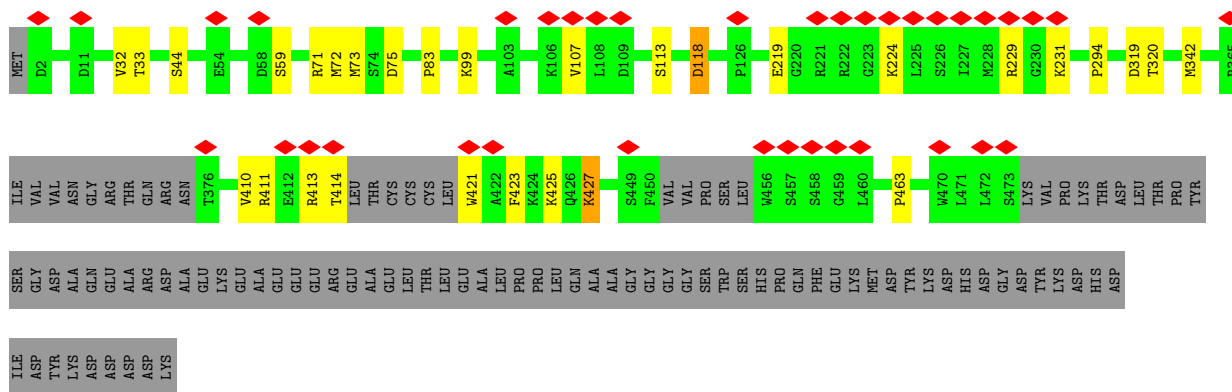


- Molecule 1: mRNA-capping enzyme nsP1

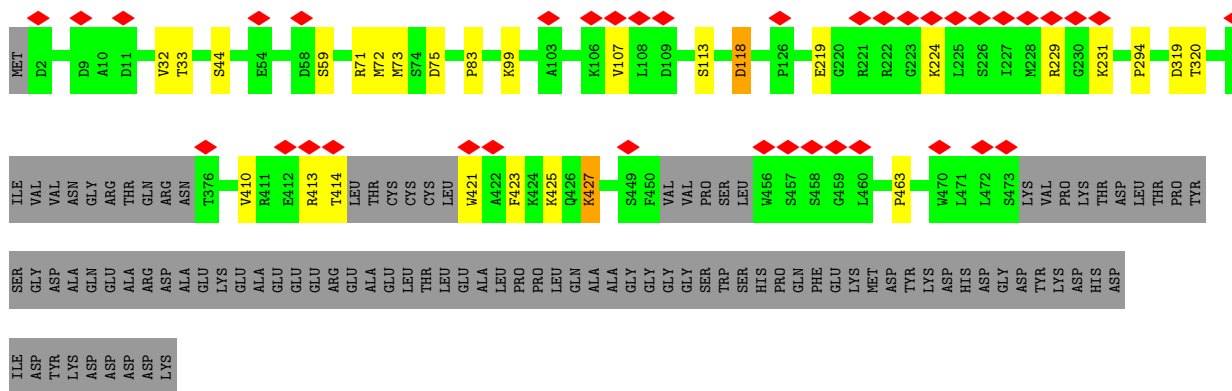
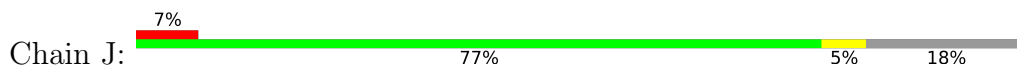


- Molecule 1: mRNA-capping enzyme nsP1

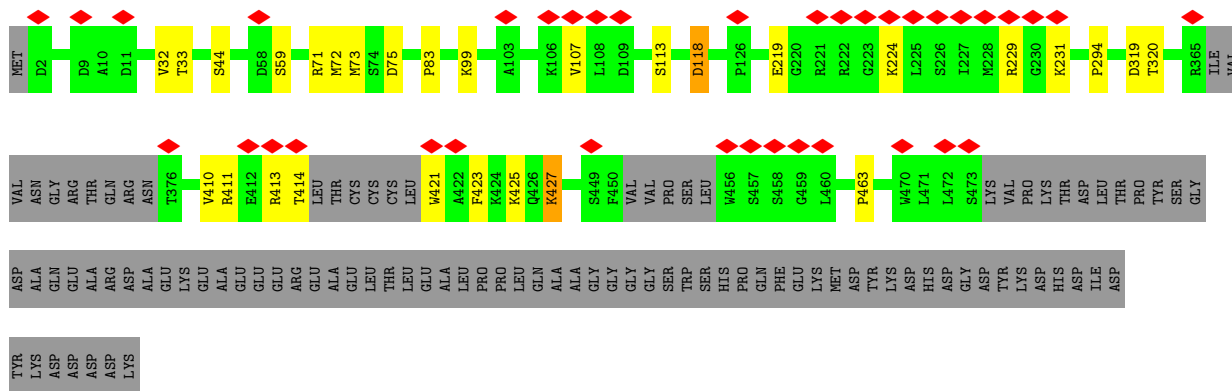
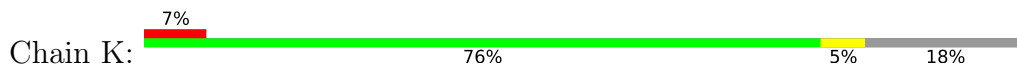




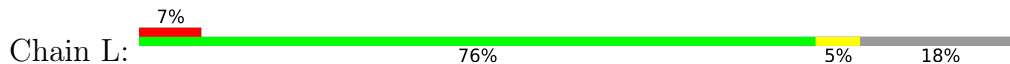
• Molecule 1: mRNA-capping enzyme nsP1

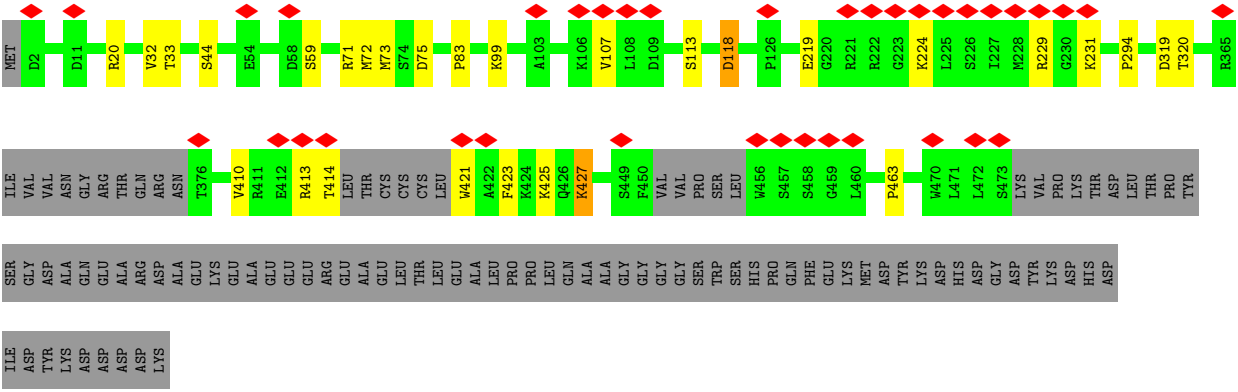


• Molecule 1: mRNA-capping enzyme nsP1



• Molecule 1: mRNA-capping enzyme nsP1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	244484	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.932	Depositor
Minimum map value	-0.975	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.3	Depositor
Map size ($\text{\AA}$)	408.0, 408.0, 408.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.31	0/3629	0.53	2/4914 (0.0%)
1	B	0.31	0/3629	0.53	2/4914 (0.0%)
1	C	0.31	0/3629	0.53	2/4914 (0.0%)
1	D	0.31	0/3629	0.53	2/4914 (0.0%)
1	E	0.31	0/3629	0.53	2/4914 (0.0%)
1	F	0.31	0/3629	0.53	2/4914 (0.0%)
1	G	0.31	0/3629	0.53	2/4914 (0.0%)
1	H	0.31	0/3629	0.53	2/4914 (0.0%)
1	I	0.31	0/3629	0.53	2/4914 (0.0%)
1	J	0.31	0/3629	0.53	2/4914 (0.0%)
1	K	0.31	0/3629	0.53	2/4914 (0.0%)
1	L	0.31	0/3629	0.53	2/4914 (0.0%)
All	All	0.31	0/43548	0.53	24/58968 (0.0%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	83	PRO	CA-C-N	-5.64	114.08	123.33
1	H	83	PRO	C-N-CA	-5.64	114.08	123.33
1	F	83	PRO	CA-C-N	-5.62	114.11	123.33
1	F	83	PRO	C-N-CA	-5.62	114.11	123.33
1	E	83	PRO	CA-C-N	-5.61	114.13	123.33
1	E	83	PRO	C-N-CA	-5.61	114.13	123.33
1	K	83	PRO	CA-C-N	-5.60	114.14	123.33
1	K	83	PRO	C-N-CA	-5.60	114.14	123.33
1	C	83	PRO	CA-C-N	-5.60	114.15	123.33
1	C	83	PRO	C-N-CA	-5.60	114.15	123.33
1	I	83	PRO	CA-C-N	-5.59	114.16	123.33
1	I	83	PRO	C-N-CA	-5.59	114.16	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	83	PRO	CA-C-N	-5.59	114.16	123.33
1	J	83	PRO	C-N-CA	-5.59	114.16	123.33
1	B	83	PRO	CA-C-N	-5.57	114.19	123.33
1	B	83	PRO	C-N-CA	-5.57	114.19	123.33
1	D	83	PRO	CA-C-N	-5.57	114.19	123.33
1	D	83	PRO	C-N-CA	-5.57	114.19	123.33
1	L	83	PRO	CA-C-N	-5.56	114.22	123.33
1	L	83	PRO	C-N-CA	-5.56	114.22	123.33
1	A	83	PRO	CA-C-N	-5.55	114.22	123.33
1	A	83	PRO	C-N-CA	-5.55	114.22	123.33
1	G	83	PRO	CA-C-N	-5.52	114.28	123.33
1	G	83	PRO	C-N-CA	-5.52	114.28	123.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3553	0	3521	25	0
1	B	3553	0	3521	24	0
1	C	3553	0	3521	25	0
1	D	3553	0	3521	25	0
1	E	3553	0	3521	26	0
1	F	3553	0	3521	24	0
1	G	3553	0	3521	23	0
1	H	3553	0	3521	26	0
1	I	3553	0	3521	25	0
1	J	3553	0	3521	24	0
1	K	3553	0	3521	23	0
1	L	3553	0	3521	25	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	26	0	19	1	0
3	B	26	0	19	1	0
3	C	26	0	19	1	0
3	D	26	0	19	1	0
3	E	26	0	19	1	0
3	F	26	0	19	1	0
3	G	26	0	19	1	0
3	H	26	0	19	1	0
3	I	26	0	19	1	0
3	J	26	0	19	1	0
3	K	26	0	19	1	0
3	L	26	0	19	1	0
4	A	33	0	15	0	0
4	B	33	0	15	0	0
4	C	33	0	15	0	0
4	D	33	0	15	0	0
4	E	33	0	15	0	0
4	F	33	0	15	0	0
4	G	33	0	15	0	0
4	H	33	0	15	0	0
4	I	33	0	15	0	0
4	J	33	0	15	0	0
4	K	33	0	15	0	0
4	L	33	0	15	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	1	0	0	0	0
6	A	147	0	0	1	0
6	B	147	0	0	1	0
6	C	147	0	0	1	0
6	D	147	0	0	1	0
6	E	147	0	0	1	0
6	F	147	0	0	1	0
6	G	147	0	0	1	0
6	H	147	0	0	1	0
6	I	147	0	0	1	0
6	J	147	0	0	1	0
6	K	147	0	0	1	0
6	L	147	0	0	1	0
All	All	45132	0	42660	227	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.

