



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 15, 2024 – 09:47 pm GMT

PDB ID : 6T6G  
Title : Bacteroides salyersiae GH164 beta-mannosidase in complex with noeuromycin  
Authors : Armstrong, Z.; Davies, G.  
Deposited on : 2019-10-18  
Resolution : 2.06 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

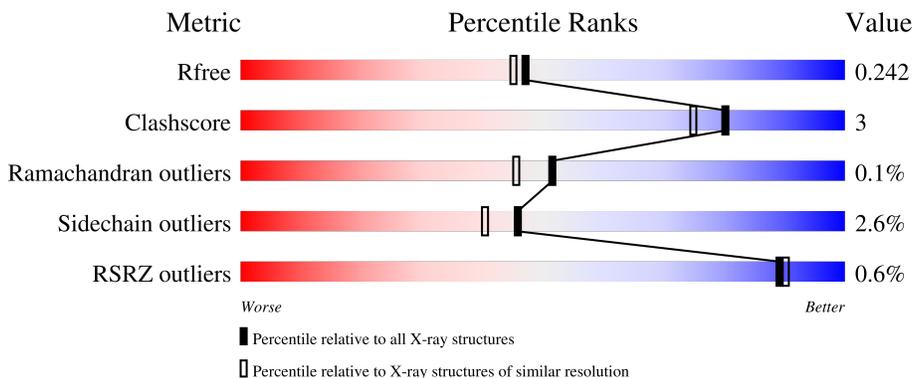
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.06 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	674	 89% 8% .
1	BBB	674	 89% 7% .
1	CCC	674	 87% 8% . .
1	DDD	674	 89% 8% . .
1	EEE	674	 88% 8% .

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Mol	Chain	Length	Quality of chain
1	FFF	674	 88% 8% ..

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 63581 atoms, of which 30974 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 Glyco\_hydro\_42M domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	AAA	655	10447	3409	5172	872	975	19	285	0	0
1	DDD	655	10435	3405	5168	871	972	19	283	0	0
1	CCC	650	10358	3378	5126	866	969	19	282	0	0
1	BBB	650	10361	3379	5128	866	969	19	283	0	0
1	FFF	651	10387	3387	5141	868	972	19	284	1	0
1	EEE	650	10354	3377	5125	865	968	19	281	0	0

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	10	MET	-	initiating methionine	UNP I9SUA3
AAA	11	GLY	-	expression tag	UNP I9SUA3
AAA	12	SER	-	expression tag	UNP I9SUA3
AAA	13	SER	-	expression tag	UNP I9SUA3
AAA	14	HIS	-	expression tag	UNP I9SUA3
AAA	15	HIS	-	expression tag	UNP I9SUA3
AAA	16	HIS	-	expression tag	UNP I9SUA3
AAA	17	HIS	-	expression tag	UNP I9SUA3
AAA	18	HIS	-	expression tag	UNP I9SUA3
AAA	19	HIS	-	expression tag	UNP I9SUA3
AAA	20	SER	-	expression tag	UNP I9SUA3
AAA	21	SER	-	expression tag	UNP I9SUA3
AAA	22	GLY	-	expression tag	UNP I9SUA3
AAA	23	LEU	-	expression tag	UNP I9SUA3
AAA	24	GLU	-	expression tag	UNP I9SUA3
AAA	25	VAL	-	expression tag	UNP I9SUA3
AAA	26	LEU	-	expression tag	UNP I9SUA3

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	27	PHE	-	expression tag	UNP I9SUA3
AAA	28	GLN	-	expression tag	UNP I9SUA3
AAA	29	GLY	-	expression tag	UNP I9SUA3
AAA	30	PRO	-	expression tag	UNP I9SUA3
AAA	31	ALA	-	expression tag	UNP I9SUA3
DDD	10	MET	-	initiating methionine	UNP I9SUA3
DDD	11	GLY	-	expression tag	UNP I9SUA3
DDD	12	SER	-	expression tag	UNP I9SUA3
DDD	13	SER	-	expression tag	UNP I9SUA3
DDD	14	HIS	-	expression tag	UNP I9SUA3
DDD	15	HIS	-	expression tag	UNP I9SUA3
DDD	16	HIS	-	expression tag	UNP I9SUA3
DDD	17	HIS	-	expression tag	UNP I9SUA3
DDD	18	HIS	-	expression tag	UNP I9SUA3
DDD	19	HIS	-	expression tag	UNP I9SUA3
DDD	20	SER	-	expression tag	UNP I9SUA3
DDD	21	SER	-	expression tag	UNP I9SUA3
DDD	22	GLY	-	expression tag	UNP I9SUA3
DDD	23	LEU	-	expression tag	UNP I9SUA3
DDD	24	GLU	-	expression tag	UNP I9SUA3
DDD	25	VAL	-	expression tag	UNP I9SUA3
DDD	26	LEU	-	expression tag	UNP I9SUA3
DDD	27	PHE	-	expression tag	UNP I9SUA3
DDD	28	GLN	-	expression tag	UNP I9SUA3
DDD	29	GLY	-	expression tag	UNP I9SUA3
DDD	30	PRO	-	expression tag	UNP I9SUA3
DDD	31	ALA	-	expression tag	UNP I9SUA3
CCC	10	MET	-	initiating methionine	UNP I9SUA3
CCC	11	GLY	-	expression tag	UNP I9SUA3
CCC	12	SER	-	expression tag	UNP I9SUA3
CCC	13	SER	-	expression tag	UNP I9SUA3
CCC	14	HIS	-	expression tag	UNP I9SUA3
CCC	15	HIS	-	expression tag	UNP I9SUA3
CCC	16	HIS	-	expression tag	UNP I9SUA3
CCC	17	HIS	-	expression tag	UNP I9SUA3
CCC	18	HIS	-	expression tag	UNP I9SUA3
CCC	19	HIS	-	expression tag	UNP I9SUA3
CCC	20	SER	-	expression tag	UNP I9SUA3
CCC	21	SER	-	expression tag	UNP I9SUA3
CCC	22	GLY	-	expression tag	UNP I9SUA3
CCC	23	LEU	-	expression tag	UNP I9SUA3
CCC	24	GLU	-	expression tag	UNP I9SUA3

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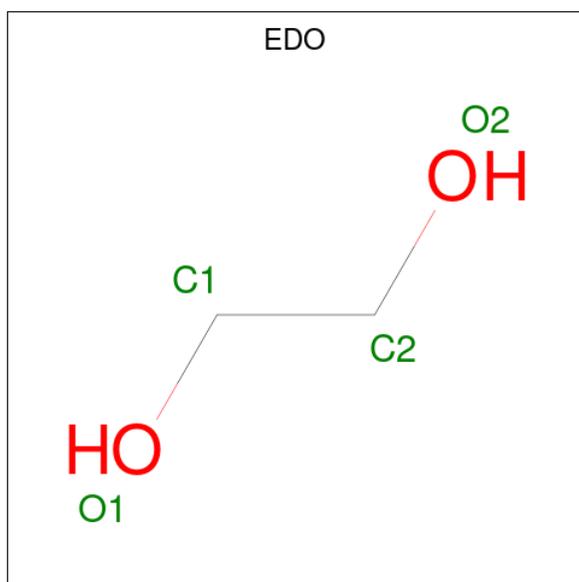
Chain	Residue	Modelled	Actual	Comment	Reference
CCC	25	VAL	-	expression tag	UNP I9SUA3
CCC	26	LEU	-	expression tag	UNP I9SUA3
CCC	27	PHE	-	expression tag	UNP I9SUA3
CCC	28	GLN	-	expression tag	UNP I9SUA3
CCC	29	GLY	-	expression tag	UNP I9SUA3
CCC	30	PRO	-	expression tag	UNP I9SUA3
CCC	31	ALA	-	expression tag	UNP I9SUA3
BBB	10	MET	-	initiating methionine	UNP I9SUA3
BBB	11	GLY	-	expression tag	UNP I9SUA3
BBB	12	SER	-	expression tag	UNP I9SUA3
BBB	13	SER	-	expression tag	UNP I9SUA3
BBB	14	HIS	-	expression tag	UNP I9SUA3
BBB	15	HIS	-	expression tag	UNP I9SUA3
BBB	16	HIS	-	expression tag	UNP I9SUA3
BBB	17	HIS	-	expression tag	UNP I9SUA3
BBB	18	HIS	-	expression tag	UNP I9SUA3
BBB	19	HIS	-	expression tag	UNP I9SUA3
BBB	20	SER	-	expression tag	UNP I9SUA3
BBB	21	SER	-	expression tag	UNP I9SUA3
BBB	22	GLY	-	expression tag	UNP I9SUA3
BBB	23	LEU	-	expression tag	UNP I9SUA3
BBB	24	GLU	-	expression tag	UNP I9SUA3
BBB	25	VAL	-	expression tag	UNP I9SUA3
BBB	26	LEU	-	expression tag	UNP I9SUA3
BBB	27	PHE	-	expression tag	UNP I9SUA3
BBB	28	GLN	-	expression tag	UNP I9SUA3
BBB	29	GLY	-	expression tag	UNP I9SUA3
BBB	30	PRO	-	expression tag	UNP I9SUA3
BBB	31	ALA	-	expression tag	UNP I9SUA3
FFF	10	MET	-	initiating methionine	UNP I9SUA3
FFF	11	GLY	-	expression tag	UNP I9SUA3
FFF	12	SER	-	expression tag	UNP I9SUA3
FFF	13	SER	-	expression tag	UNP I9SUA3
FFF	14	HIS	-	expression tag	UNP I9SUA3
FFF	15	HIS	-	expression tag	UNP I9SUA3
FFF	16	HIS	-	expression tag	UNP I9SUA3
FFF	17	HIS	-	expression tag	UNP I9SUA3
FFF	18	HIS	-	expression tag	UNP I9SUA3
FFF	19	HIS	-	expression tag	UNP I9SUA3
FFF	20	SER	-	expression tag	UNP I9SUA3
FFF	21	SER	-	expression tag	UNP I9SUA3
FFF	22	GLY	-	expression tag	UNP I9SUA3

