



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2020 – 07:49 PM BST

PDB ID : 6Y66
Title : Structure of Goose Hemorrhagic Polyomavirus VP1 in complex with 2-O-Methyl-5-N-acetyl-alpha-D-neuraminic acid
Authors : Stroh, L.J.; Rustmeier, N.H.; Stehle, T.
Deposited on : 2020-02-26
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

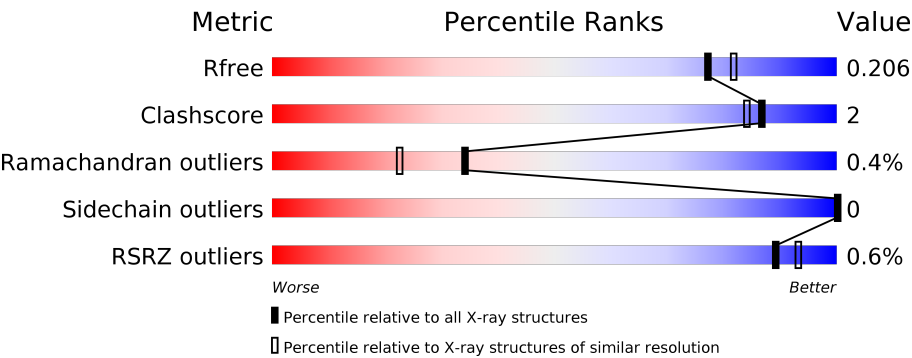
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	287	<div><div></div><div>88%•8%</div></div>
1	BBB	287	<div><div></div><div>88%5%8%</div></div>
1	CCC	287	<div><div>%</div><div>89%•7%</div></div>
1	DDD	287	<div><div></div><div>86%6%8%</div></div>
1	EEE	287	<div><div></div><div>86%6%8%</div></div>
1	FFF	287	<div><div></div><div>88%•8%</div></div>

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Mol	Chain	Length	Quality of chain
1	GGG	287	<div><div></div><div>86%</div><div>7%7%</div></div>
1	HHH	287	<div>%<div><div></div><div>87%</div><div>5%8%</div></div></div>
1	III	287	<div>%<div><div></div><div>88%</div><div>5%7%</div></div></div>
1	JJJ	287	<div>%<div><div></div><div>87%</div><div>7%7%</div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23150 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	265	Total	C	N	O	S	0	1	0
			2006	1262	341	386	17			
1	BBB	265	Total	C	N	O	S	0	1	0
			1999	1258	341	383	17			
1	CCC	267	Total	C	N	O	S	0	1	0
			2023	1271	346	388	18			
1	DDD	265	Total	C	N	O	S	0	2	0
			2008	1266	341	384	17			
1	EEE	265	Total	C	N	O	S	0	1	0
			2005	1262	342	384	17			
1	FFF	265	Total	C	N	O	S	0	1	0
			2002	1260	340	385	17			
1	GGG	268	Total	C	N	O	S	0	1	0
			2019	1270	344	387	18			
1	HHH	265	Total	C	N	O	S	0	2	0
			2010	1265	341	387	17			
1	III	267	Total	C	N	O	S	0	1	0
			2007	1263	343	383	18			
1	JJJ	268	Total	C	N	O	S	0	1	0
			2030	1275	348	389	18			

There are 210 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	0	MET	-	initiating methionine	UNP Q80FI3
AAA	1	GLY	-	expression tag	UNP Q80FI3
AAA	2	SER	-	expression tag	UNP Q80FI3
AAA	3	SER	-	expression tag	UNP Q80FI3
AAA	4	HIS	-	expression tag	UNP Q80FI3
AAA	5	HIS	-	expression tag	UNP Q80FI3
AAA	6	HIS	-	expression tag	UNP Q80FI3
AAA	7	HIS	-	expression tag	UNP Q80FI3
AAA	8	HIS	-	expression tag	UNP Q80FI3

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	9	HIS	-	expression tag	UNP Q80FI3
AAA	10	SER	-	expression tag	UNP Q80FI3
AAA	11	SER	-	expression tag	UNP Q80FI3
AAA	12	GLY	-	expression tag	UNP Q80FI3
AAA	13	LEU	-	expression tag	UNP Q80FI3
AAA	14	VAL	-	expression tag	UNP Q80FI3
AAA	15	PRO	-	expression tag	UNP Q80FI3
AAA	16	ARG	-	expression tag	UNP Q80FI3
AAA	17	GLY	-	expression tag	UNP Q80FI3
AAA	18	SER	-	expression tag	UNP Q80FI3
AAA	19	HIS	-	expression tag	UNP Q80FI3
AAA	20	MET	-	expression tag	UNP Q80FI3
BBB	0	MET	-	initiating methionine	UNP Q80FI3
BBB	1	GLY	-	expression tag	UNP Q80FI3
BBB	2	SER	-	expression tag	UNP Q80FI3
BBB	3	SER	-	expression tag	UNP Q80FI3
BBB	4	HIS	-	expression tag	UNP Q80FI3
BBB	5	HIS	-	expression tag	UNP Q80FI3
BBB	6	HIS	-	expression tag	UNP Q80FI3
BBB	7	HIS	-	expression tag	UNP Q80FI3
BBB	8	HIS	-	expression tag	UNP Q80FI3
BBB	9	HIS	-	expression tag	UNP Q80FI3
BBB	10	SER	-	expression tag	UNP Q80FI3
BBB	11	SER	-	expression tag	UNP Q80FI3
BBB	12	GLY	-	expression tag	UNP Q80FI3
BBB	13	LEU	-	expression tag	UNP Q80FI3
BBB	14	VAL	-	expression tag	UNP Q80FI3
BBB	15	PRO	-	expression tag	UNP Q80FI3
BBB	16	ARG	-	expression tag	UNP Q80FI3
BBB	17	GLY	-	expression tag	UNP Q80FI3
BBB	18	SER	-	expression tag	UNP Q80FI3
BBB	19	HIS	-	expression tag	UNP Q80FI3
BBB	20	MET	-	expression tag	UNP Q80FI3
CCC	0	MET	-	initiating methionine	UNP Q80FI3
CCC	1	GLY	-	expression tag	UNP Q80FI3
CCC	2	SER	-	expression tag	UNP Q80FI3
CCC	3	SER	-	expression tag	UNP Q80FI3
CCC	4	HIS	-	expression tag	UNP Q80FI3
CCC	5	HIS	-	expression tag	UNP Q80FI3
CCC	6	HIS	-	expression tag	UNP Q80FI3
CCC	7	HIS	-	expression tag	UNP Q80FI3
CCC	8	HIS	-	expression tag	UNP Q80FI3

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Chain	Residue	Modelled	Actual	Comment	Reference
CCC	9	HIS	-	expression tag	UNP Q80FI3
CCC	10	SER	-	expression tag	UNP Q80FI3
CCC	11	SER	-	expression tag	UNP Q80FI3
CCC	12	GLY	-	expression tag	UNP Q80FI3
CCC	13	LEU	-	expression tag	UNP Q80FI3
CCC	14	VAL	-	expression tag	UNP Q80FI3
CCC	15	PRO	-	expression tag	UNP Q80FI3
CCC	16	ARG	-	expression tag	UNP Q80FI3
CCC	17	GLY	-	expression tag	UNP Q80FI3
CCC	18	SER	-	expression tag	UNP Q80FI3
CCC	19	HIS	-	expression tag	UNP Q80FI3
CCC	20	MET	-	expression tag	UNP Q80FI3
DDD	0	MET	-	initiating methionine	UNP Q80FI3
DDD	1	GLY	-	expression tag	UNP Q80FI3
DDD	2	SER	-	expression tag	UNP Q80FI3
DDD	3	SER	-	expression tag	UNP Q80FI3
DDD	4	HIS	-	expression tag	UNP Q80FI3
DDD	5	HIS	-	expression tag	UNP Q80FI3
DDD	6	HIS	-	expression tag	UNP Q80FI3
DDD	7	HIS	-	expression tag	UNP Q80FI3
DDD	8	HIS	-	expression tag	UNP Q80FI3
DDD	9	HIS	-	expression tag	UNP Q80FI3
DDD	10	SER	-	expression tag	UNP Q80FI3
DDD	11	SER	-	expression tag	UNP Q80FI3
DDD	12	GLY	-	expression tag	UNP Q80FI3
DDD	13	LEU	-	expression tag	UNP Q80FI3
DDD	14	VAL	-	expression tag	UNP Q80FI3
DDD	15	PRO	-	expression tag	UNP Q80FI3
DDD	16	ARG	-	expression tag	UNP Q80FI3
DDD	17	GLY	-	expression tag	UNP Q80FI3
DDD	18	SER	-	expression tag	UNP Q80FI3
DDD	19	HIS	-	expression tag	UNP Q80FI3
DDD	20	MET	-	expression tag	UNP Q80FI3
EEE	0	MET	-	initiating methionine	UNP Q80FI3
EEE	1	GLY	-	expression tag	UNP Q80FI3
EEE	2	SER	-	expression tag	UNP Q80FI3
EEE	3	SER	-	expression tag	UNP Q80FI3
EEE	4	HIS	-	expression tag	UNP Q80FI3
EEE	5	HIS	-	expression tag	UNP Q80FI3
EEE	6	HIS	-	expression tag	UNP Q80FI3
EEE	7	HIS	-	expression tag	UNP Q80FI3
EEE	8	HIS	-	expression tag	UNP Q80FI3

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Chain	Residue	Modelled	Actual	Comment	Reference
EEE	9	HIS	-	expression tag	UNP Q80FI3
EEE	10	SER	-	expression tag	UNP Q80FI3
EEE	11	SER	-	expression tag	UNP Q80FI3
EEE	12	GLY	-	expression tag	UNP Q80FI3
EEE	13	LEU	-	expression tag	UNP Q80FI3
EEE	14	VAL	-	expression tag	UNP Q80FI3
EEE	15	PRO	-	expression tag	UNP Q80FI3
EEE	16	ARG	-	expression tag	UNP Q80FI3
EEE	17	GLY	-	expression tag	UNP Q80FI3
EEE	18	SER	-	expression tag	UNP Q80FI3
EEE	19	HIS	-	expression tag	UNP Q80FI3
EEE	20	MET	-	expression tag	UNP Q80FI3
FFF	0	MET	-	initiating methionine	UNP Q80FI3
FFF	1	GLY	-	expression tag	UNP Q80FI3
FFF	2	SER	-	expression tag	UNP Q80FI3
FFF	3	SER	-	expression tag	UNP Q80FI3
FFF	4	HIS	-	expression tag	UNP Q80FI3
FFF	5	HIS	-	expression tag	UNP Q80FI3
FFF	6	HIS	-	expression tag	UNP Q80FI3
FFF	7	HIS	-	expression tag	UNP Q80FI3
FFF	8	HIS	-	expression tag	UNP Q80FI3
FFF	9	HIS	-	expression tag	UNP Q80FI3
FFF	10	SER	-	expression tag	UNP Q80FI3
FFF	11	SER	-	expression tag	UNP Q80FI3
FFF	12	GLY	-	expression tag	UNP Q80FI3
FFF	13	LEU	-	expression tag	UNP Q80FI3
FFF	14	VAL	-	expression tag	UNP Q80FI3
FFF	15	PRO	-	expression tag	UNP Q80FI3
FFF	16	ARG	-	expression tag	UNP Q80FI3
FFF	17	GLY	-	expression tag	UNP Q80FI3
FFF	18	SER	-	expression tag	UNP Q80FI3
FFF	19	HIS	-	expression tag	UNP Q80FI3
FFF	20	MET	-	expression tag	UNP Q80FI3
GGG	0	MET	-	initiating methionine	UNP Q80FI3
GGG	1	GLY	-	expression tag	UNP Q80FI3
GGG	2	SER	-	expression tag	UNP Q80FI3
GGG	3	SER	-	expression tag	UNP Q80FI3
GGG	4	HIS	-	expression tag	UNP Q80FI3
GGG	5	HIS	-	expression tag	UNP Q80FI3
GGG	6	HIS	-	expression tag	UNP Q80FI3
GGG	7	HIS	-	expression tag	UNP Q80FI3
GGG	8	HIS	-	expression tag	UNP Q80FI3

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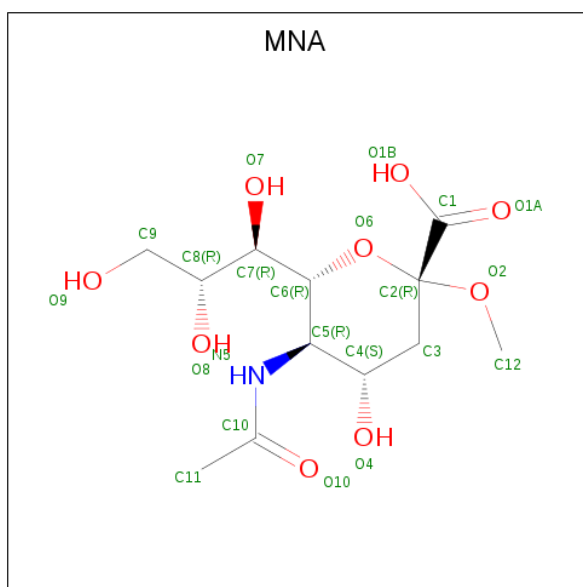
Chain	Residue	Modelled	Actual	Comment	Reference
GGG	9	HIS	-	expression tag	UNP Q80FI3
GGG	10	SER	-	expression tag	UNP Q80FI3
GGG	11	SER	-	expression tag	UNP Q80FI3
GGG	12	GLY	-	expression tag	UNP Q80FI3
GGG	13	LEU	-	expression tag	UNP Q80FI3
GGG	14	VAL	-	expression tag	UNP Q80FI3
GGG	15	PRO	-	expression tag	UNP Q80FI3
GGG	16	ARG	-	expression tag	UNP Q80FI3
GGG	17	GLY	-	expression tag	UNP Q80FI3
GGG	18	SER	-	expression tag	UNP Q80FI3
GGG	19	HIS	-	expression tag	UNP Q80FI3
GGG	20	MET	-	expression tag	UNP Q80FI3
HHH	0	MET	-	initiating methionine	UNP Q80FI3
HHH	1	GLY	-	expression tag	UNP Q80FI3
HHH	2	SER	-	expression tag	UNP Q80FI3
HHH	3	SER	-	expression tag	UNP Q80FI3
HHH	4	HIS	-	expression tag	UNP Q80FI3
HHH	5	HIS	-	expression tag	UNP Q80FI3
HHH	6	HIS	-	expression tag	UNP Q80FI3
HHH	7	HIS	-	expression tag	UNP Q80FI3
HHH	8	HIS	-	expression tag	UNP Q80FI3
HHH	9	HIS	-	expression tag	UNP Q80FI3
HHH	10	SER	-	expression tag	UNP Q80FI3
HHH	11	SER	-	expression tag	UNP Q80FI3
HHH	12	GLY	-	expression tag	UNP Q80FI3
HHH	13	LEU	-	expression tag	UNP Q80FI3
HHH	14	VAL	-	expression tag	UNP Q80FI3
HHH	15	PRO	-	expression tag	UNP Q80FI3
HHH	16	ARG	-	expression tag	UNP Q80FI3
HHH	17	GLY	-	expression tag	UNP Q80FI3
HHH	18	SER	-	expression tag	UNP Q80FI3
HHH	19	HIS	-	expression tag	UNP Q80FI3
HHH	20	MET	-	expression tag	UNP Q80FI3
III	0	MET	-	initiating methionine	UNP Q80FI3
III	1	GLY	-	expression tag	UNP Q80FI3
III	2	SER	-	expression tag	UNP Q80FI3
III	3	SER	-	expression tag	UNP Q80FI3
III	4	HIS	-	expression tag	UNP Q80FI3
III	5	HIS	-	expression tag	UNP Q80FI3
III	6	HIS	-	expression tag	UNP Q80FI3
III	7	HIS	-	expression tag	UNP Q80FI3
III	8	HIS	-	expression tag	UNP Q80FI3