All (227) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:219:GLU:O	1:H:427:LYS:HG2	2.02	0.60
1:B:219:GLU:O	1:C:427:LYS:HG2	2.03	0.59
1:J:219:GLU:O	1:K:427:LYS:HG2	2.03	0.59
1:D:219:GLU:O	1:E:427:LYS:HG2	2.03	0.59
1:I:219:GLU:O	1:J:427:LYS:HG2	2.03	0.58
1:A:219:GLU:O	1:B:427:LYS:HG2	2.04	0.58
1:A:427:LYS:HG2	1:L:219:GLU:O	2.03	0.58
1:K:219:GLU:O	1:L:427:LYS:HG2	2.04	0.58
1:E:219:GLU:O	1:F:427:LYS:HG2	2.03	0.58
1:A:425:LYS:HD2	1:L:224:LYS:HE3	1.86	0.57
1:C:219:GLU:O	1:D:427:LYS:HG2	2.04	0.57
1:F:219:GLU:O	1:G:427:LYS:HG2	2.04	0.57
1:G:224:LYS:HE3	1:H:425:LYS:HD2	1.86	0.57
1:I:224:LYS:HE3	1:J:425:LYS:HD2	1.87	0.57
1:H:219:GLU:O	1:I:427:LYS:HG2	2.04	0.57
1:J:224:LYS:HE3	1:K:425:LYS:HD2	1.87	0.57
1:B:224:LYS:HE3	1:C:425:LYS:HD2	1.86	0.57
1:H:224:LYS:HE3	1:I:425:LYS:HD2	1.88	0.56
1:K:224:LYS:HE3	1:L:425:LYS:HD2	1.87	0.56
1:A:224:LYS:HE3	1:B:425:LYS:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ARG:NH1	6:A:1103:HOH:O	2.35	0.56
1:C:224:LYS:HE3	1:D:425:LYS:HZ3	1.70	0.56
1:E:463:PRO:HB2	1:F:294:PRO:HB2	1.87	0.56
1:A:294:PRO:HB2	1:L:463:PRO:HB2	1.88	0.56
1:E:224:LYS:HE3	1:F:425:LYS:HD2	1.87	0.56
1:F:224:LYS:HE3	1:G:425:LYS:HD2	1.87	0.56
1:I:71:ARG:NH1	6:I:1103:HOH:O	2.35	0.56
1:C:224:LYS:HE3	1:D:425:LYS:HD2	1.87	0.55
1:D:224:LYS:HE3	1:E:425:LYS:HD2	1.87	0.55
1:J:463:PRO:HB2	1:K:294:PRO:HB2	1.88	0.55
1:A:425:LYS:HZ3	1:L:224:LYS:HE3	1.71	0.55
1:L:71:ARG:NH1	6:L:1103:HOH:O	2.35	0.55
1:A:463:PRO:HB2	1:B:294:PRO:HB2	1.89	0.54
1:K:463:PRO:HB2	1:L:294:PRO:HB2	1.89	0.54
1:H:463:PRO:HB2	1:I:294:PRO:HB2	1.88	0.54
1:B:463:PRO:HB2	1:C:294:PRO:HB2	1.88	0.54
1:G:463:PRO:HB2	1:H:294:PRO:HB2	1.88	0.54
1:K:224:LYS:HE3	1:L:425:LYS:HZ3	1.72	0.54
1:G:71:ARG:NH1	6:G:1103:HOH:O	2.35	0.54
1:E:224:LYS:HE3	1:F:425:LYS:HZ3	1.73	0.54
1:D:463:PRO:HB2	1:E:294:PRO:HB2	1.89	0.54
1:A:224:LYS:HE3	1:B:425:LYS:HZ3	1.72	0.54
1:F:463:PRO:HB2	1:G:294:PRO:HB2	1.89	0.54
1:C:463:PRO:HB2	1:D:294:PRO:HB2	1.88	0.54
1:I:463:PRO:HB2	1:J:294:PRO:HB2	1.89	0.54
1:G:224:LYS:HE3	1:H:425:LYS:HZ3	1.74	0.53
1:F:71:ARG:NH1	6:F:1103:HOH:O	2.35	0.53
1:H:71:ARG:NH1	6:H:1103:HOH:O	2.35	0.53
1:K:71:ARG:NH1	6:K:1103:HOH:O	2.35	0.53
1:B:224:LYS:HE3	1:C:425:LYS:HZ3	1.75	0.52
1:H:224:LYS:HE3	1:I:425:LYS:HZ3	1.73	0.52
1:E:71:ARG:NH1	6:E:1103:HOH:O	2.35	0.52
1:J:224:LYS:HE3	1:K:425:LYS:HZ3	1.74	0.52
1:F:224:LYS:HE3	1:G:425:LYS:HZ3	1.74	0.52
1:I:224:LYS:HE3	1:J:425:LYS:HZ3	1.76	0.51
1:D:224:LYS:HE3	1:E:425:LYS:HZ3	1.75	0.51
1:J:71:ARG:NH1	6:J:1103:HOH:O	2.35	0.50
1:D:71:ARG:NH1	6:D:1103:HOH:O	2.35	0.50
1:G:224:LYS:HE3	1:H:425:LYS:CD	2.43	0.49
1:E:224:LYS:HE3	1:F:425:LYS:CD	2.43	0.49
1:D:73:MET:HE1	1:D:107:VAL:HG11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:LYS:HB3	1:A:427:LYS:HE2	1.58	0.49
1:F:73:MET:HE1	1:F:107:VAL:HG11	1.95	0.49
1:K:73:MET:HE1	1:K:107:VAL:HG11	1.95	0.49
1:B:224:LYS:HE3	1:C:425:LYS:CD	2.43	0.49
1:I:73:MET:HE1	1:I:107:VAL:HG11	1.95	0.48
1:A:425:LYS:CD	1:L:224:LYS:HE3	2.43	0.48
1:B:73:MET:HE1	1:B:107:VAL:HG11	1.95	0.48
1:H:73:MET:HE1	1:H:107:VAL:HG11	1.95	0.48
1:J:427:LYS:HB3	1:J:427:LYS:HE2	1.58	0.48
1:C:224:LYS:HE3	1:D:425:LYS:CD	2.44	0.48
1:H:224:LYS:HE3	1:I:425:LYS:CD	2.44	0.48
1:J:73:MET:HE1	1:J:107:VAL:HG11	1.95	0.48
1:J:224:LYS:HE3	1:K:425:LYS:CD	2.43	0.48
1:L:73:MET:HE1	1:L:107:VAL:HG11	1.95	0.48
1:A:73:MET:HE1	1:A:107:VAL:HG11	1.95	0.48
1:D:99:LYS:HE2	1:D:99:LYS:HB3	1.56	0.48
1:C:71:ARG:NH1	6:C:1103:HOH:O	2.35	0.48
1:A:224:LYS:HE3	1:B:425:LYS:CD	2.44	0.48
1:D:224:LYS:HE3	1:E:425:LYS:CD	2.43	0.48
1:I:224:LYS:HE3	1:J:425:LYS:CD	2.43	0.48
1:G:73:MET:HE1	1:G:107:VAL:HG11	1.95	0.48
1:C:73:MET:HE1	1:C:107:VAL:HG11	1.95	0.47
1:H:99:LYS:HE2	1:H:99:LYS:HB3	1.55	0.47
1:C:99:LYS:HB3	1:C:99:LYS:HE2	1.56	0.47
3:C:1002:SAH:H4'	3:C:1002:SAH:HG1	1.75	0.47
1:E:73:MET:HE1	1:E:107:VAL:HG11	1.95	0.47
1:F:224:LYS:HE3	1:G:425:LYS:CD	2.44	0.47
1:J:99:LYS:HB3	1:J:99:LYS:HE2	1.56	0.47
1:K:224:LYS:HE3	1:L:425:LYS:CD	2.44	0.46
1:B:71:ARG:NH1	6:B:1103:HOH:O	2.35	0.46
3:I:1002:SAH:HG1	3:I:1002:SAH:H4'	1.75	0.46
3:L:1002:SAH:H4'	3:L:1002:SAH:HG1	1.75	0.45
3:B:1002:SAH:HG1	3:B:1002:SAH:H4'	1.75	0.45
1:C:118:ASP:OD1	1:C:118:ASP:N	2.50	0.45
1:B:99:LYS:HE2	1:B:99:LYS:HB3	1.56	0.45
1:D:118:ASP:OD1	1:D:118:ASP:N	2.50	0.45
1:F:99:LYS:HB3	1:F:99:LYS:HE2	1.55	0.45
1:G:118:ASP:N	1:G:118:ASP:OD1	2.50	0.45
1:C:32:VAL:HG23	1:C:33:THR:HG23	1.99	0.44
1:D:32:VAL:HG23	1:D:33:THR:HG23	1.99	0.44
1:E:32:VAL:HG23	1:E:33:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LYS:HE2	1:A:99:LYS:HB3	1.55	0.44
1:H:118:ASP:OD1	1:H:118:ASP:N	2.50	0.44
1:J:118:ASP:N	1:J:118:ASP:OD1	2.50	0.44
1:B:32:VAL:HG23	1:B:33:THR:HG23	1.99	0.44
1:E:229:ARG:HG2	1:E:229:ARG:HH11	1.83	0.44
1:H:229:ARG:HG2	1:H:229:ARG:HH11	1.83	0.44
1:I:118:ASP:OD1	1:I:118:ASP:N	2.50	0.44
1:J:32:VAL:HG23	1:J:33:THR:HG23	1.99	0.44
3:D:1002:SAH:HG1	3:D:1002:SAH:H4'	1.75	0.44
1:E:118:ASP:OD1	1:E:118:ASP:N	2.50	0.44
1:F:32:VAL:HG23	1:F:33:THR:HG23	1.99	0.44
1:I:427:LYS:HB3	1:I:427:LYS:HE2	1.58	0.44
1:D:427:LYS:HB3	1:D:427:LYS:HE2	1.58	0.44
1:I:32:VAL:HG23	1:I:33:THR:HG23	1.99	0.44
1:L:231:LYS:O	1:L:231:LYS:HG2	2.18	0.44
1:A:118:ASP:OD1	1:A:118:ASP:N	2.50	0.43
1:D:229:ARG:HH11	1:D:229:ARG:HG2	1.83	0.43
1:G:413:ARG:HG2	1:G:423:PHE:HB3	2.01	0.43
1:H:413:ARG:HG2	1:H:423:PHE:HB3	2.00	0.43
1:L:319:ASP:OD1	1:L:320:THR:N	2.50	0.43
1:A:32:VAL:HG23	1:A:33:THR:HG23	1.99	0.43
1:F:413:ARG:HG2	1:F:423:PHE:HB3	2.01	0.43
1:G:32:VAL:HG23	1:G:33:THR:HG23	1.99	0.43
1:G:229:ARG:HG2	1:G:229:ARG:HH11	1.83	0.43
1:I:229:ARG:HH11	1:I:229:ARG:HG2	1.83	0.43
1:K:32:VAL:HG23	1:K:33:THR:HG23	1.99	0.43
1:K:319:ASP:OD1	1:K:320:THR:N	2.50	0.43
1:L:229:ARG:HG2	1:L:229:ARG:HH11	1.83	0.43
1:L:427:LYS:HB3	1:L:427:LYS:HE2	1.58	0.43
1:B:231:LYS:O	1:B:231:LYS:HG2	2.18	0.43
1:J:231:LYS:O	1:J:231:LYS:HG2	2.18	0.43
1:K:229:ARG:HH11	1:K:229:ARG:HG2	1.83	0.43
1:F:229:ARG:HH11	1:F:229:ARG:HG2	1.83	0.43
1:I:413:ARG:HG2	1:I:423:PHE:HB3	2.00	0.43
1:J:413:ARG:HG2	1:J:423:PHE:HB3	2.00	0.43
1:A:319:ASP:OD1	1:A:320:THR:N	2.50	0.43
1:E:413:ARG:HG2	1:E:423:PHE:HB3	2.00	0.43
1:I:231:LYS:O	1:I:231:LYS:HG2	2.18	0.43
1:J:229:ARG:HG2	1:J:229:ARG:HH11	1.83	0.43
1:K:413:ARG:HG2	1:K:423:PHE:HB3	2.01	0.43
1:K:231:LYS:O	1:K:231:LYS:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ARG:HG2	1:A:229:ARG:HH11	1.83	0.43
3:E:1002:SAH:HG1	3:E:1002:SAH:H4'	1.75	0.43
1:F:427:LYS:HB3	1:F:427:LYS:HE2	1.57	0.43
1:J:319:ASP:OD1	1:J:320:THR:N	2.50	0.43
3:K:1002:SAH:H4'	3:K:1002:SAH:HG1	1.75	0.43
1:L:32:VAL:HG23	1:L:33:THR:HG23	1.99	0.43
1:L:413:ARG:HG2	1:L:423:PHE:HB3	2.00	0.43
1:D:413:ARG:HG2	1:D:423:PHE:HB3	2.00	0.43
1:H:32:VAL:HG23	1:H:33:THR:HG23	1.99	0.43
1:A:231:LYS:O	1:A:231:LYS:HG2	2.18	0.42
1:B:229:ARG:HG2	1:B:229:ARG:HH11	1.83	0.42
1:B:427:LYS:HB3	1:B:427:LYS:HE2	1.57	0.42
1:E:99:LYS:HB3	1:E:99:LYS:HE2	1.56	0.42
1:C:229:ARG:HG2	1:C:229:ARG:HH11	1.83	0.42
1:F:118:ASP:OD1	1:F:118:ASP:N	2.50	0.42
1:A:413:ARG:HG2	1:A:423:PHE:HB3	2.00	0.42
1:B:118:ASP:OD1	1:B:118:ASP:N	2.50	0.42
1:B:319:ASP:OD1	1:B:320:THR:N	2.51	0.42
1:B:413:ARG:HG2	1:B:423:PHE:HB3	2.00	0.42
1:H:231:LYS:O	1:H:231:LYS:HG2	2.18	0.42
3:H:1002:SAH:HG1	3:H:1002:SAH:H4'	1.75	0.42
1:C:231:LYS:O	1:C:231:LYS:HG2	2.18	0.42
1:D:231:LYS:O	1:D:231:LYS:HG2	2.18	0.42
3:G:1002:SAH:HG1	3:G:1002:SAH:H4'	1.75	0.42
1:C:413:ARG:HG2	1:C:423:PHE:HB3	2.00	0.42
1:J:229:ARG:NH2	1:K:421:TRP:CE3	2.88	0.42
1:L:72:MET:HE2	1:L:73:MET:HG2	2.02	0.42
3:A:1002:SAH:H4'	3:A:1002:SAH:HG1	1.75	0.42
1:I:319:ASP:OD1	1:I:320:THR:N	2.50	0.42
1:J:72:MET:HE2	1:J:73:MET:HG2	2.02	0.42
1:K:72:MET:HE2	1:K:73:MET:HG2	2.02	0.42
1:K:118:ASP:OD1	1:K:118:ASP:N	2.50	0.42
1:E:229:ARG:NH2	1:F:421:TRP:CE3	2.88	0.42
1:A:20:ARG:HE	1:A:20:ARG:HB3	1.71	0.42
1:A:72:MET:HE2	1:A:73:MET:HG2	2.02	0.42
1:C:427:LYS:HE2	1:C:427:LYS:HB3	1.58	0.42
1:G:72:MET:HE2	1:G:73:MET:HG2	2.02	0.42
1:H:72:MET:HE2	1:H:73:MET:HG2	2.02	0.42
1:H:229:ARG:NH2	1:I:421:TRP:CE3	2.88	0.42
1:I:72:MET:HE2	1:I:73:MET:HG2	2.02	0.42
1:I:99:LYS:HE2	1:I:99:LYS:HB3	1.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:99:LYS:HB3	1:K:99:LYS:HE2	1.56	0.42
1:G:231:LYS:O	1:G:231:LYS:HG2	2.18	0.42
1:L:99:LYS:HB3	1:L:99:LYS:HE2	1.56	0.42
1:B:229:ARG:NH2	1:C:421:TRP:CE3	2.88	0.42
1:C:319:ASP:OD1	1:C:320:THR:N	2.50	0.42
1:E:28:GLU:HA	1:E:29:PRO:HD3	1.94	0.42
1:F:72:MET:HE2	1:F:73:MET:HG2	2.02	0.42
1:F:231:LYS:O	1:F:231:LYS:HG2	2.18	0.42
1:G:231:LYS:HA	1:H:411:ARG:O	2.20	0.42
1:C:72:MET:HE2	1:C:73:MET:HG2	2.02	0.41
1:D:72:MET:HE2	1:D:73:MET:HG2	2.02	0.41
1:E:72:MET:HE2	1:E:73:MET:HG2	2.02	0.41
1:E:231:LYS:HG2	1:E:231:LYS:O	2.18	0.41
1:A:421:TRP:CE3	1:L:229:ARG:NH2	2.88	0.41
1:B:72:MET:HE2	1:B:73:MET:HG2	2.02	0.41
1:C:229:ARG:NH2	1:D:421:TRP:CE3	2.88	0.41
1:G:229:ARG:NH2	1:H:421:TRP:CE3	2.88	0.41
1:E:231:LYS:HA	1:F:411:ARG:O	2.20	0.41
1:H:319:ASP:OD1	1:H:320:THR:N	2.51	0.41
1:H:427:LYS:HE2	1:H:427:LYS:HB3	1.58	0.41
1:K:229:ARG:NH2	1:L:421:TRP:CE3	2.89	0.41
1:A:229:ARG:NH2	1:B:421:TRP:CE3	2.88	0.41
1:J:231:LYS:HA	1:K:411:ARG:O	2.20	0.41
1:L:118:ASP:OD1	1:L:118:ASP:N	2.50	0.41
3:J:1002:SAH:H4'	3:J:1002:SAH:HG1	1.75	0.41
1:D:319:ASP:OD1	1:D:320:THR:N	2.50	0.41
1:F:229:ARG:NH2	1:G:421:TRP:CE3	2.89	0.41
3:F:1002:SAH:HG1	3:F:1002:SAH:H4'	1.75	0.41
1:I:229:ARG:NH2	1:J:421:TRP:CE3	2.89	0.41
1:D:231:LYS:HA	1:E:411:ARG:O	2.21	0.41
1:E:20:ARG:HE	1:E:20:ARG:HB3	1.71	0.41
1:G:319:ASP:OD1	1:G:320:THR:N	2.50	0.41
1:A:411:ARG:O	1:L:231:LYS:HA	2.21	0.41
1:H:231:LYS:HA	1:I:411:ARG:O	2.21	0.41
1:L:20:ARG:HE	1:L:20:ARG:HB3	1.71	0.41
1:C:231:LYS:HA	1:D:411:ARG:O	2.21	0.40
1:G:342:MET:HE3	1:G:342:MET:HB3	2.01	0.40
1:H:342:MET:HE3	1:H:342:MET:HB3	2.01	0.40
1:D:229:ARG:NH2	1:E:421:TRP:CE3	2.89	0.40
1:E:319:ASP:OD1	1:E:320:THR:N	2.51	0.40
1:I:342:MET:HE3	1:I:342:MET:HB3	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:319:ASP:OD1	1:F:320:THR:N	2.51	0.40
1:B:231:LYS:HA	1:C:411:ARG:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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	385/475 (81%)	377 (98%)	8 (2%)	47	63
1	B	385/475 (81%)	377 (98%)	8 (2%)	47	63
1	C	385/475 (81%)	377 (98%)	8 (2%)	47	63
1	D	385/475 (81%)	377 (98%)	8 (2%)	47	63
1	E	385/475 (81%)	377 (98%)	8 (2%)	47	63
1	F	385/475 (81%)	377 (98%)	8 (2%)	47	63
1	G	385/475 (81%)	377 (98%)	8 (2%)	47	63
1	H	385/475 (81%)	377 (98%)	8 (2%)	47	63
1	I	385/475 (81%)	377 (98%)	8 (2%)	47	63
1	J	385/475 (81%)	377 (98%)	8 (2%)	47	63
1	K	385/475 (81%)	377 (98%)	8 (2%)	47	63
1	L	385/475 (81%)	377 (98%)	8 (2%)	47	63
All	All	4620/5700 (81%)	4524 (98%)	96 (2%)	46	63

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	SER
1	A	59	SER
1	A	75	ASP
1	A	113	SER
1	A	118	ASP
1	A	410	VAL
1	A	414	THR
1	A	427	LYS
1	B	44	SER
1	B	59	SER
1	B	75	ASP
1	B	113	SER
1	B	118	ASP
1	B	410	VAL
1	B	414	THR
1	B	427	LYS
1	C	44	SER
1	C	59	SER
1	C	75	ASP
1	C	113	SER
1	C	118	ASP
1	C	410	VAL
1	C	414	THR
1	C	427	LYS
1	D	44	SER
1	D	59	SER
1	D	75	ASP
1	D	113	SER
1	D	118	ASP
1	D	410	VAL
1	D	414	THR
1	D	427	LYS
1	E	44	SER
1	E	59	SER
1	E	75	ASP
1	E	113	SER
1	E	118	ASP
1	E	410	VAL
1	E	414	THR
1	E	427	LYS
1	F	44	SER
1	F	59	SER
1	F	75	ASP

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Mol	Chain	Res	Type
1	F	113	SER
1	F	118	ASP
1	F	410	VAL
1	F	414	THR
1	F	427	LYS
1	G	44	SER
1	G	59	SER
1	G	75	ASP
1	G	113	SER
1	G	118	ASP
1	G	410	VAL
1	G	414	THR
1	G	427	LYS
1	H	44	SER
1	H	59	SER
1	H	75	ASP
1	H	113	SER
1	H	118	ASP
1	H	410	VAL
1	H	414	THR
1	H	427	LYS
1	I	44	SER
1	I	59	SER
1	I	75	ASP
1	I	113	SER
1	I	118	ASP
1	I	410	VAL
1	I	414	THR
1	I	427	LYS
1	J	44	SER
1	J	59	SER
1	J	75	ASP
1	J	113	SER
1	J	118	ASP
1	J	410	VAL
1	J	414	THR
1	J	427	LYS
1	K	44	SER
1	K	59	SER
1	K	75	ASP
1	K	113	SER
1	K	118	ASP

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Mol	Chain	Res	Type
1	K	410	VAL
1	K	414	THR
1	K	427	LYS
1	L	44	SER
1	L	59	SER
1	L	75	ASP
1	L	113	SER
1	L	118	ASP
1	L	410	VAL
1	L	414	THR
1	L	427	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	198	ASN
1	A	426	GLN
1	A	429	HIS
1	A	438	GLN
1	B	165	GLN
1	B	198	ASN
1	B	429	HIS
1	B	438	GLN
1	C	198	ASN
1	C	429	HIS
1	C	438	GLN
1	D	198	ASN
1	D	429	HIS
1	D	438	GLN
1	E	198	ASN
1	E	429	HIS
1	E	438	GLN
1	F	165	GLN
1	F	198	ASN
1	F	429	HIS
1	F	438	GLN
1	G	165	GLN
1	G	198	ASN
1	G	429	HIS
1	G	438	GLN
1	H	165	GLN

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Mol	Chain	Res	Type
1	H	198	ASN
1	H	426	GLN
1	H	429	HIS
1	H	438	GLN
1	I	198	ASN
1	I	429	HIS
1	I	438	GLN
1	J	165	GLN
1	J	198	ASN
1	J	429	HIS
1	J	438	GLN
1	K	165	GLN
1	K	198	ASN
1	K	429	HIS
1	K	438	GLN
1	L	198	ASN
1	L	429	HIS
1	L	438	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 48 ligands modelled in this entry, 24 are monoatomic - leaving 24 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	SAH	G	1002	-	27,28,28	1.05	4 (14%)	36,40,40	2.08	10 (27%)
3	SAH	D	1002	-	27,28,28	1.04	4 (14%)	36,40,40	2.09	10 (27%)
3	SAH	C	1002	-	27,28,28	1.04	4 (14%)	36,40,40	2.09	10 (27%)
4	MGP	H	1003	5	34,35,35	1.44	4 (11%)	52,56,56	1.60	7 (13%)
4	MGP	J	1003	5	34,35,35	1.44	4 (11%)	52,56,56	1.60	7 (13%)
4	MGP	B	1003	5	34,35,35	1.44	4 (11%)	52,56,56	1.60	7 (13%)
4	MGP	K	1003	5	34,35,35	1.43	4 (11%)	52,56,56	1.60	7 (13%)
4	MGP	L	1003	5	34,35,35	1.43	4 (11%)	52,56,56	1.60	7 (13%)
4	MGP	C	1003	5	34,35,35	1.43	4 (11%)	52,56,56	1.60	7 (13%)
3	SAH	L	1002	-	27,28,28	1.04	4 (14%)	36,40,40	2.08	10 (27%)
4	MGP	D	1003	5	34,35,35	1.44	4 (11%)	52,56,56	1.60	7 (13%)
3	SAH	F	1002	-	27,28,28	1.04	3 (11%)	36,40,40	2.07	10 (27%)
3	SAH	I	1002	-	27,28,28	1.05	4 (14%)	36,40,40	2.08	10 (27%)
4	MGP	A	1003	5	34,35,35	1.45	4 (11%)	52,56,56	1.60	7 (13%)
4	MGP	G	1003	5	34,35,35	1.43	4 (11%)	52,56,56	1.59	7 (13%)
3	SAH	A	1002	-	27,28,28	1.05	5 (18%)	36,40,40	2.08	10 (27%)
4	MGP	E	1003	5	34,35,35	1.44	4 (11%)	52,56,56	1.60	7 (13%)
3	SAH	H	1002	-	27,28,28	1.04	4 (14%)	36,40,40	2.08	10 (27%)
3	SAH	E	1002	-	27,28,28	1.05	4 (14%)	36,40,40	2.08	10 (27%)
3	SAH	J	1002	-	27,28,28	1.05	5 (18%)	36,40,40	2.07	10 (27%)
4	MGP	F	1003	5	34,35,35	1.44	4 (11%)	52,56,56	1.60	7 (13%)
3	SAH	B	1002	-	27,28,28	1.05	5 (18%)	36,40,40	2.08	10 (27%)
4	MGP	I	1003	5	34,35,35	1.43	4 (11%)	52,56,56	1.59	7 (13%)
3	SAH	K	1002	-	27,28,28	1.05	4 (14%)	36,40,40	2.08	10 (27%)

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	SAH	G	1002	-	-	3/15/31/31	0/3/3/3
3	SAH	D	1002	-	-	3/15/31/31	0/3/3/3
3	SAH	C	1002	-	-	3/15/31/31	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MGP	H	1003	5	-	0/22/38/38	0/3/3/3
4	MGP	J	1003	5	-	0/22/38/38	0/3/3/3
4	MGP	B	1003	5	-	0/22/38/38	0/3/3/3
4	MGP	K	1003	5	-	0/22/38/38	0/3/3/3
4	MGP	L	1003	5	-	0/22/38/38	0/3/3/3
4	MGP	C	1003	5	-	0/22/38/38	0/3/3/3
3	SAH	L	1002	-	-	3/15/31/31	0/3/3/3
4	MGP	D	1003	5	-	0/22/38/38	0/3/3/3
3	SAH	F	1002	-	-	3/15/31/31	0/3/3/3
3	SAH	I	1002	-	-	3/15/31/31	0/3/3/3
4	MGP	A	1003	5	-	0/22/38/38	0/3/3/3
4	MGP	G	1003	5	-	0/22/38/38	0/3/3/3
3	SAH	A	1002	-	-	3/15/31/31	0/3/3/3
4	MGP	E	1003	5	-	0/22/38/38	0/3/3/3
3	SAH	H	1002	-	-	3/15/31/31	0/3/3/3
3	SAH	E	1002	-	-	3/15/31/31	0/3/3/3
3	SAH	J	1002	-	-	3/15/31/31	0/3/3/3
4	MGP	F	1003	5	-	0/22/38/38	0/3/3/3
3	SAH	B	1002	-	-	3/15/31/31	0/3/3/3
4	MGP	I	1003	5	-	0/22/38/38	0/3/3/3
3	SAH	K	1002	-	-	3/15/31/31	0/3/3/3