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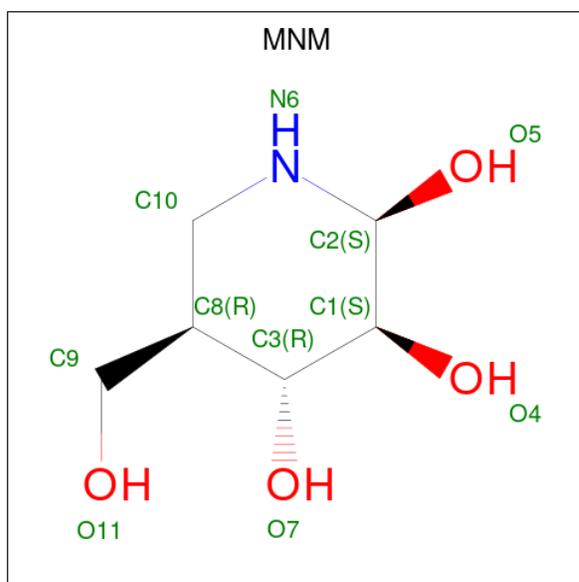
Chain	Residue	Modelled	Actual	Comment	Reference
FFF	23	LEU	-	expression tag	UNP I9SUA3
FFF	24	GLU	-	expression tag	UNP I9SUA3
FFF	25	VAL	-	expression tag	UNP I9SUA3
FFF	26	LEU	-	expression tag	UNP I9SUA3
FFF	27	PHE	-	expression tag	UNP I9SUA3
FFF	28	GLN	-	expression tag	UNP I9SUA3
FFF	29	GLY	-	expression tag	UNP I9SUA3
FFF	30	PRO	-	expression tag	UNP I9SUA3
FFF	31	ALA	-	expression tag	UNP I9SUA3
EEE	10	MET	-	initiating methionine	UNP I9SUA3
EEE	11	GLY	-	expression tag	UNP I9SUA3
EEE	12	SER	-	expression tag	UNP I9SUA3
EEE	13	SER	-	expression tag	UNP I9SUA3
EEE	14	HIS	-	expression tag	UNP I9SUA3
EEE	15	HIS	-	expression tag	UNP I9SUA3
EEE	16	HIS	-	expression tag	UNP I9SUA3
EEE	17	HIS	-	expression tag	UNP I9SUA3
EEE	18	HIS	-	expression tag	UNP I9SUA3
EEE	19	HIS	-	expression tag	UNP I9SUA3
EEE	20	SER	-	expression tag	UNP I9SUA3
EEE	21	SER	-	expression tag	UNP I9SUA3
EEE	22	GLY	-	expression tag	UNP I9SUA3
EEE	23	LEU	-	expression tag	UNP I9SUA3
EEE	24	GLU	-	expression tag	UNP I9SUA3
EEE	25	VAL	-	expression tag	UNP I9SUA3
EEE	26	LEU	-	expression tag	UNP I9SUA3
EEE	27	PHE	-	expression tag	UNP I9SUA3
EEE	28	GLN	-	expression tag	UNP I9SUA3
EEE	29	GLY	-	expression tag	UNP I9SUA3
EEE	30	PRO	-	expression tag	UNP I9SUA3
EEE	31	ALA	-	expression tag	UNP I9SUA3

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	AAA	1	10	2	6	2	1	0
2	DDD	1	10	2	6	2	1	0
2	CCC	1	10	2	6	2	1	0
2	BBB	1	10	2	6	2	1	0
2	FFF	1	10	2	6	2	1	0
2	EEE	1	10	2	6	2	1	0

- Molecule 3 is (2S,3S,4R,5R)-2,3,4-TRIHYDROXY-5-HYDROXYMETHYL-PIPERIDINE (three-letter code: MNM) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	H	N			O
3	AAA	1	Total	C	H	N	O	3	0
			24	6	13	1	4		
3	DDD	1	Total	C	H	N	O	3	0
			24	6	13	1	4		
3	CCC	1	Total	C	H	N	O	3	0
			24	6	13	1	4		
3	BBB	1	Total	C	H	N	O	3	0
			24	6	13	1	4		
3	FFF	1	Total	C	H	N	O	3	0
			24	6	13	1	4		
3	EEE	1	Total	C	H	N	O	3	0
			24	6	13	1	4		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total 1 Cl	0	0
4	DDD	1	Total 1 Cl	0	0
4	CCC	1	Total 1 Cl	0	0
4	BBB	1	Total 1 Cl	0	0
4	FFF	1	Total 1 Cl	0	0
4	EEE	1	Total 1 Cl	0	0

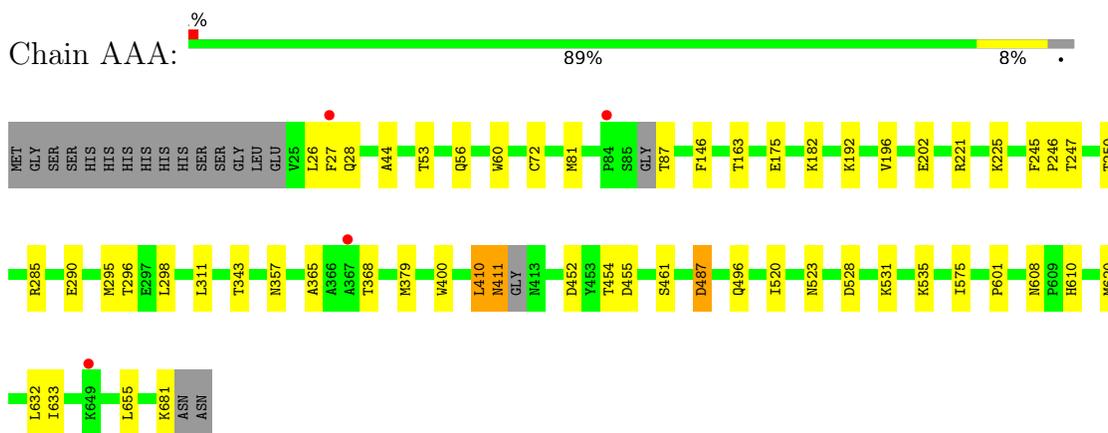
- Molecule 5 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	AAA	168	Total 168	O 168	0	0
5	DDD	131	Total 131	O 131	0	0
5	CCC	160	Total 160	O 160	0	0
5	BBB	212	Total 212	O 212	0	0
5	FFF	228	Total 228	O 228	0	0
5	EEE	130	Total 130	O 130	0	0