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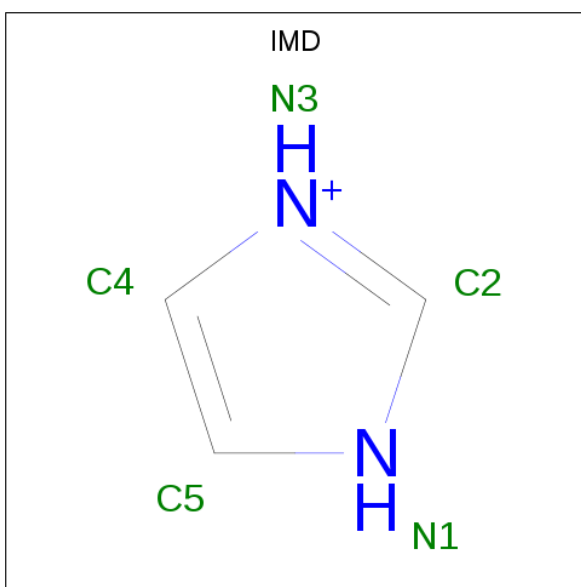
Chain	Residue	Modelled	Actual	Comment	Reference
III	9	HIS	-	expression tag	UNP Q80FI3
III	10	SER	-	expression tag	UNP Q80FI3
III	11	SER	-	expression tag	UNP Q80FI3
III	12	GLY	-	expression tag	UNP Q80FI3
III	13	LEU	-	expression tag	UNP Q80FI3
III	14	VAL	-	expression tag	UNP Q80FI3
III	15	PRO	-	expression tag	UNP Q80FI3
III	16	ARG	-	expression tag	UNP Q80FI3
III	17	GLY	-	expression tag	UNP Q80FI3
III	18	SER	-	expression tag	UNP Q80FI3
III	19	HIS	-	expression tag	UNP Q80FI3
III	20	MET	-	expression tag	UNP Q80FI3
JJJ	0	MET	-	initiating methionine	UNP Q80FI3
JJJ	1	GLY	-	expression tag	UNP Q80FI3
JJJ	2	SER	-	expression tag	UNP Q80FI3
JJJ	3	SER	-	expression tag	UNP Q80FI3
JJJ	4	HIS	-	expression tag	UNP Q80FI3
JJJ	5	HIS	-	expression tag	UNP Q80FI3
JJJ	6	HIS	-	expression tag	UNP Q80FI3
JJJ	7	HIS	-	expression tag	UNP Q80FI3
JJJ	8	HIS	-	expression tag	UNP Q80FI3
JJJ	9	HIS	-	expression tag	UNP Q80FI3
JJJ	10	SER	-	expression tag	UNP Q80FI3
JJJ	11	SER	-	expression tag	UNP Q80FI3
JJJ	12	GLY	-	expression tag	UNP Q80FI3
JJJ	13	LEU	-	expression tag	UNP Q80FI3
JJJ	14	VAL	-	expression tag	UNP Q80FI3
JJJ	15	PRO	-	expression tag	UNP Q80FI3
JJJ	16	ARG	-	expression tag	UNP Q80FI3
JJJ	17	GLY	-	expression tag	UNP Q80FI3
JJJ	18	SER	-	expression tag	UNP Q80FI3
JJJ	19	HIS	-	expression tag	UNP Q80FI3
JJJ	20	MET	-	expression tag	UNP Q80FI3

- Molecule 2 is 2-O-methyl-5-N-acetyl-alpha-D-neuraminic acid (three-letter code: MNA) (formula: C₁₂H₂₁NO₉) (labeled as "Ligand of Interest" by author).



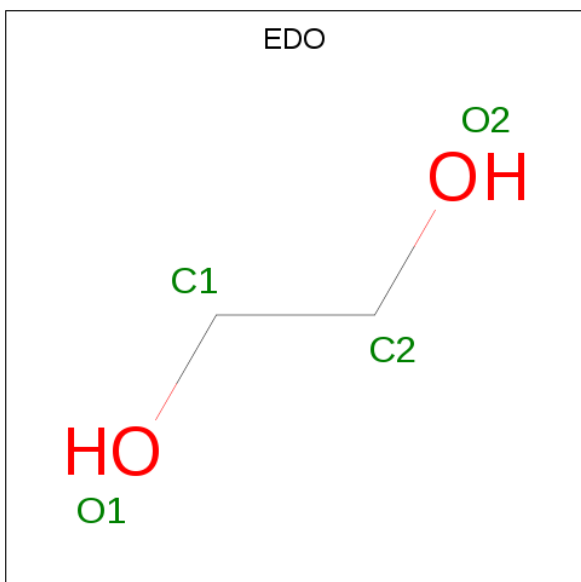
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	0	0
			22	12	1	9		
2	BBB	1	Total	C	N	O	0	0
			22	12	1	9		
2	CCC	1	Total	C	N	O	0	0
			22	12	1	9		
2	DDD	1	Total	C	N	O	0	0
			22	12	1	9		
2	EEE	1	Total	C	N	O	0	0
			22	12	1	9		
2	FFF	1	Total	C	N	O	0	0
			22	12	1	9		
2	GGG	1	Total	C	N	O	0	0
			22	12	1	9		
2	HHH	1	Total	C	N	O	0	0
			22	12	1	9		
2	III	1	Total	C	N	O	0	0
			22	12	1	9		
2	JJJ	1	Total	C	N	O	0	0
			22	12	1	9		

- Molecule 3 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	C	N	0	0
			5	3	2		
3	CCC	1	Total	C	N	0	0
			5	3	2		
3	DDD	1	Total	C	N	0	0
			5	3	2		
3	EEE	1	Total	C	N	0	0
			5	3	2		
3	GGG	1	Total	C	N	0	0
			5	3	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	BBB	1	Total C O 4 2 2	0	0
4	CCC	1	Total C O 4 2 2	0	0
4	CCC	1	Total C O 4 2 2	0	0
4	DDD	1	Total C O 4 2 2	0	0
4	DDD	1	Total C O 4 2 2	0	0
4	EEE	1	Total C O 4 2 2	0	0
4	EEE	1	Total C O 4 2 2	0	0
4	EEE	1	Total C O 4 2 2	0	0
4	EEE	1	Total C O 4 2 2	0	0
4	EEE	1	Total C O 4 2 2	0	0
4	FFF	1	Total C O 4 2 2	0	0
4	FFF	1	Total C O 4 2 2	0	0
4	GGG	1	Total C O 4 2 2	0	0
4	GGG	1	Total C O 4 2 2	0	0
4	HHH	1	Total C O 4 2 2	0	0
4	HHH	1	Total C O 4 2 2	0	0
4	III	1	Total C O 4 2 2	0	0
4	JJJ	1	Total C O 4 2 2	0	0
4	JJJ	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

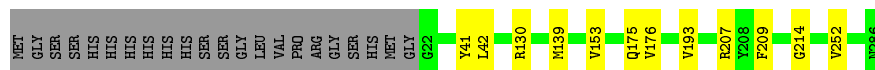
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	264	Total 264	O 264	0	0
5	BBB	256	Total 261	O 261	0	5
5	CCC	265	Total 271	O 271	0	6
5	DDD	279	Total 284	O 284	0	5
5	EEE	255	Total 260	O 260	0	5
5	FFF	281	Total 284	O 284	0	3
5	GGG	265	Total 272	O 272	0	7
5	HHH	256	Total 261	O 261	0	5
5	III	261	Total 264	O 264	0	3
5	JJJ	283	Total 287	O 287	0	4

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Capsid protein VP1

Chain AAA: 



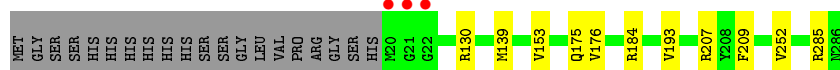
- Molecule 1: Capsid protein VP1

Chain BBB: 



- Molecule 1: Capsid protein VP1

Chain CCC: 



- Molecule 1: Capsid protein VP1

Chain DDD: 



- Molecule 1: Capsid protein VP1

Chain EEE: 



- Molecule 1: Capsid protein VP1

Chain FFF:  88% 8%




- Molecule 1: Capsid protein VP1

Chain GGG:  86% 7% 7%




- Molecule 1: Capsid protein VP1

Chain HHH:  87% 5% 8%




- Molecule 1: Capsid protein VP1

Chain III:  88% 5% 7%



- Molecule 1: Capsid protein VP1

Chain JJJ:  87% 7% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	87.46 Å 90.54 Å 101.22 Å 94.23° 98.09° 107.87°	Depositor
Resolution (Å)	49.58 – 1.95 49.58 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.7 (49.58-1.95) 97.7 (49.58-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 1.95 Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.165 , 0.201 0.173 , 0.206	Depositor DCC
R_{free} test set	2069 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	23150	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MNA, IMD, EDO

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	AAA	0.67	0/2054	0.82	4/2804 (0.1%)
1	BBB	0.65	0/2047	0.80	3/2797 (0.1%)
1	CCC	0.64	0/2071	0.81	4/2825 (0.1%)
1	DDD	0.65	0/2059	0.83	1/2811 (0.0%)
1	EEE	0.64	0/2053	0.79	1/2802 (0.0%)
1	FFF	0.65	0/2050	0.81	3/2800 (0.1%)
1	GGG	0.66	0/2067	0.79	2/2821 (0.1%)
1	HHH	0.66	0/2058	0.82	3/2811 (0.1%)
1	III	0.67	0/2055	0.81	1/2805 (0.0%)
1	JJJ	0.67	0/2079	0.82	2/2837 (0.1%)
All	All	0.66	0/20593	0.81	24/28113 (0.1%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	HHH	207	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	III	285	ARG	CG-CD-NE	6.40	125.25	111.80
1	FFF	130	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	AAA	130	ARG	CB-CA-C	-6.13	98.14	110.40
1	CCC	130	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	AAA	130	ARG	NE-CZ-NH1	-6.03	117.28	120.30
1	BBB	130	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	BBB	130	ARG	CB-CA-C	-5.98	98.44	110.40
1	HHH	207	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	FFF	130	ARG	CB-CA-C	-5.86	98.68	110.40
1	CCC	130	ARG	CB-CA-C	-5.85	98.71	110.40
1	GGG	130	ARG	CB-CA-C	-5.79	98.81	110.40
1	DDD	130	ARG	CB-CA-C	-5.76	98.88	110.40
1	BBB	207	ARG	NE-CZ-NH1	5.74	123.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	EEE	130	ARG	CB-CA-C	-5.74	98.93	110.40
1	AAA	207	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	AAA	207	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	HHH	130	ARG	CB-CA-C	-5.66	99.08	110.40
1	JJJ	130	ARG	CB-CA-C	-5.62	99.17	110.40
1	CCC	207	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	JJJ	207	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	CCC	184	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	GGG	130	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	FFF	207	ARG	NE-CZ-NH2	-5.01	117.79	120.30

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	AAA	2006	0	1957	5	0
1	BBB	1999	0	1946	6	0
1	CCC	2023	0	1978	4	0
1	DDD	2008	0	1963	13	0
1	EEE	2005	0	1959	10	0
1	FFF	2002	0	1945	7	0
1	GGG	2019	0	1967	13	0
1	HHH	2010	0	1956	8	0
1	III	2007	0	1951	9	0
1	JJJ	2030	0	1976	12	0
2	AAA	22	0	20	0	0
2	BBB	22	0	20	0	0
2	CCC	22	0	20	0	0
2	DDD	22	0	20	0	0
2	EEE	22	0	20	0	0
2	FFF	22	0	20	0	0
2	GGG	22	0	20	0	0
2	HHH	22	0	20	0	0
2	III	22	0	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	JJJ	22	0	20	0	0
3	AAA	5	0	5	0	0
3	CCC	5	0	5	0	0
3	DDD	5	0	5	0	0
3	EEE	5	0	5	0	0
3	GGG	5	0	5	0	0
4	AAA	12	0	18	0	0
4	BBB	4	0	6	0	0
4	CCC	8	0	12	0	0
4	DDD	8	0	12	0	0
4	EEE	20	0	30	1	0
4	FFF	8	0	12	0	0
4	GGG	8	0	12	0	0
4	HHH	8	0	12	0	0
4	III	4	0	6	0	0
4	JJJ	8	0	12	0	0
5	AAA	264	0	0	0	0
5	BBB	261	0	0	1	0
5	CCC	271	0	0	1	0
5	DDD	284	0	0	3	0
5	EEE	260	0	0	3	0
5	FFF	284	0	0	4	0
5	GGG	272	0	0	4	0
5	HHH	261	0	0	1	0
5	III	264	0	0	5	0
5	JJJ	287	0	0	4	0
All	All	23150	0	19955	85	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 2.