All (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1003	MGP	C5-N7	-5.16	1.33	1.39
4	F	1003	MGP	C5-N7	-5.11	1.33	1.39
4	D	1003	MGP	C5-N7	-5.09	1.33	1.39
4	B	1003	MGP	C5-N7	-5.09	1.33	1.39
4	E	1003	MGP	C5-N7	-5.09	1.33	1.39
4	G	1003	MGP	C5-N7	-5.08	1.33	1.39
4	H	1003	MGP	C5-N7	-5.08	1.33	1.39
4	C	1003	MGP	C5-N7	-5.06	1.33	1.39
4	L	1003	MGP	C5-N7	-5.06	1.33	1.39
4	J	1003	MGP	C5-N7	-5.04	1.33	1.39
4	K	1003	MGP	C5-N7	-5.04	1.33	1.39
4	I	1003	MGP	C5-N7	-5.02	1.33	1.39
4	F	1003	MGP	C5-C4	3.11	1.46	1.38
4	K	1003	MGP	C5-C4	3.10	1.46	1.38
4	B	1003	MGP	C5-C4	3.10	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1003	MGP	C5-C4	3.10	1.46	1.38
4	C	1003	MGP	C5-C4	3.10	1.46	1.38
4	L	1003	MGP	C5-C4	3.10	1.46	1.38
4	A	1003	MGP	C5-C4	3.07	1.45	1.38
4	J	1003	MGP	C5-C4	3.07	1.45	1.38
4	G	1003	MGP	C5-C4	3.06	1.45	1.38
4	I	1003	MGP	C5-C4	3.06	1.45	1.38
4	D	1003	MGP	C5-C4	3.05	1.45	1.38
4	E	1003	MGP	C5-C4	3.03	1.45	1.38
4	I	1003	MGP	C6-N1	-3.00	1.33	1.38
4	D	1003	MGP	C6-N1	-3.00	1.33	1.38
4	B	1003	MGP	C6-N1	-2.97	1.33	1.38
4	C	1003	MGP	C6-N1	-2.96	1.33	1.38
4	A	1003	MGP	C6-N1	-2.96	1.33	1.38
4	G	1003	MGP	C6-N1	-2.96	1.33	1.38
4	H	1003	MGP	C6-N1	-2.96	1.33	1.38
4	J	1003	MGP	C6-N1	-2.95	1.33	1.38
4	F	1003	MGP	C6-N1	-2.94	1.33	1.38
4	E	1003	MGP	C6-N1	-2.94	1.33	1.38
4	L	1003	MGP	C6-N1	-2.94	1.33	1.38
4	K	1003	MGP	C6-N1	-2.94	1.33	1.38
3	G	1002	SAH	OXT-C	-2.38	1.23	1.30
3	I	1002	SAH	OXT-C	-2.37	1.23	1.30
3	D	1002	SAH	OXT-C	-2.36	1.23	1.30
3	H	1002	SAH	OXT-C	-2.36	1.23	1.30
3	K	1002	SAH	OXT-C	-2.35	1.23	1.30
3	C	1002	SAH	OXT-C	-2.35	1.23	1.30
3	L	1002	SAH	OXT-C	-2.34	1.23	1.30
3	E	1002	SAH	OXT-C	-2.34	1.23	1.30
3	F	1002	SAH	OXT-C	-2.33	1.23	1.30
3	A	1002	SAH	OXT-C	-2.33	1.23	1.30
3	J	1002	SAH	OXT-C	-2.33	1.23	1.30
3	B	1002	SAH	OXT-C	-2.33	1.23	1.30
3	I	1002	SAH	C5-N7	-2.15	1.35	1.39
3	E	1002	SAH	C5-N7	-2.15	1.35	1.39
3	A	1002	SAH	C5-N7	-2.14	1.35	1.39
3	K	1002	SAH	C2-N3	2.14	1.37	1.33
3	C	1002	SAH	C2-N3	2.14	1.37	1.33
3	G	1002	SAH	C5-N7	-2.13	1.35	1.39
3	J	1002	SAH	C5-N7	-2.13	1.35	1.39
3	B	1002	SAH	C5-N7	-2.13	1.35	1.39
3	F	1002	SAH	C5-N7	-2.13	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1002	SAH	C2-N3	2.12	1.37	1.33
3	K	1002	SAH	C5-N7	-2.11	1.35	1.39
3	L	1002	SAH	C5-N7	-2.11	1.35	1.39
3	F	1002	SAH	C2-N3	2.11	1.37	1.33
3	D	1002	SAH	C2-N3	2.11	1.37	1.33
3	H	1002	SAH	C5-N7	-2.11	1.35	1.39
3	L	1002	SAH	C2-N3	2.11	1.37	1.33
3	D	1002	SAH	C5-N7	-2.10	1.35	1.39
3	B	1002	SAH	C2-N3	2.10	1.37	1.33
3	J	1002	SAH	C2-N3	2.10	1.37	1.33
3	E	1002	SAH	C2-N3	2.10	1.37	1.33
3	H	1002	SAH	C2-N3	2.10	1.37	1.33
3	C	1002	SAH	C5-N7	-2.10	1.35	1.39
3	A	1002	SAH	C2-N3	2.09	1.37	1.33
4	L	1003	MGP	C4-N9	-2.08	1.32	1.38
4	A	1003	MGP	C4-N9	-2.08	1.32	1.38
4	H	1003	MGP	C4-N9	-2.08	1.32	1.38
3	I	1002	SAH	C2-N3	2.08	1.37	1.33
4	C	1003	MGP	C4-N9	-2.07	1.32	1.38
4	K	1003	MGP	C4-N9	-2.07	1.32	1.38
4	J	1003	MGP	C4-N9	-2.07	1.32	1.38
3	K	1002	SAH	C2-N1	2.07	1.37	1.33
4	I	1003	MGP	C4-N9	-2.06	1.32	1.38
3	J	1002	SAH	C2-N1	2.06	1.37	1.33
4	D	1003	MGP	C4-N9	-2.06	1.32	1.38
3	I	1002	SAH	C2-N1	2.06	1.37	1.33
4	E	1003	MGP	C4-N9	-2.06	1.32	1.38
4	F	1003	MGP	C4-N9	-2.05	1.32	1.38
3	J	1002	SAH	C8-N7	2.04	1.35	1.31
3	E	1002	SAH	C2-N1	2.04	1.37	1.33
4	G	1003	MGP	C4-N9	-2.04	1.32	1.38
4	B	1003	MGP	C4-N9	-2.03	1.32	1.38
3	A	1002	SAH	C2-N1	2.03	1.37	1.33
3	G	1002	SAH	C2-N1	2.03	1.37	1.33
3	L	1002	SAH	C2-N1	2.03	1.37	1.33
3	H	1002	SAH	C2-N1	2.03	1.37	1.33
3	C	1002	SAH	C2-N1	2.02	1.37	1.33
3	B	1002	SAH	C2-N1	2.01	1.37	1.33
3	A	1002	SAH	C8-N7	2.01	1.35	1.31
3	B	1002	SAH	C8-N7	2.00	1.35	1.31
3	D	1002	SAH	C2-N1	2.00	1.37	1.33

All (204) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1002	SAH	N3-C2-N1	-5.77	119.85	128.58
3	D	1002	SAH	N3-C2-N1	-5.77	119.85	128.58
3	C	1002	SAH	N3-C2-N1	-5.77	119.85	128.58
3	B	1002	SAH	N3-C2-N1	-5.76	119.86	128.58
3	K	1002	SAH	N3-C2-N1	-5.75	119.88	128.58
3	L	1002	SAH	N3-C2-N1	-5.75	119.88	128.58
3	A	1002	SAH	N3-C2-N1	-5.74	119.89	128.58
3	G	1002	SAH	N3-C2-N1	-5.74	119.90	128.58
3	H	1002	SAH	N3-C2-N1	-5.73	119.91	128.58
3	F	1002	SAH	N3-C2-N1	-5.73	119.91	128.58
3	I	1002	SAH	N3-C2-N1	-5.71	119.93	128.58
3	J	1002	SAH	N3-C2-N1	-5.71	119.94	128.58
4	L	1003	MGP	N9-C4-N3	5.18	136.32	125.95
4	K	1003	MGP	N9-C4-N3	5.17	136.29	125.95
4	C	1003	MGP	N9-C4-N3	5.17	136.29	125.95
4	B	1003	MGP	N9-C4-N3	5.17	136.29	125.95
4	F	1003	MGP	N9-C4-N3	5.16	136.27	125.95
4	J	1003	MGP	N9-C4-N3	5.16	136.27	125.95
4	I	1003	MGP	N9-C4-N3	5.16	136.27	125.95
4	E	1003	MGP	N9-C4-N3	5.15	136.26	125.95
4	D	1003	MGP	N9-C4-N3	5.15	136.26	125.95
4	A	1003	MGP	N9-C4-N3	5.15	136.26	125.95
4	H	1003	MGP	N9-C4-N3	5.15	136.25	125.95
4	G	1003	MGP	N9-C4-N3	5.13	136.21	125.95
4	L	1003	MGP	C5-C4-N3	-5.01	118.69	128.15
4	C	1003	MGP	C5-C4-N3	-4.99	118.72	128.15
4	K	1003	MGP	C5-C4-N3	-4.99	118.72	128.15
4	J	1003	MGP	C5-C4-N3	-4.98	118.74	128.15
4	A	1003	MGP	C5-C4-N3	-4.98	118.75	128.15
4	H	1003	MGP	C5-C4-N3	-4.97	118.75	128.15
4	B	1003	MGP	C5-C4-N3	-4.97	118.75	128.15
4	D	1003	MGP	C5-C4-N3	-4.97	118.77	128.15
4	E	1003	MGP	C5-C4-N3	-4.96	118.77	128.15
4	I	1003	MGP	C5-C4-N3	-4.96	118.78	128.15
4	F	1003	MGP	C5-C4-N3	-4.95	118.79	128.15
4	G	1003	MGP	C5-C4-N3	-4.93	118.83	128.15
3	E	1002	SAH	C5-C4-N3	-4.74	120.19	126.72
3	G	1002	SAH	C5-C4-N3	-4.73	120.20	126.72
3	D	1002	SAH	C5-C4-N3	-4.73	120.20	126.72
3	H	1002	SAH	C5-C4-N3	-4.71	120.23	126.72
3	C	1002	SAH	C5-C4-N3	-4.71	120.23	126.72
3	L	1002	SAH	C5-C4-N3	-4.70	120.24	126.72
3	B	1002	SAH	C5-C4-N3	-4.70	120.25	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1002	SAH	C5-C4-N3	-4.69	120.26	126.72
3	A	1002	SAH	C5-C4-N3	-4.68	120.27	126.72
4	C	1003	MGP	C2-N3-C4	4.68	120.36	112.30
4	K	1003	MGP	C2-N3-C4	4.68	120.36	112.30
4	L	1003	MGP	C2-N3-C4	4.68	120.35	112.30
4	B	1003	MGP	C2-N3-C4	4.67	120.35	112.30
3	J	1002	SAH	C5-C4-N3	-4.67	120.28	126.72
3	F	1002	SAH	C5-C4-N3	-4.67	120.29	126.72
4	A	1003	MGP	C2-N3-C4	4.66	120.33	112.30
3	K	1002	SAH	C5-C4-N3	-4.65	120.32	126.72
4	D	1003	MGP	C2-N3-C4	4.64	120.29	112.30
4	H	1003	MGP	C2-N3-C4	4.63	120.28	112.30
4	J	1003	MGP	C2-N3-C4	4.63	120.27	112.30
4	F	1003	MGP	C2-N3-C4	4.62	120.25	112.30
4	G	1003	MGP	C2-N3-C4	4.62	120.25	112.30
4	E	1003	MGP	C2-N3-C4	4.62	120.25	112.30
4	I	1003	MGP	C2-N3-C4	4.60	120.23	112.30
3	K	1002	SAH	N9-C8-N7	-3.91	108.39	113.94
3	C	1002	SAH	N9-C8-N7	-3.90	108.40	113.94
3	B	1002	SAH	N9-C8-N7	-3.89	108.41	113.94
3	I	1002	SAH	N9-C8-N7	-3.89	108.42	113.94
3	J	1002	SAH	N9-C8-N7	-3.88	108.43	113.94
3	D	1002	SAH	N9-C8-N7	-3.88	108.43	113.94
3	F	1002	SAH	N9-C8-N7	-3.88	108.44	113.94
3	A	1002	SAH	N9-C8-N7	-3.87	108.44	113.94
3	G	1002	SAH	N9-C8-N7	-3.87	108.44	113.94
3	H	1002	SAH	N9-C8-N7	-3.85	108.48	113.94
3	L	1002	SAH	N9-C8-N7	-3.84	108.48	113.94
3	E	1002	SAH	N9-C8-N7	-3.84	108.48	113.94
3	E	1002	SAH	C2-N3-C4	3.67	120.78	111.83
3	D	1002	SAH	C2-N3-C4	3.66	120.76	111.83
3	G	1002	SAH	C2-N3-C4	3.65	120.74	111.83
3	B	1002	SAH	C2-N3-C4	3.64	120.71	111.83
3	I	1002	SAH	C2-N3-C4	3.63	120.71	111.83
3	L	1002	SAH	C2-N3-C4	3.63	120.71	111.83
3	H	1002	SAH	C2-N3-C4	3.63	120.70	111.83
3	C	1002	SAH	C2-N3-C4	3.63	120.69	111.83
3	A	1002	SAH	C2-N3-C4	3.63	120.69	111.83
3	K	1002	SAH	C2-N3-C4	3.61	120.65	111.83
3	J	1002	SAH	C2-N3-C4	3.61	120.64	111.83
3	F	1002	SAH	C2-N3-C4	3.60	120.63	111.83
3	C	1002	SAH	C5-N7-C8	3.56	109.04	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1002	SAH	C5-N7-C8	3.54	109.02	103.45
3	K	1002	SAH	C5-N7-C8	3.53	109.00	103.45
3	I	1002	SAH	C5-N7-C8	3.53	109.00	103.45
3	A	1002	SAH	C5-N7-C8	3.53	109.00	103.45
3	B	1002	SAH	C5-N7-C8	3.53	109.00	103.45
3	D	1002	SAH	C5-N7-C8	3.52	108.97	103.45
3	L	1002	SAH	C5-N7-C8	3.52	108.97	103.45
3	H	1002	SAH	C5-N7-C8	3.50	108.96	103.45
3	E	1002	SAH	C5-N7-C8	3.50	108.96	103.45
3	J	1002	SAH	C5-N7-C8	3.50	108.94	103.45
3	G	1002	SAH	C5-N7-C8	3.48	108.92	103.45
3	J	1002	SAH	C5'-SD-CG	-3.15	92.91	102.26
3	C	1002	SAH	C5'-SD-CG	-3.15	92.91	102.26
3	E	1002	SAH	C5'-SD-CG	-3.15	92.91	102.26
3	L	1002	SAH	C5'-SD-CG	-3.14	92.94	102.26
3	K	1002	SAH	C5'-SD-CG	-3.14	92.94	102.26
3	G	1002	SAH	C5'-SD-CG	-3.14	92.94	102.26
3	B	1002	SAH	C5'-SD-CG	-3.14	92.94	102.26
3	D	1002	SAH	C5'-SD-CG	-3.13	92.96	102.26
3	A	1002	SAH	C5'-SD-CG	-3.13	92.96	102.26
3	F	1002	SAH	C5'-SD-CG	-3.13	92.97	102.26
3	H	1002	SAH	C5'-SD-CG	-3.13	92.97	102.26
3	I	1002	SAH	C5'-SD-CG	-3.13	92.99	102.26
3	B	1002	SAH	O4'-C1'-N9	2.83	113.53	108.09
3	G	1002	SAH	N3-C4-N9	2.82	131.96	127.17
3	A	1002	SAH	O4'-C1'-N9	2.82	113.50	108.09
3	D	1002	SAH	O4'-C1'-N9	2.82	113.50	108.09
3	C	1002	SAH	O4'-C1'-N9	2.81	113.49	108.09
3	C	1002	SAH	C4-C5-N7	-2.81	107.36	110.58
3	H	1002	SAH	O4'-C1'-N9	2.81	113.49	108.09
3	I	1002	SAH	O4'-C1'-N9	2.81	113.49	108.09
3	L	1002	SAH	O4'-C1'-N9	2.81	113.48	108.09
3	E	1002	SAH	N3-C4-N9	2.81	131.94	127.17
3	E	1002	SAH	O4'-C1'-N9	2.81	113.48	108.09
3	D	1002	SAH	N3-C4-N9	2.81	131.94	127.17
3	L	1002	SAH	N3-C4-N9	2.80	131.93	127.17
3	K	1002	SAH	O4'-C1'-N9	2.80	113.47	108.09
3	J	1002	SAH	O4'-C1'-N9	2.80	113.46	108.09
3	B	1002	SAH	N3-C4-N9	2.79	131.91	127.17
3	H	1002	SAH	N3-C4-N9	2.79	131.91	127.17
3	F	1002	SAH	O4'-C1'-N9	2.78	113.44	108.09
3	I	1002	SAH	N3-C4-N9	2.78	131.90	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1002	SAH	C4-C5-N7	-2.78	107.41	110.58
3	C	1002	SAH	N3-C4-N9	2.77	131.88	127.17
3	A	1002	SAH	N3-C4-N9	2.76	131.87	127.17
3	I	1002	SAH	C4-C5-N7	-2.76	107.42	110.58
3	H	1002	SAH	C4-C5-N7	-2.76	107.42	110.58
3	K	1002	SAH	C4-C5-N7	-2.76	107.42	110.58
3	G	1002	SAH	O4'-C1'-N9	2.76	113.39	108.09
3	A	1002	SAH	C4-C5-N7	-2.76	107.43	110.58
3	L	1002	SAH	C4-C5-N7	-2.76	107.43	110.58
3	B	1002	SAH	C4-C5-N7	-2.75	107.44	110.58
3	D	1002	SAH	C4-C5-N7	-2.75	107.44	110.58
3	E	1002	SAH	C4-C5-N7	-2.74	107.45	110.58
3	J	1002	SAH	N3-C4-N9	2.74	131.83	127.17
3	F	1002	SAH	N3-C4-N9	2.73	131.81	127.17
3	J	1002	SAH	OXT-C-O	-2.73	117.88	124.08
3	K	1002	SAH	OXT-C-O	-2.73	117.88	124.08
3	H	1002	SAH	OXT-C-O	-2.73	117.89	124.08
3	I	1002	SAH	OXT-C-O	-2.73	117.89	124.08
3	B	1002	SAH	OXT-C-O	-2.73	117.89	124.08
3	J	1002	SAH	C4-C5-N7	-2.73	107.46	110.58
3	D	1002	SAH	OXT-C-O	-2.73	117.90	124.08
3	K	1002	SAH	N3-C4-N9	2.72	131.79	127.17
3	L	1002	SAH	OXT-C-O	-2.72	117.91	124.08
3	G	1002	SAH	C4-C5-N7	-2.71	107.48	110.58
3	F	1002	SAH	OXT-C-O	-2.71	117.92	124.08
3	A	1002	SAH	OXT-C-O	-2.71	117.94	124.08
3	E	1002	SAH	OXT-C-O	-2.70	117.95	124.08
4	D	1003	MGP	C3'-C2'-C1'	2.70	106.56	101.46
3	C	1002	SAH	OXT-C-O	-2.70	117.96	124.08
4	E	1003	MGP	C3'-C2'-C1'	2.69	106.56	101.46
4	I	1003	MGP	C3'-C2'-C1'	2.69	106.55	101.46
4	F	1003	MGP	C3'-C2'-C1'	2.68	106.54	101.46
4	B	1003	MGP	C3'-C2'-C1'	2.68	106.54	101.46
3	G	1002	SAH	OXT-C-O	-2.68	117.99	124.08
4	J	1003	MGP	C3'-C2'-C1'	2.68	106.54	101.46
4	H	1003	MGP	C3'-C2'-C1'	2.68	106.54	101.46
4	L	1003	MGP	C3'-C2'-C1'	2.68	106.53	101.46
4	G	1003	MGP	C3'-C2'-C1'	2.68	106.53	101.46
4	A	1003	MGP	C3'-C2'-C1'	2.68	106.53	101.46
4	K	1003	MGP	C3'-C2'-C1'	2.68	106.53	101.46
4	C	1003	MGP	C3'-C2'-C1'	2.64	106.46	101.46
4	C	1003	MGP	CM7-N7-C5	2.47	129.87	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1003	MGP	C5-C6-N1	2.46	116.92	111.84
4	C	1003	MGP	C5-C6-N1	2.45	116.91	111.84
4	A	1003	MGP	CM7-N7-C5	2.45	129.85	126.80
4	D	1003	MGP	CM7-N7-C5	2.45	129.85	126.80
4	E	1003	MGP	CM7-N7-C5	2.44	129.84	126.80
4	D	1003	MGP	C5-C6-N1	2.44	116.88	111.84
4	L	1003	MGP	C5-C6-N1	2.44	116.88	111.84
4	I	1003	MGP	CM7-N7-C5	2.44	129.83	126.80
4	A	1003	MGP	C5-C6-N1	2.43	116.87	111.84
4	F	1003	MGP	C5-C6-N1	2.43	116.87	111.84
4	K	1003	MGP	C5-C6-N1	2.43	116.87	111.84
4	J	1003	MGP	C5-C6-N1	2.43	116.87	111.84
4	H	1003	MGP	C5-C6-N1	2.43	116.86	111.84
4	L	1003	MGP	CM7-N7-C5	2.42	129.82	126.80
4	G	1003	MGP	C5-C6-N1	2.42	116.84	111.84
4	E	1003	MGP	C5-C6-N1	2.42	116.84	111.84
4	I	1003	MGP	C5-C6-N1	2.41	116.83	111.84
4	J	1003	MGP	CM7-N7-C5	2.41	129.80	126.80
4	H	1003	MGP	CM7-N7-C5	2.40	129.79	126.80
4	B	1003	MGP	CM7-N7-C5	2.39	129.77	126.80
4	F	1003	MGP	CM7-N7-C5	2.39	129.77	126.80
4	K	1003	MGP	CM7-N7-C5	2.39	129.77	126.80
4	G	1003	MGP	CM7-N7-C5	2.37	129.75	126.80
4	E	1003	MGP	O3B-PB-O2B	-2.28	103.86	110.70
4	B	1003	MGP	O3B-PB-O2B	-2.27	103.87	110.70
4	A	1003	MGP	O3B-PB-O2B	-2.27	103.88	110.70
4	L	1003	MGP	O3B-PB-O2B	-2.27	103.88	110.70
4	C	1003	MGP	O3B-PB-O2B	-2.27	103.89	110.70
4	F	1003	MGP	O3B-PB-O2B	-2.26	103.89	110.70
4	J	1003	MGP	O3B-PB-O2B	-2.26	103.90	110.70
4	H	1003	MGP	O3B-PB-O2B	-2.26	103.90	110.70
4	G	1003	MGP	O3B-PB-O2B	-2.26	103.90	110.70
4	K	1003	MGP	O3B-PB-O2B	-2.26	103.90	110.70
4	I	1003	MGP	O3B-PB-O2B	-2.26	103.91	110.70
4	D	1003	MGP	O3B-PB-O2B	-2.25	103.93	110.70

