



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 10, 2025 – 09:20 pm GMT

PDB ID : 9QM6 / pdb\_00009qm6  
Title : Crystal structure of highly stable methionine gamma-lyase from *Thermobrachium celere* in complex with PLP and norleucine  
Authors : Kopecny, D.; Ferchaud, N.; Briozzo, P.  
Deposited on : 2025-03-21  
Resolution : 2.61 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](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	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

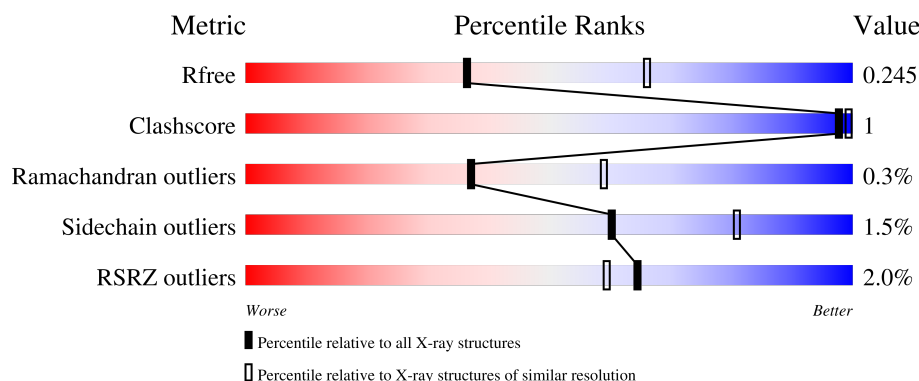
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 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))
$R_{free}$	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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	A	419	<div> <div></div> <div>92%</div> <div>5%</div> </div>
1	B	419	<div> <div></div> <div>93%</div> <div>5%</div> </div>
1	C	419	<div> <div></div> <div>93%</div> <div>•</div> </div>
1	D	419	<div> <div>5%</div> <div>89%</div> <div>6%</div> <div>5%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24756 atoms, of which 12386 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 L-methionine gamma-lyase.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
1	A	400	Total	C	H	N	O	P	S		0	0	0
			6163	1955	3083	520	587	1	17				
1	B	400	Total	C	H	N	O	P	S		0	0	0
			6164	1955	3084	520	587	1	17				
1	C	401	Total	C	H	N	O	P	S		0	0	0
			6174	1958	3088	521	589	1	17				
1	D	400	Total	C	H	N	O	P	S		0	0	0
			6154	1952	3077	520	587	1	17				

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP R7RTI8
A	-18	GLY	-	expression tag	UNP R7RTI8
A	-17	SER	-	expression tag	UNP R7RTI8
A	-16	SER	-	expression tag	UNP R7RTI8
A	-15	HIS	-	expression tag	UNP R7RTI8
A	-14	HIS	-	expression tag	UNP R7RTI8
A	-13	HIS	-	expression tag	UNP R7RTI8
A	-12	HIS	-	expression tag	UNP R7RTI8
A	-11	HIS	-	expression tag	UNP R7RTI8
A	-10	HIS	-	expression tag	UNP R7RTI8
A	-9	SER	-	expression tag	UNP R7RTI8
A	-8	SER	-	expression tag	UNP R7RTI8
A	-7	GLY	-	expression tag	UNP R7RTI8
A	-6	LEU	-	expression tag	UNP R7RTI8
A	-5	VAL	-	expression tag	UNP R7RTI8
A	-4	PRO	-	expression tag	UNP R7RTI8
A	-3	ARG	-	expression tag	UNP R7RTI8
A	-2	GLY	-	expression tag	UNP R7RTI8
A	-1	SER	-	expression tag	UNP R7RTI8
A	0	HIS	-	expression tag	UNP R7RTI8
B	-19	MET	-	initiating methionine	UNP R7RTI8