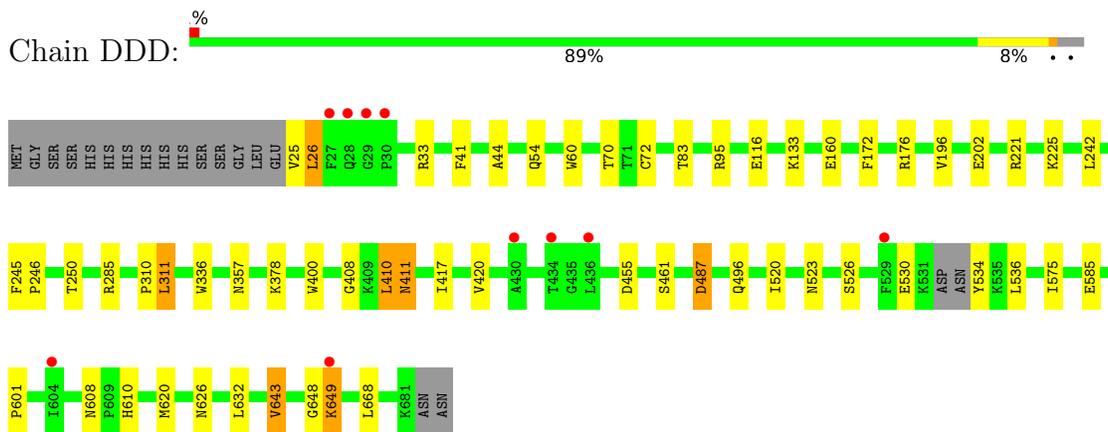
### 3 Residue-property plots [i](#)

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

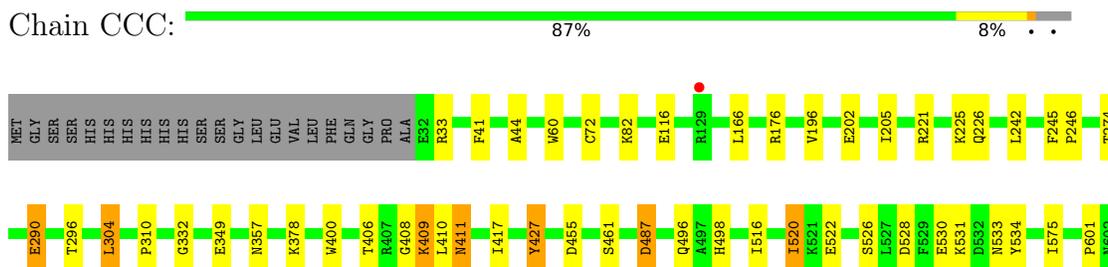
- Molecule 1: Glyco\_hydro\_42M domain-containing protein



- Molecule 1: Glyco\_hydro\_42M domain-containing protein



- Molecule 1: Glyco\_hydro\_42M domain-containing protein





- Molecule 1: Glyco\_hydro\_42M domain-containing protein

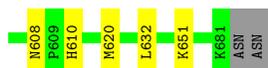
Chain BBB: 89% 7%



ASN

- Molecule 1: Glyco\_hydro\_42M domain-containing protein

Chain FFF: 88% 8%



- Molecule 1: Glyco\_hydro\_42M domain-containing protein

Chain EEE: 88% 8%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.75Å 105.10Å 170.54Å 92.60° 97.21° 105.10°	Depositor
Resolution (Å)	90.19 – 2.06 101.13 – 2.06	Depositor EDS
% Data completeness (in resolution range)	98.2 (90.19-2.06) 98.3 (101.13-2.06)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 2.07Å)	Xtrriage
Refinement program	REFMAC 5.8.0257	Depositor
R, $R_{free}$	0.212 , 0.240 0.217 , 0.242	Depositor DCC
$R_{free}$ test set	13971 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.0	Xtrriage
Anisotropy	0.687	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 28.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	63581	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.77	1/5419 (0.0%)	0.86	2/7334 (0.0%)
1	BBB	0.81	2/5376 (0.0%)	0.88	5/7276 (0.1%)
1	CCC	0.79	0/5376	0.88	2/7277 (0.0%)
1	DDD	0.76	1/5412 (0.0%)	0.86	3/7325 (0.0%)
1	EEE	0.78	1/5372 (0.0%)	0.86	2/7270 (0.0%)
1	FFF	0.78	3/5390 (0.1%)	0.87	3/7295 (0.0%)
All	All	0.78	8/32345 (0.0%)	0.87	17/43777 (0.0%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	EEE	627	GLY	C-O	-13.49	1.02	1.23
1	AAA	290	GLU	CD-OE1	6.90	1.33	1.25
1	BBB	66	GLU	CD-OE1	5.70	1.31	1.25
1	FFF	240[A]	SER	CA-CB	-5.47	1.44	1.52
1	FFF	240[B]	SER	CA-CB	-5.47	1.44	1.52

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	285	ARG	NE-CZ-NH1	-9.95	115.32	120.30
1	AAA	285	ARG	NE-CZ-NH2	-7.59	116.51	120.30
1	DDD	285	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	BBB	626	ASN	CB-CA-C	6.62	123.65	110.40
1	BBB	285	ARG	NE-CZ-NH2	6.30	123.45	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	5275	5172	5151	38	0
1	BBB	5233	5128	5108	22	0
1	CCC	5232	5126	5107	33	0
1	DDD	5267	5168	5148	34	0
1	EEE	5229	5125	5105	26	0
1	FFF	5246	5141	5120	28	0
2	AAA	4	6	6	0	0
2	BBB	4	6	6	0	0
2	CCC	4	6	6	0	0
2	DDD	4	6	6	0	0
2	EEE	4	6	6	0	0
2	FFF	4	6	6	0	0
3	AAA	11	13	13	0	0
3	BBB	11	13	13	0	0
3	CCC	11	13	13	0	0
3	DDD	11	13	13	1	0
3	EEE	11	13	13	0	0
3	FFF	11	13	13	0	0
4	AAA	1	0	0	0	0
4	BBB	1	0	0	0	0
4	CCC	1	0	0	0	0
4	DDD	1	0	0	0	0
4	EEE	1	0	0	0	0
4	FFF	1	0	0	0	0
5	AAA	168	0	0	0	0
5	BBB	212	0	0	1	0
5	CCC	160	0	0	0	0
5	DDD	131	0	0	0	0
5	EEE	130	0	0	0	0
5	FFF	228	0	0	0	0
All	All	32607	30974	30853	171	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 171 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:AAA:53:THR:H	1:AAA:56:GLN:HE21	1.05	0.98
1:AAA:365:ALA:O	1:AAA:368:THR:HG22	1.68	0.93
1:AAA:620:MET:SD	1:AAA:633:ILE:CD1	2.60	0.90
1:AAA:53:THR:N	1:AAA:56:GLN:HE21	1.78	0.81
1:AAA:620:MET:SD	1:AAA:633:ILE:HD11	2.26	0.75

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	649/674 (96%)	630 (97%)	19 (3%)	0	100	100
1	BBB	646/674 (96%)	630 (98%)	16 (2%)	0	100	100
1	CCC	648/674 (96%)	631 (97%)	16 (2%)	1 (0%)	47	39
1	DDD	651/674 (97%)	631 (97%)	18 (3%)	2 (0%)	41	32
1	EEE	646/674 (96%)	625 (97%)	21 (3%)	0	100	100
1	FFF	648/674 (96%)	625 (96%)	22 (3%)	1 (0%)	47	39
All	All	3888/4044 (96%)	3772 (97%)	112 (3%)	4 (0%)	51	45

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	DDD	411	ASN
1	CCC	411	ASN
1	FFF	407	ARG
1	DDD	530	GLU

### 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 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	567/582 (97%)	555 (98%)	12 (2%)	53	48
1	BBB	562/582 (97%)	553 (98%)	9 (2%)	62	59
1	CCC	562/582 (97%)	541 (96%)	21 (4%)	34	27
1	DDD	565/582 (97%)	550 (97%)	15 (3%)	44	39
1	EEE	561/582 (96%)	549 (98%)	12 (2%)	53	48
1	FFF	564/582 (97%)	545 (97%)	19 (3%)	37	30
All	All	3381/3492 (97%)	3293 (97%)	88 (3%)	46	40

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	FFF	32	GLU
1	FFF	487	ASP
1	FFF	56	GLN
1	FFF	225	LYS
1	FFF	651	LYS

