



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 25, 2022 – 02:56 pm BST

PDB ID : 7OA4
Title : Crystal structure of the N-terminal endonuclease domain of La Crosse virus L-protein bound to compound L-742,001
Authors : Feracci, M.; Hernandez, S.; Vincentelli, R.; Ferron, F.; Reguera, J.; Canard, B.; Alvarez, K.
Deposited on : 2021-04-19
Resolution : 2.90 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 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:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.29
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

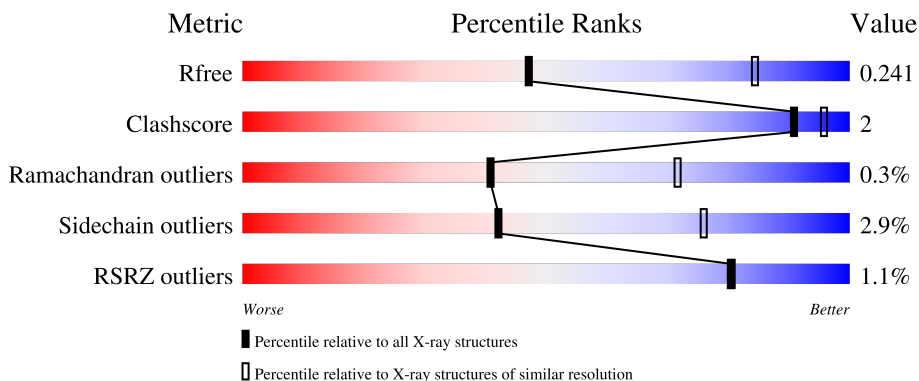
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

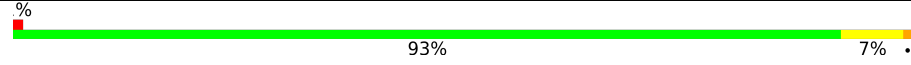
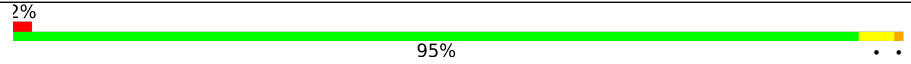
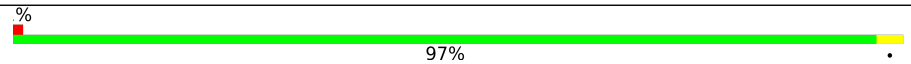
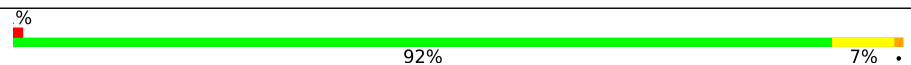
The reported resolution of this entry is 2.90 Å.

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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 ≥ 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	184	
1	BBB	184	
1	DDD	184	
1	GGG	184	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12540 atoms, of which 6154 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.

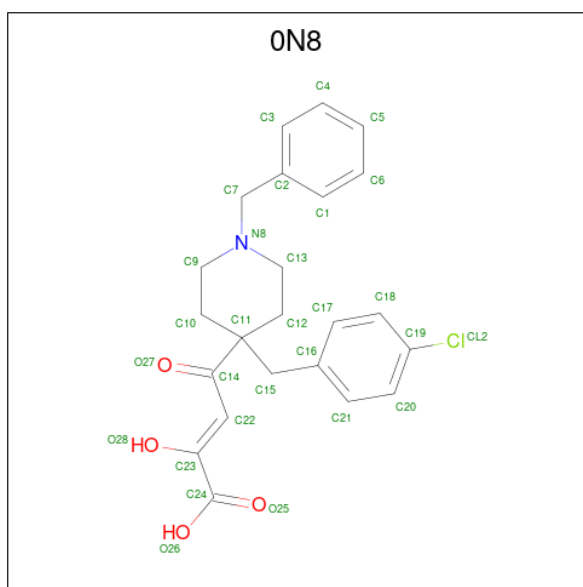
- Molecule 1 is a protein called N-terminal endonuclease domain of La Crosse virus L-protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	AAA	184	3044	987	1511	246	296	4	35	0	0
1	BBB	184	3045	987	1512	246	296	4	36	0	0
1	DDD	184	3062	993	1519	249	297	4	37	1	0
1	GGG	184	3045	987	1512	246	296	4	36	0	0

There are 4 discrepancies between the modelled and reference sequences:

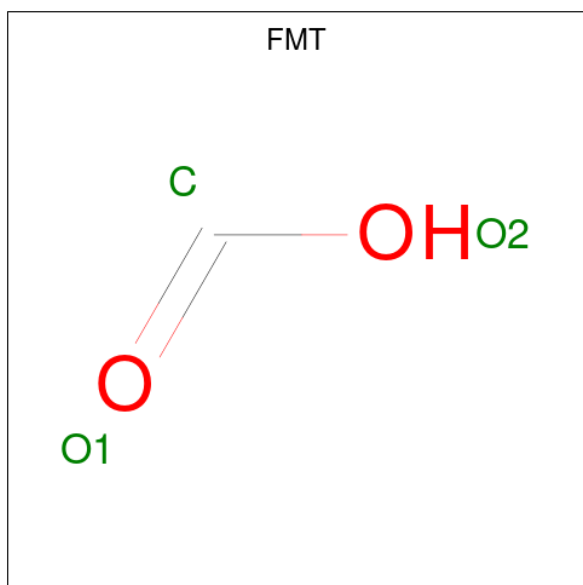
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	0	GLY	-	cloning artifact	UNP A5HC98
BBB	0	GLY	-	cloning artifact	UNP A5HC98
DDD	0	GLY	-	cloning artifact	UNP A5HC98
GGG	0	GLY	-	cloning artifact	UNP A5HC98

- Molecule 2 is (2Z)-4-[1-benzyl-4-(4-chlorobenzyl)piperidin-4-yl]-2-hydroxy-4-oxobut-2-enic acid (three-letter code: ON8) (formula: C₂₃H₂₄ClNO₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	H	N			O
2	AAA	1	Total 51	C 23	Cl 1	H 22	N 1	O 4	0	0
2	BBB	1	Total 51	C 23	Cl 1	H 22	N 1	O 4	0	0
2	DDD	1	Total 51	C 23	Cl 1	H 22	N 1	O 4	0	0
2	GGG	1	Total 51	C 23	Cl 1	H 22	N 1	O 4	0	0

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	H	O	1	0
			5	1	2	2		
3	AAA	1	Total	C	H	O	1	0
			5	1	2	2		
3	BBB	1	Total	C	H	O	1	0
			5	1	2	2		
3	DDD	1	Total	C	H	O	1	0
			5	1	2	2		
3	DDD	1	Total	C	H	O	1	0
			5	1	2	2		
3	GGG	1	Total	C	H	O	1	0
			5	1	2	2		

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	2	Total	Mn	0	0
			2	2		
4	BBB	2	Total	Mn	0	0
			2	2		
4	DDD	2	Total	Mn	0	0
			2	2		
4	GGG	2	Total	Mn	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	28	Total	O	0	0
			28	28		
5	BBB	32	Total	O	0	0
			32	32		
5	DDD	28	Total	O	0	0
			28	28		
5	GGG	14	Total	O	0	0
			14	14		

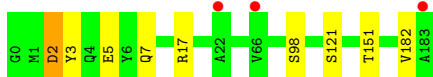
3 Residue-property plots [i](#)

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: N-terminal endonuclease domain of La Crosse virus L-protein



- Molecule 1: N-terminal endonuclease domain of La Crosse virus L-protein



- Molecule 1: N-terminal endonuclease domain of La Crosse virus L-protein



- Molecule 1: N-terminal endonuclease domain of La Crosse virus L-protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	124.79Å 124.79Å 295.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	108.07 – 2.90 108.07 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (108.07-2.90) 100.0 (108.07-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.197 , 0.239 0.206 , 0.241	Depositor DCC
R_{free} test set	1549 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12540	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FMT, MN, ON8

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	0.63	0/1565	0.71	0/2126
1	BBB	0.63	0/1565	0.72	0/2126
1	DDD	0.63	0/1576	0.72	0/2141
1	GGG	0.63	0/1565	0.70	0/2126
All	All	0.63	0/6271	0.71	0/8519

There are no bond length outliers.

There are no bond angle outliers.