All (85) 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:DDD:85[A]:LEU:HD11	1:DDD:281:LYS:HE2	1.44	0.99
1:DDD:85[A]:LEU:CD1	1:DDD:281:LYS:HE2	2.22	0.68
1:GGG:19:HIS:N	5:GGG:502:HOH:O	2.26	0.68
1:HHH:49:ASP:OD1	5:HHH:501:HOH:O	2.13	0.66
1:FFF:130:ARG:HG3	5:FFF:598:HOH:O	2.01	0.61
1:HHH:193:VAL:HG21	1:HHH:252:VAL:HG21	1.83	0.61
1:JJJ:173:LYS:CG	5:JJJ:695:HOH:O	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JJJ:84:MET:CE	5:JJJ:549:HOH:O	2.49	0.60
1:CCC:193:VAL:HG21	1:CCC:252:VAL:HG21	1.83	0.60
1:JJJ:193:VAL:HG21	1:JJJ:252:VAL:HG21	1.83	0.60
1:AAA:193:VAL:HG21	1:AAA:252:VAL:HG21	1.84	0.60
1:EEE:193:VAL:HG21	1:EEE:252:VAL:HG21	1.83	0.60
1:DDD:193:VAL:HG21	1:DDD:252:VAL:HG21	1.84	0.59
1:GGG:193:VAL:HG21	1:GGG:252:VAL:HG21	1.83	0.59
1:BBB:193:VAL:HG21	1:BBB:252:VAL:HG21	1.84	0.59
1:III:193:VAL:HG21	1:III:252:VAL:HG21	1.84	0.58
1:FFF:193:VAL:HG21	1:FFF:252:VAL:HG21	1.84	0.58
1:EEE:86:ASN:HB2	4:EEE:403:EDO:H21	1.87	0.57
1:DDD:85[A]:LEU:HD11	1:DDD:281:LYS:CE	2.27	0.56
1:HHH:24:GLU:OE1	1:HHH:285:ARG:HG3	2.06	0.55
1:GGG:24:GLU:OE1	1:GGG:285:ARG:HG3	2.06	0.55
1:GGG:49:ASP:O	5:GGG:501:HOH:O	2.19	0.54
1:FFF:49:ASP:O	5:FFF:501:HOH:O	2.19	0.53
1:DDD:42:LEU:HD21	1:DDD:78:ALA:HB2	1.90	0.53
1:HHH:24:GLU:HB3	1:HHH:285:ARG:HB2	1.90	0.52
1:JJJ:84:MET:HE2	5:JJJ:549:HOH:O	2.10	0.51
1:III:20:MET:HG3	5:III:621[B]:HOH:O	2.10	0.51
1:GGG:24:GLU:HB3	1:GGG:285:ARG:HB2	1.93	0.50
1:III:49:ASP:O	5:III:501:HOH:O	2.19	0.50
1:BBB:105:GLU:CD	5:BBB:536:HOH:O	2.52	0.48
1:III:184:ARG:NE	5:III:507:HOH:O	2.46	0.48
1:CCC:285:ARG:HD2	5:CCC:700:HOH:O	2.14	0.47
1:FFF:153:VAL:O	1:FFF:175:GLN:HA	2.14	0.47
1:AAA:41:TYR:C	1:AAA:42:LEU:HD12	2.35	0.47
1:AAA:153:VAL:O	1:AAA:175:GLN:HA	2.14	0.47
1:HHH:153:VAL:O	1:HHH:175:GLN:HA	2.14	0.47
1:GGG:153:VAL:O	1:GGG:175:GLN:HA	2.15	0.47
1:EEE:41:TYR:C	1:EEE:42:LEU:HD12	2.35	0.47
1:III:153:VAL:O	1:III:175:GLN:HA	2.15	0.47
1:EEE:153:VAL:O	1:EEE:175:GLN:HA	2.15	0.47
1:JJJ:41:TYR:C	1:JJJ:42:LEU:HD12	2.35	0.46
1:BBB:41:TYR:C	1:BBB:42:LEU:HD12	2.36	0.46
1:CCC:153:VAL:O	1:CCC:175:GLN:HA	2.15	0.46
1:BBB:153:VAL:O	1:BBB:175:GLN:HA	2.15	0.46
1:EEE:184:ARG:NE	5:EEE:510:HOH:O	2.49	0.46
1:III:173:LYS:HE2	5:III:508:HOH:O	2.16	0.46
1:FFF:41:TYR:C	1:FFF:42:LEU:HD12	2.36	0.46
1:BBB:105:GLU:OE2	1:BBB:224:PHE:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:153:VAL:O	1:DDD:175:GLN:HA	2.15	0.46
1:JJJ:19:HIS:HA	1:JJJ:23:ILE:O	2.16	0.45
1:DDD:49:ASP:O	5:DDD:501:HOH:O	2.21	0.45
1:JJJ:153:VAL:O	1:JJJ:175:GLN:HA	2.15	0.45
1:JJJ:21:GLY:HA2	5:JJJ:536:HOH:O	2.16	0.45
1:HHH:41:TYR:C	1:HHH:42[A]:LEU:HD12	2.36	0.45
1:DDD:85[B]:LEU:HD21	1:DDD:245:ASP:OD1	2.16	0.45
1:DDD:235:GLU:CB	5:DDD:529:HOH:O	2.65	0.44
1:DDD:128:VAL:HG12	1:EEE:56:VAL:HB	2.00	0.44
5:III:534:HOH:O	1:JJJ:214:GLY:HA3	2.17	0.44
1:GGG:278:SER:HB2	5:GGG:504:HOH:O	2.17	0.44
1:GGG:19:HIS:HA	1:GGG:23:ILE:O	2.17	0.43
1:GGG:105:GLU:OE2	1:GGG:224:PHE:HB2	2.19	0.43
5:FFF:516:HOH:O	1:GGG:214:GLY:HA3	2.19	0.43
1:EEE:204:GLU:CB	5:EEE:750:HOH:O	2.66	0.43
1:JJJ:139:MET:HA	1:JJJ:209:PHE:O	2.19	0.43
1:CCC:139:MET:HA	1:CCC:209:PHE:O	2.19	0.43
1:DDD:85[A]:LEU:HD12	1:DDD:85[A]:LEU:HA	1.46	0.43
1:EEE:105:GLU:OE2	1:EEE:224:PHE:HB2	2.18	0.43
1:AAA:139:MET:HA	1:AAA:209:PHE:O	2.19	0.43
5:DDD:532:HOH:O	1:EEE:214:GLY:HA3	2.18	0.42
1:FFF:184:ARG:CD	5:FFF:701:HOH:O	2.67	0.42
1:GGG:20:MET:HG3	5:GGG:702:HOH:O	2.19	0.42
1:FFF:139:MET:HA	1:FFF:209:PHE:O	2.19	0.42
1:HHH:139:MET:HA	1:HHH:209:PHE:O	2.19	0.42
1:DDD:139:MET:HA	1:DDD:209:PHE:O	2.20	0.42
1:GGG:139:MET:HA	1:GGG:209:PHE:O	2.20	0.42
1:AAA:214:GLY:HA3	5:EEE:523:HOH:O	2.20	0.42
1:EEE:139:MET:HA	1:EEE:209:PHE:O	2.20	0.41
1:BBB:139:MET:HA	1:BBB:209:PHE:O	2.20	0.41
1:III:139:MET:HA	1:III:209:PHE:O	2.19	0.41
1:GGG:42:LEU:HD21	1:GGG:78:ALA:HB2	2.02	0.41
1:III:42:LEU:HD21	1:III:78:ALA:HB2	2.01	0.41
1:JJJ:85:LEU:HD23	1:JJJ:85:LEU:HA	1.86	0.41
1:III:128:VAL:HG12	1:JJJ:56:VAL:HB	2.03	0.40
1:DDD:152:CYS:O	1:DDD:195:CYS:HA	2.22	0.40
1:HHH:42[B]:LEU:HD21	1:HHH:78:ALA:HB2	2.03	0.40

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 X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	264/287 (92%)	256 (97%)	7 (3%)	1 (0%)	34	22
1	BBB	264/287 (92%)	255 (97%)	8 (3%)	1 (0%)	34	22
1	CCC	266/287 (93%)	257 (97%)	8 (3%)	1 (0%)	34	22
1	DDD	265/287 (92%)	255 (96%)	9 (3%)	1 (0%)	34	22
1	EEE	264/287 (92%)	254 (96%)	9 (3%)	1 (0%)	34	22
1	FFF	264/287 (92%)	255 (97%)	8 (3%)	1 (0%)	34	22
1	GGG	267/287 (93%)	258 (97%)	8 (3%)	1 (0%)	34	22
1	HHH	265/287 (92%)	256 (97%)	8 (3%)	1 (0%)	34	22
1	III	266/287 (93%)	257 (97%)	8 (3%)	1 (0%)	34	22
1	JJJ	267/287 (93%)	257 (96%)	9 (3%)	1 (0%)	34	22
All	All	2652/2870 (92%)	2560 (96%)	82 (3%)	10 (0%)	34	22

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	FFF	176	VAL
1	AAA	176	VAL
1	BBB	176	VAL
1	CCC	176	VAL
1	DDD	176	VAL
1	EEE	176	VAL
1	GGG	176	VAL
1	HHH	176	VAL
1	III	176	VAL
1	JJJ	176	VAL

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 X-ray entries followed by that with respect to entries of similar resolution.

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	AAA	222/243 (91%)	222 (100%)	0	100	100
1	BBB	220/243 (90%)	220 (100%)	0	100	100
1	CCC	224/243 (92%)	224 (100%)	0	100	100
1	DDD	221/243 (91%)	221 (100%)	0	100	100
1	EEE	221/243 (91%)	221 (100%)	0	100	100
1	FFF	220/243 (90%)	220 (100%)	0	100	100
1	GGG	222/243 (91%)	222 (100%)	0	100	100
1	HHH	222/243 (91%)	222 (100%)	0	100	100
1	III	219/243 (90%)	219 (100%)	0	100	100
1	JJJ	224/243 (92%)	224 (100%)	0	100	100
All	All	2215/2430 (91%)	2215 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

37 ligands are modelled in this entry.

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
4	EDO	AAA	404	-	3,3,3	0.21	0	2,2,2	0.26	0
4	EDO	HHH	402	-	3,3,3	0.08	0	2,2,2	0.17	0
3	IMD	AAA	402	-	3,5,5	0.37	0	4,5,5	0.84	0
2	MNA	JJJ	401	-	19,22,22	0.80	1 (5%)	25,32,32	0.91	0
4	EDO	HHH	403	-	3,3,3	0.27	0	2,2,2	0.19	0
4	EDO	CCC	404	-	3,3,3	0.19	0	2,2,2	0.25	0
2	MNA	FFF	401	-	19,22,22	0.75	0	25,32,32	0.88	0
4	EDO	GGG	403	-	3,3,3	0.16	0	2,2,2	0.39	0
4	EDO	DDD	404	-	3,3,3	0.05	0	2,2,2	0.24	0
3	IMD	EEE	402	-	3,5,5	0.42	0	4,5,5	0.71	0
2	MNA	GGG	401	-	19,22,22	0.92	1 (5%)	25,32,32	0.80	0
2	MNA	BBB	401	-	19,22,22	0.68	0	25,32,32	0.89	1 (4%)
3	IMD	DDD	402	-	3,5,5	0.43	0	4,5,5	0.76	0
4	EDO	EEE	407	-	3,3,3	0.25	0	2,2,2	0.26	0
2	MNA	HHH	401	-	19,22,22	0.83	1 (5%)	25,32,32	0.88	1 (4%)
4	EDO	FFF	402	-	3,3,3	0.22	0	2,2,2	0.08	0
4	EDO	FFF	403	-	3,3,3	0.21	0	2,2,2	0.21	0
4	EDO	GGG	404	-	3,3,3	0.21	0	2,2,2	0.13	0
4	EDO	DDD	403	-	3,3,3	0.20	0	2,2,2	0.19	0
4	EDO	AAA	405	-	3,3,3	0.20	0	2,2,2	0.08	0
3	IMD	GGG	402	-	3,5,5	0.36	0	4,5,5	0.80	0
4	EDO	EEE	404	-	3,3,3	0.19	0	2,2,2	0.32	0
2	MNA	CCC	401	-	19,22,22	0.83	1 (5%)	25,32,32	0.70	0
4	EDO	CCC	403	-	3,3,3	0.10	0	2,2,2	0.03	0
4	EDO	AAA	403	-	3,3,3	0.17	0	2,2,2	0.46	0
3	IMD	CCC	402	-	3,5,5	0.40	0	4,5,5	0.87	0
4	EDO	EEE	403	-	3,3,3	0.34	0	2,2,2	0.33	0
2	MNA	EEE	401	-	19,22,22	1.04	1 (5%)	25,32,32	0.92	0
4	EDO	JJJ	402	-	3,3,3	0.27	0	2,2,2	0.12	0
2	MNA	AAA	401	-	19,22,22	0.76	1 (5%)	25,32,32	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	III	402	-	3,3,3	0.34	0	2,2,2	0.34	0
4	EDO	EEE	406	-	3,3,3	0.21	0	2,2,2	0.22	0
4	EDO	EEE	405	-	3,3,3	0.08	0	2,2,2	0.10	0
2	MNA	DDD	401	-	19,22,22	0.82	2 (10%)	25,32,32	0.83	0
4	EDO	JJJ	403	-	3,3,3	0.08	0	2,2,2	0.11	0
4	EDO	BBB	402	-	3,3,3	0.17	0	2,2,2	0.19	0
2	MNA	III	401	-	19,22,22	0.70	0	25,32,32	0.85	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
4	EDO	AAA	404	-	-	0/1/1/1	-
4	EDO	HHH	402	-	-	0/1/1/1	-
3	IMD	AAA	402	-	-	-	0/1/1/1
2	MNA	JJJ	401	-	-	0/17/41/41	0/1/1/1
4	EDO	HHH	403	-	-	0/1/1/1	-
4	EDO	CCC	404	-	-	0/1/1/1	-
2	MNA	FFF	401	-	-	0/17/41/41	0/1/1/1
4	EDO	GGG	403	-	-	1/1/1/1	-
4	EDO	DDD	404	-	-	0/1/1/1	-
3	IMD	EEE	402	-	-	-	0/1/1/1
2	MNA	GGG	401	-	-	0/17/41/41	0/1/1/1
2	MNA	BBB	401	-	-	0/17/41/41	0/1/1/1
3	IMD	DDD	402	-	-	-	0/1/1/1
4	EDO	EEE	407	-	-	1/1/1/1	-
2	MNA	HHH	401	-	-	0/17/41/41	0/1/1/1
4	EDO	FFF	402	-	-	0/1/1/1	-
4	EDO	FFF	403	-	-	1/1/1/1	-
4	EDO	GGG	404	-	-	1/1/1/1	-
4	EDO	DDD	403	-	-	0/1/1/1	-
4	EDO	AAA	405	-	-	1/1/1/1	-
3	IMD	GGG	402	-	-	-	0/1/1/1
4	EDO	EEE	404	-	-	1/1/1/1	-
2	MNA	CCC	401	-	-	1/17/41/41	0/1/1/1
4	EDO	CCC	403	-	-	0/1/1/1	-
4	EDO	AAA	403	-	-	1/1/1/1	-
3	IMD	CCC	402	-	-	-	0/1/1/1
4	EDO	EEE	403	-	-	1/1/1/1	-
2	MNA	EEE	401	-	-	0/17/41/41	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	JJJ	402	-	-	1/1/1/1	-
2	MNA	AAA	401	-	-	0/17/41/41	0/1/1/1
4	EDO	III	402	-	-	1/1/1/1	-
4	EDO	EEE	406	-	-	0/1/1/1	-
4	EDO	EEE	405	-	-	1/1/1/1	-
2	MNA	DDD	401	-	-	0/17/41/41	0/1/1/1
4	EDO	JJJ	403	-	-	1/1/1/1	-
4	EDO	BBB	402	-	-	0/1/1/1	-
2	MNA	III	401	-	-	0/17/41/41	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	CCC	401	MNA	O2-C2	3.04	1.45	1.41
2	EEE	401	MNA	O2-C2	2.97	1.45	1.41
2	GGG	401	MNA	O2-C2	2.53	1.44	1.41
2	HHH	401	MNA	O2-C2	2.43	1.44	1.41
2	DDD	401	MNA	O2-C2	2.14	1.44	1.41
2	AAA	401	MNA	O6-C2	2.12	1.45	1.42
2	DDD	401	MNA	O6-C2	2.07	1.45	1.42
2	JJJ	401	MNA	O2-C2	2.02	1.44	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	HHH	401	MNA	C3-C4-C5	2.13	113.26	109.98
2	BBB	401	MNA	O6-C6-C7	-2.00	104.20	107.29