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

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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	MNM	DDD	702	-	9,11,11	0.61	0	10,15,15	1.50	1 (10%)
2	EDO	BBB	701	-	3,3,3	1.41	0	2,2,2	0.92	0
3	MNM	CCC	702	-	9,11,11	0.85	0	10,15,15	1.28	2 (20%)
2	EDO	EEE	701	-	3,3,3	0.44	0	2,2,2	0.46	0
2	EDO	FFF	701	-	3,3,3	0.62	0	2,2,2	0.30	0
3	MNM	BBB	702	-	9,11,11	0.74	0	10,15,15	1.59	1 (10%)
3	MNM	FFF	702	-	9,11,11	0.50	0	10,15,15	1.61	1 (10%)
3	MNM	EEE	702	-	9,11,11	0.50	0	10,15,15	1.84	1 (10%)
2	EDO	AAA	701	-	3,3,3	0.62	0	2,2,2	0.33	0
3	MNM	AAA	702	-	9,11,11	0.70	0	10,15,15	1.19	1 (10%)
2	EDO	DDD	701	-	3,3,3	0.62	0	2,2,2	0.40	0
2	EDO	CCC	701	-	3,3,3	0.44	0	2,2,2	0.47	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MNM	DDD	702	-	-	0/2/19/19	0/1/1/1
2	EDO	BBB	701	-	-	1/1/1/1	-
3	MNM	CCC	702	-	-	0/2/19/19	0/1/1/1
2	EDO	EEE	701	-	-	1/1/1/1	-
2	EDO	FFF	701	-	-	1/1/1/1	-
3	MNM	BBB	702	-	-	0/2/19/19	0/1/1/1
3	MNM	FFF	702	-	-	0/2/19/19	0/1/1/1
3	MNM	EEE	702	-	-	0/2/19/19	0/1/1/1
2	EDO	AAA	701	-	-	1/1/1/1	-
3	MNM	AAA	702	-	-	0/2/19/19	0/1/1/1
2	EDO	DDD	701	-	-	0/1/1/1	-

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*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	CCC	701	-	-	0/1/1/1	-

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	EEE	702	MNM	C10-N6-C2	5.07	118.75	108.98
3	FFF	702	MNM	C10-N6-C2	4.28	117.23	108.98
3	DDD	702	MNM	C10-N6-C2	3.81	116.33	108.98
3	BBB	702	MNM	C10-N6-C2	3.64	116.00	108.98
3	CCC	702	MNM	O11-C9-C8	2.33	116.71	111.36

There are no chirality outliers.

All (4) torsion outliers are listed below:

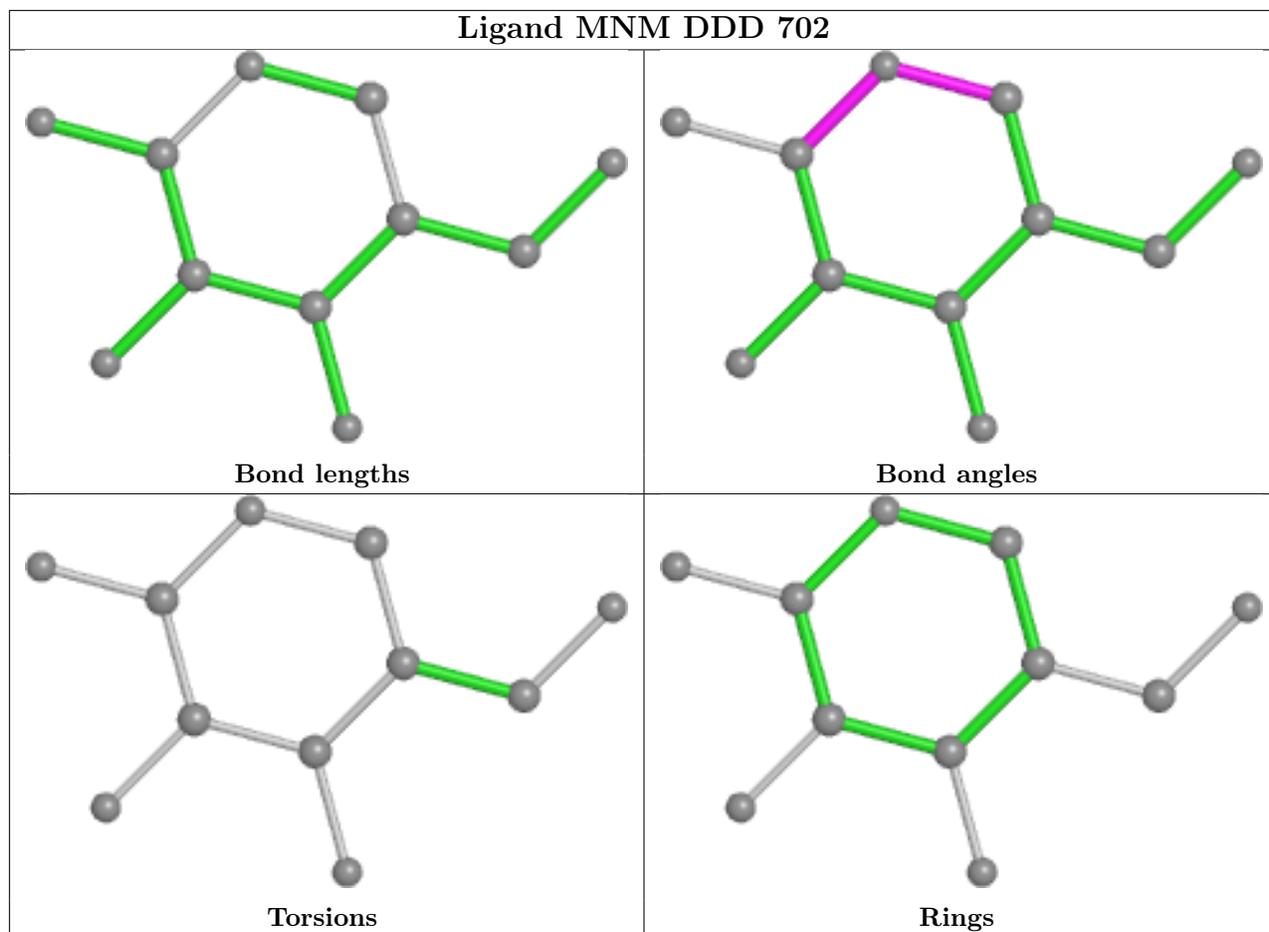
Mol	Chain	Res	Type	Atoms
2	BBB	701	EDO	O1-C1-C2-O2
2	AAA	701	EDO	O1-C1-C2-O2
2	FFF	701	EDO	O1-C1-C2-O2
2	EEE	701	EDO	O1-C1-C2-O2

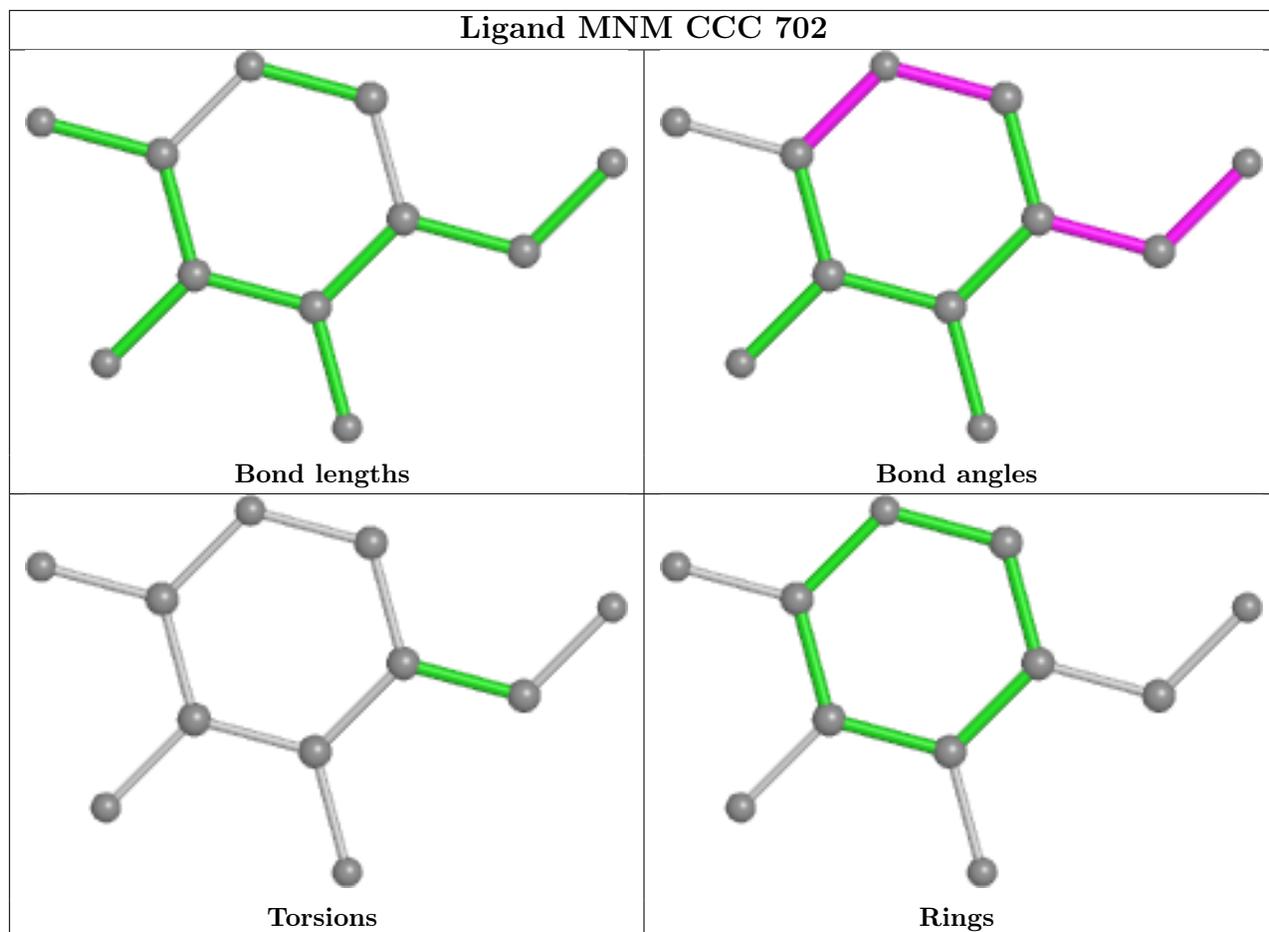
There are no ring outliers.