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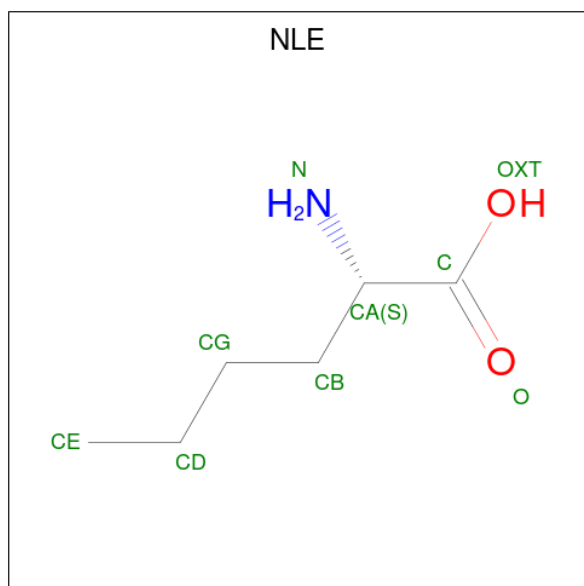
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP R7RTI8
B	-17	SER	-	expression tag	UNP R7RTI8
B	-16	SER	-	expression tag	UNP R7RTI8
B	-15	HIS	-	expression tag	UNP R7RTI8
B	-14	HIS	-	expression tag	UNP R7RTI8
B	-13	HIS	-	expression tag	UNP R7RTI8
B	-12	HIS	-	expression tag	UNP R7RTI8
B	-11	HIS	-	expression tag	UNP R7RTI8
B	-10	HIS	-	expression tag	UNP R7RTI8
B	-9	SER	-	expression tag	UNP R7RTI8
B	-8	SER	-	expression tag	UNP R7RTI8
B	-7	GLY	-	expression tag	UNP R7RTI8
B	-6	LEU	-	expression tag	UNP R7RTI8
B	-5	VAL	-	expression tag	UNP R7RTI8
B	-4	PRO	-	expression tag	UNP R7RTI8
B	-3	ARG	-	expression tag	UNP R7RTI8
B	-2	GLY	-	expression tag	UNP R7RTI8
B	-1	SER	-	expression tag	UNP R7RTI8
B	0	HIS	-	expression tag	UNP R7RTI8
C	-19	MET	-	initiating methionine	UNP R7RTI8
C	-18	GLY	-	expression tag	UNP R7RTI8
C	-17	SER	-	expression tag	UNP R7RTI8
C	-16	SER	-	expression tag	UNP R7RTI8
C	-15	HIS	-	expression tag	UNP R7RTI8
C	-14	HIS	-	expression tag	UNP R7RTI8
C	-13	HIS	-	expression tag	UNP R7RTI8
C	-12	HIS	-	expression tag	UNP R7RTI8
C	-11	HIS	-	expression tag	UNP R7RTI8
C	-10	HIS	-	expression tag	UNP R7RTI8
C	-9	SER	-	expression tag	UNP R7RTI8
C	-8	SER	-	expression tag	UNP R7RTI8
C	-7	GLY	-	expression tag	UNP R7RTI8
C	-6	LEU	-	expression tag	UNP R7RTI8
C	-5	VAL	-	expression tag	UNP R7RTI8
C	-4	PRO	-	expression tag	UNP R7RTI8
C	-3	ARG	-	expression tag	UNP R7RTI8
C	-2	GLY	-	expression tag	UNP R7RTI8
C	-1	SER	-	expression tag	UNP R7RTI8
C	0	HIS	-	expression tag	UNP R7RTI8
D	-19	MET	-	initiating methionine	UNP R7RTI8
D	-18	GLY	-	expression tag	UNP R7RTI8
D	-17	SER	-	expression tag	UNP R7RTI8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP R7RTI8
D	-15	HIS	-	expression tag	UNP R7RTI8
D	-14	HIS	-	expression tag	UNP R7RTI8
D	-13	HIS	-	expression tag	UNP R7RTI8
D	-12	HIS	-	expression tag	UNP R7RTI8
D	-11	HIS	-	expression tag	UNP R7RTI8
D	-10	HIS	-	expression tag	UNP R7RTI8
D	-9	SER	-	expression tag	UNP R7RTI8
D	-8	SER	-	expression tag	UNP R7RTI8
D	-7	GLY	-	expression tag	UNP R7RTI8
D	-6	LEU	-	expression tag	UNP R7RTI8
D	-5	VAL	-	expression tag	UNP R7RTI8
D	-4	PRO	-	expression tag	UNP R7RTI8
D	-3	ARG	-	expression tag	UNP R7RTI8
D	-2	GLY	-	expression tag	UNP R7RTI8
D	-1	SER	-	expression tag	UNP R7RTI8
D	0	HIS	-	expression tag	UNP R7RTI8

- Molecule 2 is NORLEUCINE (CCD ID: NLE) (formula:  $C_6H_{13}NO_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			21	6	12	1	2		
2	B	1	Total	C	H	N	O	0	0
			21	6	12	1	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	H	N	O	0	0
			21	6	12	1	2		
2	D	1	Total	C	H	N	O	0	0
			21	6	12	1	2		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		

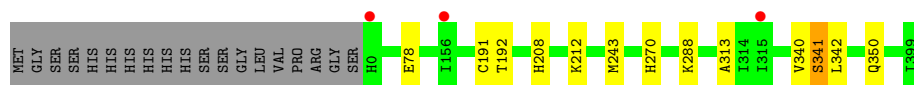
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	O	0	0
			6	6		
4	D	1	Total	O	0	0
			1	1		

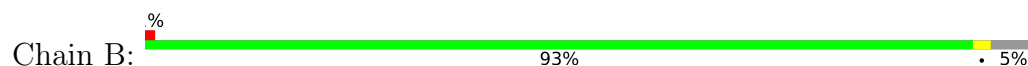
### 3 Residue-property plots [i](#)

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: L-methionine gamma-lyase



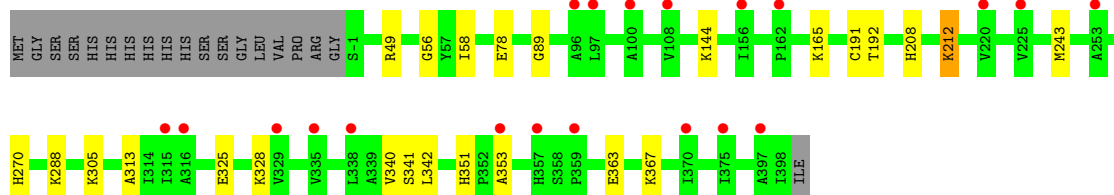
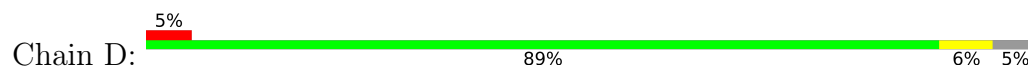
- Molecule 1: L-methionine gamma-lyase