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	III	402	EDO	O1-C1-C2-O2
4	EEE	404	EDO	O1-C1-C2-O2
4	AAA	403	EDO	O1-C1-C2-O2
4	EEE	405	EDO	O1-C1-C2-O2
4	GGG	404	EDO	O1-C1-C2-O2
4	EEE	403	EDO	O1-C1-C2-O2
4	JJJ	402	EDO	O1-C1-C2-O2
2	CCC	401	MNA	O8-C8-C9-O9
4	GGG	403	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	AAA	405	EDO	O1-C1-C2-O2
4	JJJ	403	EDO	O1-C1-C2-O2
4	FFF	403	EDO	O1-C1-C2-O2
4	EEE	407	EDO	O1-C1-C2-O2

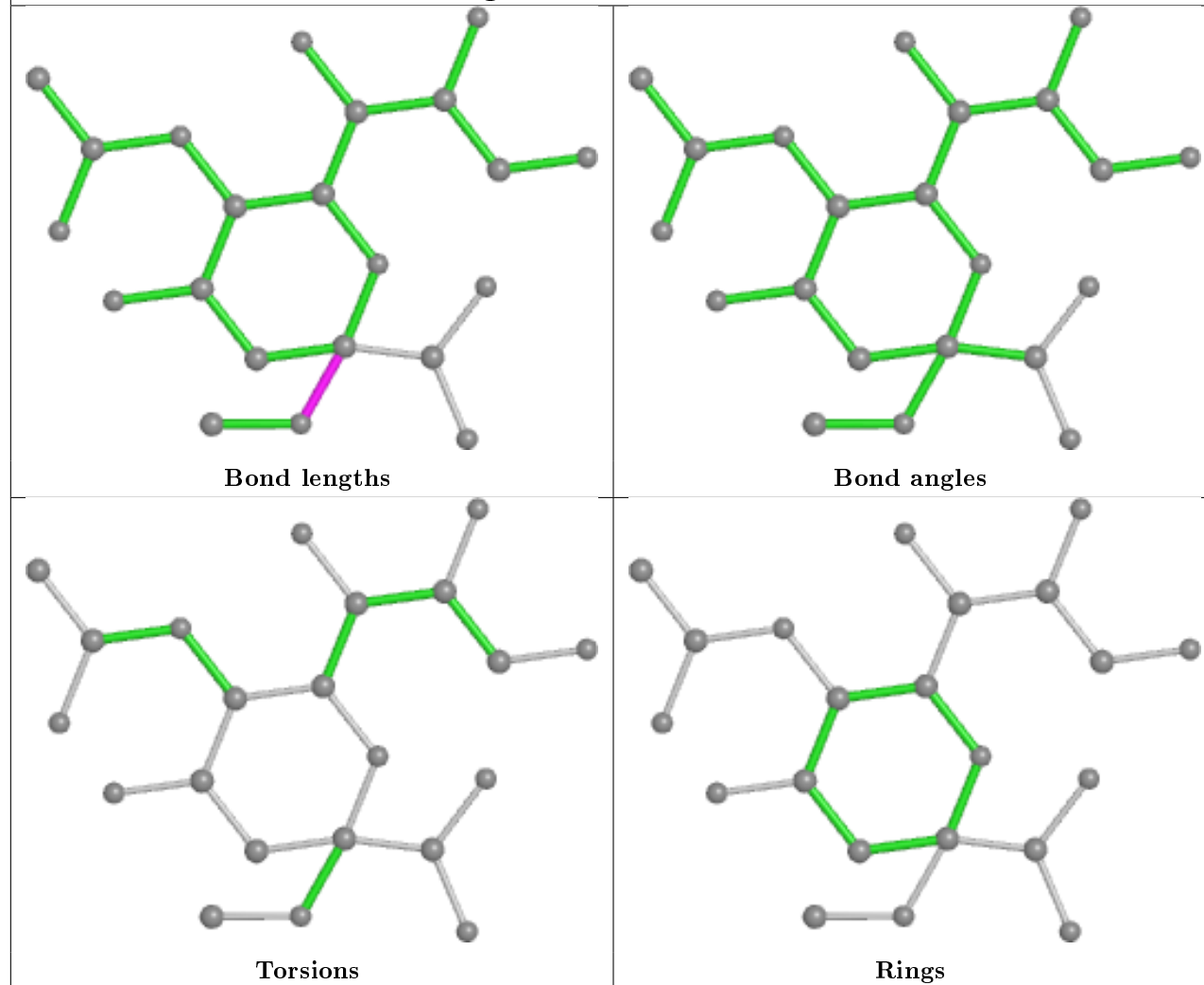
There are no ring outliers.

1 monomer is involved in 1 short contact:

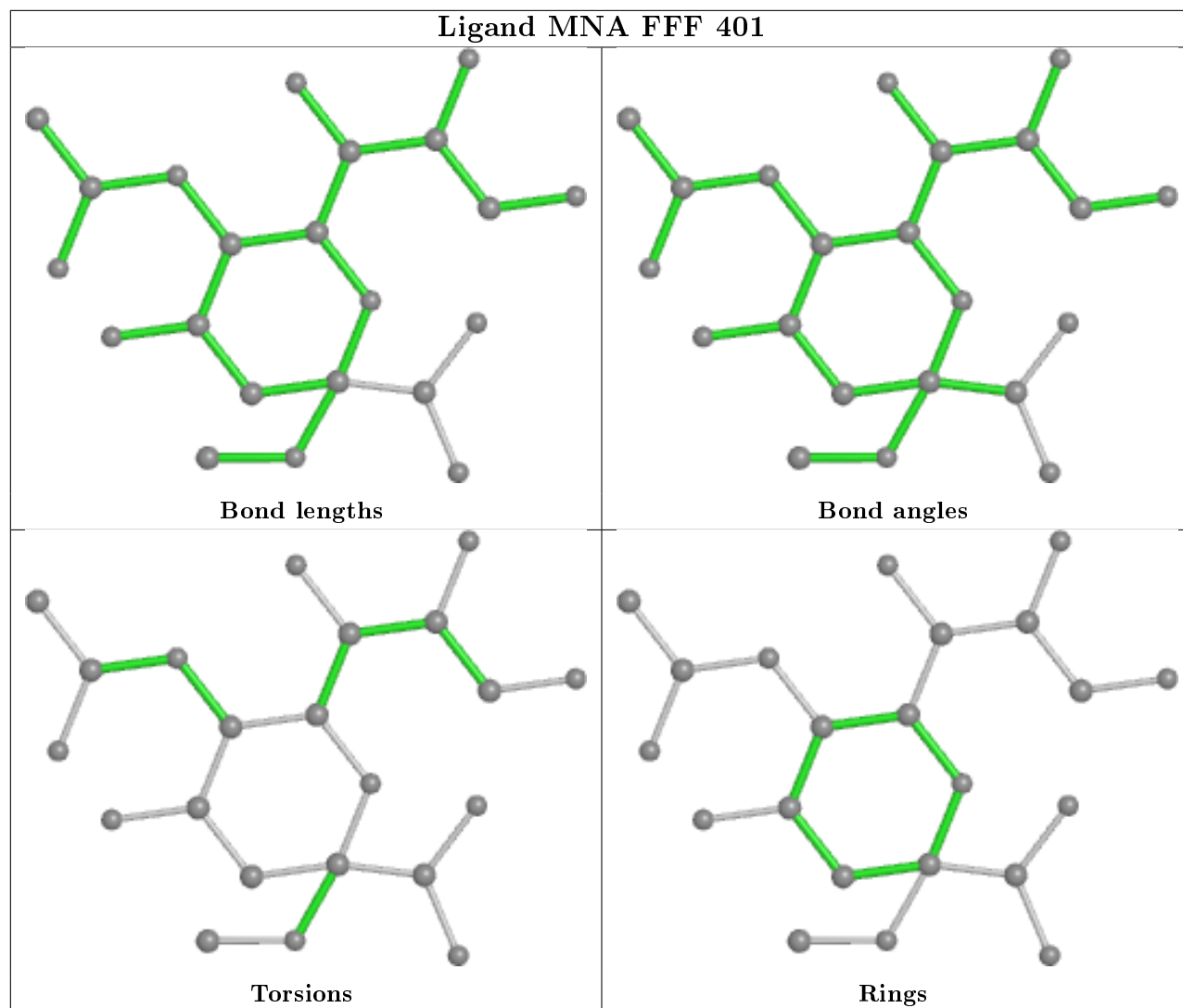
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	EEE	403	EDO	1	0

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.