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	SAH	N-CA-CB-CG
3	A	1002	SAH	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
3	B	1002	SAH	N-CA-CB-CG
3	B	1002	SAH	C-CA-CB-CG
3	C	1002	SAH	N-CA-CB-CG
3	C	1002	SAH	C-CA-CB-CG
3	D	1002	SAH	N-CA-CB-CG
3	D	1002	SAH	C-CA-CB-CG
3	E	1002	SAH	N-CA-CB-CG
3	E	1002	SAH	C-CA-CB-CG
3	F	1002	SAH	N-CA-CB-CG
3	F	1002	SAH	C-CA-CB-CG
3	G	1002	SAH	N-CA-CB-CG
3	G	1002	SAH	C-CA-CB-CG
3	H	1002	SAH	N-CA-CB-CG
3	H	1002	SAH	C-CA-CB-CG
3	I	1002	SAH	N-CA-CB-CG
3	I	1002	SAH	C-CA-CB-CG
3	J	1002	SAH	N-CA-CB-CG
3	J	1002	SAH	C-CA-CB-CG
3	K	1002	SAH	N-CA-CB-CG
3	K	1002	SAH	C-CA-CB-CG
3	L	1002	SAH	N-CA-CB-CG
3	L	1002	SAH	C-CA-CB-CG
3	A	1002	SAH	C2'-C1'-N9-C8
3	B	1002	SAH	C2'-C1'-N9-C8
3	C	1002	SAH	C2'-C1'-N9-C8
3	D	1002	SAH	C2'-C1'-N9-C8
3	E	1002	SAH	C2'-C1'-N9-C8
3	F	1002	SAH	C2'-C1'-N9-C8
3	G	1002	SAH	C2'-C1'-N9-C8
3	H	1002	SAH	C2'-C1'-N9-C8
3	I	1002	SAH	C2'-C1'-N9-C8
3	J	1002	SAH	C2'-C1'-N9-C8
3	K	1002	SAH	C2'-C1'-N9-C8
3	L	1002	SAH	C2'-C1'-N9-C8

There are no ring outliers.

12 monomers are involved in 12 short contacts:

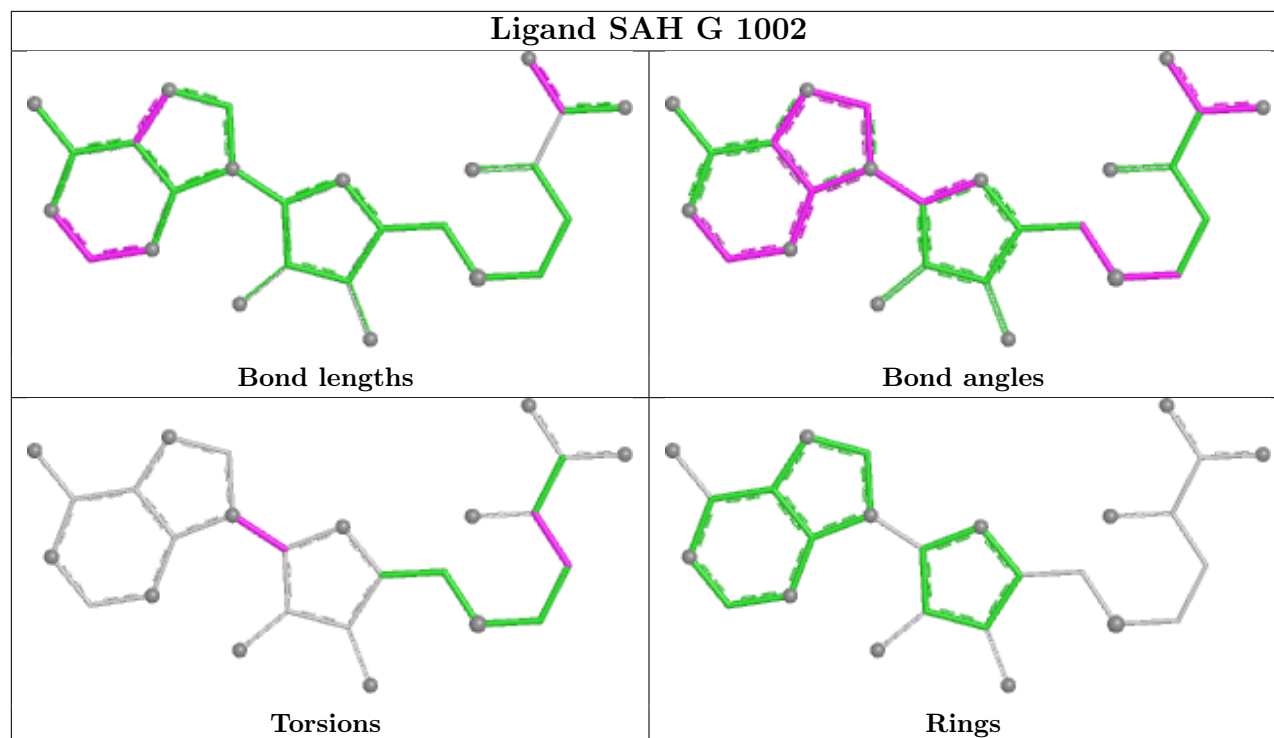
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1002	SAH	1	0
3	D	1002	SAH	1	0
3	C	1002	SAH	1	0

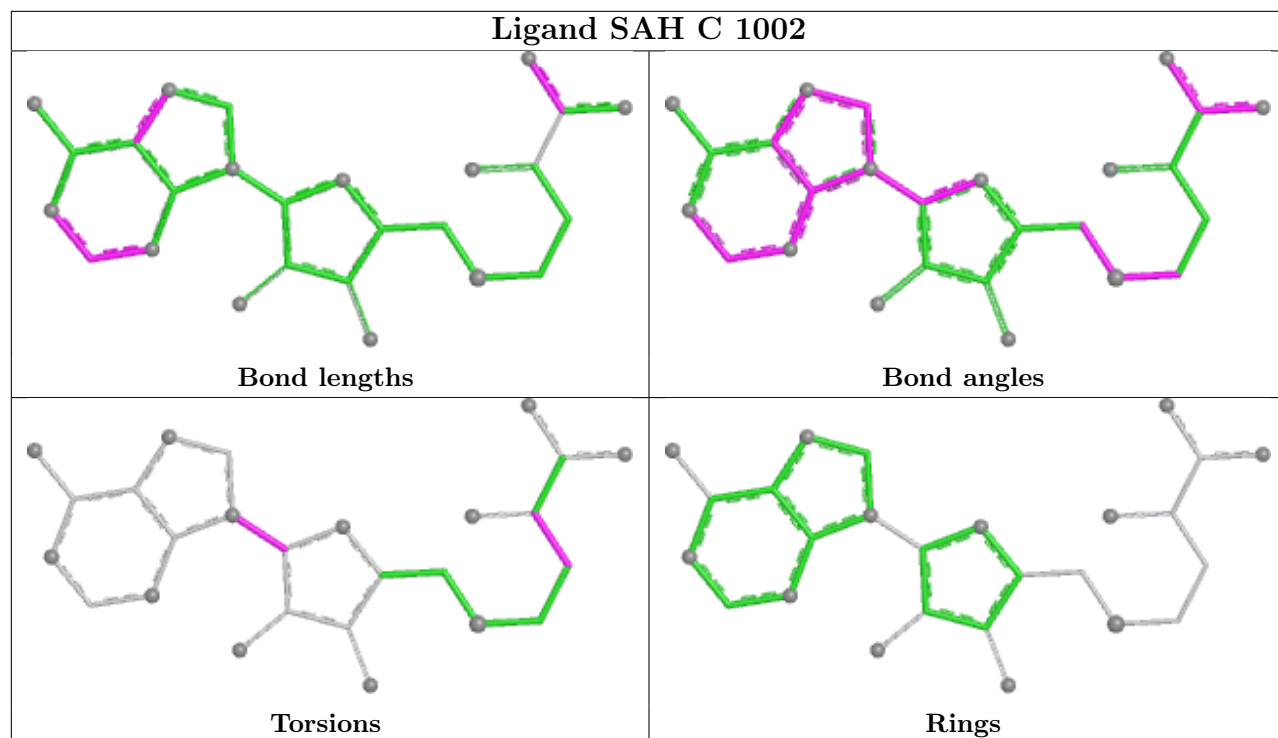
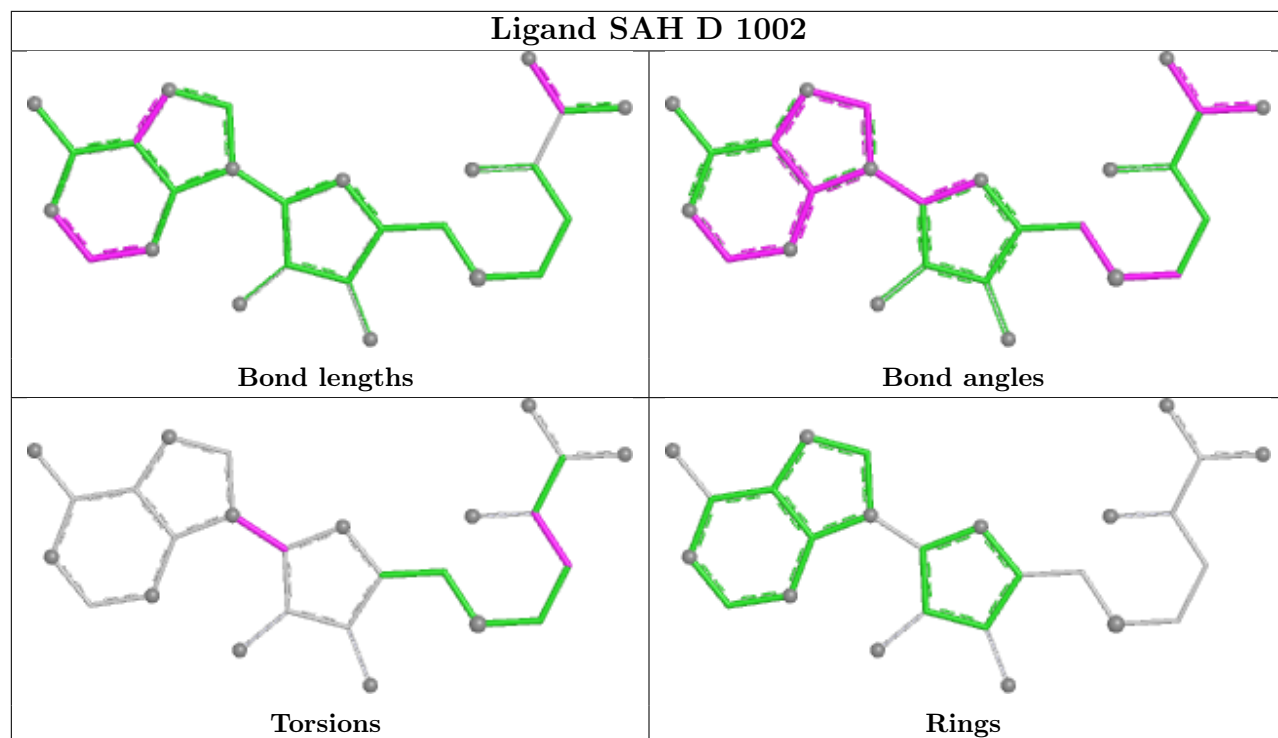
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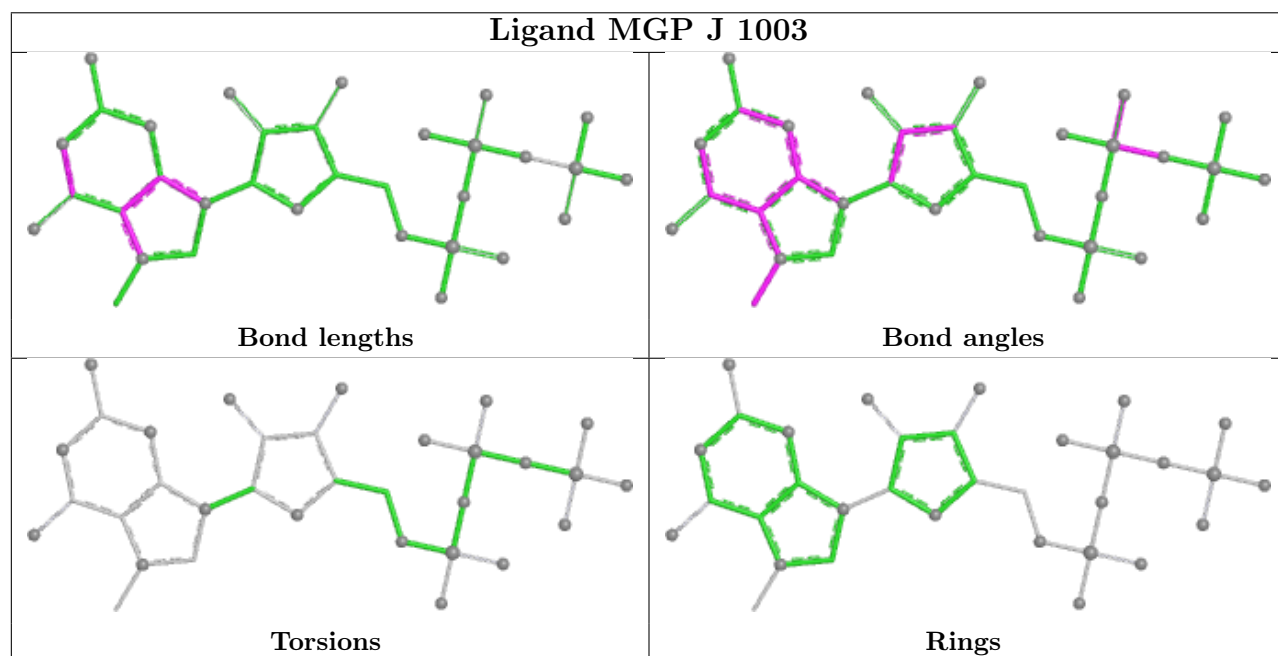
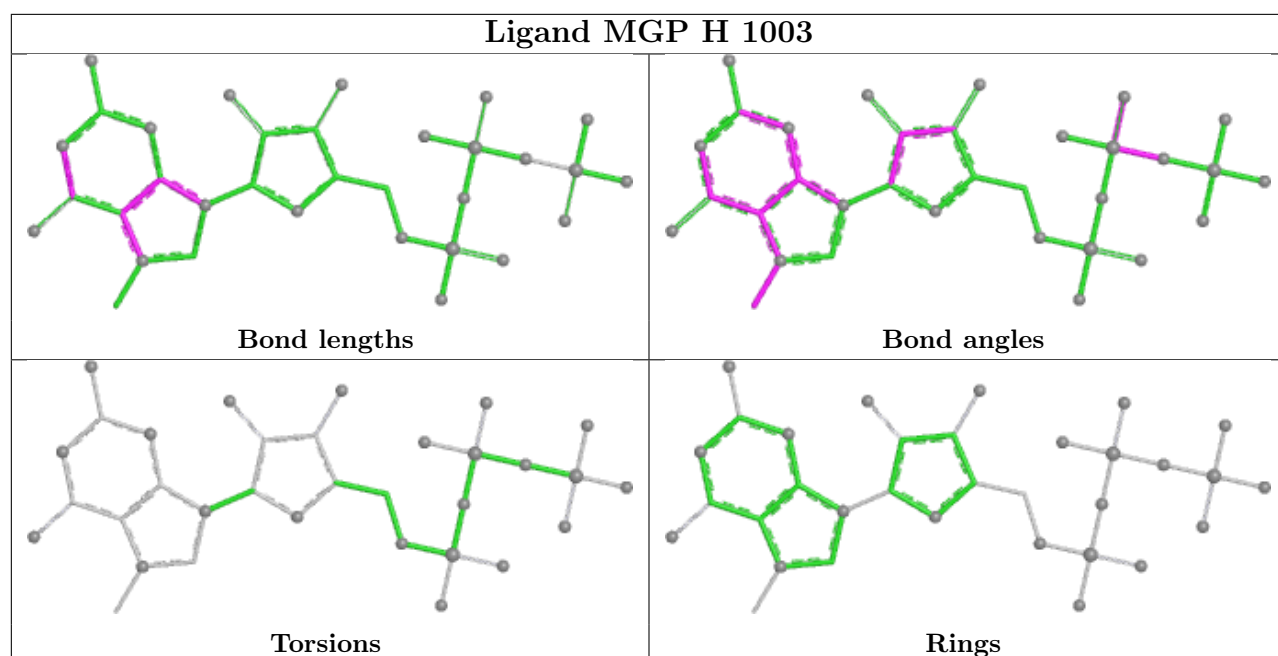
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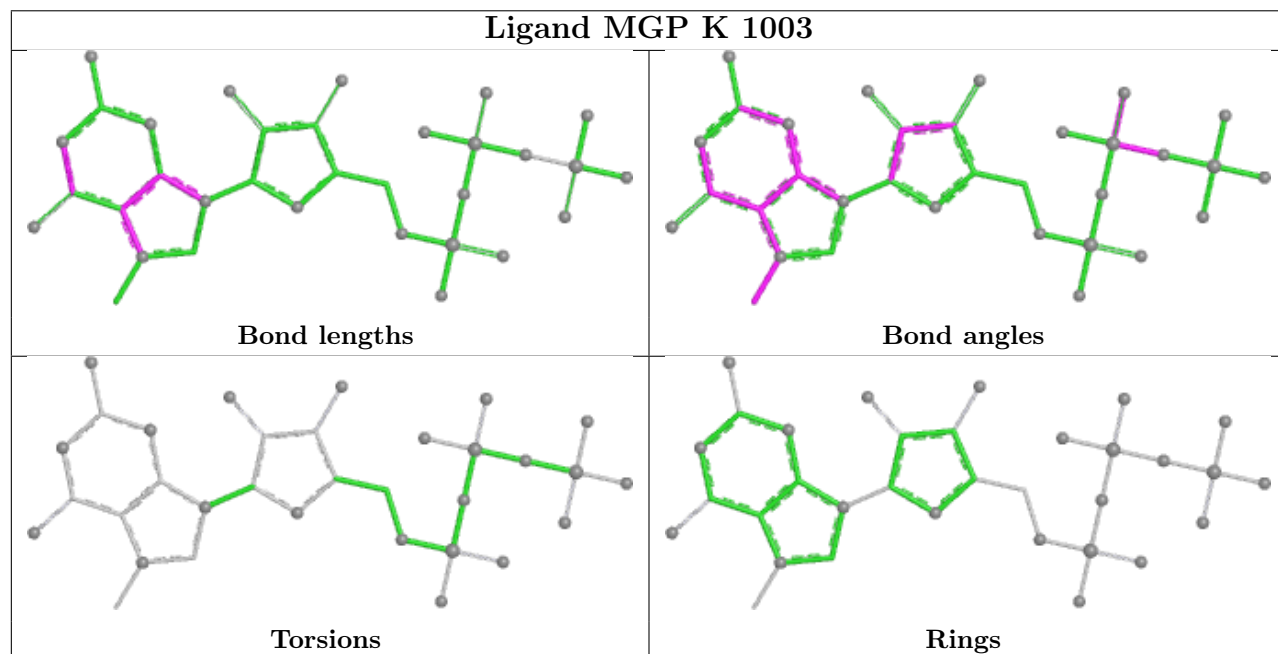
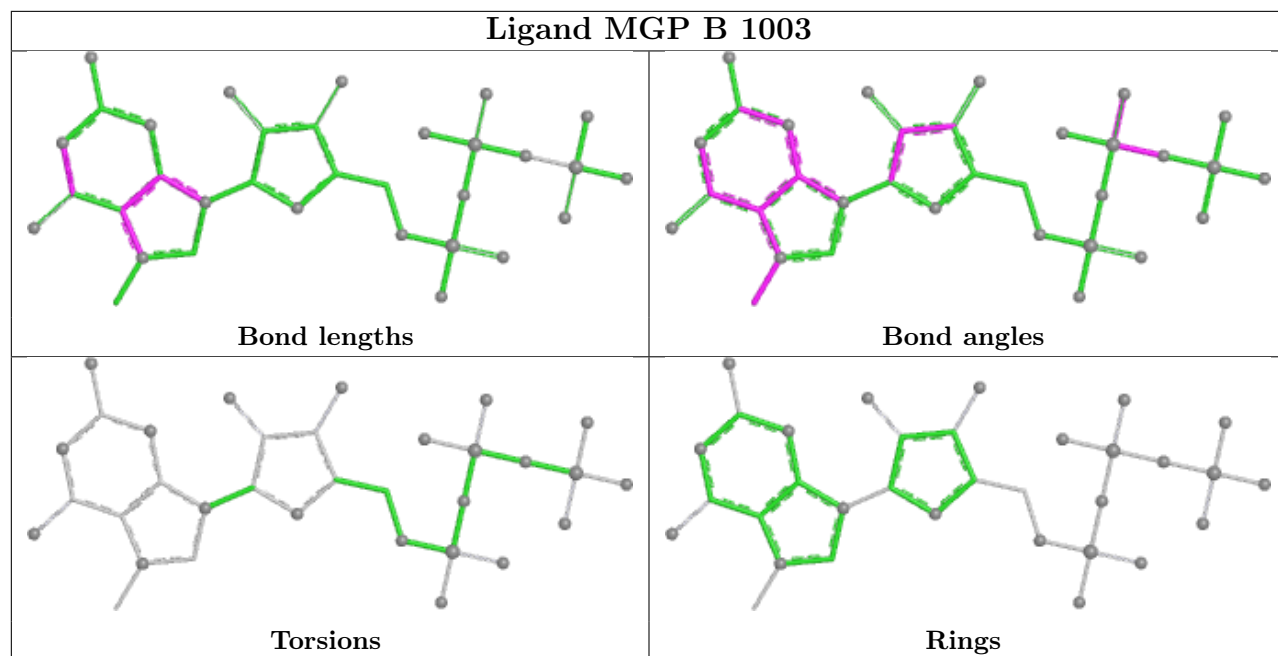
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	1002	SAH	1	0
3	F	1002	SAH	1	0
3	I	1002	SAH	1	0
3	A	1002	SAH	1	0
3	H	1002	SAH	1	0
3	E	1002	SAH	1	0
3	J	1002	SAH	1	0
3	B	1002	SAH	1	0
3	K	1002	SAH	1	0