- Molecule 1: L-methionine gamma-lyase



- Molecule 1: L-methionine gamma-lyase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.43Å 86.43Å 862.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.84 – 2.61 37.84 – 2.61	Depositor EDS
% Data completeness (in resolution range)	65.7 (37.84-2.61) 65.6 (37.84-2.61)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, $R_{free}$	0.250 , 0.268 0.233 , 0.245	Depositor DCC
$R_{free}$ test set	1998 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.4	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 40.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	24756	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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: NLE, EDO, LLP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.70	0/3111	0.95	1/4205 (0.0%)
1	B	0.71	0/3111	0.96	1/4205 (0.0%)
1	C	0.70	0/3117	0.95	2/4213 (0.0%)
1	D	0.72	0/3108	0.97	1/4202 (0.0%)
All	All	0.71	0/12447	0.96	5/16825 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	243	MET	N-CA-C	5.22	117.05	111.36
1	C	243	MET	N-CA-C	5.15	116.97	111.36
1	D	243	MET	N-CA-C	5.09	116.91	111.36
1	C	372	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	243	MET	N-CA-C	5.06	116.88	111.36

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3080	3083	3086	4	0
1	B	3080	3084	3086	3	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3086	3088	3091	1	1
1	D	3077	3077	3080	8	0
2	A	9	12	12	0	0
2	B	9	12	12	1	0
2	C	9	12	12	0	0
2	D	9	12	12	1	0
3	A	4	6	6	0	0
4	A	6	0	0	0	0
4	D	1	0	0	0	0
All	All	12370	12386	12397	16	1

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 1.

All (16) 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:D:212:LLP:C4'	2:D:401:NLE:H	2.14	0.60
1:B:212:LLP:C4'	2:B:401:NLE:H	2.18	0.56
1:D:351:HIS:CE1	1:D:353:ALA:HB3	2.42	0.54
1:D:49:ARG:NE	1:D:56:GLY:HA3	2.26	0.50
1:C:270:HIS:HB3	1:C:313:ALA:HB2	1.96	0.48
1:A:270:HIS:HB3	1:A:313:ALA:HB2	1.96	0.48
1:B:270:HIS:HB3	1:B:313:ALA:HB2	1.96	0.47
1:D:270:HIS:HB3	1:D:313:ALA:HB2	1.96	0.47
1:B:78:GLU:OE2	1:B:208:HIS:NE2	2.50	0.43
1:D:78:GLU:OE2	1:D:208:HIS:NE2	2.50	0.43
1:A:78:GLU:OE2	1:A:208:HIS:NE2	2.51	0.42
1:A:340:VAL:O	1:A:341:SER:HB3	2.20	0.42
1:D:191:CYS:O	1:D:192:THR:OG1	2.35	0.41
1:A:191:CYS:O	1:A:192:THR:OG1	2.36	0.41
1:D:49:ARG:HB3	1:D:58:ILE:HD11	2.02	0.40
1:D:89:GLY:HA3	1:D:212:LLP:OP4	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:TYR:HH	1:C:212:LLP:OP3[8_675]	1.54	0.06

## 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	A	397/419 (95%)	380 (96%)	16 (4%)	1 (0%)	37	59
1	B	397/419 (95%)	376 (95%)	19 (5%)	2 (0%)	25	47
1	C	398/419 (95%)	380 (96%)	17 (4%)	1 (0%)	37	59
1	D	397/419 (95%)	375 (94%)	21 (5%)	1 (0%)	37	59
All	All	1589/1676 (95%)	1511 (95%)	73 (5%)	5 (0%)	37	59

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	341	SER
1	C	341	SER
1	A	341	SER
1	D	341	SER
1	B	321	GLY

### 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	A	323/339 (95%)	320 (99%)	3 (1%)	75	90
1	B	323/339 (95%)	321 (99%)	2 (1%)	84	94
1	C	324/339 (96%)	319 (98%)	5 (2%)	60	81
1	D	323/339 (95%)	313 (97%)	10 (3%)	35	62
All	All	1293/1356 (95%)	1273 (98%)	20 (2%)	60	81

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

Mol	Chain	Res	Type
1	A	288	LYS
1	A	342	LEU
1	A	350	GLN
1	B	22	LYS
1	B	342	LEU
1	C	131	GLU
1	C	144	LYS
1	C	288	LYS
1	C	342	LEU
1	C	350	GLN
1	D	144	LYS
1	D	165	LYS
1	D	288	LYS
1	D	305	LYS
1	D	325	GLU
1	D	328	LYS
1	D	340	VAL
1	D	342	LEU
1	D	363	GLU
1	D	367	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	23	ASN
1	A	64	ASN
1	A	383	ASN
1	B	23	ASN
1	B	64	ASN
1	B	234	GLN
1	C	23	ASN
1	C	64	ASN
1	C	234	GLN
1	D	64	ASN
1	D	139	ASN
1	D	234	GLN
1	D	383	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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
1	LLP	A	212	1	23,24,25	1.41	1 (4%)	25,32,34	0.95	1 (4%)
1	LLP	C	212	1	23,24,25	1.42	1 (4%)	25,32,34	0.96	1 (4%)
1	LLP	B	212	1	23,24,25	1.47	1 (4%)	25,32,34	0.93	1 (4%)
1	LLP	D	212	1	23,24,25	1.46	1 (4%)	25,32,34	0.88	1 (4%)