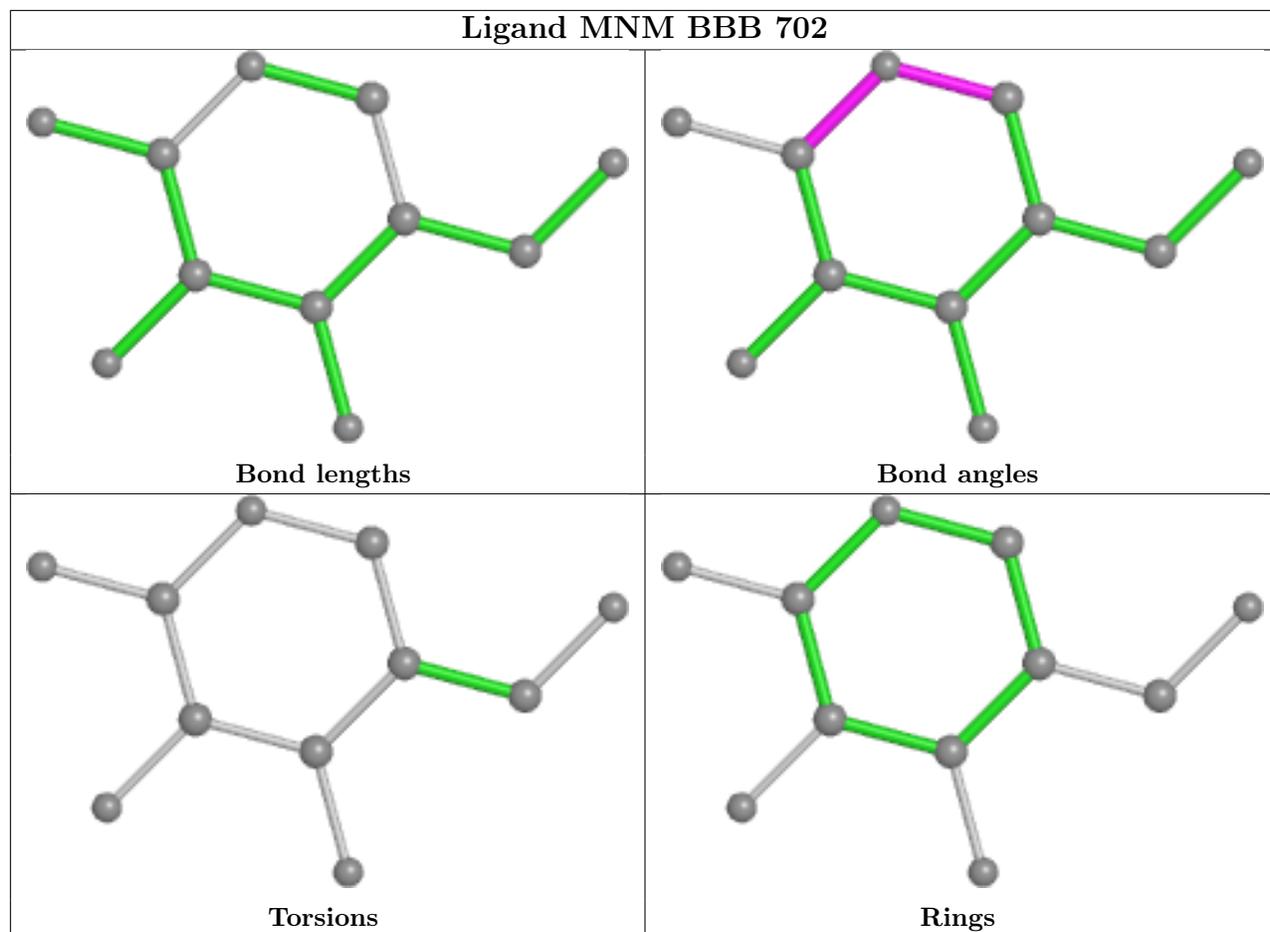
1 monomer is involved in 1 short contact:

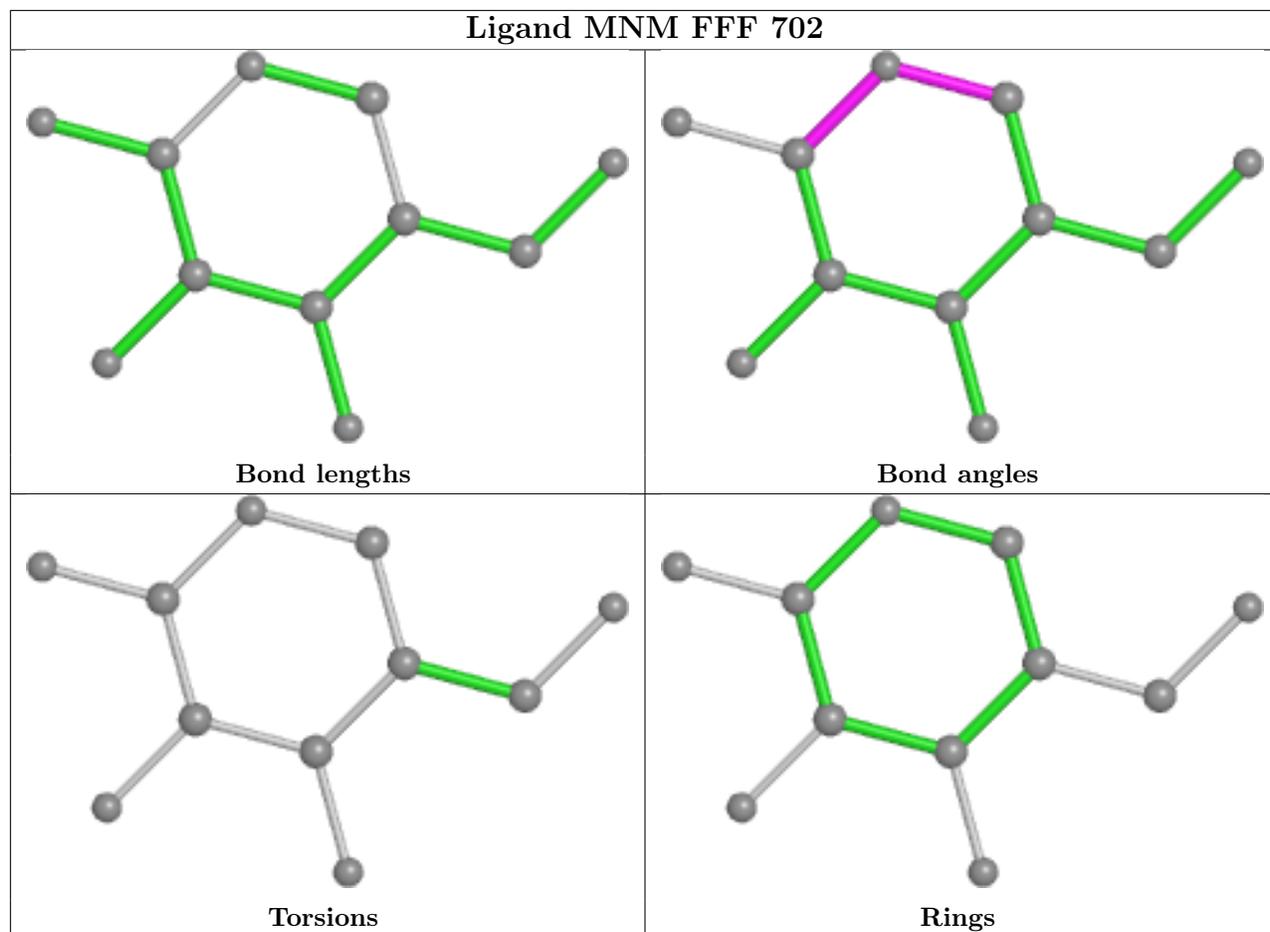
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	DDD	702	MNM	1	0