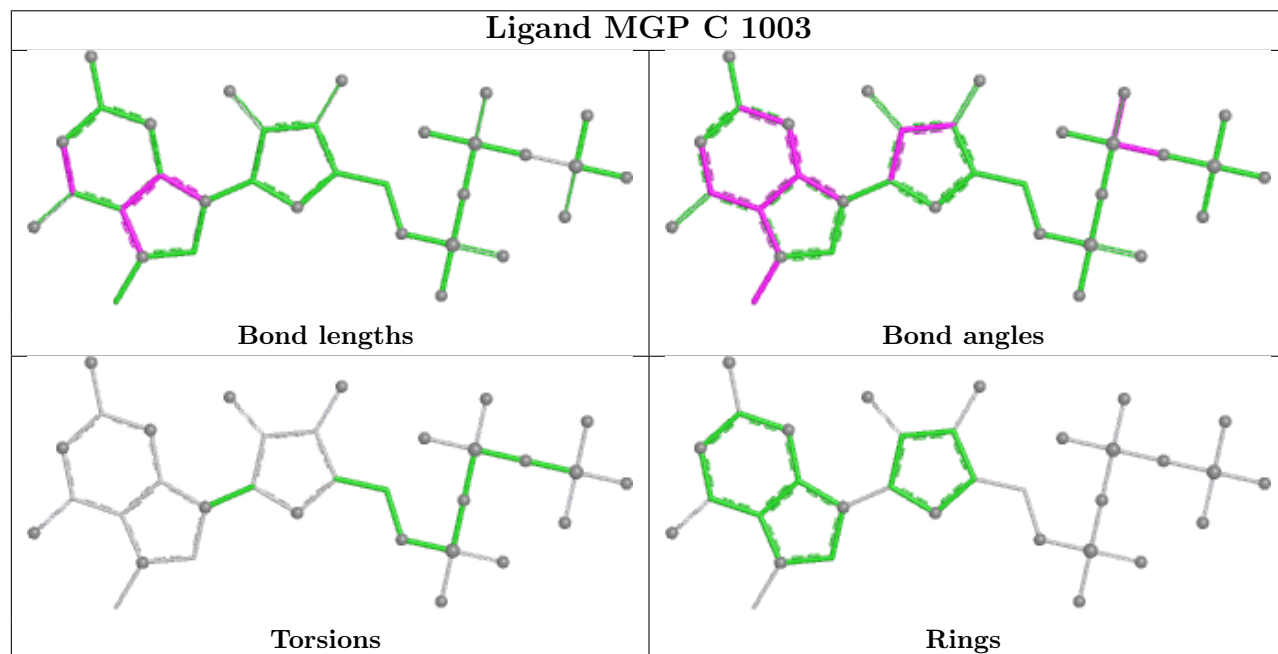
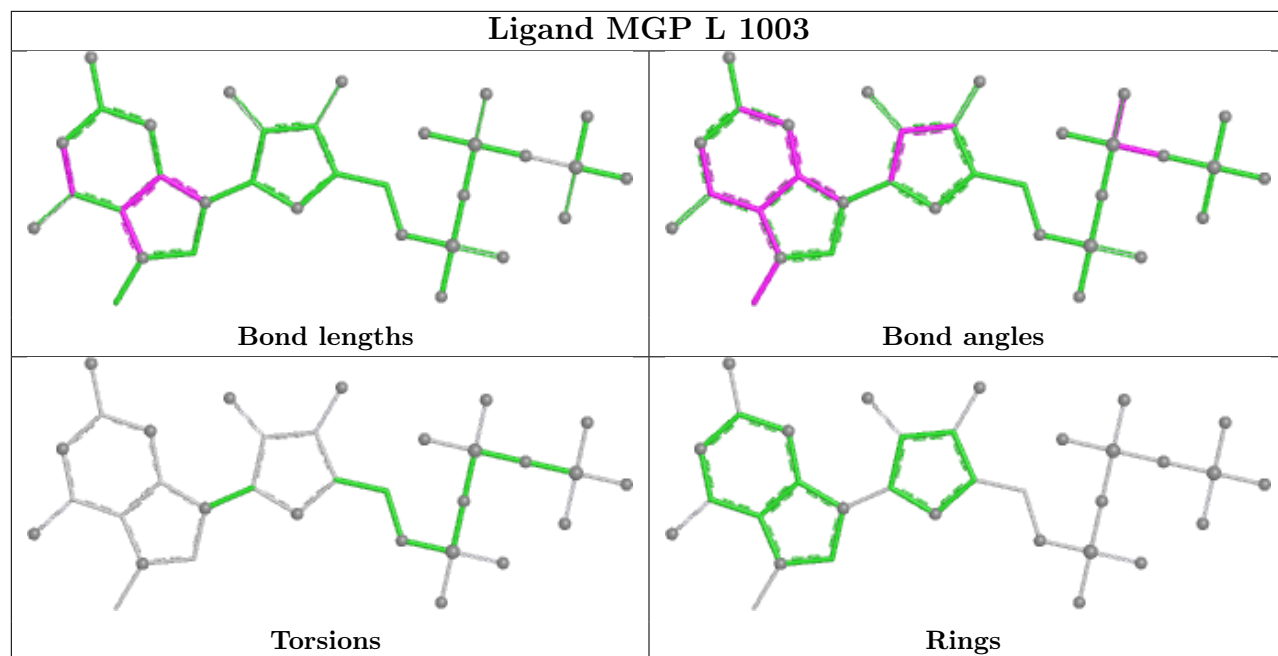
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

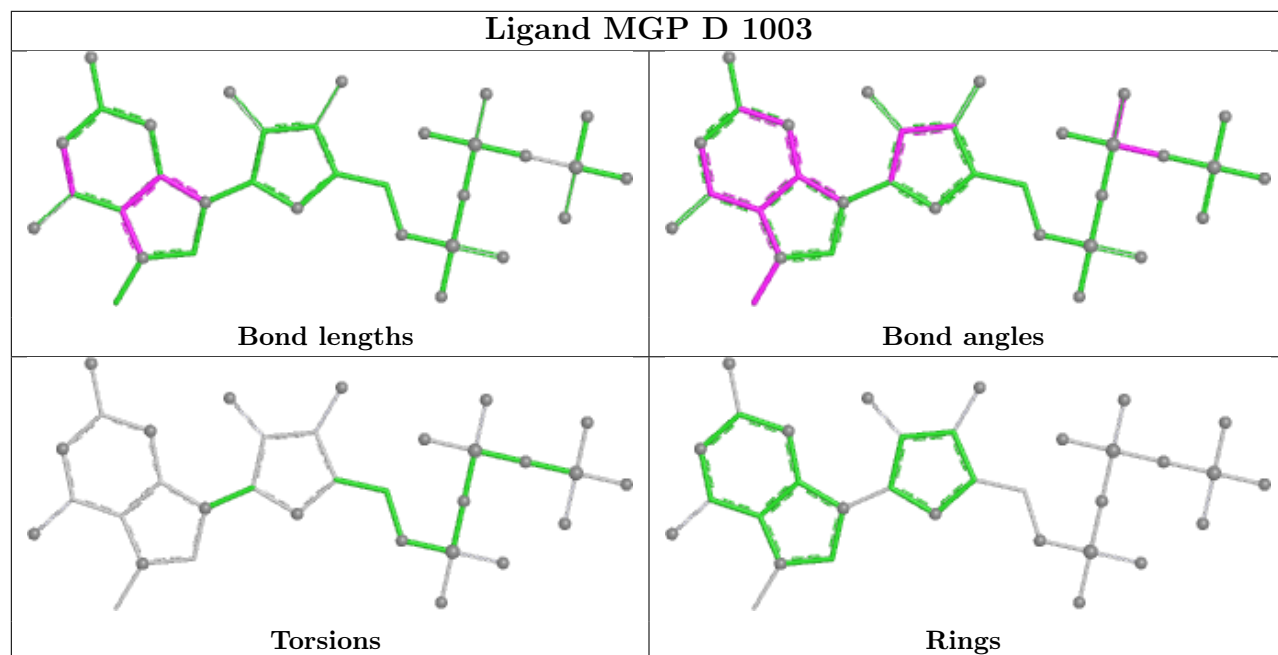
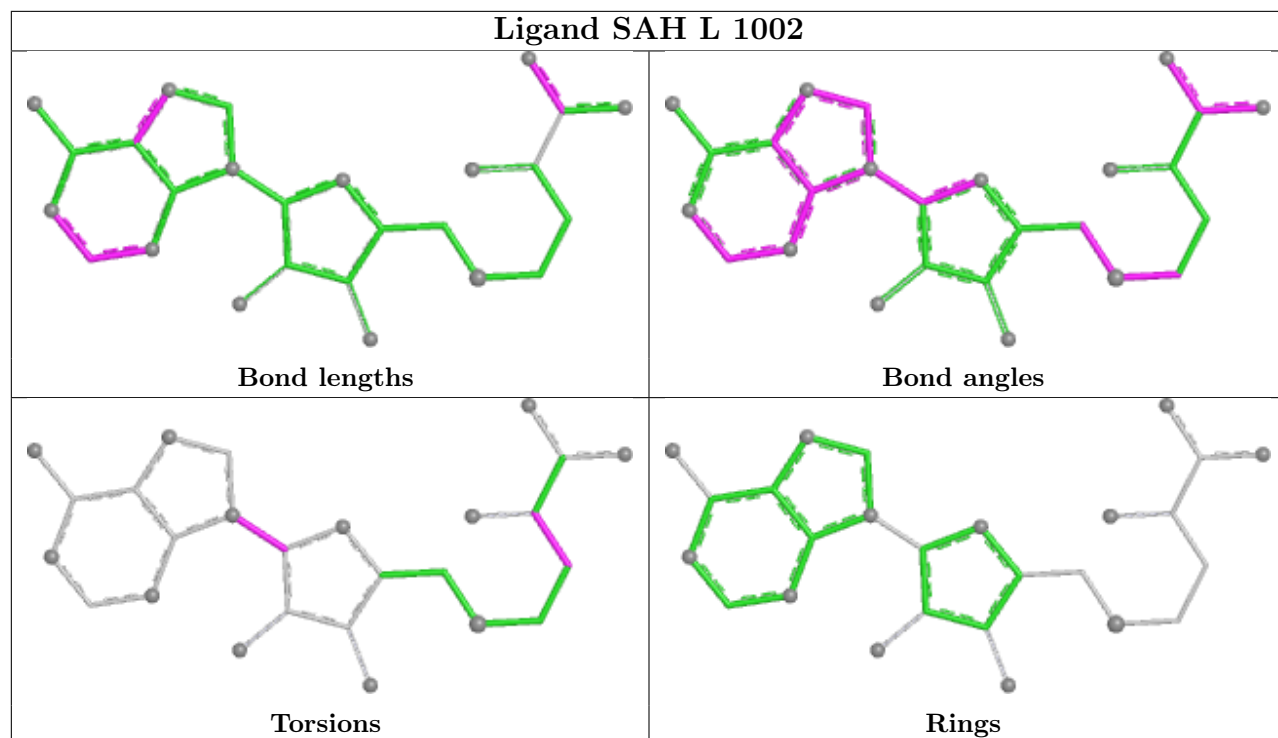


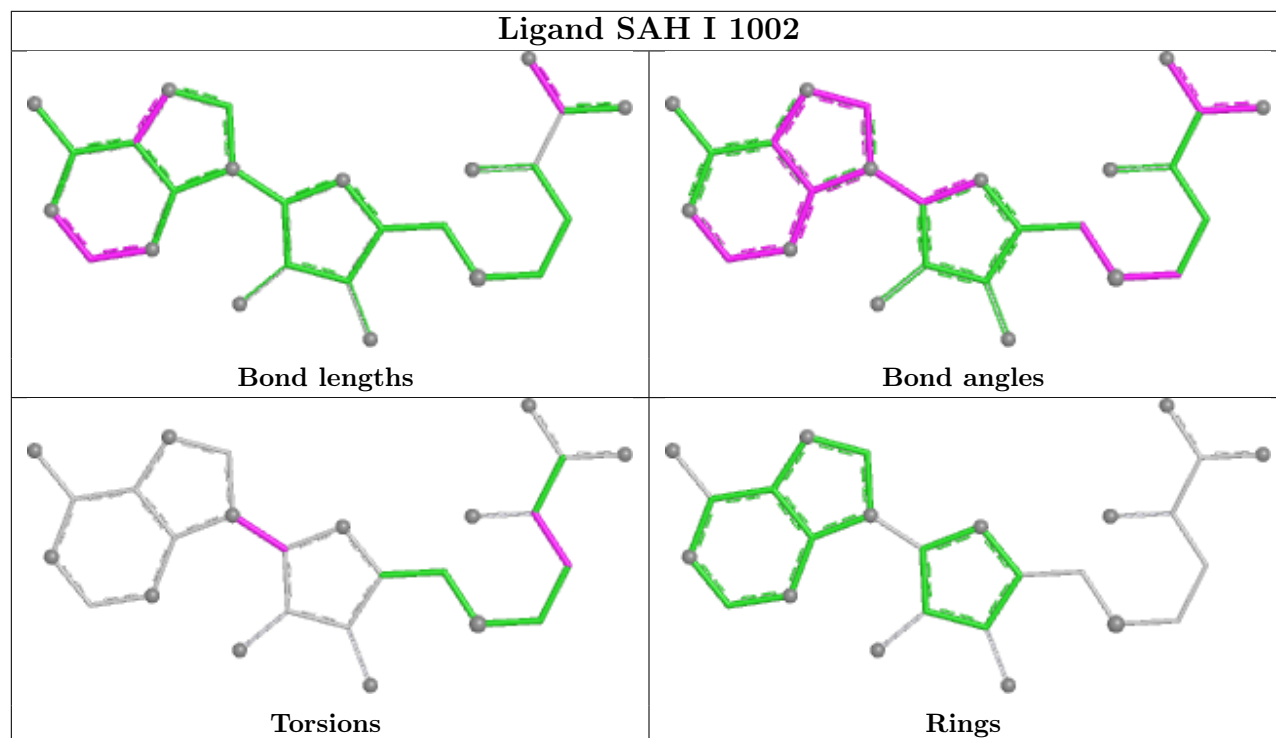
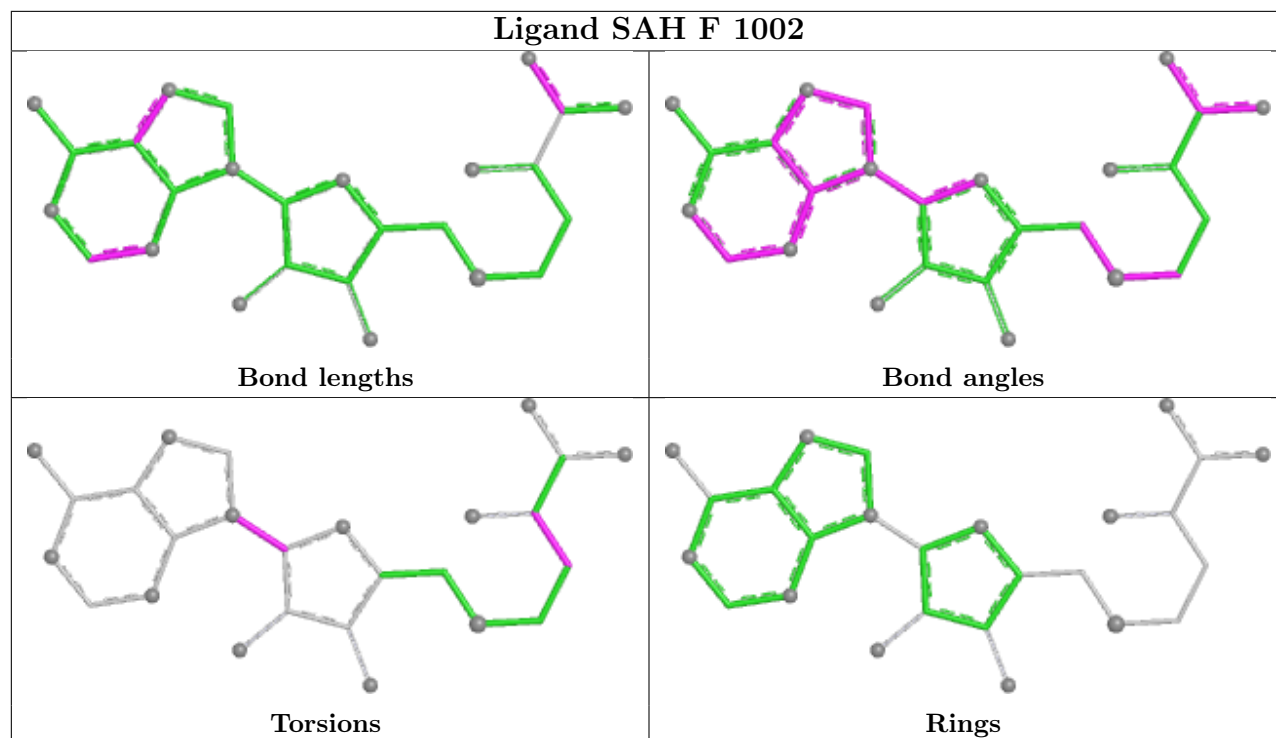