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
1	LLP	A	212	1	-	5/16/17/19	0/1/1/1
1	LLP	C	212	1	-	4/16/17/19	0/1/1/1
1	LLP	B	212	1	-	5/16/17/19	0/1/1/1
1	LLP	D	212	1	-	4/16/17/19	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	212	LLP	C4'-NZ	6.17	1.48	1.27
1	D	212	LLP	C4'-NZ	6.17	1.48	1.27
1	C	212	LLP	C4'-NZ	6.07	1.47	1.27
1	A	212	LLP	C4'-NZ	6.04	1.47	1.27

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	212	LLP	OP4-C5'-C5	2.48	114.08	109.35
1	A	212	LLP	OP4-C5'-C5	2.37	113.86	109.35
1	C	212	LLP	OP4-C5'-C5	2.35	113.83	109.35
1	D	212	LLP	OP4-C5'-C5	2.12	113.39	109.35

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	212	LLP	C4-C4'-NZ-CE
1	A	212	LLP	O-C-CA-CB
1	B	212	LLP	C4-C4'-NZ-CE
1	B	212	LLP	O-C-CA-CB
1	C	212	LLP	C4-C4'-NZ-CE
1	C	212	LLP	O-C-CA-CB
1	D	212	LLP	C4-C4'-NZ-CE
1	D	212	LLP	O-C-CA-CB
1	B	212	LLP	CA-CB-CG-CD
1	C	212	LLP	CA-CB-CG-CD
1	A	212	LLP	CA-CB-CG-CD
1	D	212	LLP	CA-CB-CG-CD
1	A	212	LLP	CD-CE-NZ-C4'
1	C	212	LLP	CD-CE-NZ-C4'
1	B	212	LLP	CD-CE-NZ-C4'
1	D	212	LLP	CD-CE-NZ-C4'
1	A	212	LLP	C3-C4-C4'-NZ
1	B	212	LLP	N-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	212	LLP	0	1
1	B	212	LLP	1	0
1	D	212	LLP	2	0

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

5 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	$\# Z  > 2$
2	NLE	D	401	-	7,8,8	1.39	1 (14%)	8,9,9	1.25	1 (12%)
3	EDO	A	402	-	3,3,3	0.28	0	2,2,2	0.23	0
2	NLE	A	401	-	7,8,8	1.14	1 (14%)	8,9,9	0.64	0
2	NLE	C	401	-	7,8,8	1.07	0	8,9,9	0.72	0
2	NLE	B	401	-	7,8,8	1.20	1 (14%)	8,9,9	0.80	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	NLE	D	401	-	-	2/8/8/8	-
3	EDO	A	402	-	-	1/1/1/1	-
2	NLE	A	401	-	-	2/8/8/8	-
2	NLE	C	401	-	-	1/8/8/8	-
2	NLE	B	401	-	-	1/8/8/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	NLE	CB-CA	2.90	1.59	1.53
2	B	401	NLE	CB-CA	2.38	1.58	1.53
2	A	401	NLE	CB-CA	2.07	1.57	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	NLE	CB-CA-C	2.01	115.08	110.30

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	NLE	CA-CB-CG-CD
2	C	401	NLE	CE-CD-CG-CB
2	A	401	NLE	OXT-C-CA-CB
2	A	401	NLE	O-C-CA-CB
3	A	402	EDO	O1-C1-C2-O2
2	D	401	NLE	C-CA-CB-CG
2	B	401	NLE	N-CA-CB-CG