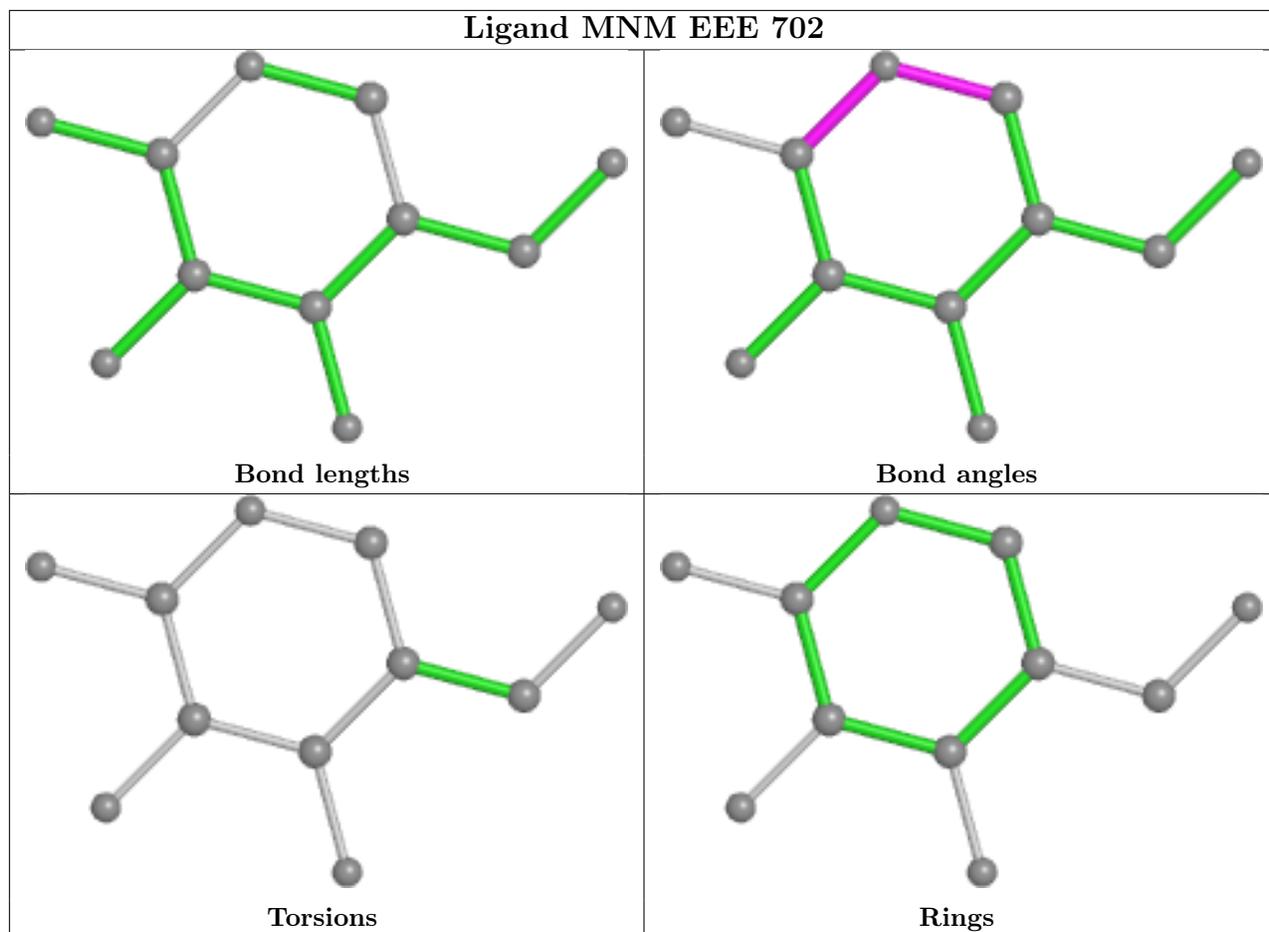
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

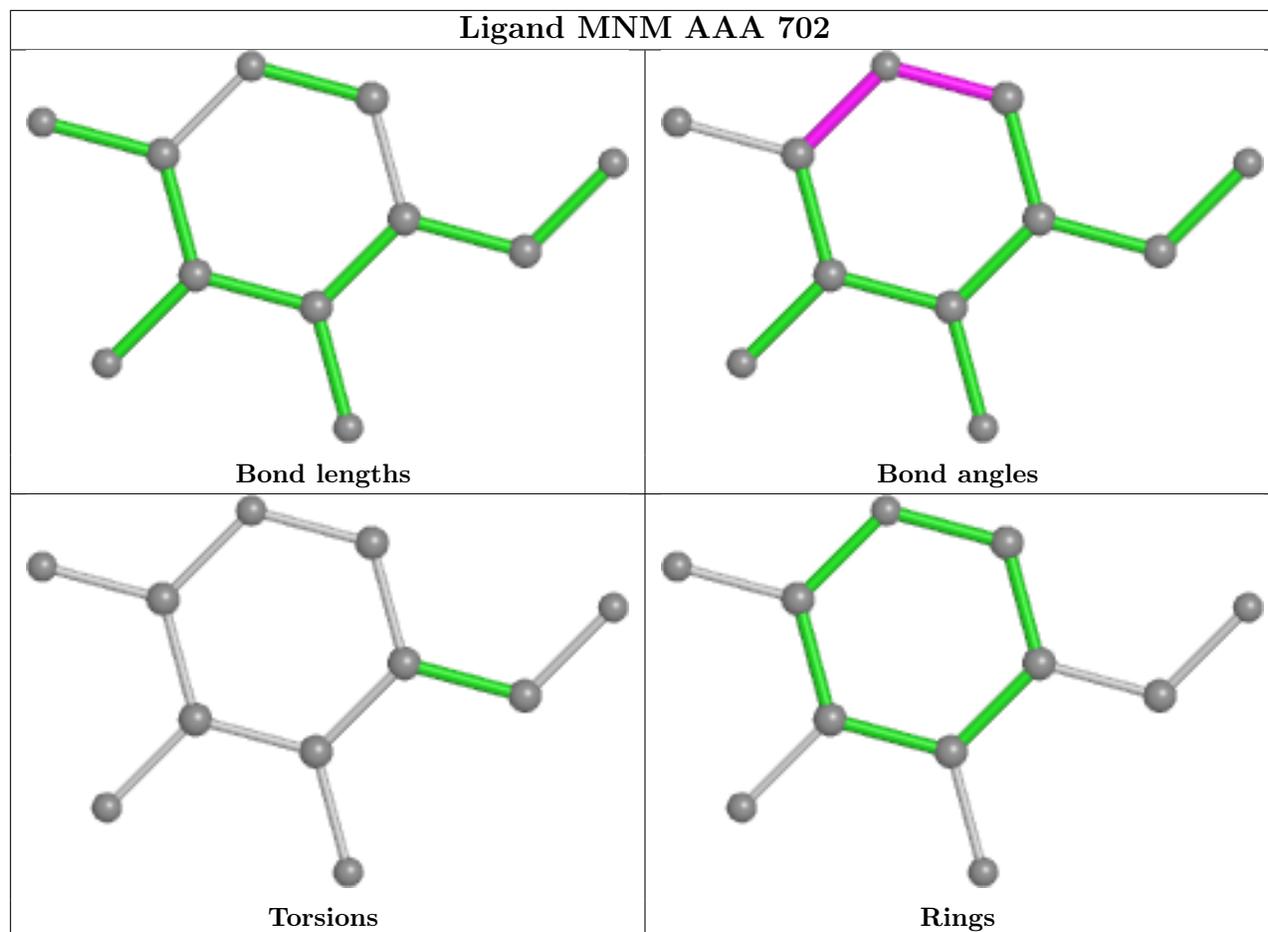












## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AAA	655/674 (97%)	0.05	4 (0%) 89 90	28, 48, 78, 115	0
1	BBB	650/674 (96%)	-0.05	2 (0%) 94 94	21, 38, 63, 90	0
1	CCC	650/674 (96%)	0.03	1 (0%) 95 95	31, 47, 73, 97	0
1	DDD	655/674 (97%)	0.09	10 (1%) 73 75	30, 52, 82, 101	0
1	EEE	650/674 (96%)	0.05	5 (0%) 86 87	31, 51, 77, 104	0
1	FFF	651/674 (96%)	-0.03	3 (0%) 91 91	25, 41, 66, 109	0
All	All	3911/4044 (96%)	0.02	25 (0%) 89 90	21, 46, 75, 115	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	84	PRO	5.3
1	EEE	385	THR	3.9
1	DDD	30	PRO	3.8
1	FFF	532	ASP	3.7
1	DDD	529	PHE	3.6