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	AAA	1533	1511	1508	8	0
1	BBB	1533	1512	1509	2	0
1	DDD	1543	1519	1514	2	0
1	GGG	1533	1512	1509	5	0
2	AAA	29	22	22	0	0
2	BBB	29	22	22	1	0
2	DDD	29	22	22	1	0
2	GGG	29	22	22	2	0
3	AAA	6	4	2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	BBB	3	2	1	0	0
3	DDD	6	4	2	0	0
3	GGG	3	2	1	0	0
4	AAA	2	0	0	0	0
4	BBB	2	0	0	0	0
4	DDD	2	0	0	0	0
4	GGG	2	0	0	0	0
5	AAA	28	0	0	0	0
5	BBB	32	0	0	0	0
5	DDD	28	0	0	0	0
5	GGG	14	0	0	1	0
All	All	6386	6154	6134	21	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 (21) 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:GGG:60:LEU:HD11	1:GGG:68:PRO:HB3	1.88	0.56
1:AAA:84:ILE:HD12	1:AAA:148:LEU:HD23	1.91	0.52
1:AAA:82:LEU:HD13	1:AAA:84:ILE:HD11	1.92	0.51
2:BBB:201:0N8:C14	2:BBB:201:0N8:C17	2.89	0.50
2:GGG:201:0N8:H10	2:GGG:201:0N8:H27	1.94	0.50
1:AAA:82:LEU:HD22	1:AAA:84:ILE:CG1	2.42	0.49
1:BBB:3:TYR:O	1:BBB:7:GLN:HG2	2.13	0.48
1:GGG:75:HIS:HB3	5:GGG:314:HOH:O	2.16	0.47
1:AAA:82:LEU:CD1	1:AAA:84:ILE:HD11	2.47	0.44
1:AAA:102:SER:HB3	1:AAA:128:ILE:HG21	2.00	0.43
1:DDD:10:LEU:HD23	1:DDD:10:LEU:HA	1.91	0.43
1:GGG:51:ASN:O	1:GGG:52:ASP:C	2.58	0.42
1:GGG:177:GLU:O	1:GGG:181:LYS:HB2	2.20	0.42
1:DDD:84:ILE:HG21	1:DDD:148:LEU:HD21	2.01	0.42
2:DDD:201:0N8:C17	2:DDD:201:0N8:C14	2.96	0.42
1:AAA:79:ASP:HB3	1:AAA:93:TYR:CE2	2.55	0.41
1:AAA:92:ASP:OD2	1:AAA:94:LYS:NZ	2.53	0.41
2:GGG:201:0N8:H10	2:GGG:201:0N8:C1	2.49	0.41
1:GGG:0:GLY:HA3	1:GGG:160:GLN:OE1	2.21	0.41
1:AAA:82:LEU:HD22	1:AAA:84:ILE:HG12	2.02	0.40
1:BBB:2:ASP:HB2	1:BBB:5:GLU:H	1.86	0.40

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	182/184 (99%)	177 (97%)	5 (3%)	0	100	100
1	BBB	182/184 (99%)	175 (96%)	7 (4%)	0	100	100
1	DDD	183/184 (100%)	174 (95%)	8 (4%)	1 (0%)	29	61
1	GGG	182/184 (99%)	176 (97%)	5 (3%)	1 (0%)	29	61
All	All	729/736 (99%)	702 (96%)	25 (3%)	2 (0%)	41	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	GGG	150	PRO
1	DDD	52	ASP

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	174/174 (100%)	169 (97%)	5 (3%)	42	76
1	BBB	174/174 (100%)	168 (97%)	6 (3%)	37	71
1	DDD	175/174 (101%)	173 (99%)	2 (1%)	73	92
1	GGG	174/174 (100%)	167 (96%)	7 (4%)	31	65
All	All	697/696 (100%)	677 (97%)	20 (3%)	42	76

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	82	LEU
1	AAA	98	SER
1	AAA	136	ARG
1	AAA	151	THR
1	AAA	182	VAL
1	BBB	2	ASP
1	BBB	17	ARG
1	BBB	98	SER
1	BBB	121	SER
1	BBB	151	THR
1	BBB	182	VAL
1	DDD	24	ASP
1	DDD	182	VAL
1	GGG	10	LEU
1	GGG	51	ASN
1	GGG	93	TYR
1	GGG	98	SER
1	GGG	121	SER
1	GGG	177	GLU
1	GGG	182	VAL

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 [i](#)