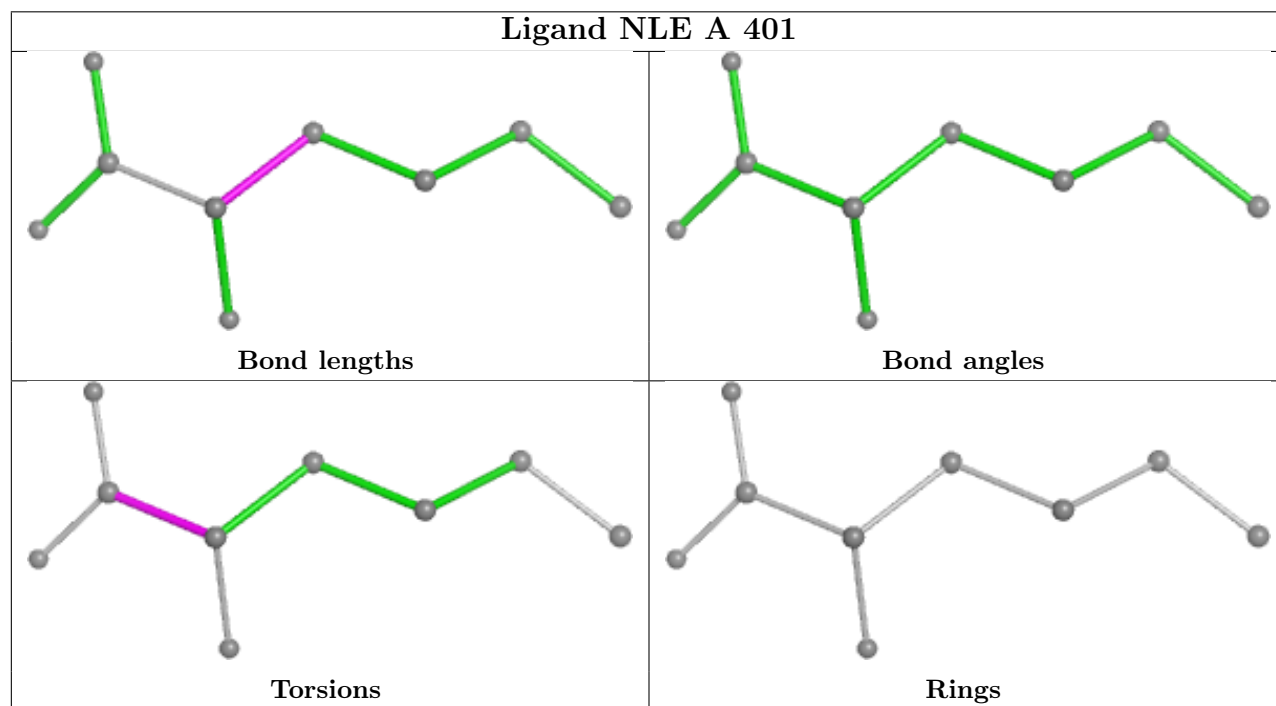
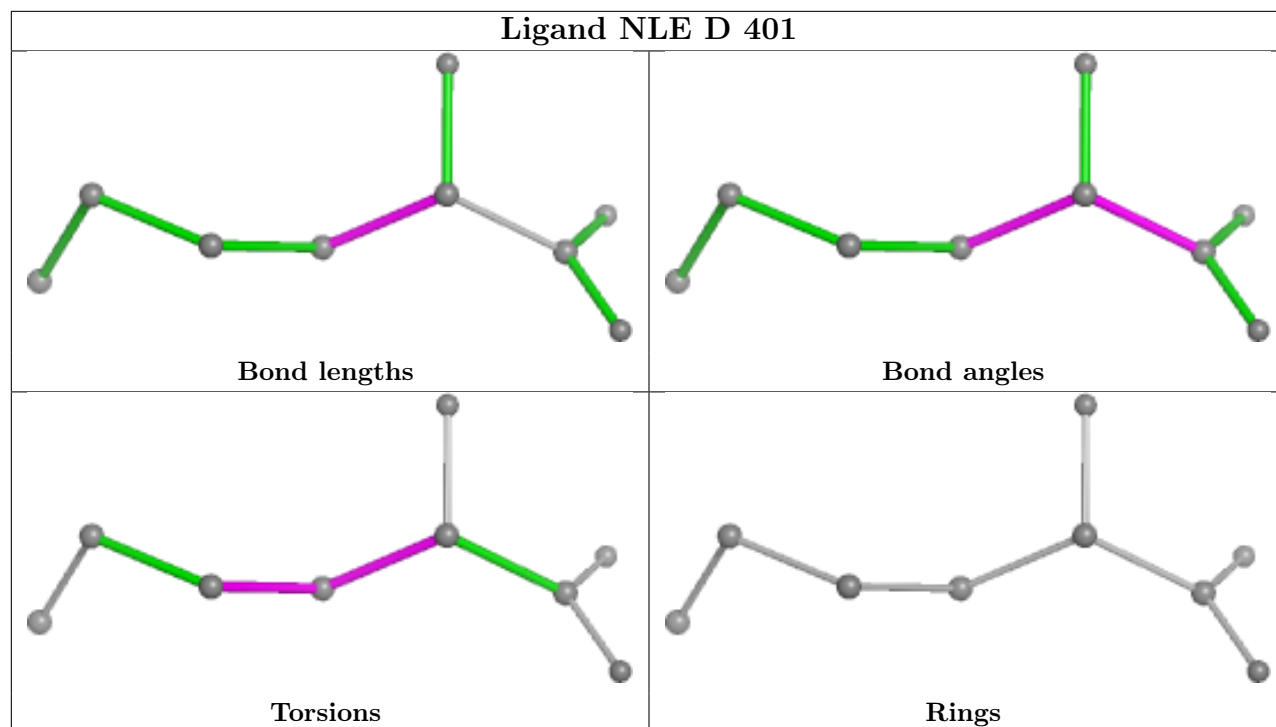
There are no ring outliers.