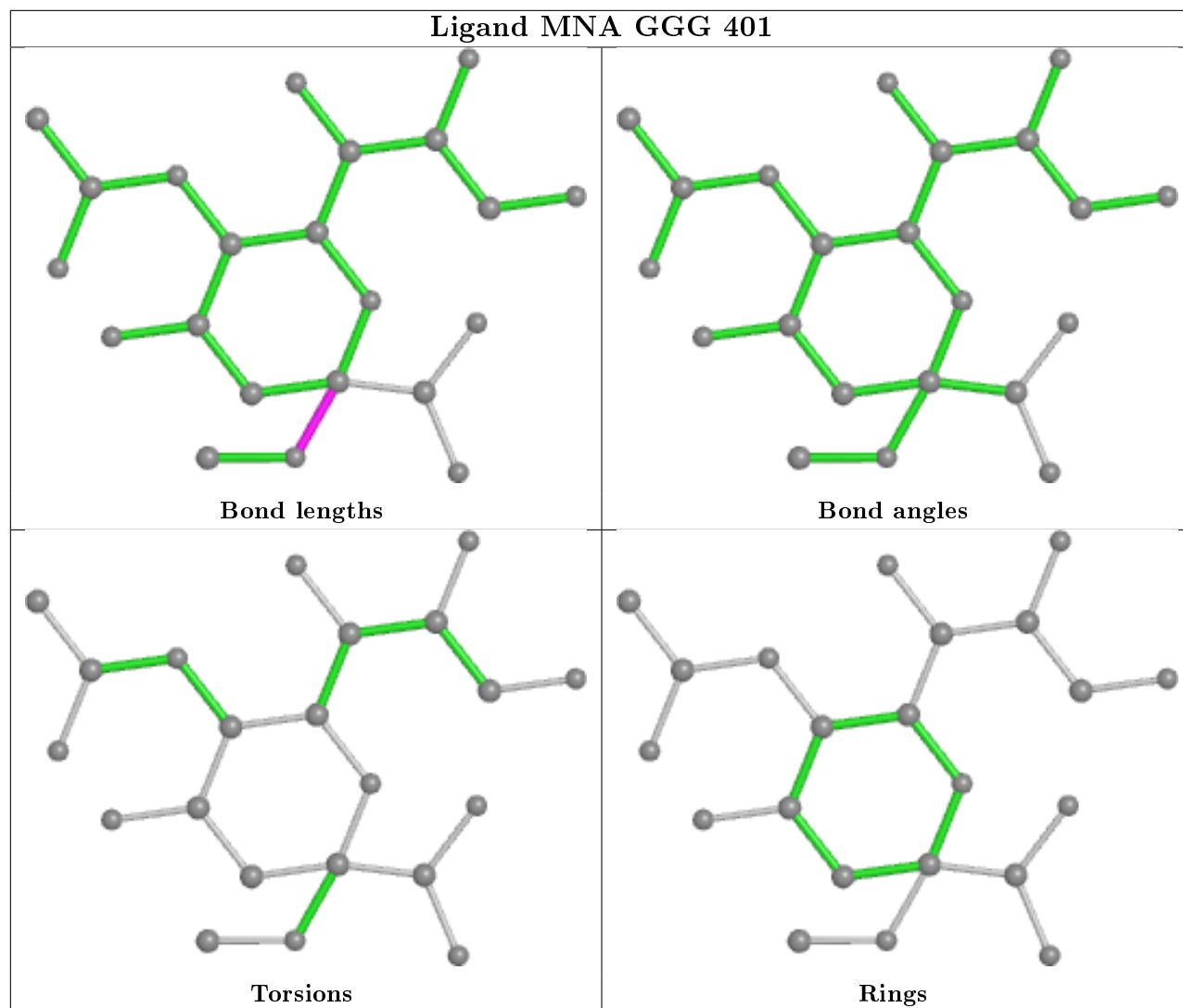
Ligand MNA JJJ 401



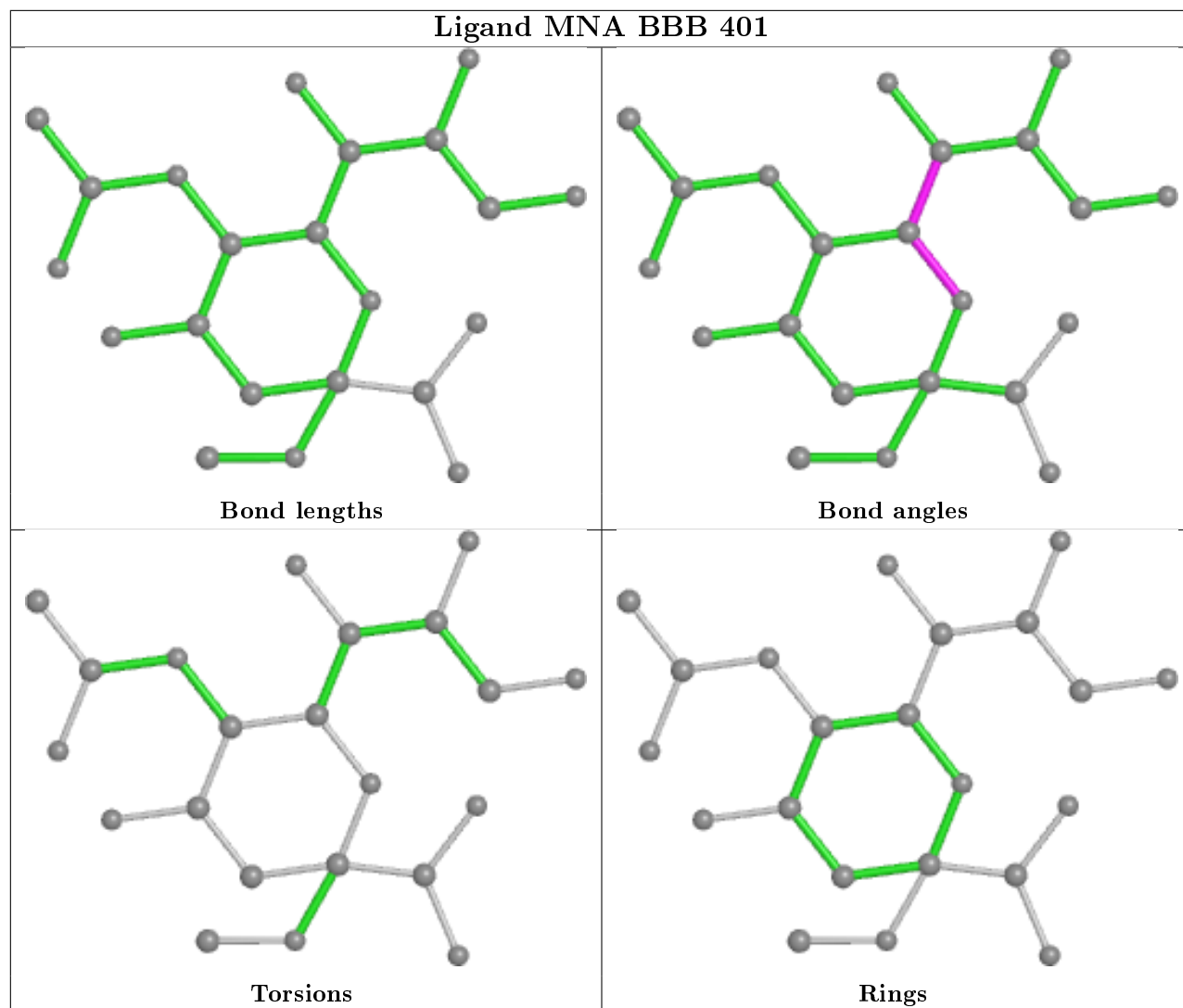
Ligand MNA FFF 401



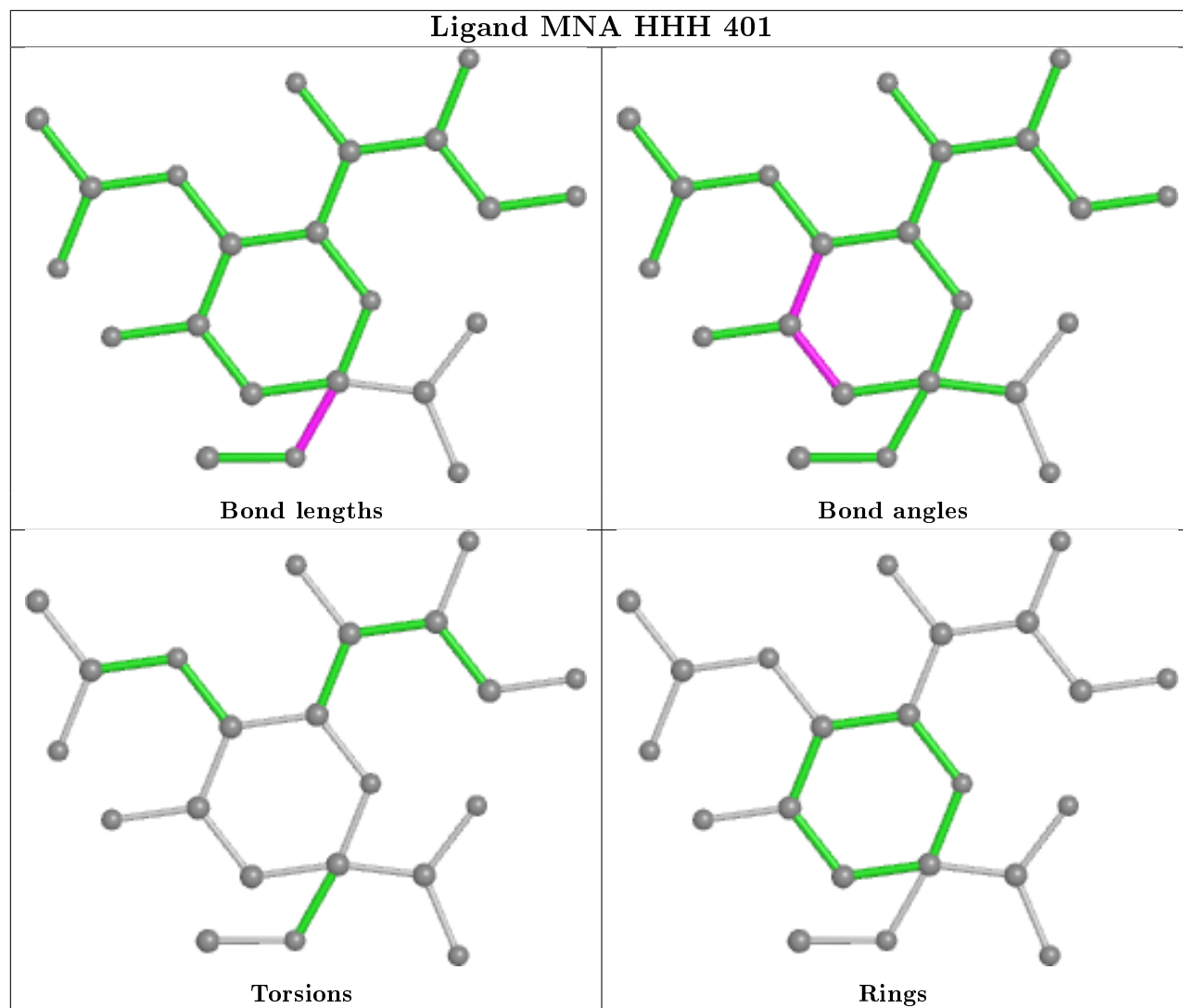
Ligand MNA GGG 401



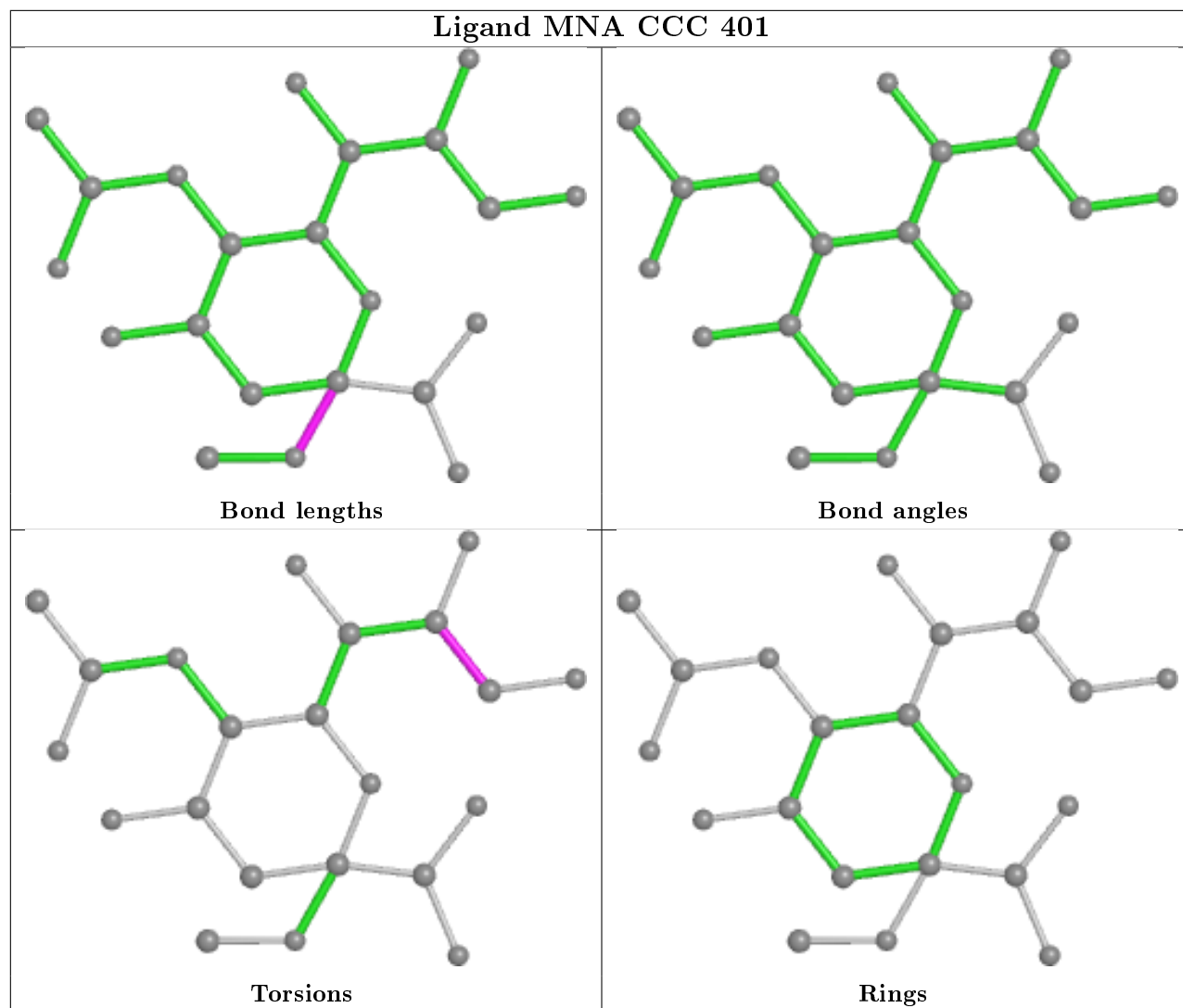
Ligand MNA BBB 401



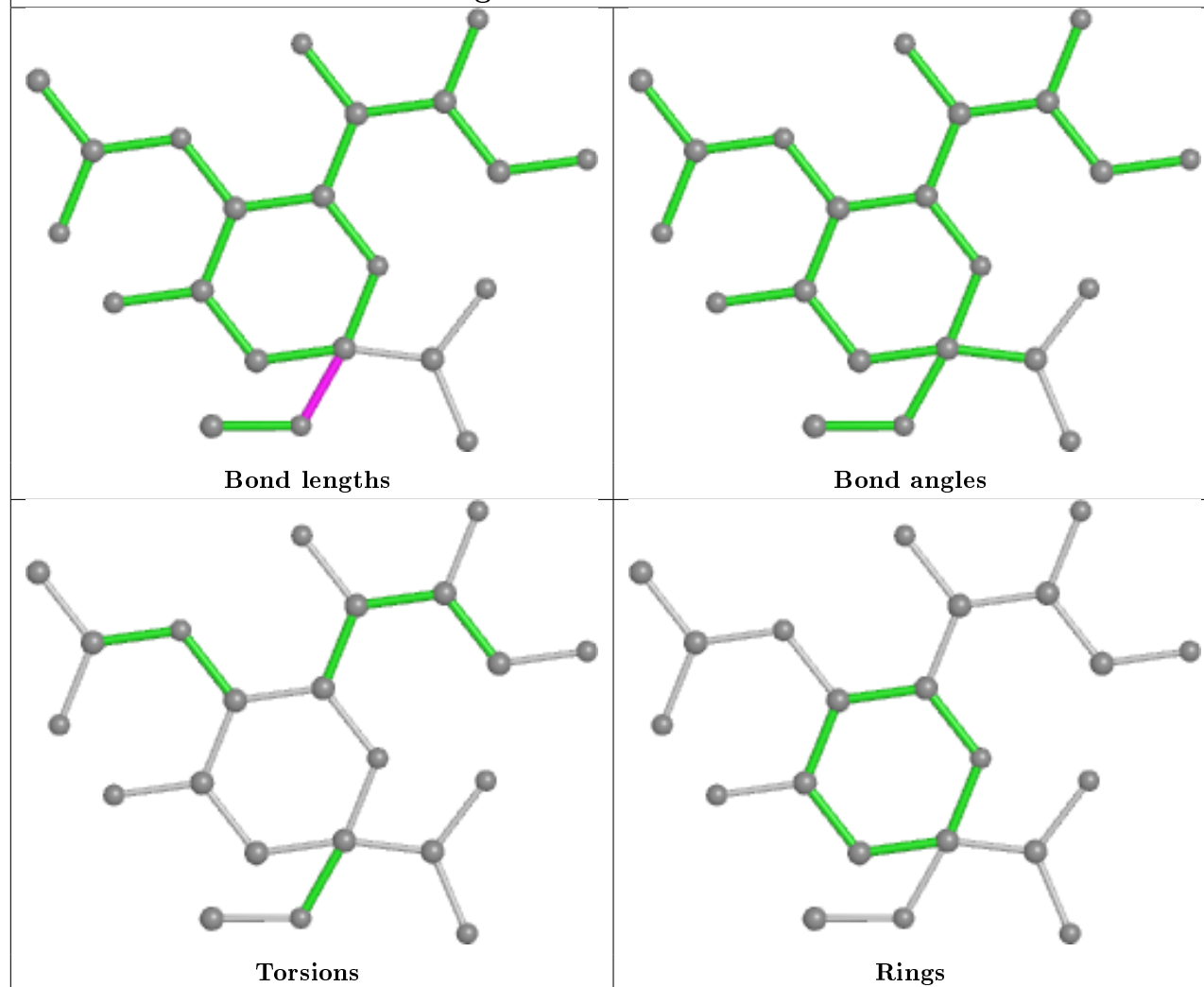
Ligand MNA HHH 401



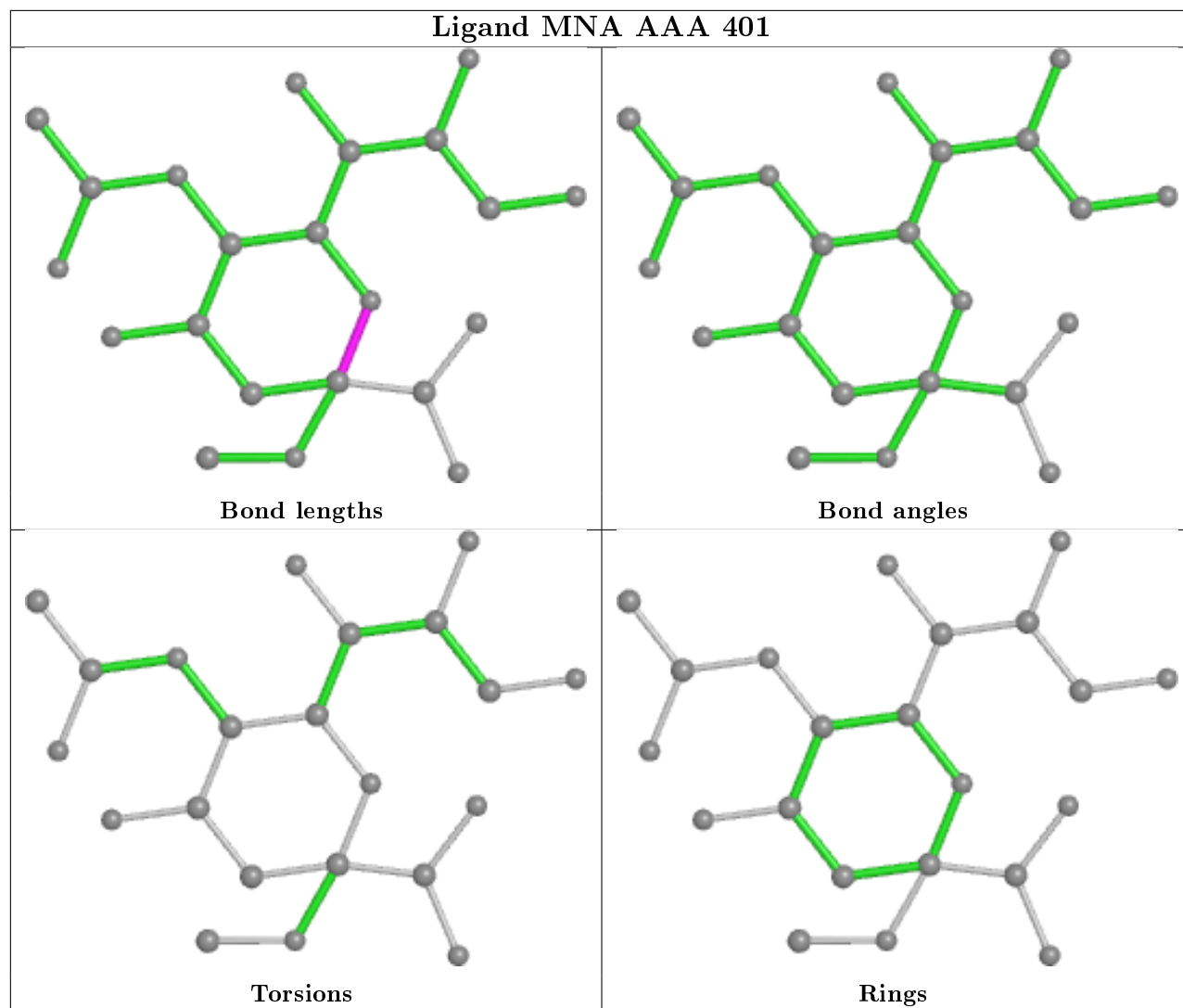
Ligand MNA CCC 401



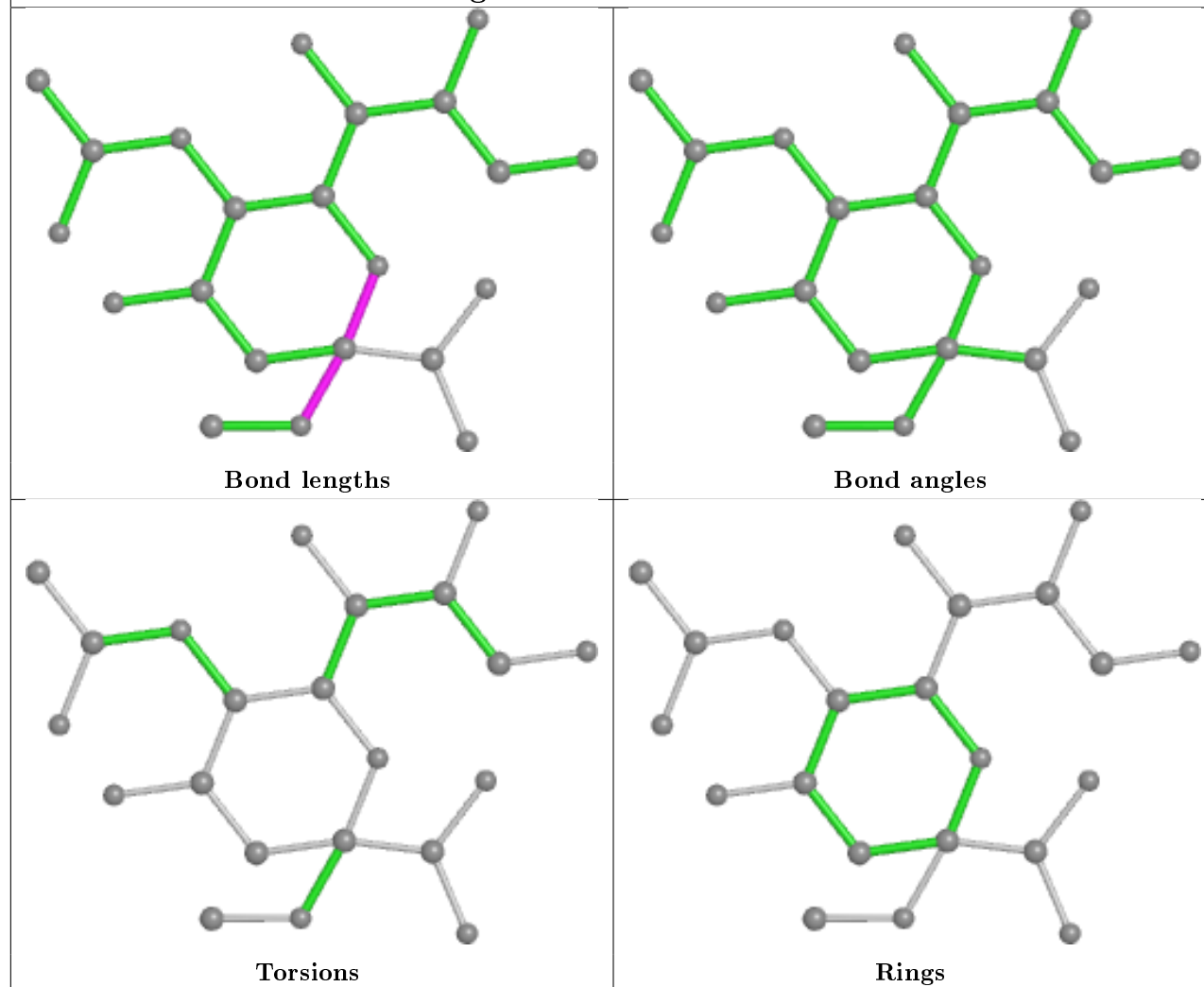
Ligand MNA EEE 401

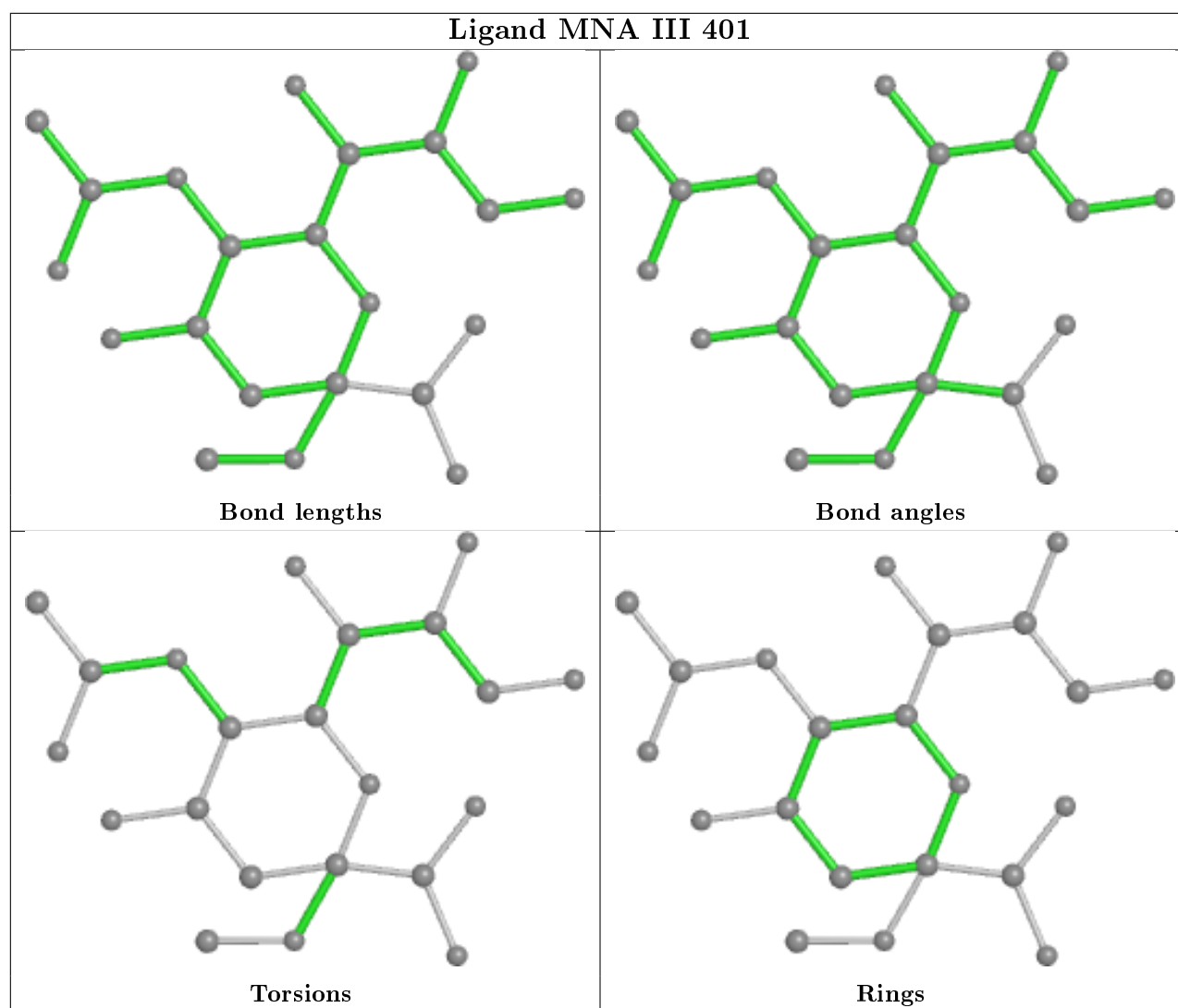


Ligand MNA AAA 401



Ligand MNA DDD 401





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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	265/287 (92%)	-0.53	0 100 100	13, 18, 26, 44	0
1	BBB	265/287 (92%)	-0.44	1 (0%) 92 95	12, 18, 31, 45	0
1	CCC	267/287 (93%)	-0.46	3 (1%) 80 85	11, 16, 29, 60	0
1	DDD	265/287 (92%)	-0.51	1 (0%) 92 95	10, 15, 30, 49	0
1	EEE	265/287 (92%)	-0.53	0 100 100	12, 16, 28, 41	0
1	FFF	265/287 (92%)	-0.47	1 (0%) 92 95	12, 17, 29, 40	0
1	GGG	268/287 (93%)	-0.45	1 (0%) 92 95	11, 16, 33, 54	0
1	HHH	265/287 (92%)	-0.49	2 (0%) 86 90	10, 15, 33, 53	0
1	III	267/287 (93%)	-0.42	4 (1%) 73 81	11, 15, 35, 65	0
1	JJJ	268/287 (93%)	-0.52	2 (0%) 87 92	12, 17, 26, 50	0
All	All	2660/2870 (92%)	-0.48	15 (0%) 89 93	10, 16, 30, 65	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	III	21	GLY	6.0