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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	FMT	BBB	202	-	2,2,2	0.42	0	1,1,1	0.06	0
3	FMT	DDD	203	-	2,2,2	0.35	0	1,1,1	0.14	0
2	0N8	AAA	201	4	31,31,31	1.06	2 (6%)	40,43,43	1.49	8 (20%)
3	FMT	AAA	203	-	2,2,2	0.31	0	1,1,1	0.13	0
2	0N8	BBB	201	4	31,31,31	1.10	2 (6%)	40,43,43	1.68	9 (22%)
3	FMT	DDD	202	-	2,2,2	0.45	0	1,1,1	0.05	0
3	FMT	AAA	202	-	2,2,2	0.35	0	1,1,1	0.15	0
2	0N8	DDD	201	4	31,31,31	1.14	2 (6%)	40,43,43	1.49	6 (15%)
2	0N8	GGG	201	4	31,31,31	1.09	3 (9%)	40,43,43	1.87	7 (17%)
3	FMT	GGG	202	-	2,2,2	0.31	0	1,1,1	0.13	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
2	0N8	AAA	201	4	-	5/23/35/35	1/3/3/3
2	0N8	BBB	201	4	-	10/23/35/35	1/3/3/3
2	0N8	GGG	201	4	-	7/23/35/35	0/3/3/3
2	0N8	DDD	201	4	-	5/23/35/35	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	201	0N8	O28-C23	-4.19	1.23	1.34
2	GGG	201	0N8	O28-C23	-4.15	1.23	1.34
2	DDD	201	0N8	O28-C23	-4.13	1.23	1.34
2	BBB	201	0N8	O28-C23	-4.11	1.23	1.34
2	DDD	201	0N8	O26-C24	-2.90	1.22	1.30
2	AAA	201	0N8	O26-C24	-2.57	1.23	1.30
2	BBB	201	0N8	O26-C24	-2.50	1.23	1.30
2	GGG	201	0N8	O26-C24	-2.35	1.23	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	GGG	201	0N8	C22-C23	2.10	1.41	1.36

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	GGG	201	0N8	C23-C22-C14	6.63	127.67	120.73
2	GGG	201	0N8	O28-C23-C24	6.17	117.74	114.01
2	DDD	201	0N8	C23-C22-C14	5.46	126.44	120.73
2	BBB	201	0N8	C23-C22-C14	5.38	126.36	120.73
2	BBB	201	0N8	C13-C12-C11	4.46	114.41	109.17
2	AAA	201	0N8	C23-C22-C14	4.31	125.23	120.73
2	DDD	201	0N8	O28-C23-C24	4.04	116.46	114.01
2	AAA	201	0N8	O28-C23-C24	3.97	116.42	114.01
2	BBB	201	0N8	O26-C24-C23	3.69	119.47	115.91
2	AAA	201	0N8	C13-C12-C11	3.38	113.15	109.17
2	GGG	201	0N8	C9-C10-C11	3.21	112.95	109.17
2	GGG	201	0N8	O26-C24-C23	3.10	118.91	115.91
2	BBB	201	0N8	O28-C23-C24	3.05	115.86	114.01
2	DDD	201	0N8	C13-C12-C11	3.03	112.74	109.17
2	AAA	201	0N8	C11-C15-C16	-2.74	112.47	116.29
2	BBB	201	0N8	O25-C24-C23	-2.65	117.03	120.08
2	DDD	201	0N8	C9-C10-C11	2.61	112.24	109.17
2	DDD	201	0N8	O27-C14-C22	-2.55	117.53	126.25
2	BBB	201	0N8	O27-C14-C22	-2.53	117.61	126.25
2	AAA	201	0N8	O27-C14-C22	-2.51	117.67	126.25
2	GGG	201	0N8	O27-C14-C22	-2.43	117.96	126.25
2	GGG	201	0N8	O25-C24-C23	-2.40	117.31	120.08
2	GGG	201	0N8	C13-C12-C11	2.37	111.96	109.17
2	BBB	201	0N8	C12-C13-N8	2.36	113.56	111.23
2	AAA	201	0N8	O28-C23-C22	-2.31	118.90	122.92
2	BBB	201	0N8	C9-C10-C11	2.15	111.70	109.17
2	AAA	201	0N8	C12-C13-N8	2.15	113.35	111.23
2	BBB	201	0N8	O28-C23-C22	-2.09	119.27	122.92
2	DDD	201	0N8	C11-C14-C22	2.02	124.57	119.44
2	AAA	201	0N8	C11-C14-C22	2.02	124.57	119.44

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	201	0N8	C14-C22-C23-O28
2	AAA	201	0N8	C14-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	BBB	201	0N8	C14-C11-C15-C16
2	DDD	201	0N8	C14-C22-C23-O28
2	DDD	201	0N8	C14-C22-C23-C24
2	GGG	201	0N8	C14-C11-C15-C16
2	GGG	201	0N8	C12-C11-C14-O27
2	BBB	201	0N8	C14-C22-C23-O28
2	GGG	201	0N8	C14-C22-C23-O28
2	AAA	201	0N8	C12-C11-C14-O27
2	BBB	201	0N8	C15-C11-C14-O27
2	BBB	201	0N8	C12-C11-C14-O27
2	DDD	201	0N8	C12-C11-C14-O27
2	GGG	201	0N8	C15-C11-C14-O27
2	BBB	201	0N8	C10-C11-C14-C22
2	GGG	201	0N8	C10-C11-C14-C22
2	AAA	201	0N8	C15-C11-C14-O27
2	AAA	201	0N8	C10-C11-C14-O27
2	BBB	201	0N8	C10-C11-C14-O27
2	DDD	201	0N8	C15-C11-C14-O27
2	DDD	201	0N8	C10-C11-C14-O27
2	GGG	201	0N8	C10-C11-C14-O27
2	BBB	201	0N8	C10-C11-C15-C16
2	BBB	201	0N8	C14-C22-C23-C24
2	BBB	201	0N8	C15-C11-C14-C22
2	BBB	201	0N8	C12-C11-C14-C22
2	GGG	201	0N8	C15-C11-C14-C22