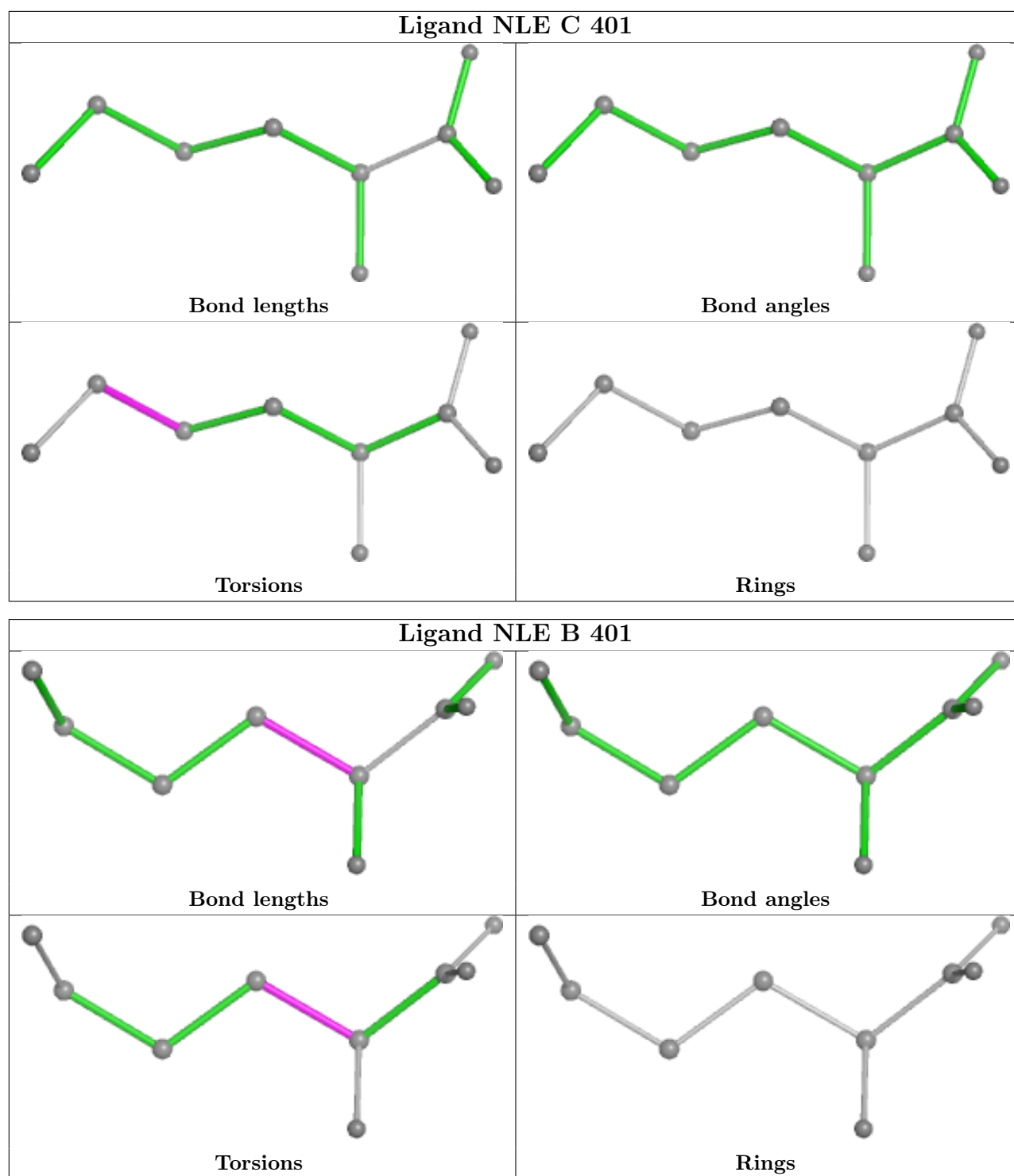
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	NLE	1	0
2	B	401	NLE	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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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, 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	A	399/419 (95%)	0.15	3 (0%) 82 79	58, 77, 99, 120	0
1	B	399/419 (95%)	0.07	4 (1%) 79 75	58, 80, 104, 115	0
1	C	400/419 (95%)	0.11	5 (1%) 74 70	60, 78, 104, 114	0
1	D	399/419 (95%)	0.39	20 (5%) 35 30	66, 96, 130, 147	0
All	All	1597/1676 (95%)	0.18	32 (2%) 64 59	58, 81, 115, 147	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	381	LEU	3.7
1	D	338	LEU	3.5
1	A	315	ILE	3.4
1	D	316	ALA	3.3
1	D	108	VAL	3.2
1	D	156	ILE	3.1
1	C	353	ALA	3.0
1	D	97	LEU	2.9
1	A	0	HIS	2.8
1	D	162	PRO	2.7
1	D	353	ALA	2.7
1	D	357	HIS	2.7
1	D	375	ILE	2.6
1	C	143	ILE	2.5
1	C	265	ILE	2.5
1	B	370	ILE	2.4
1	D	315	ILE	2.4
1	D	100	ALA	2.3
1	D	329	VAL	2.3
1	D	96	ALA	2.3
1	D	359	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	253	ALA	2.2
1	D	397	ALA	2.2
1	D	335	VAL	2.2
1	C	186	VAL	2.1
1	D	220	VAL	2.1
1	D	225	VAL	2.1
1	B	162	PRO	2.1
1	A	156	ILE	2.0
1	C	156	ILE	2.0
1	B	357	HIS	2.0
1	D	370	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 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
1	LLP	D	212	24/25	0.93	0.09	75,87,88,88	0
1	LLP	C	212	24/25	0.94	0.10	62,70,71,71	0
1	LLP	B	212	24/25	0.94	0.10	64,74,74,74	0
1	LLP	A	212	24/25	0.95	0.08	59,64,65,65	0

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 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.