1	CCC	21	GLY	5.3
1	GGG	21	GLY	3.7
1	HHH	90	THR	3.6
1	FFF	22	GLY	2.8
1	HHH	22	GLY	2.8
1	JJJ	21	GLY	2.6
1	DDD	22	GLY	2.5
1	CCC	22	GLY	2.4
1	JJJ	19	HIS	2.4
1	BBB	22	GLY	2.2
1	III	90	THR	2.2
1	III	88	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	CCC	20	MET	2.1
1	III	22	GLY	2.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	EEE	404	4/4	0.66	0.15	45,46,46,49	0
2	MNA	EEE	401	22/22	0.78	0.22	24,39,54,56	0
4	EDO	HHH	402	4/4	0.84	0.15	46,46,48,49	0
4	EDO	EEE	405	4/4	0.85	0.13	35,39,40,44	0
4	EDO	FFF	402	4/4	0.88	0.17	40,40,41,44	0
4	EDO	DDD	404	4/4	0.89	0.13	40,43,44,45	0
4	EDO	EEE	403	4/4	0.89	0.13	34,35,36,36	0
3	IMD	DDD	402	5/5	0.89	0.11	22,22,24,25	0
4	EDO	HHH	403	4/4	0.89	0.17	41,42,44,44	0
2	MNA	CCC	401	22/22	0.91	0.13	16,22,26,31	0
4	EDO	JJJ	402	4/4	0.91	0.17	35,36,37,40	0
2	MNA	AAA	401	22/22	0.91	0.12	18,23,30,35	0
2	MNA	BBB	401	22/22	0.91	0.13	21,24,31,32	0
2	MNA	III	401	22/22	0.91	0.12	21,26,32,34	0
4	EDO	AAA	405	4/4	0.92	0.13	42,43,44,45	0
4	EDO	III	402	4/4	0.92	0.11	25,30,33,33	0
4	EDO	EEE	406	4/4	0.92	0.15	43,44,44,44	0
2	MNA	GGG	401	22/22	0.92	0.11	16,22,30,32	0
4	EDO	JJJ	403	4/4	0.92	0.11	42,42,43,43	0
4	EDO	BBB	402	4/4	0.92	0.11	35,35,36,37	0
4	EDO	CCC	404	4/4	0.92	0.14	33,37,41,43	0