All (2) ring outliers are listed below:

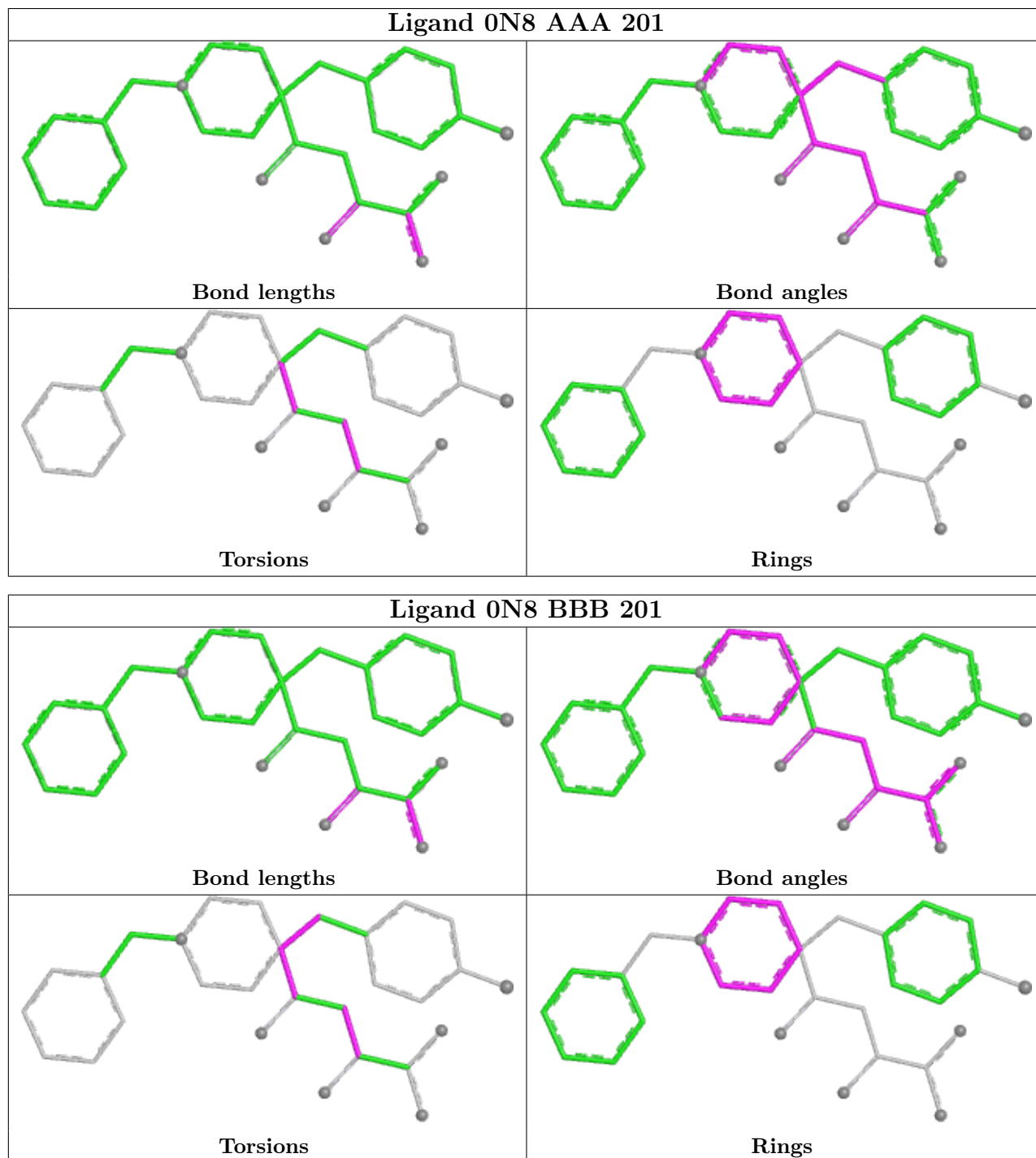
Mol	Chain	Res	Type	Atoms
2	BBB	201	0N8	C10-C11-C12-C13-C9-N8
2	AAA	201	0N8	C10-C11-C12-C13-C9-N8