### 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

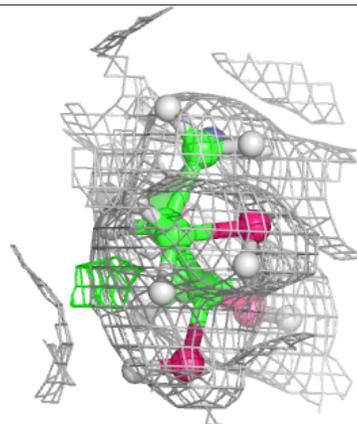
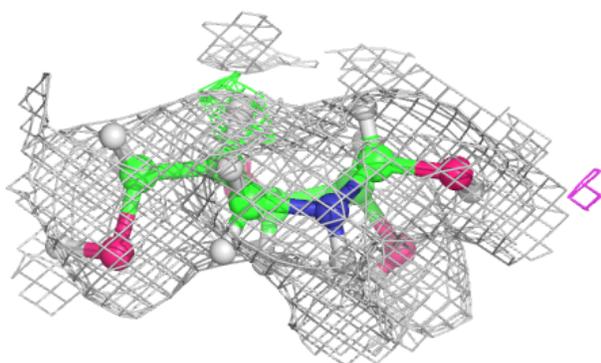
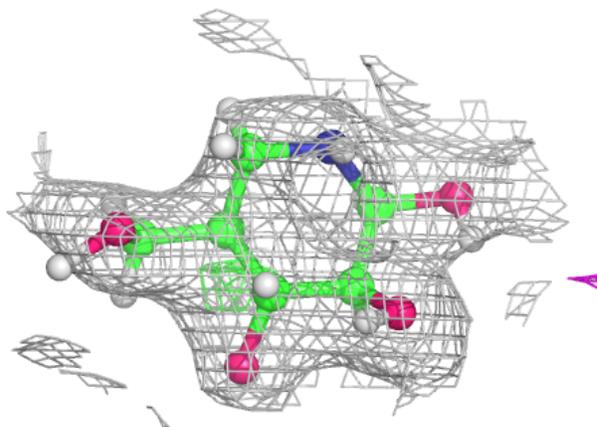
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MNM	AAA	702	11/11	0.91	0.12	37,40,40,43	3
2	EDO	CCC	701	4/4	0.95	0.11	36,37,38,39	1
3	MNM	DDD	702	11/11	0.95	0.11	33,34,34,34	3
2	EDO	BBB	701	4/4	0.96	0.09	29,29,29,30	1
2	EDO	EEE	701	4/4	0.96	0.12	35,36,36,37	1
3	MNM	CCC	702	11/11	0.96	0.09	32,33,34,35	3
4	CL	AAA	703	1/1	0.96	0.08	37,37,37,37	0
2	EDO	DDD	701	4/4	0.97	0.10	29,29,30,30	1
3	MNM	FFF	702	11/11	0.97	0.10	24,24,25,25	3
2	EDO	AAA	701	4/4	0.97	0.13	37,38,38,38	1
2	EDO	FFF	701	4/4	0.98	0.10	22,22,22,23	1
3	MNM	EEE	702	11/11	0.98	0.10	34,35,36,39	3
3	MNM	BBB	702	11/11	0.98	0.11	27,28,28,28	3
4	CL	CCC	703	1/1	0.98	0.10	32,32,32,32	0
4	CL	EEE	703	1/1	0.98	0.07	44,44,44,44	0
4	CL	BBB	703	1/1	0.99	0.07	31,31,31,31	0
4	CL	FFF	703	1/1	0.99	0.11	26,26,26,26	0
4	CL	DDD	703	1/1	0.99	0.08	35,35,35,35	0

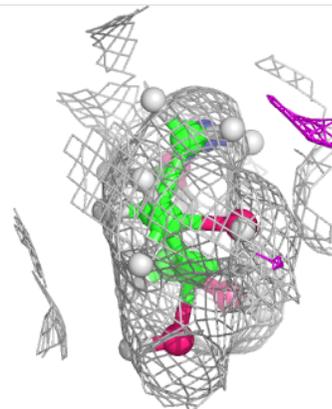
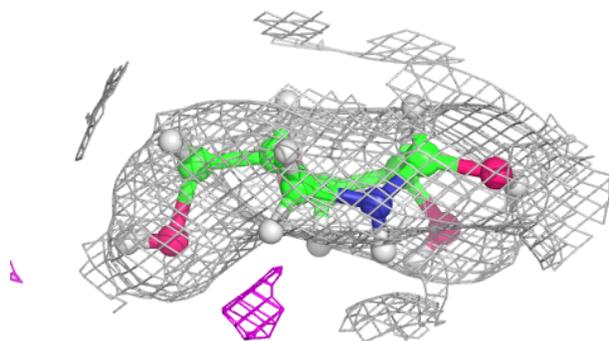
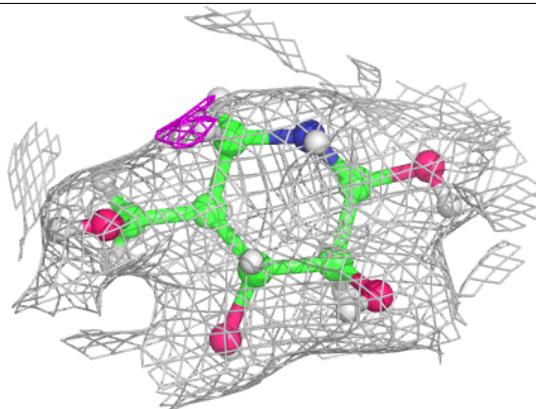
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around MNM AAA 702:**

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

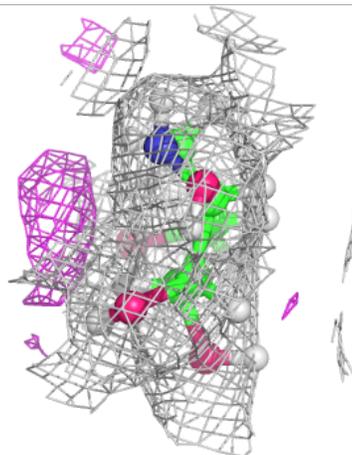
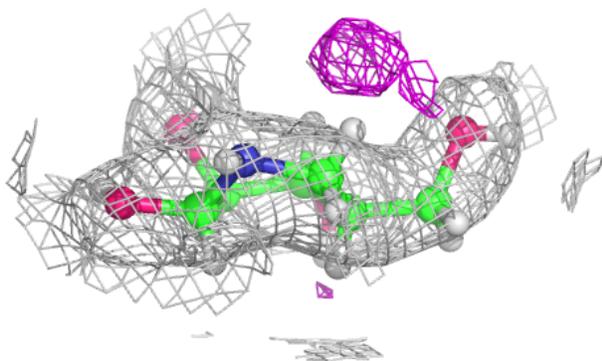
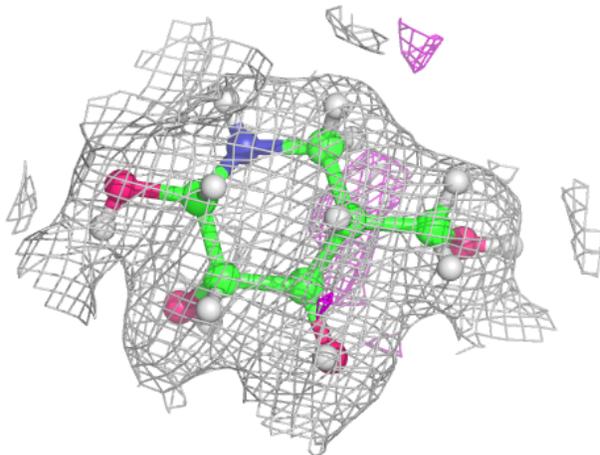
**Electron density around MNM DDD 702:**