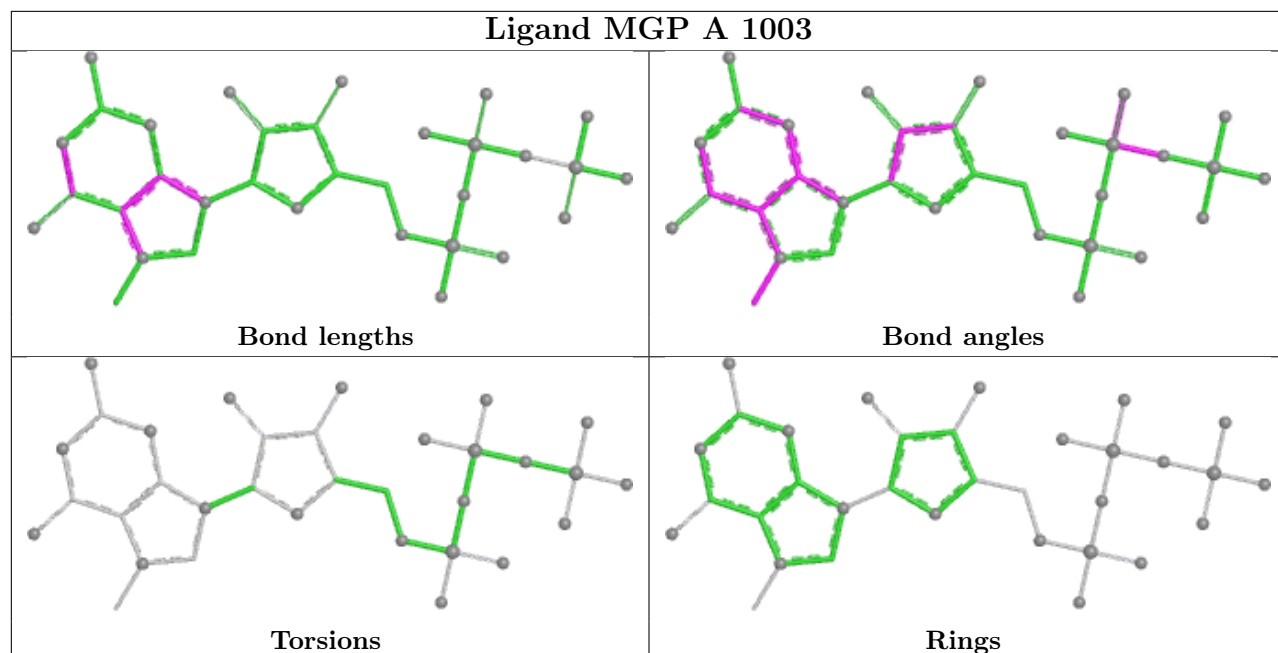




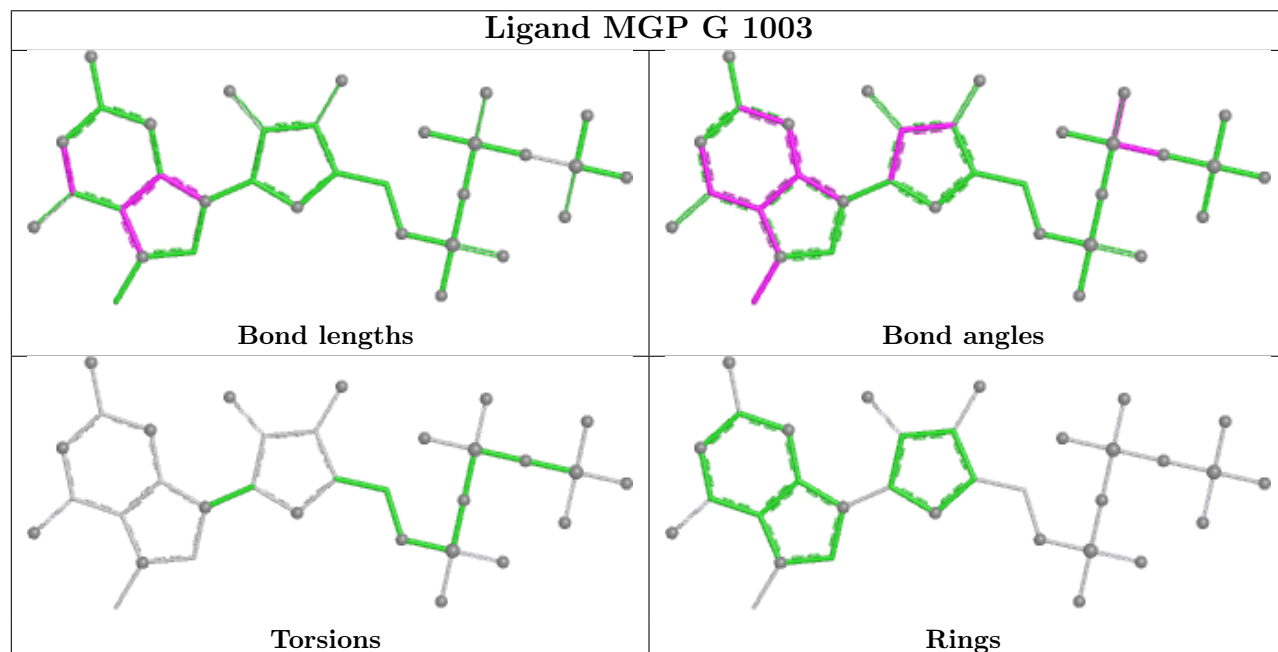


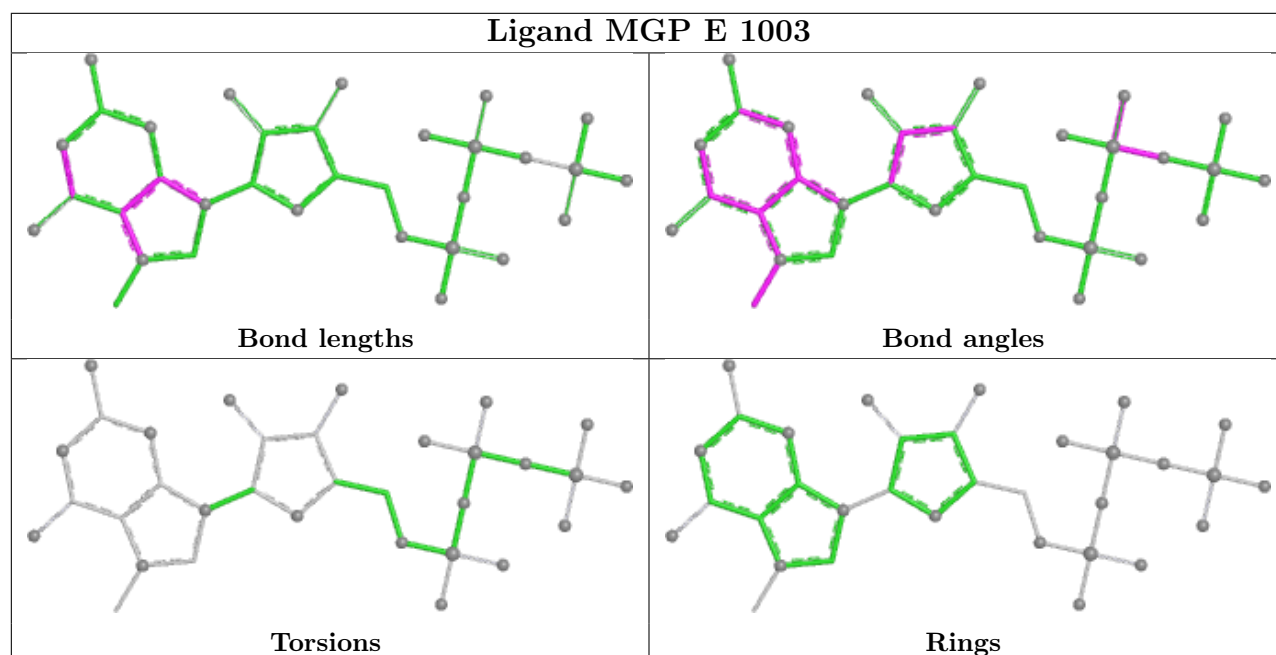
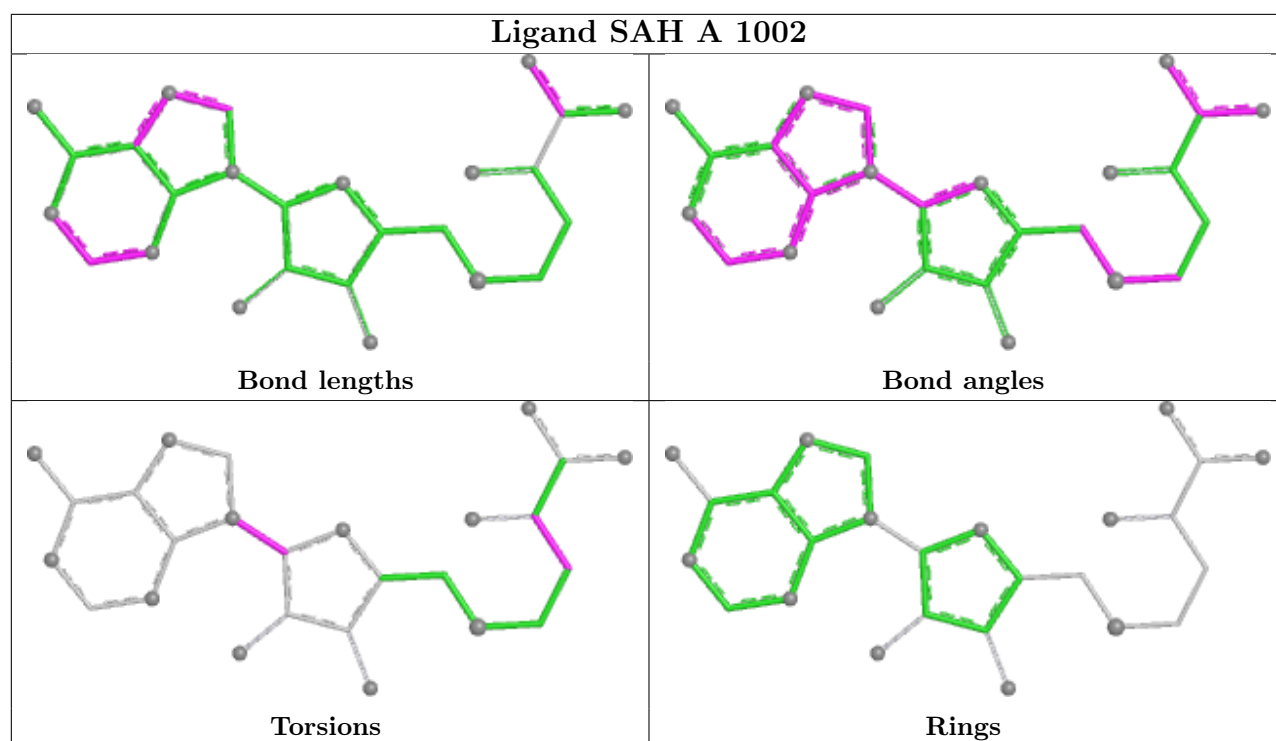


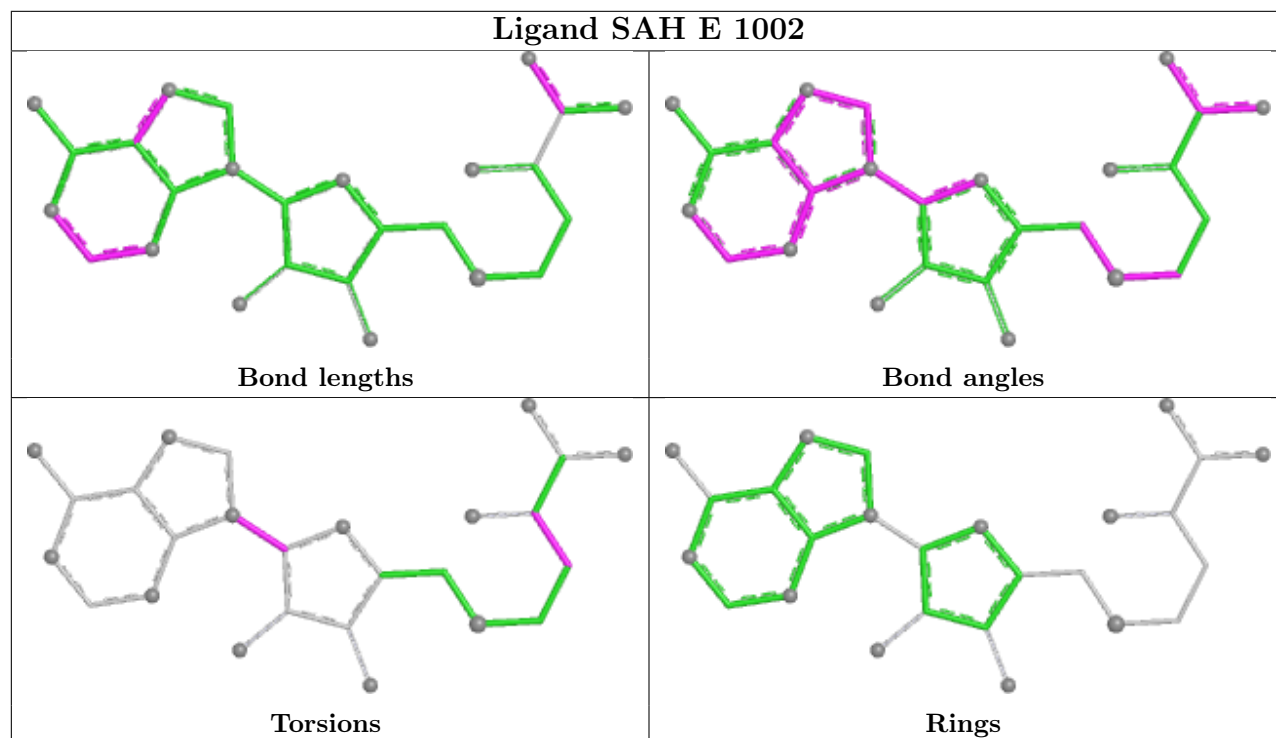
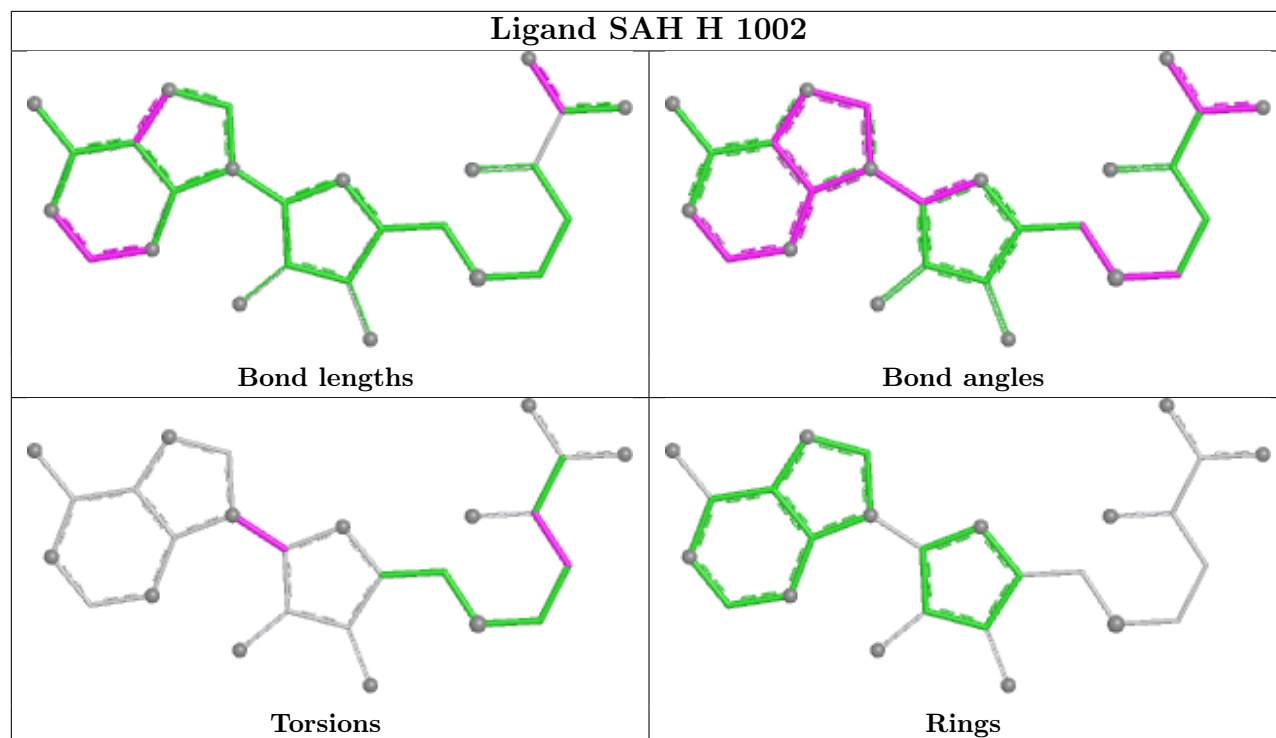
Ligand MGP A 1003

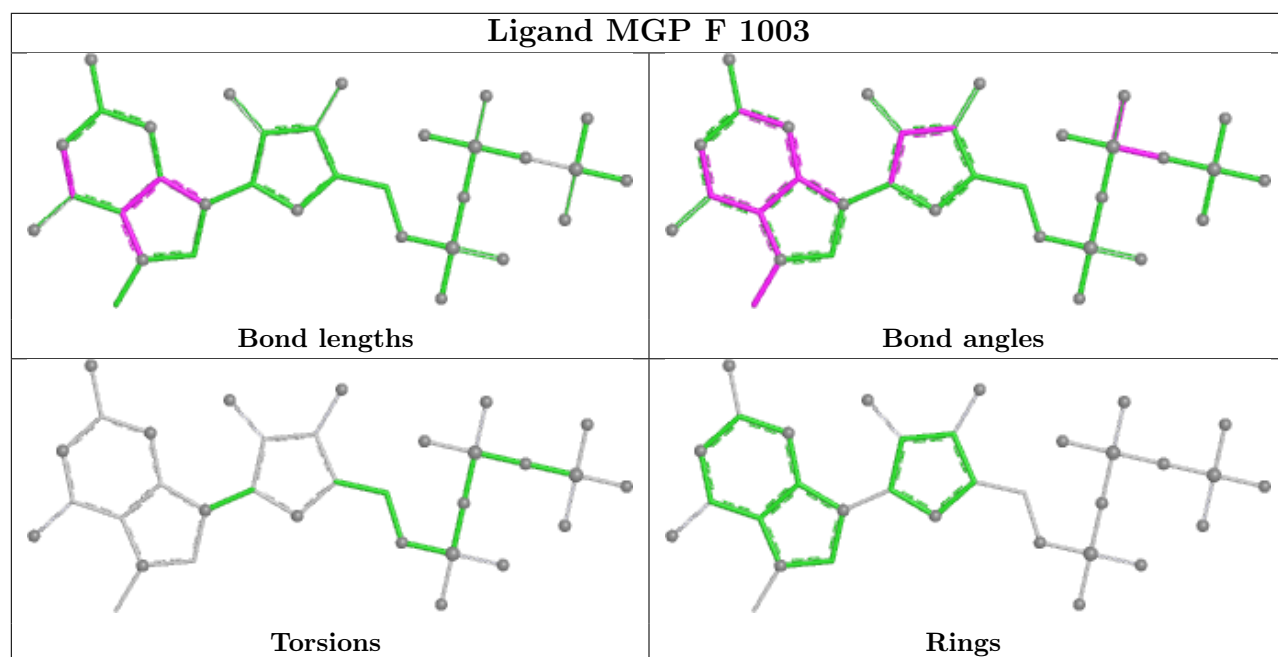
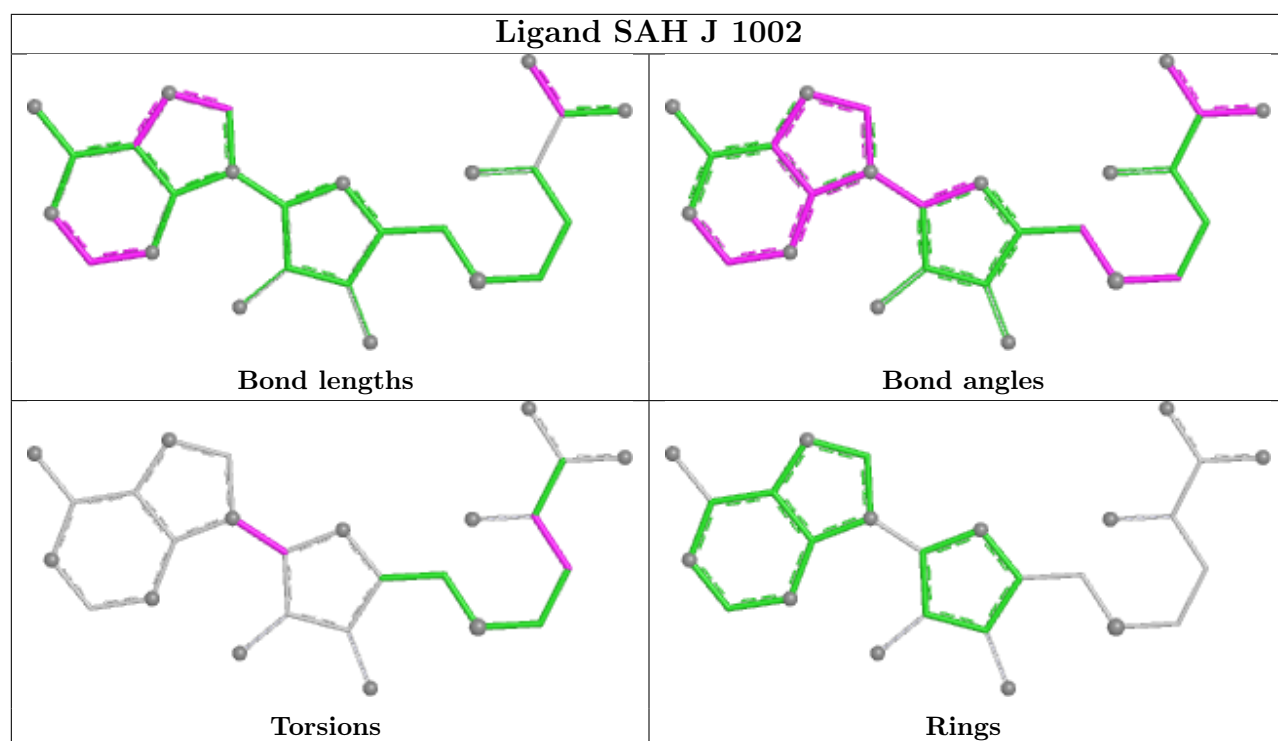