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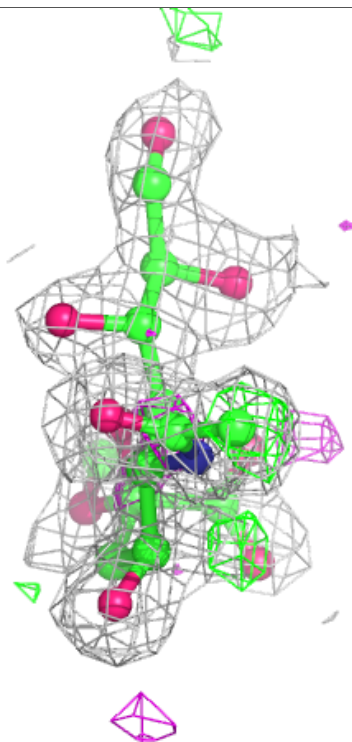
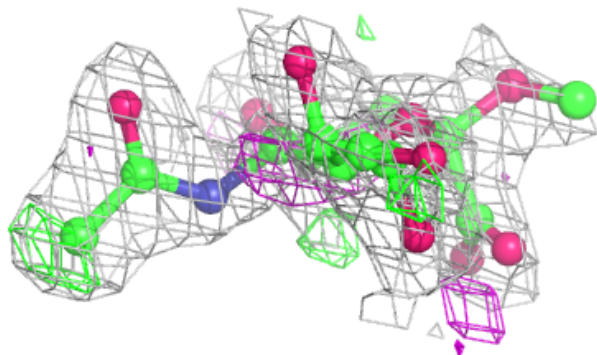
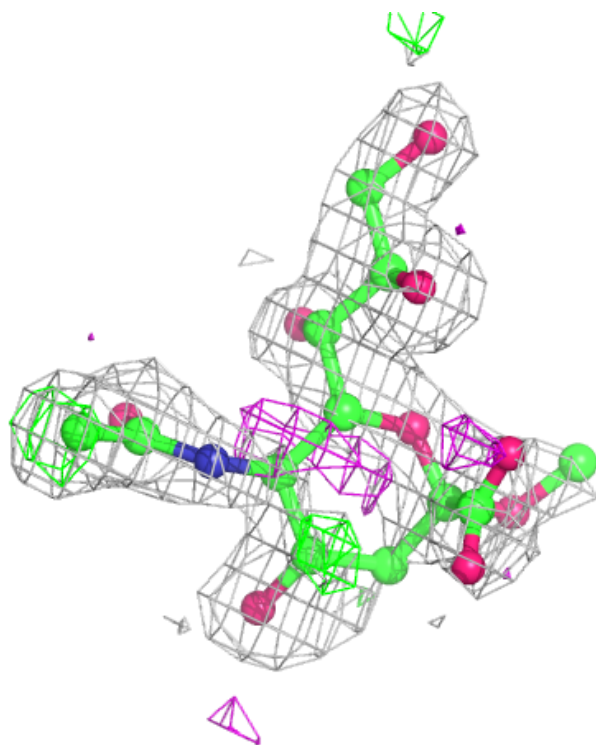
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	EEE	407	4/4	0.93	0.10	31,32,33,34	0
4	EDO	AAA	404	4/4	0.93	0.13	33,34,35,35	0
2	MNA	JJJ	401	22/22	0.93	0.14	16,23,32,36	0
2	MNA	DDD	401	22/22	0.94	0.12	15,20,26,31	0
4	EDO	GGG	404	4/4	0.94	0.11	43,44,45,46	0
4	EDO	DDD	403	4/4	0.94	0.09	36,40,42,44	0
2	MNA	FFF	401	22/22	0.94	0.11	17,22,28,31	0
3	IMD	EEE	402	5/5	0.95	0.08	24,24,25,26	0
2	MNA	HHH	401	22/22	0.95	0.11	16,20,26,29	0
3	IMD	AAA	402	5/5	0.95	0.08	20,21,22,23	0
4	EDO	FFF	403	4/4	0.95	0.13	38,39,39,42	0
3	IMD	GGG	402	5/5	0.96	0.08	20,20,21,21	0
3	IMD	CCC	402	5/5	0.97	0.08	20,21,22,22	0
4	EDO	GGG	403	4/4	0.97	0.12	29,32,33,36	0
4	EDO	CCC	403	4/4	0.97	0.08	22,27,28,30	0
4	EDO	AAA	403	4/4	0.97	0.09	25,28,30,30	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

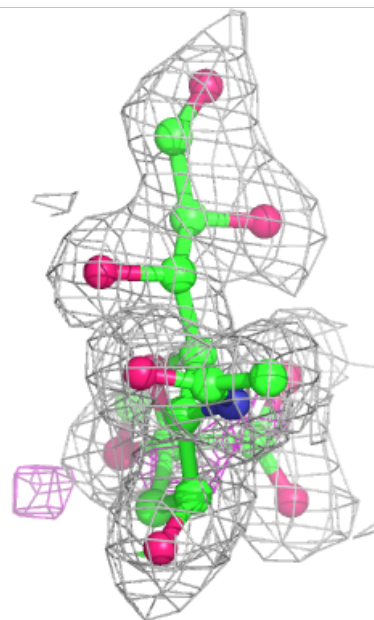
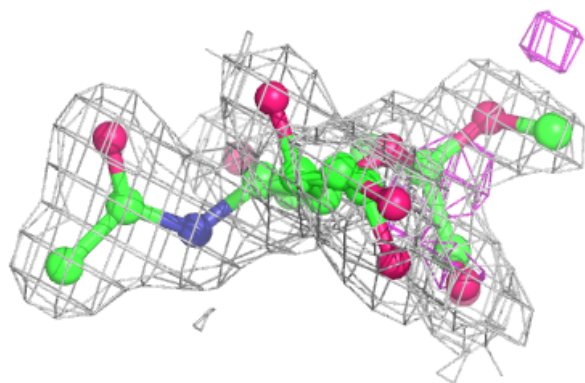
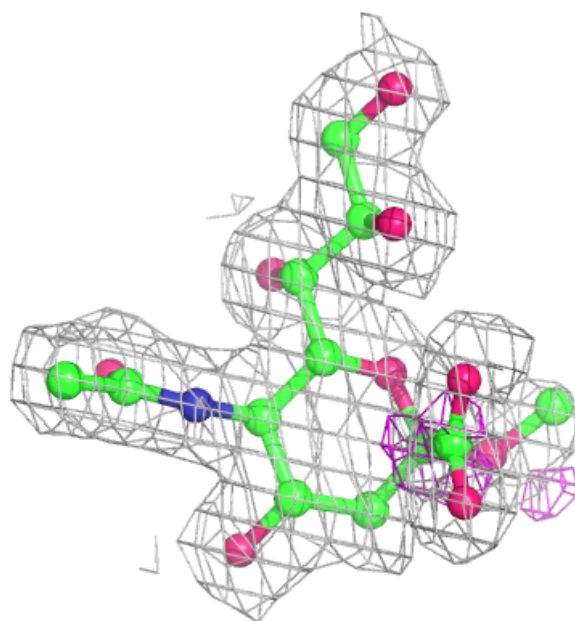
Electron density around MNA EEE 401:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



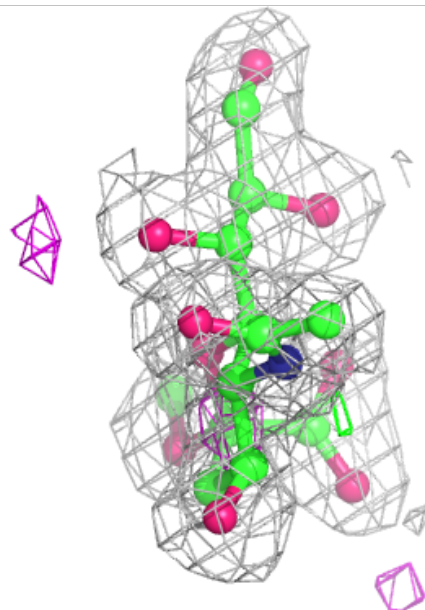
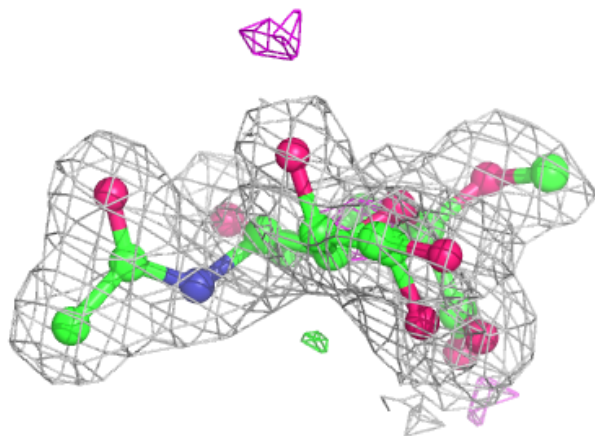
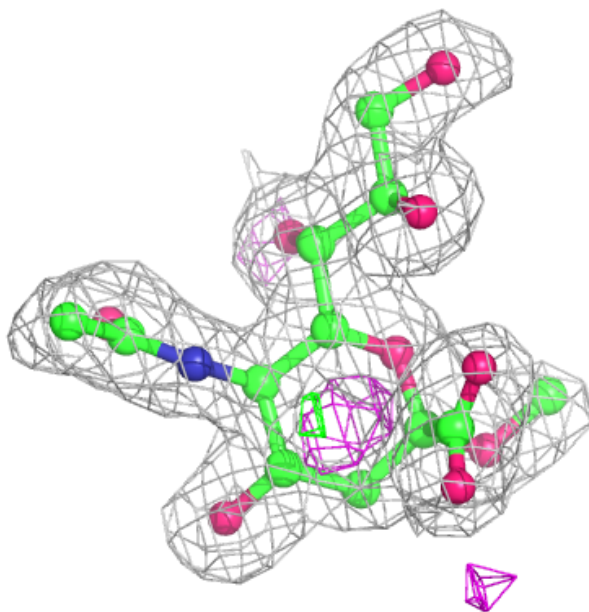
Electron density around MNA CCC 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



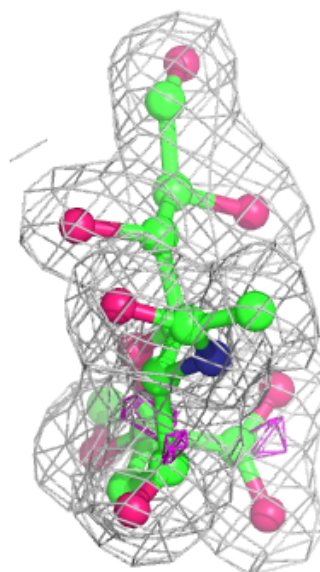
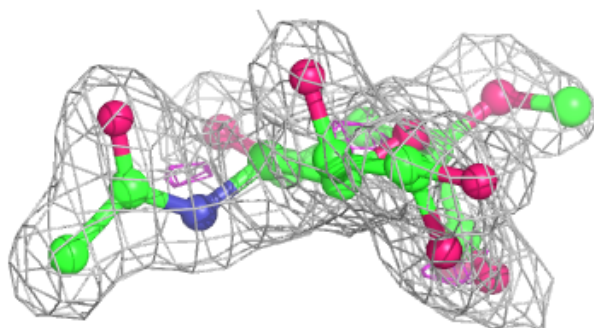
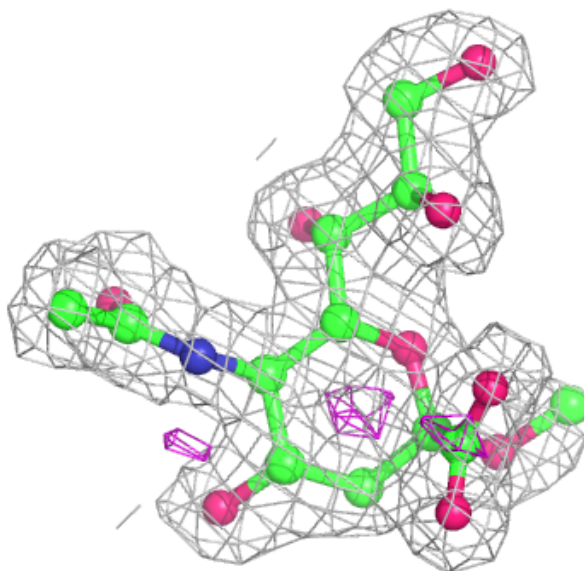
Electron density around MNA AAA 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