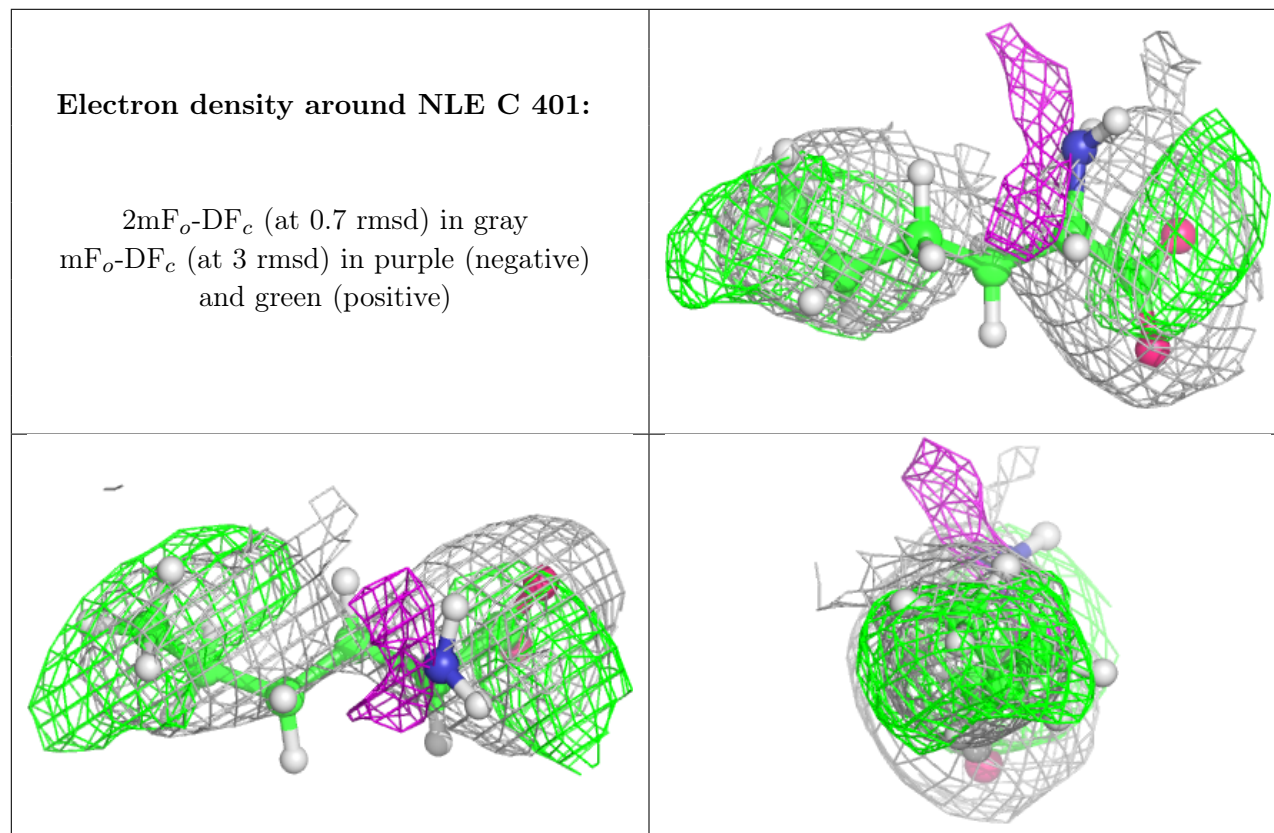
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	EDO	A	402	4/4	0.71	0.20	91,91,91,91	0
2	NLE	C	401	9/9	0.73	0.26	66,67,68,68	0
2	NLE	A	401	9/9	0.76	0.23	51,54,55,55	0

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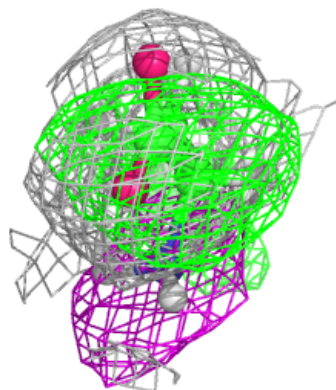
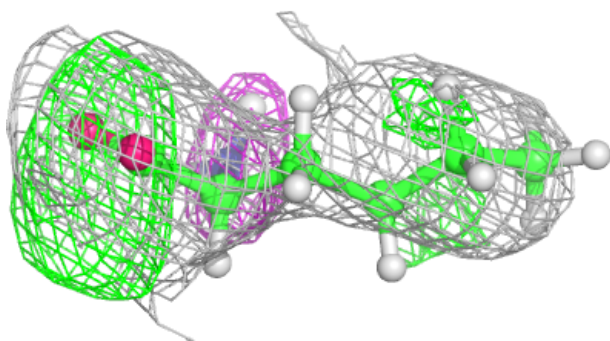
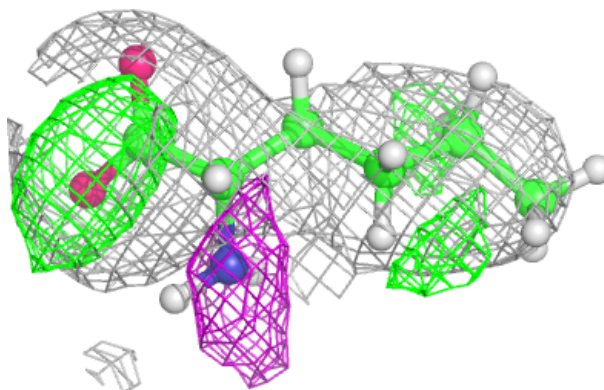
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NLE	D	401	9/9	0.77	0.24	85,85,87,87	0
2	NLE	B	401	9/9	0.81	0.21	67,68,70,70	0