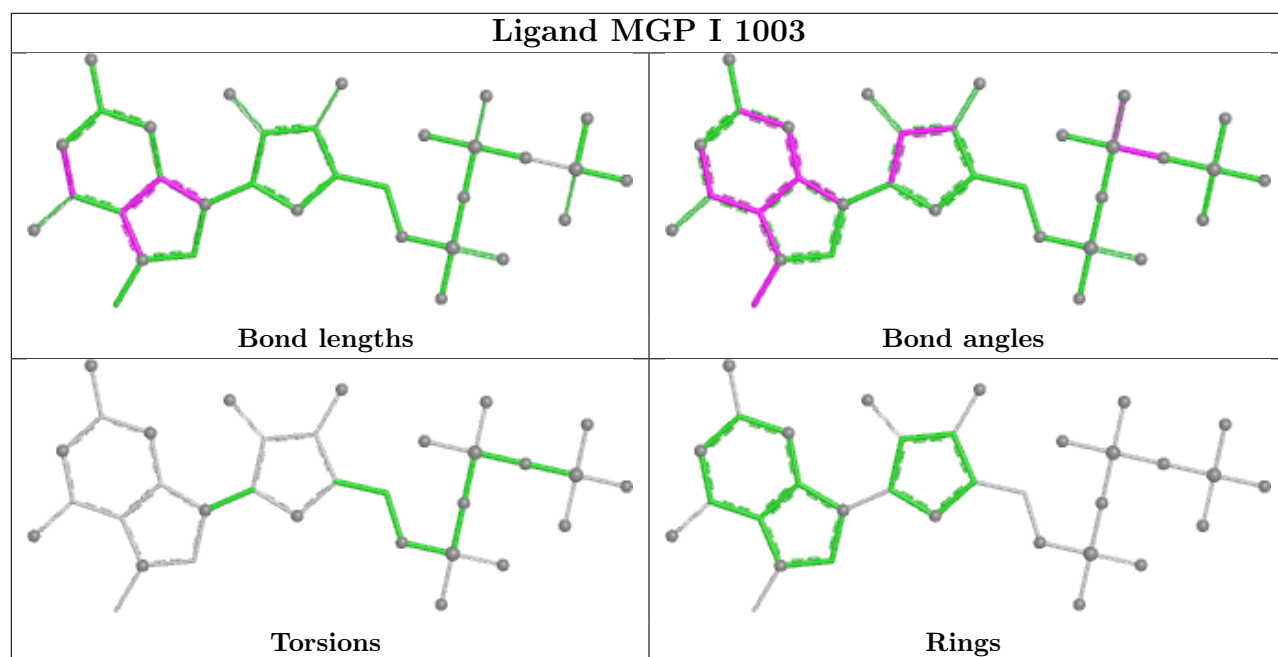
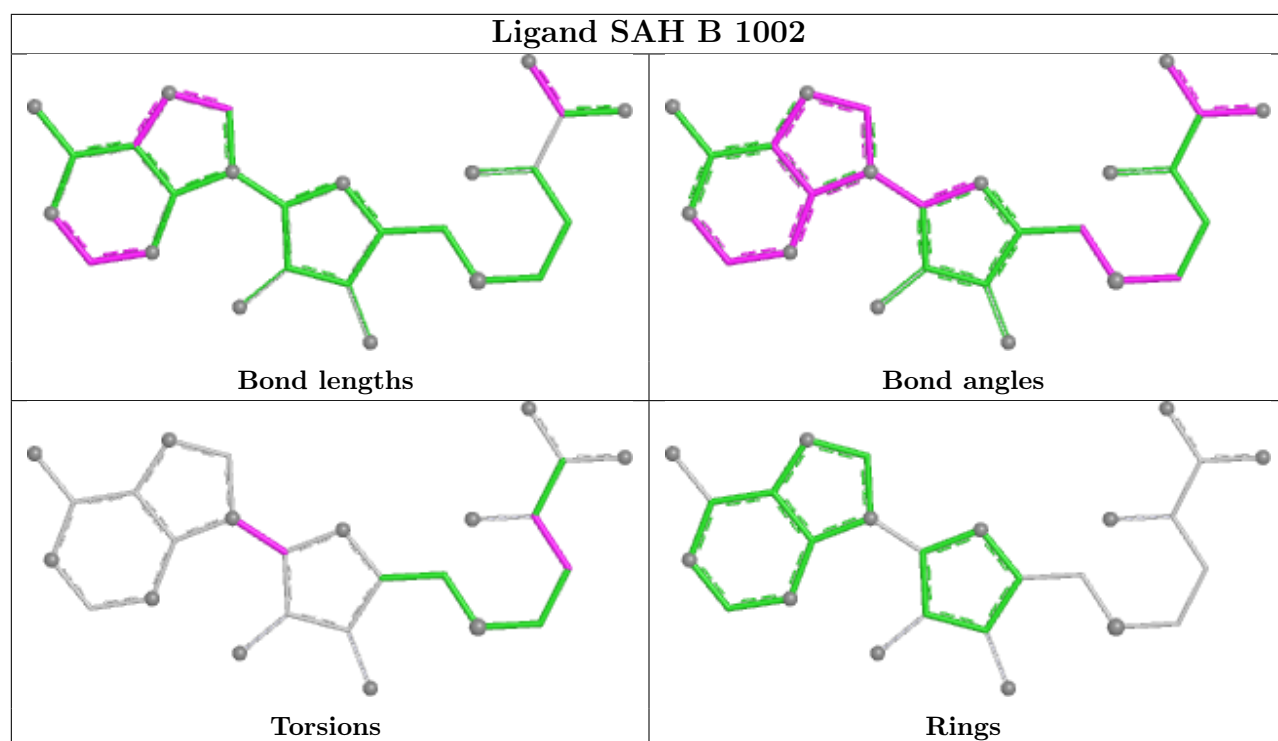
Ligand MGP G 1003

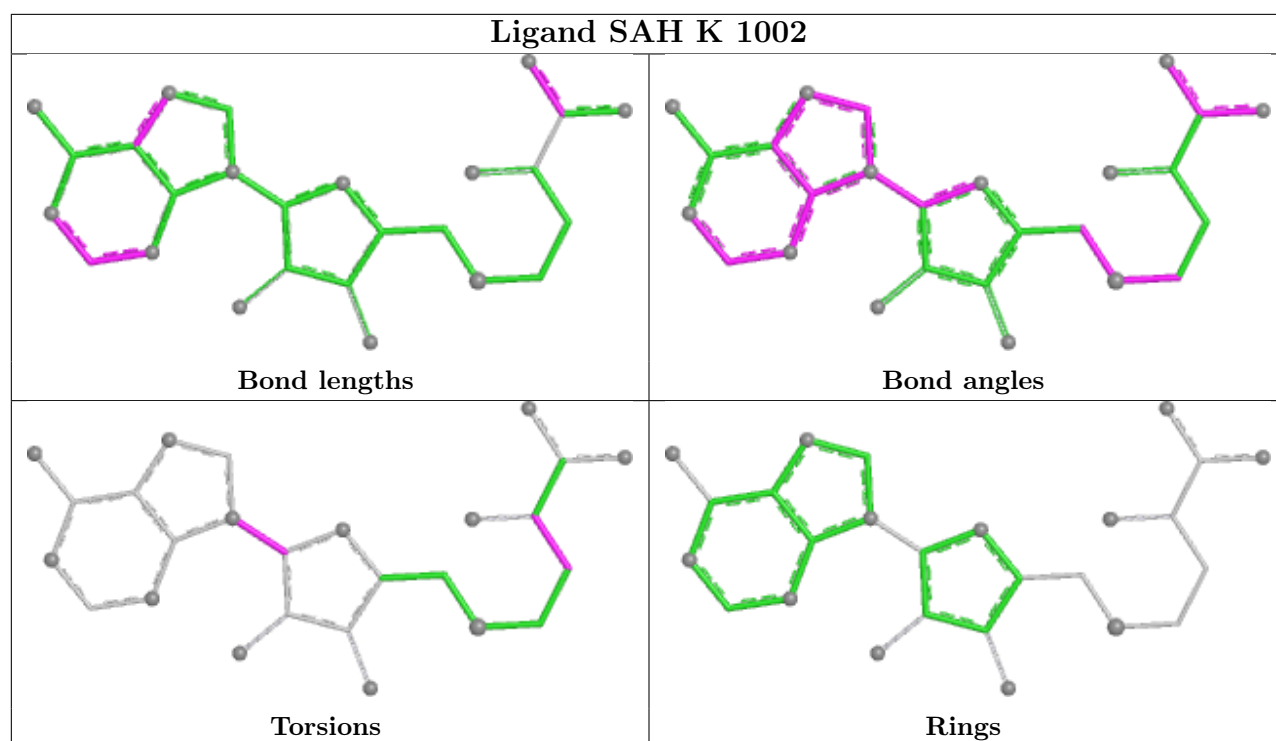












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

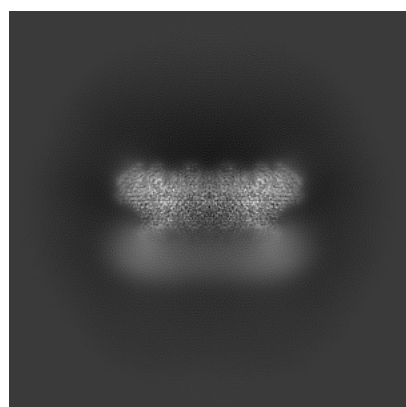
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31580. These allow visual inspection of the internal detail of the map and identification of artifacts.

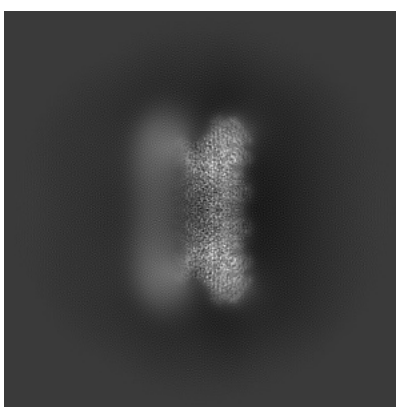
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

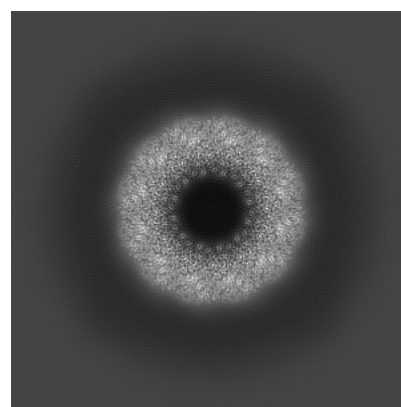
6.1.1 Primary map



X



Y

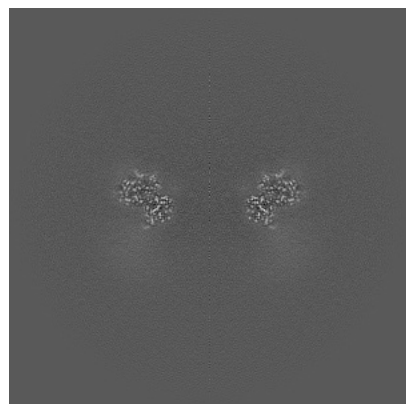


Z

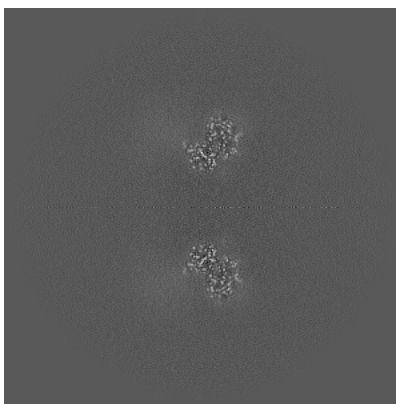
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

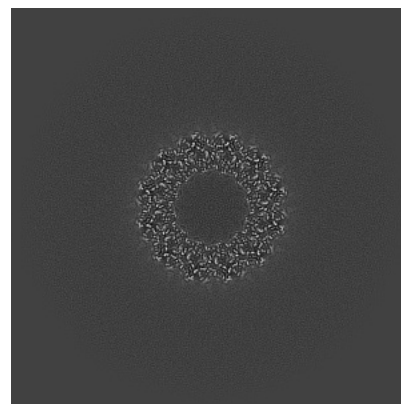
6.2.1 Primary map



X Index: 240



Y Index: 240

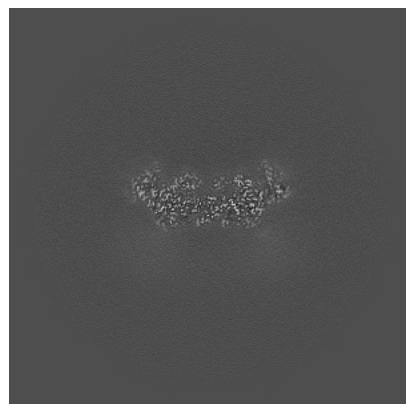


Z Index: 240

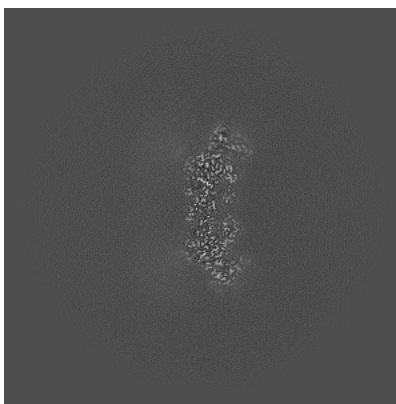
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

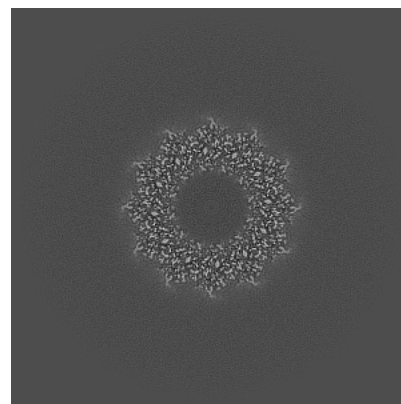
6.3.1 Primary map



X Index: 297



Y Index: 183

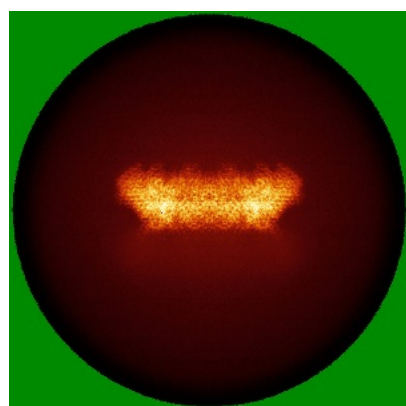


Z Index: 249

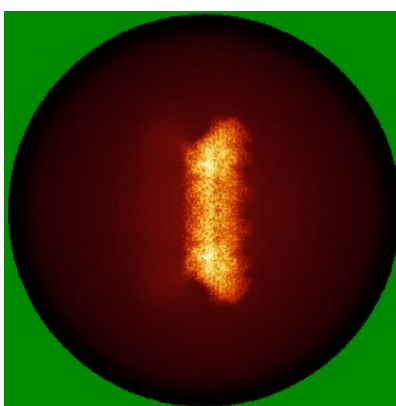
The images above show the largest variance slices of the map in three orthogonal directions.