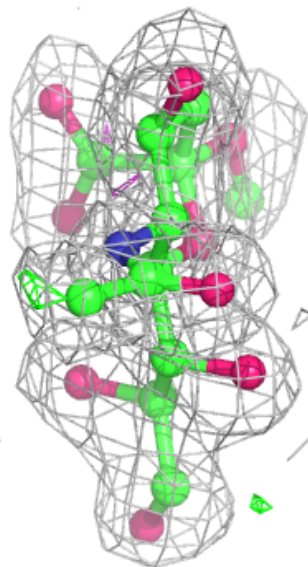
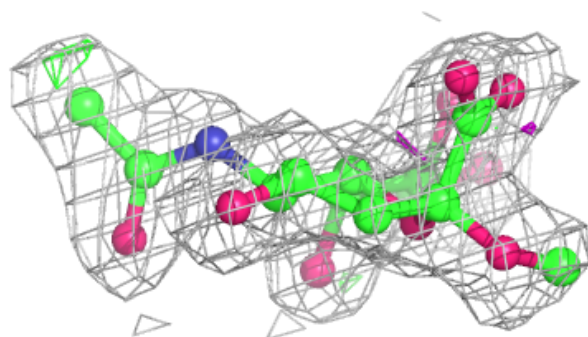
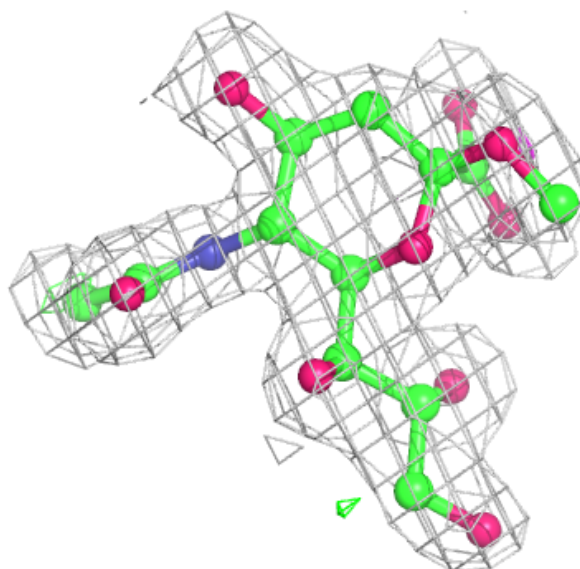
Electron density around MNA BBB 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



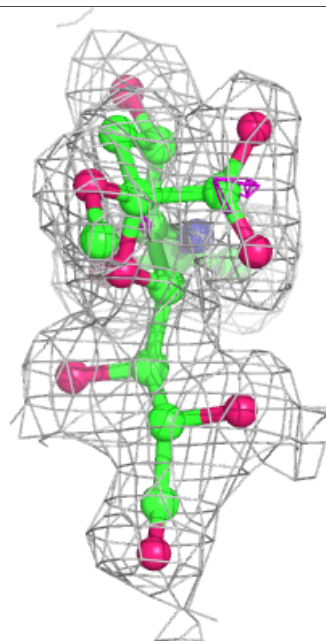
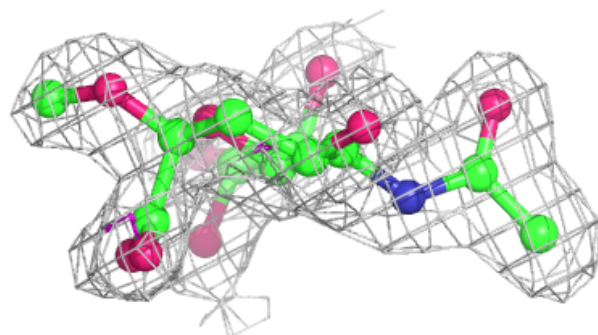
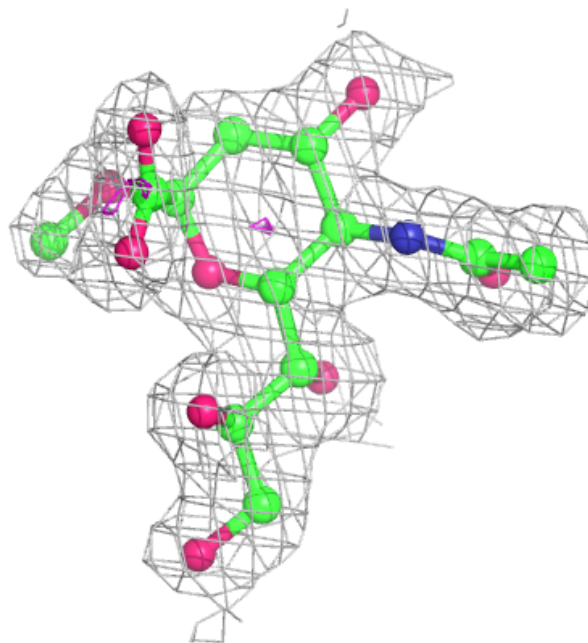
Electron density around MNA III 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



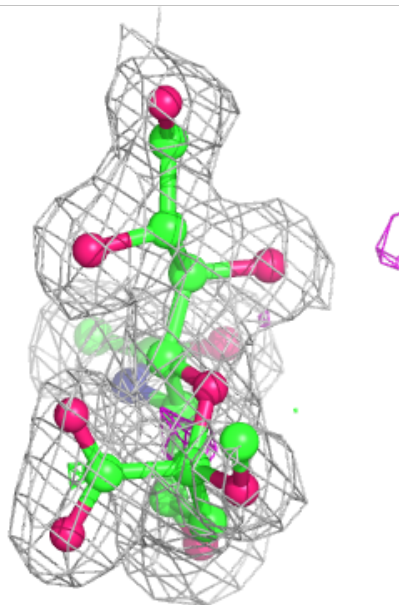
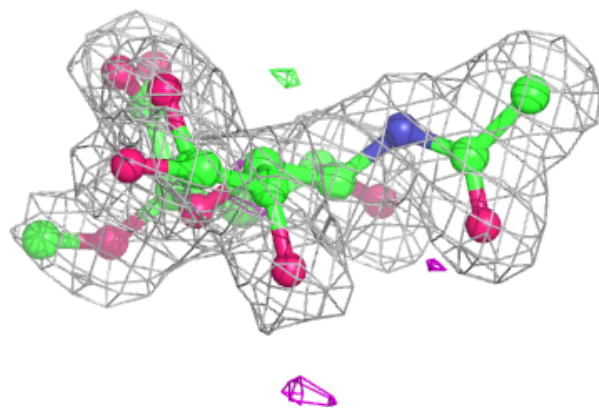
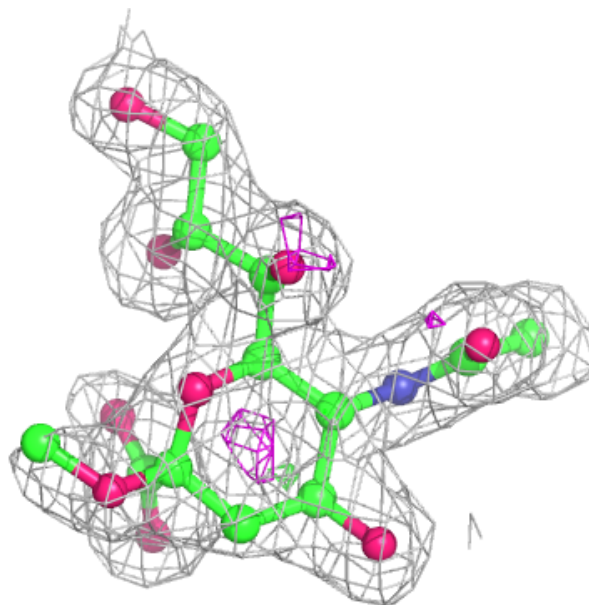
Electron density around MNA GGG 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



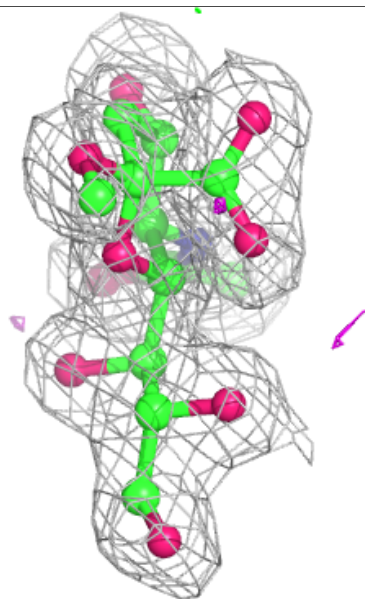
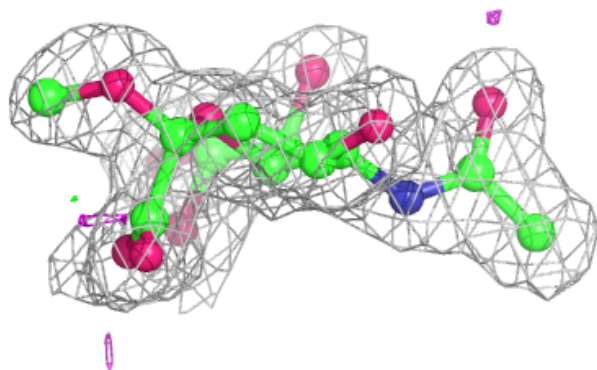
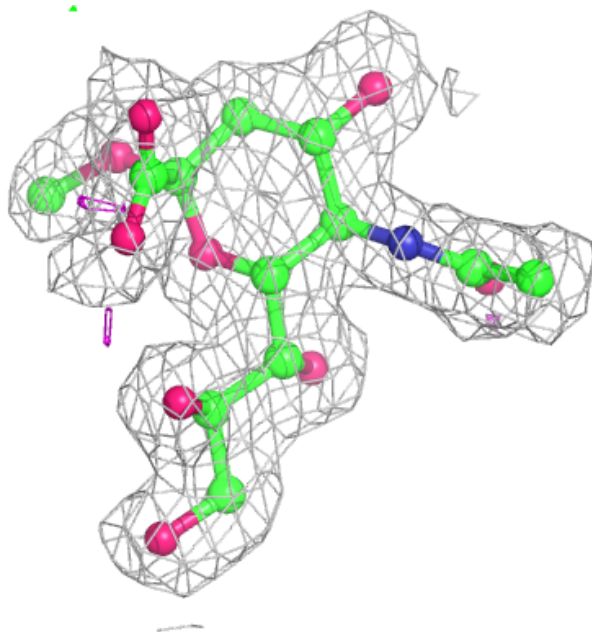
Electron density around MNA JJJ 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



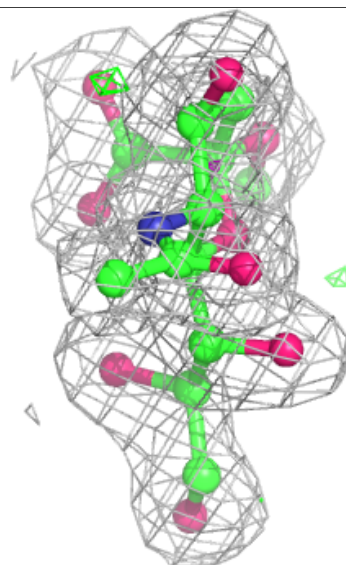
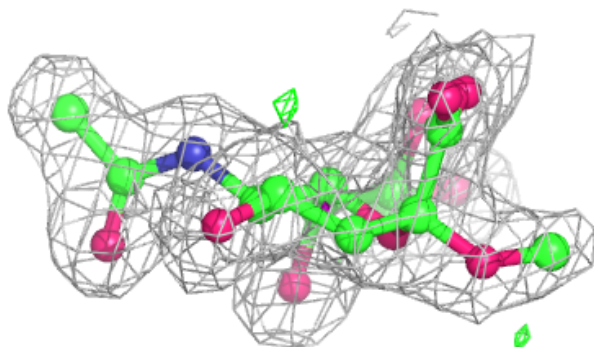
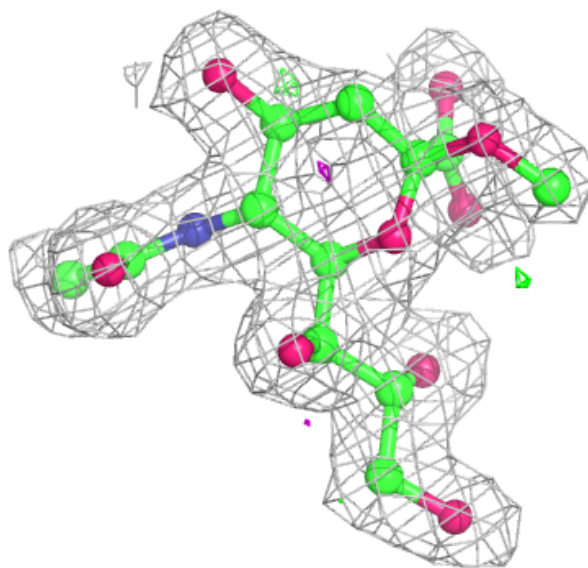
Electron density around MNA DDD 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



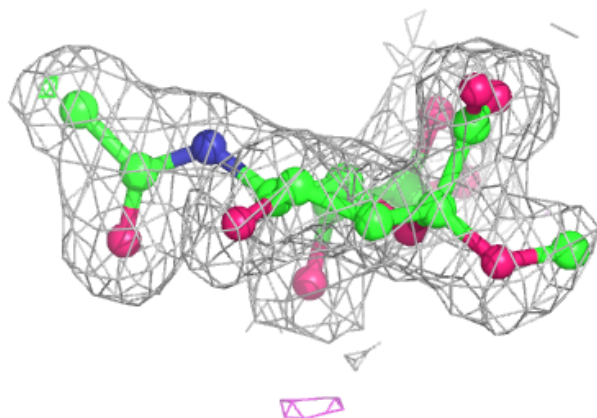
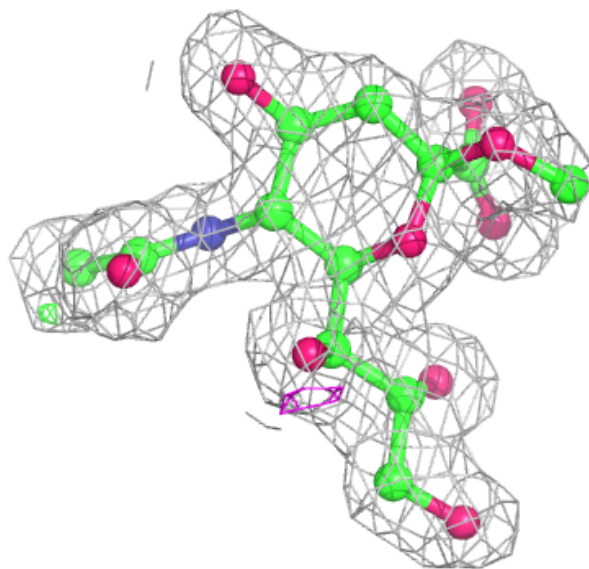
Electron density around MNA FFF 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MNA HHH 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.