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 NLE A 401:**

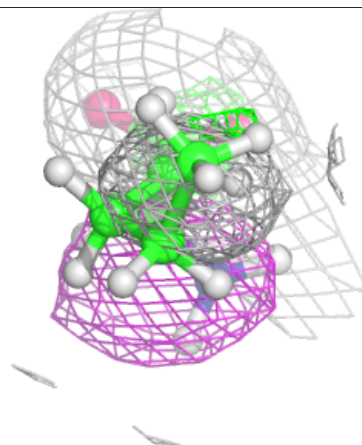
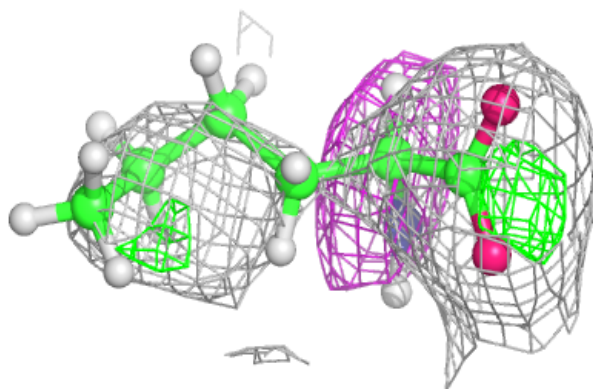
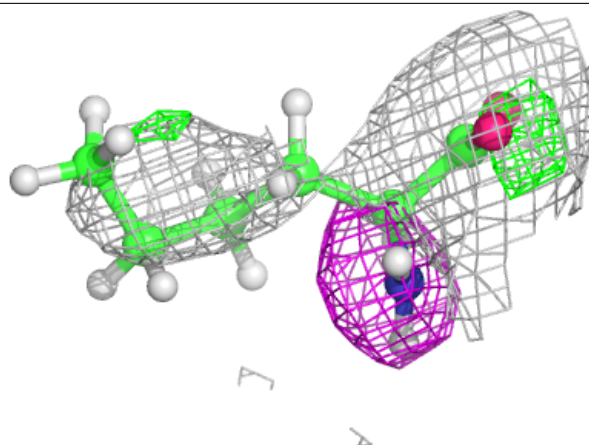
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



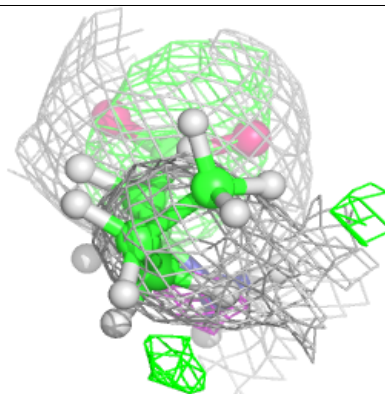
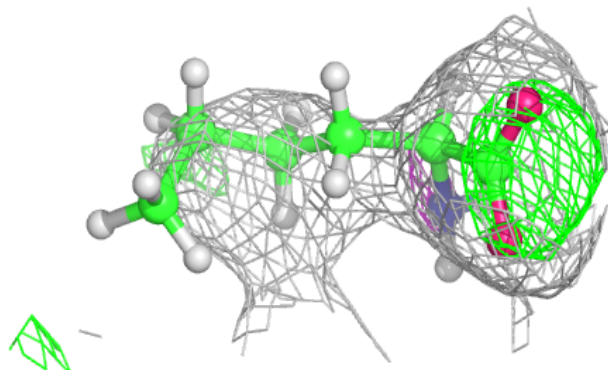
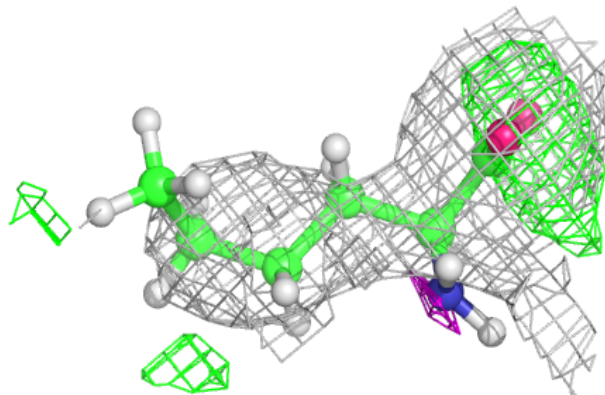


**Electron density around NLE D 401:**

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

**Electron density around NLE B 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 [i](#)

There are no such residues in this entry.