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

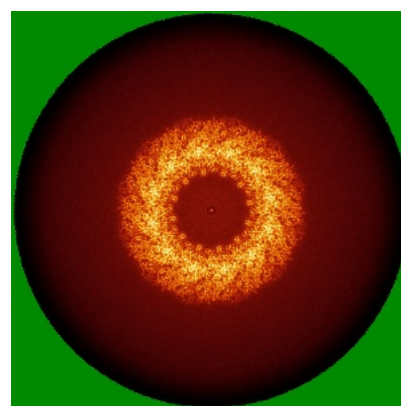
6.4.1 Primary map



X



Y

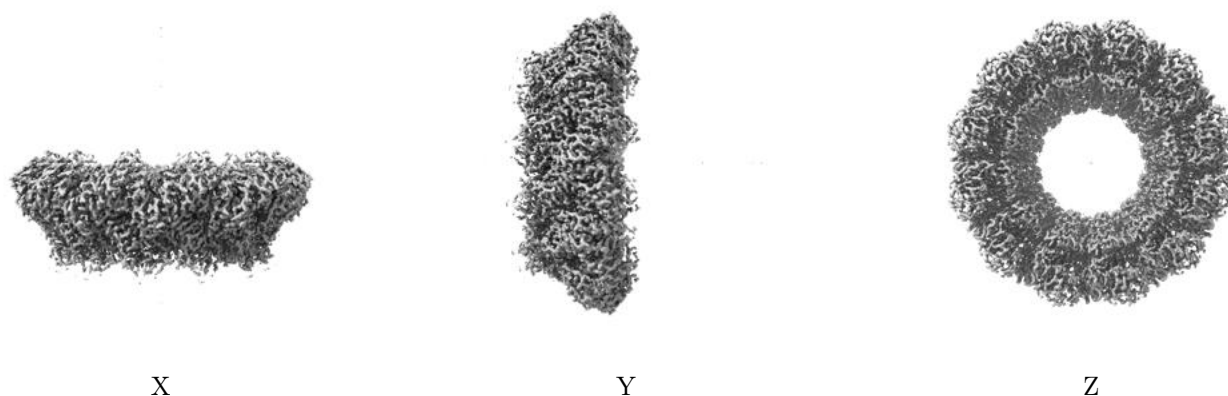


Z

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

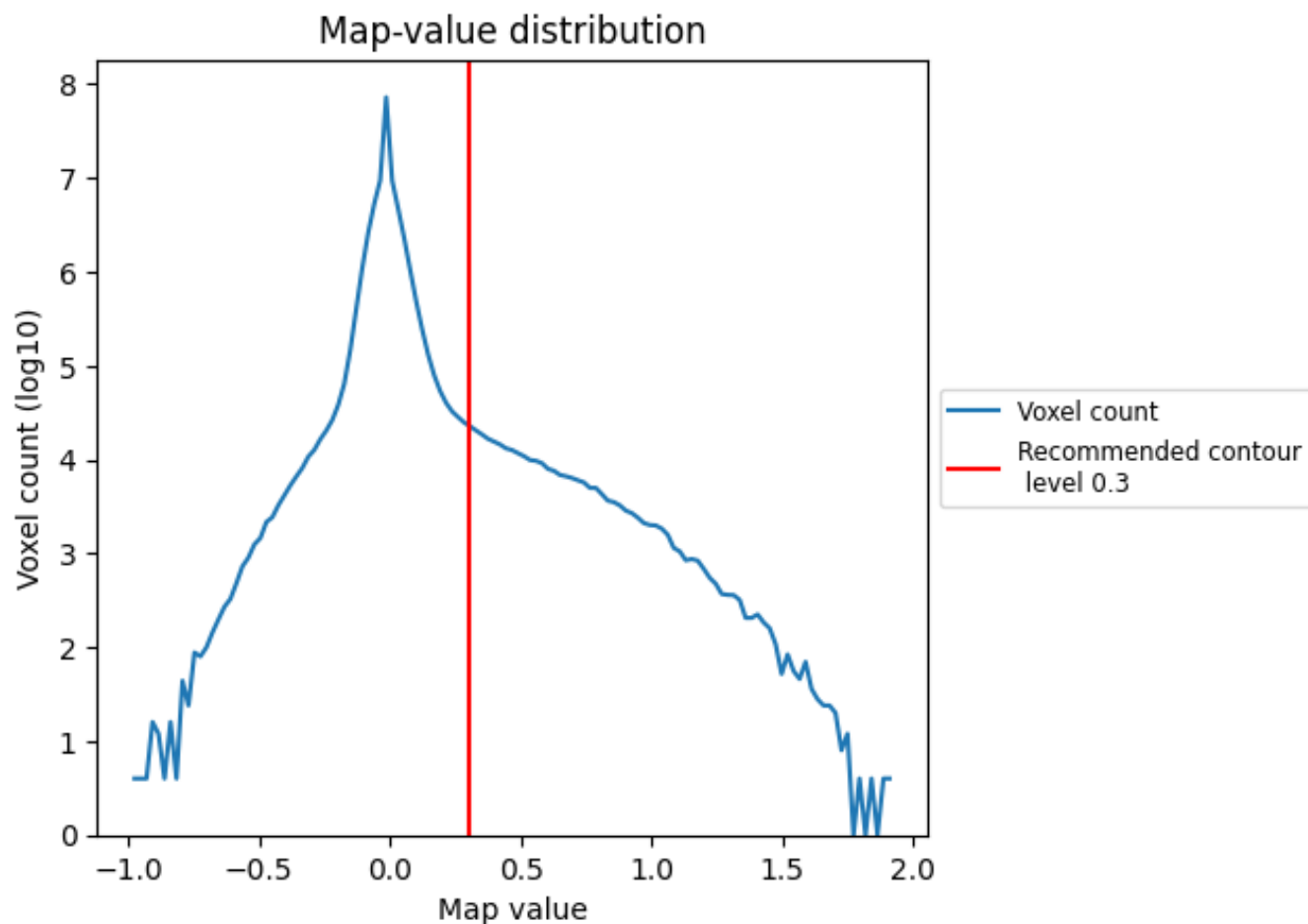
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

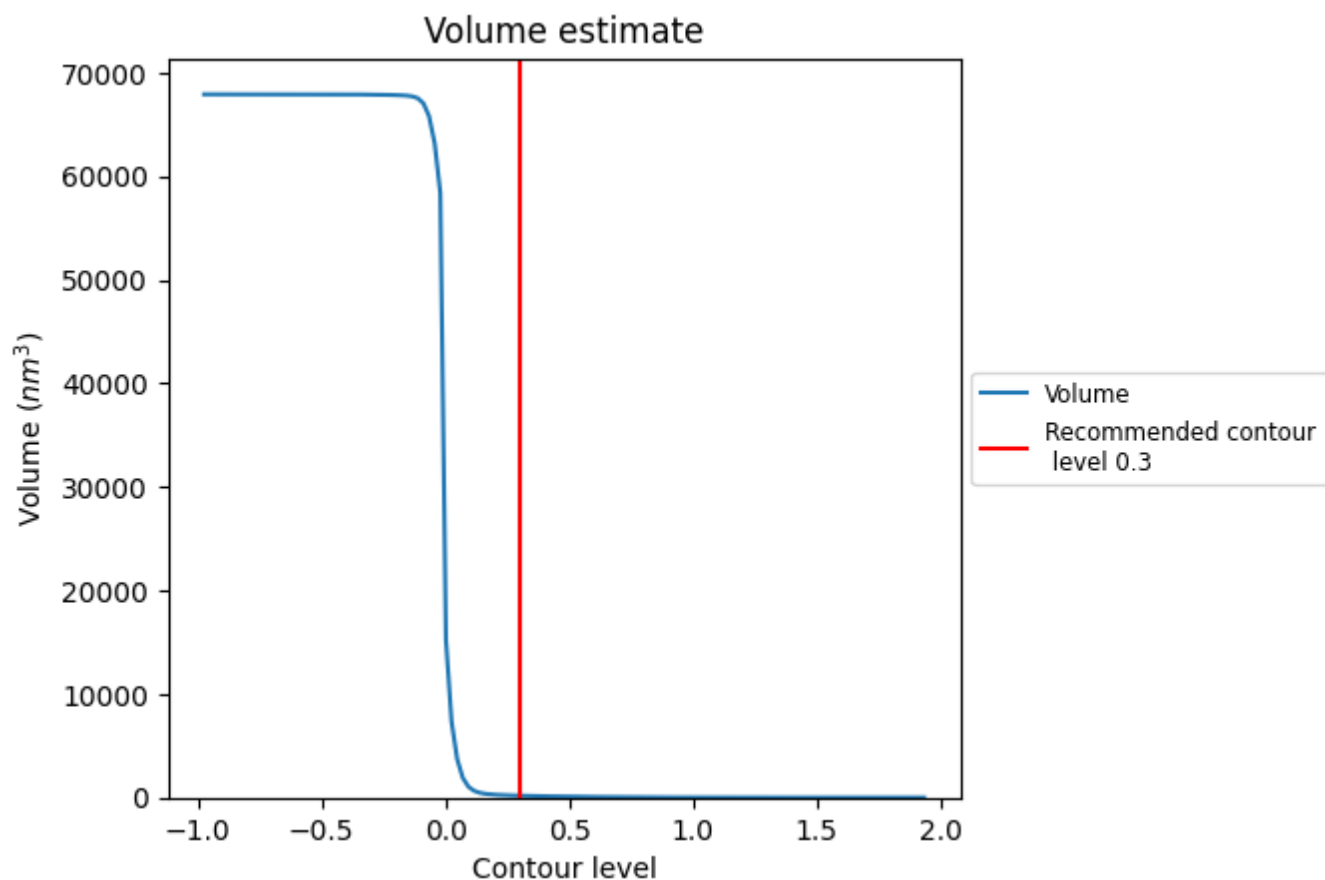
This section contains the results of statistical analysis of the map.

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.

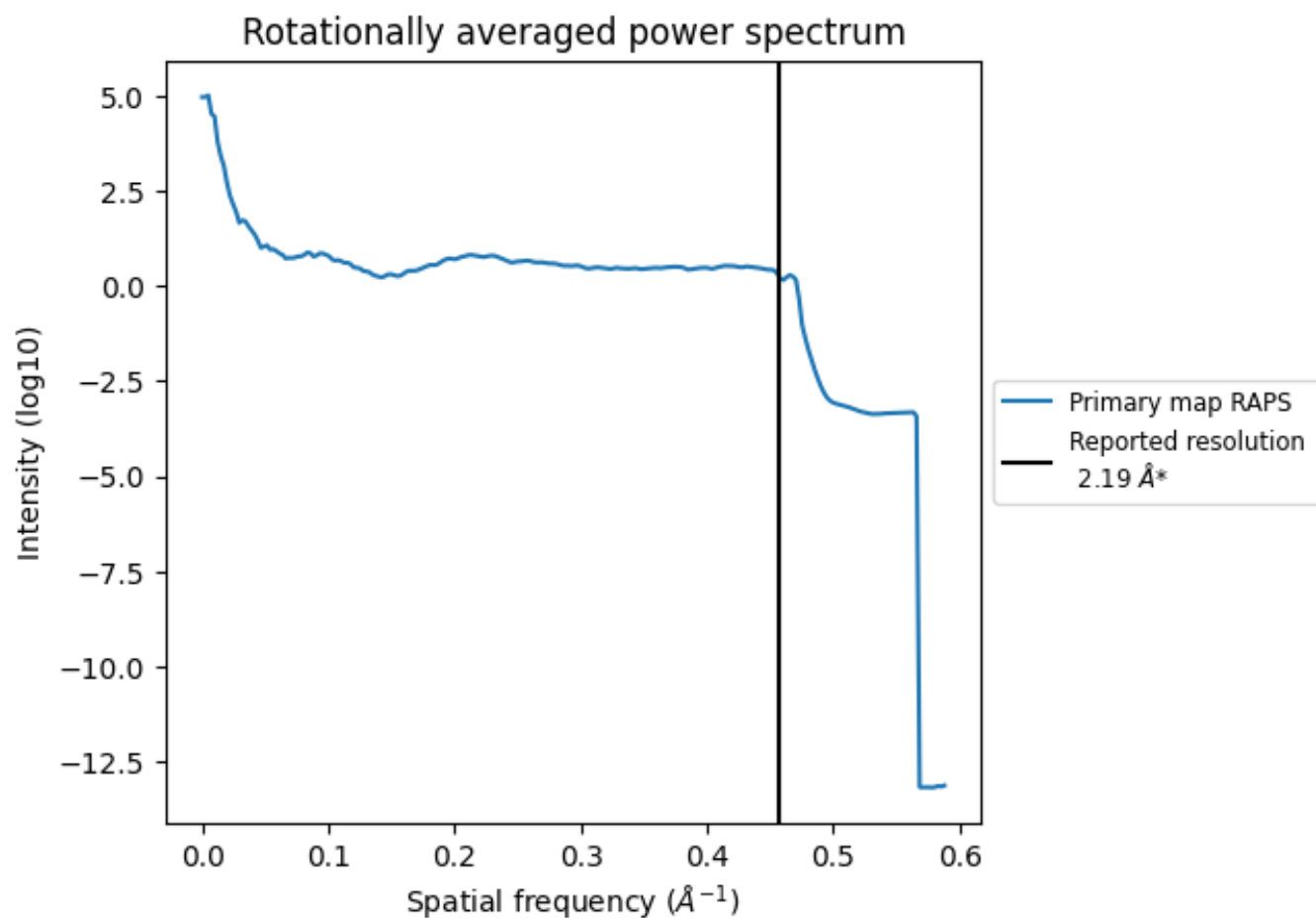
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 179 nm³; this corresponds to an approximate mass of 162 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 0.457 Å⁻¹

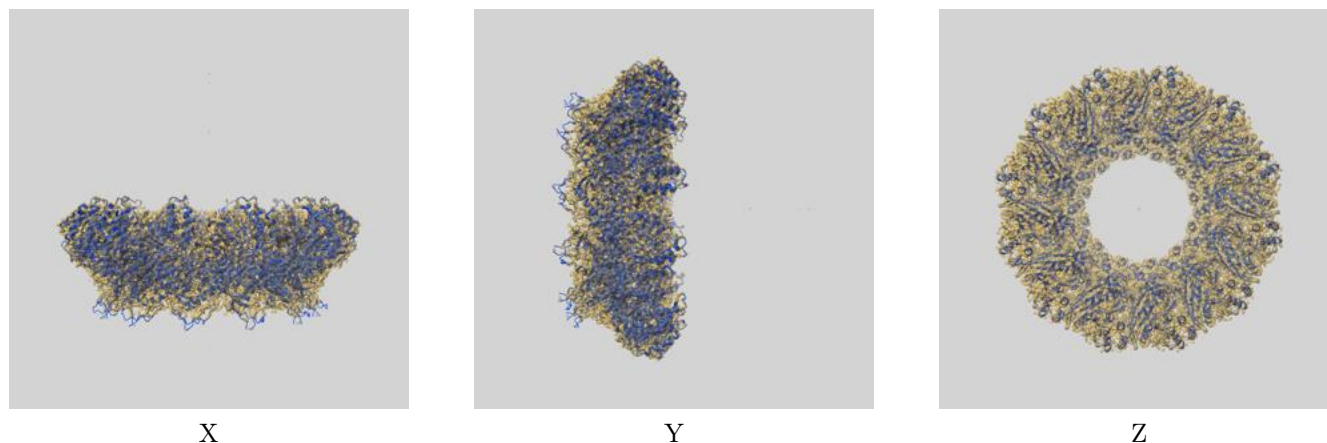
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

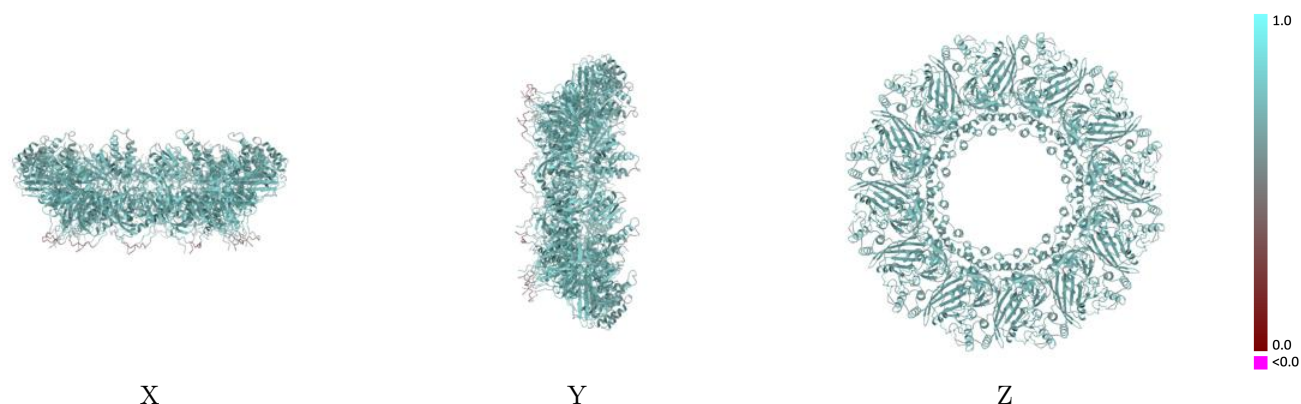
This section contains information regarding the fit between EMDB map EMD-31580 and PDB model 7FGG. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



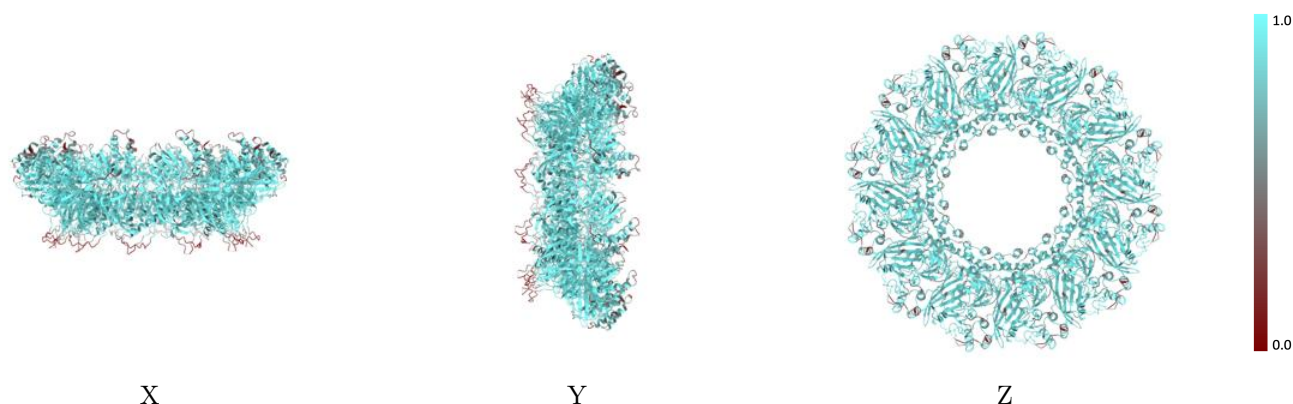
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



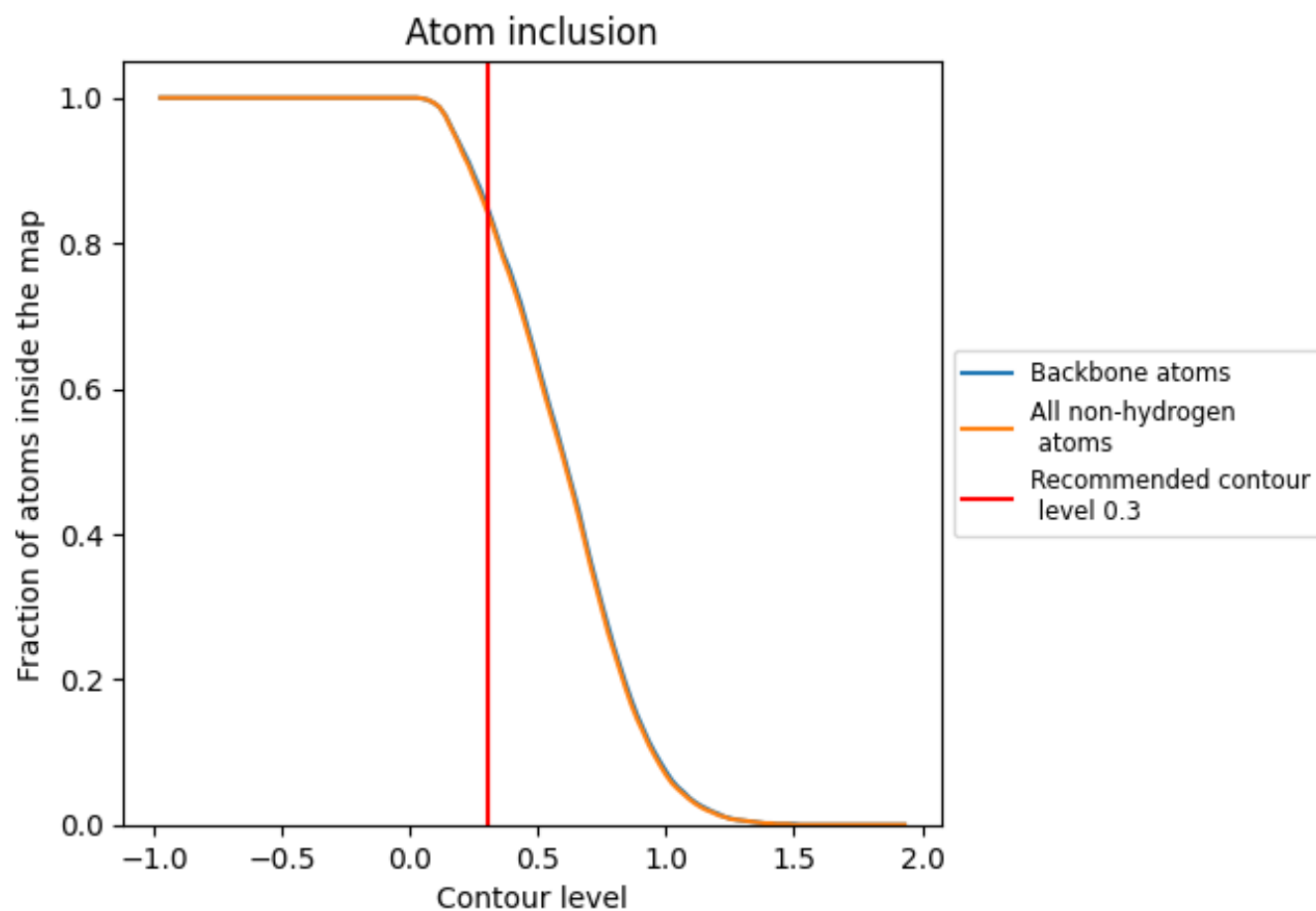
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 84% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8450	0.6980
A	0.8500	0.6950
B	0.8530	0.6980
C	0.8520	0.7000
D	0.8510	0.7010
E	0.8530	0.7020
F	0.8510	0.7010
G	0.8520	0.7000
H	0.8520	0.6990
I	0.8510	0.6980
J	0.8510	0.6970
K	0.8510	0.6950
L	0.8480	0.6940