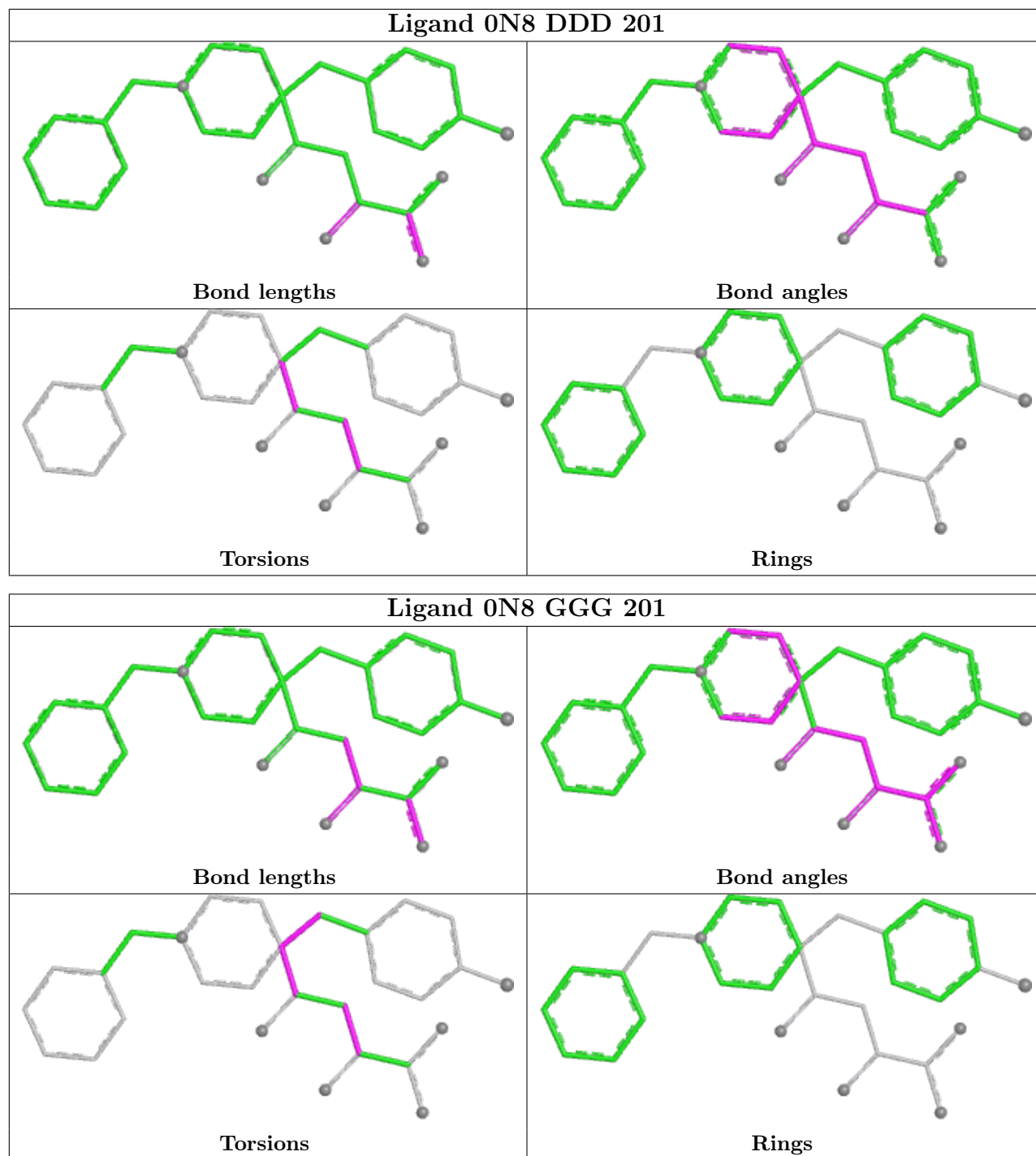
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	201	0N8	1	0
2	DDD	201	0N8	1	0
2	GGG	201	0N8	2	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, 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	184/184 (100%)	0.69	1 (0%) 91 91	43, 53, 66, 88	0
1	BBB	184/184 (100%)	0.78	3 (1%) 72 71	42, 54, 75, 92	0
1	DDD	184/184 (100%)	0.64	2 (1%) 80 80	42, 51, 71, 107	0
1	GGG	184/184 (100%)	0.70	2 (1%) 80 80	44, 58, 81, 107	0
All	All	736/736 (100%)	0.70	8 (1%) 80 80	42, 54, 77, 107	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	GGG	183	ALA	7.8
1	DDD	183	ALA	5.3
1	AAA	183	ALA	3.7
1	BBB	183	ALA	3.3
1	DDD	182	VAL	2.4
1	BBB	22	ALA	2.4
1	GGG	75	HIS	2.0
1	BBB	66	VAL	2.0