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



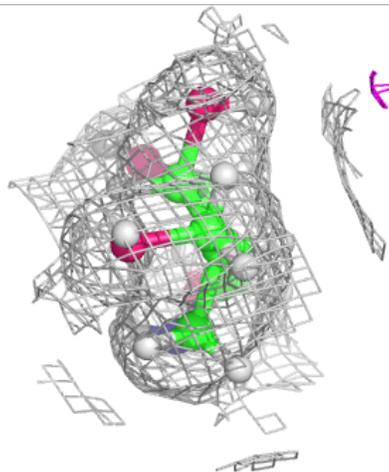
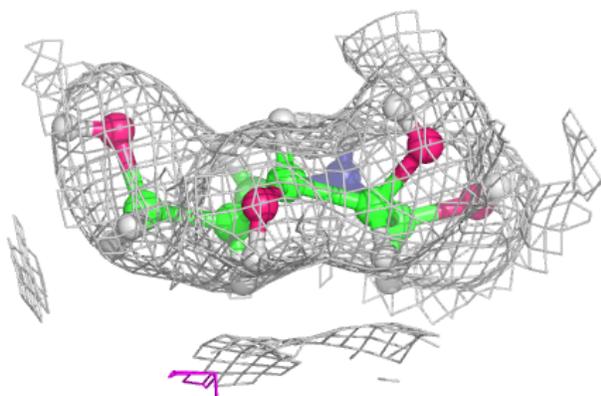
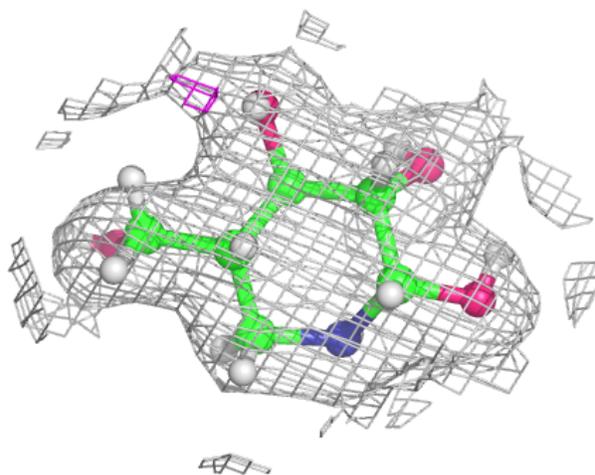
**Electron density around MNM CCC 702:**

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



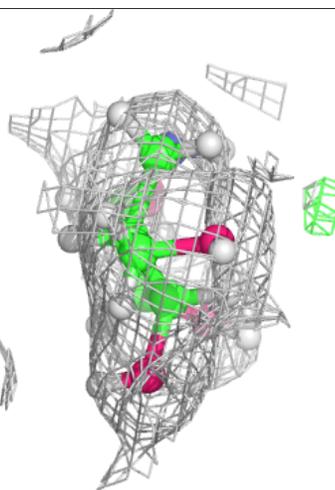
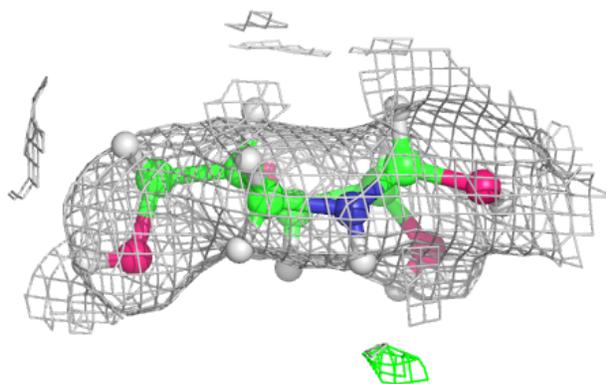
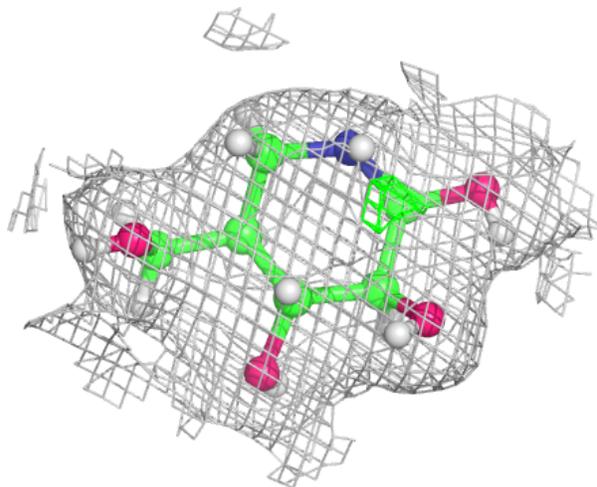
**Electron density around MNM FFF 702:**

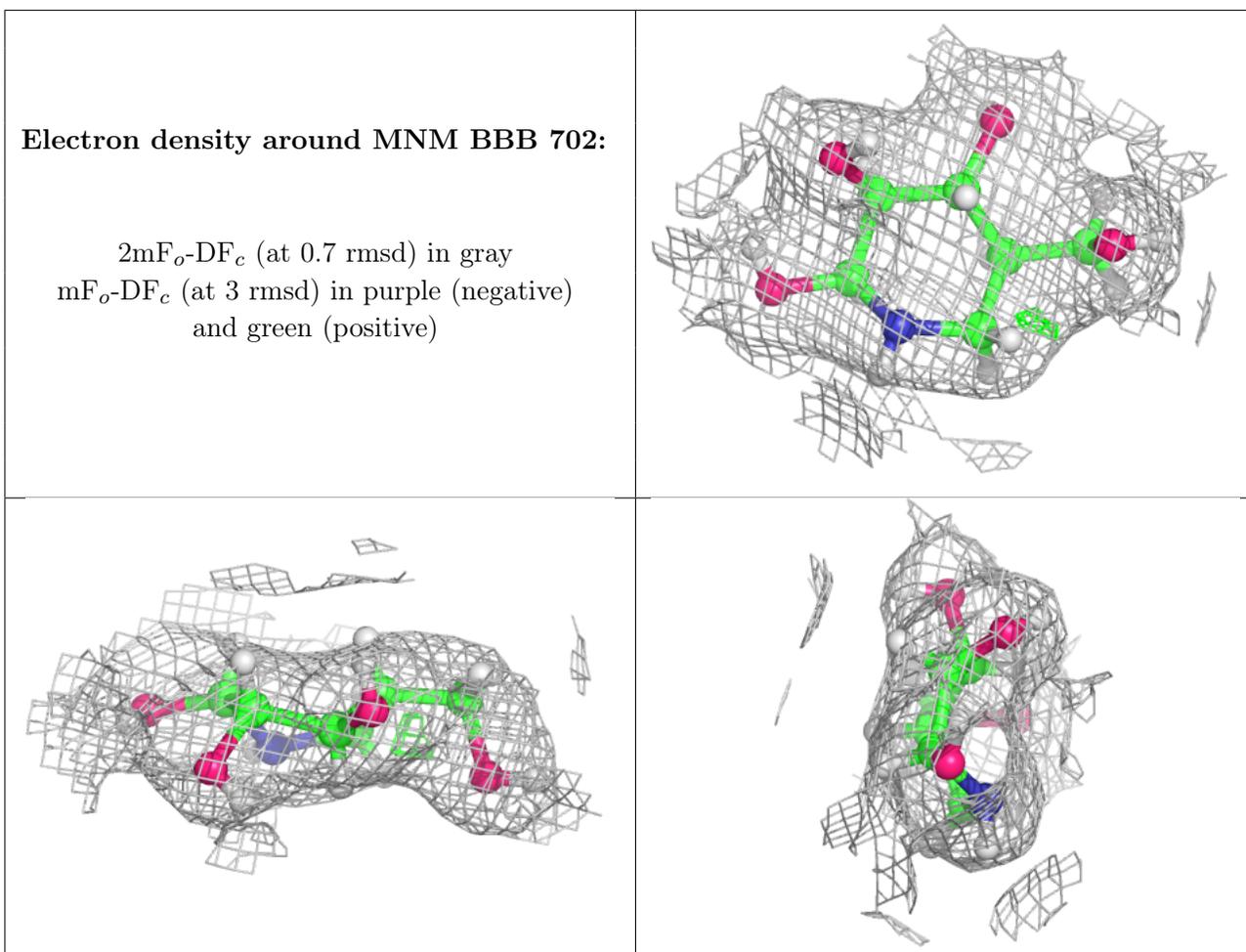
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around MNM EEE 702:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.