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

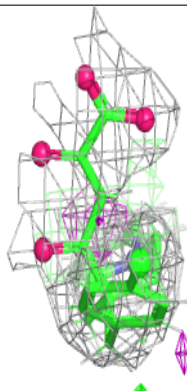
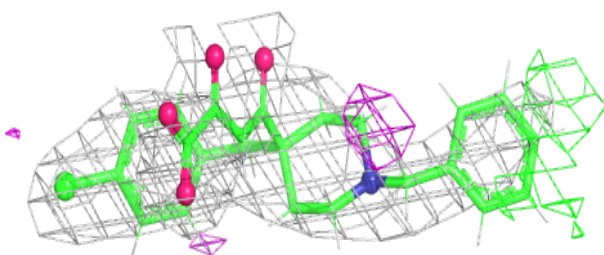
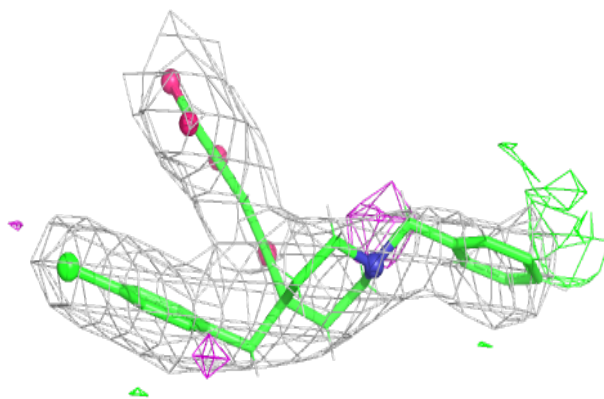
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FMT	BBB	202	3/3	0.83	0.15	45,47,47,48	1
3	FMT	AAA	202	3/3	0.88	0.18	50,50,51,51	1
3	FMT	GGG	202	3/3	0.88	0.20	59,60,61,61	1
3	FMT	DDD	202	3/3	0.92	0.30	52,52,54,55	1
3	FMT	AAA	203	3/3	0.93	0.20	60,60,61,61	1
2	0N8	GGG	201	29/29	0.94	0.32	55,68,84,84	0
2	0N8	AAA	201	29/29	0.95	0.30	49,67,87,88	0
2	0N8	BBB	201	29/29	0.95	0.27	56,64,78,78	0
2	0N8	DDD	201	29/29	0.95	0.28	51,60,78,79	0
3	FMT	DDD	203	3/3	0.96	0.14	49,49,50,50	1
4	MN	AAA	205	1/1	0.99	0.24	51,51,51,51	0
4	MN	BBB	203	1/1	0.99	0.24	48,48,48,48	0
4	MN	DDD	204	1/1	0.99	0.24	44,44,44,44	0
4	MN	GGG	204	1/1	0.99	0.25	54,54,54,54	0
4	MN	AAA	204	1/1	1.00	0.24	40,40,40,40	0
4	MN	DDD	205	1/1	1.00	0.25	47,47,47,47	0
4	MN	GGG	203	1/1	1.00	0.24	49,49,49,49	0
4	MN	BBB	204	1/1	1.00	0.24	47,47,47,47	0

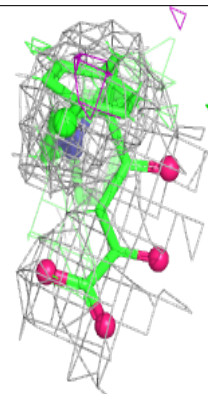
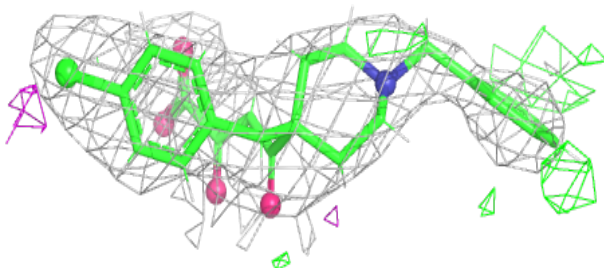
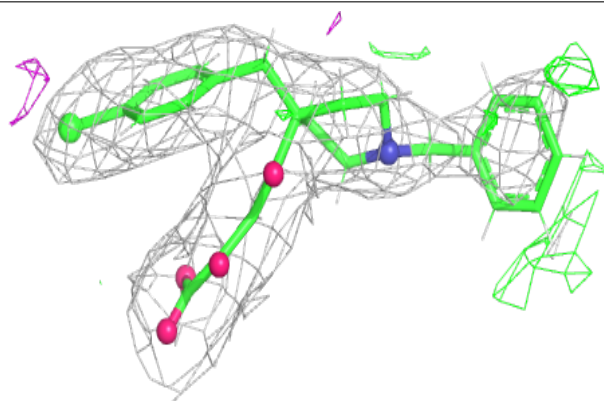
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 0N8 GGG 201:

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

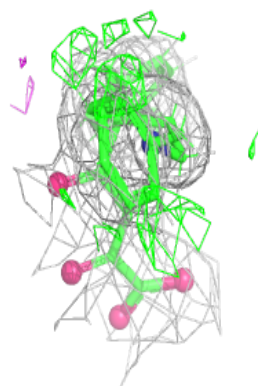
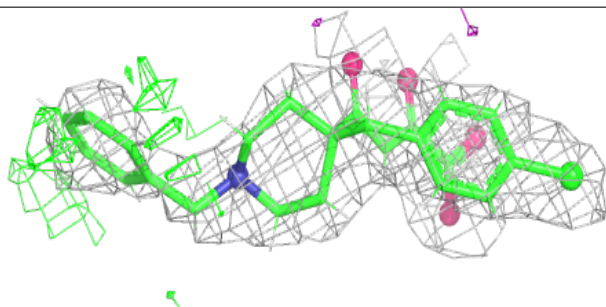
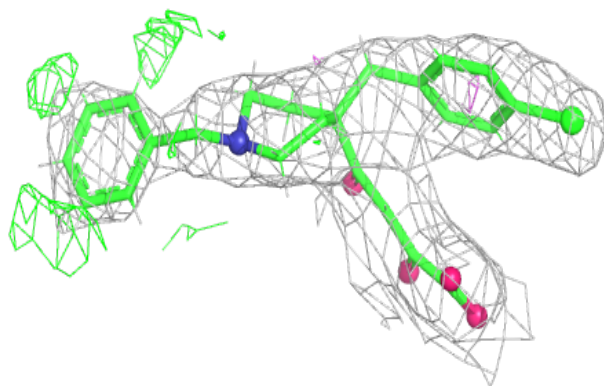
**Electron density around 0N8 AAA 201:**

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

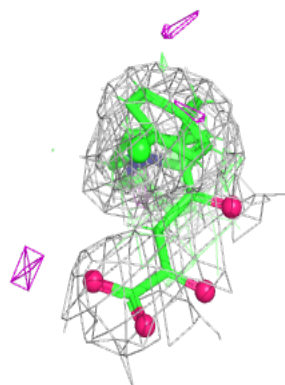
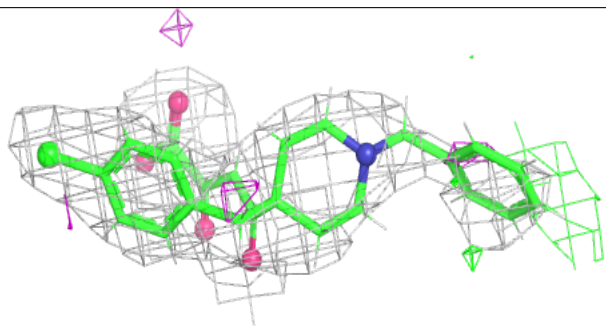
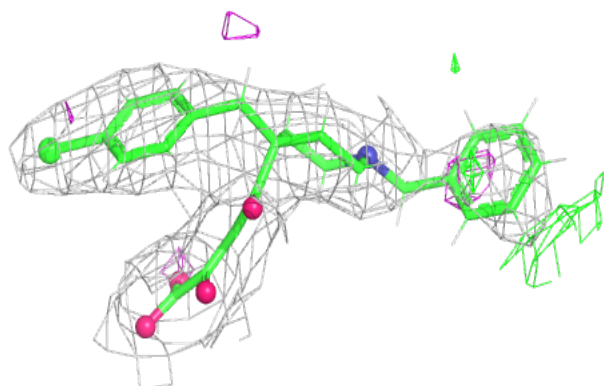


Electron density around 0N8 BBB 201:

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

**Electron density around 0N8 DDD 201:**

$2mF_o-DF_c$ (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.