



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2022 – 03:46 PM EDT

PDB ID : 8E8V
Title : Structure of the short LOR domain of human AASS bound to N-ethylsuccinimide
Authors : Khamrui, S.; Lazarus, M.B.
Deposited on : 2022-08-25
Resolution : 2.45 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
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)	:	2.31.2

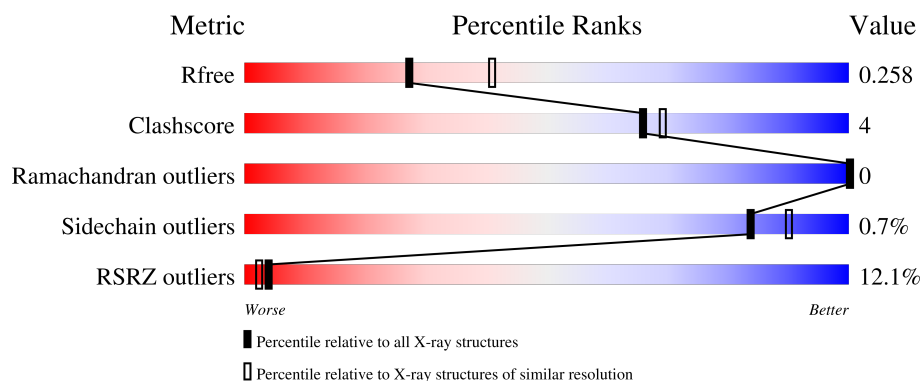
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	A	434	
1	B	434	
1	C	434	
1	D	434	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12739 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

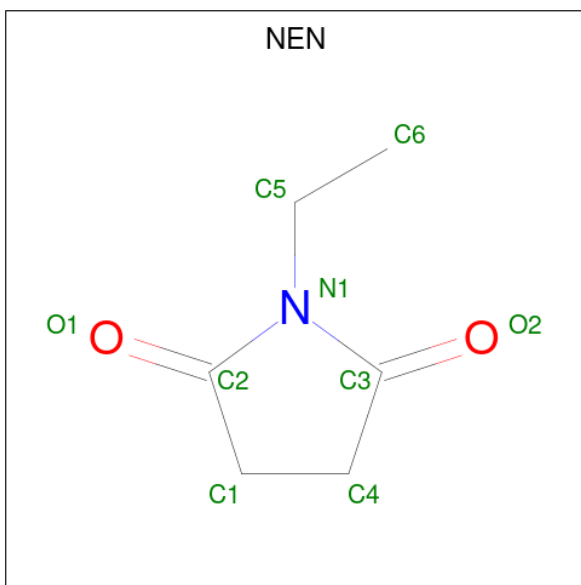
- Molecule 1 is a protein called Alpha-aminoadipic semialdehyde synthase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			3177	2013	552	591	21			
1	B	406	Total	C	N	O	S	0	0	0
			3188	2019	554	594	21			
1	C	404	Total	C	N	O	S	0	0	0
			3177	2013	552	591	21			
1	D	402	Total	C	N	O	S	0	0	0
			3161	2003	550	587	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	GLY	-	expression tag	UNP Q9UDR5
A	20	SER	-	expression tag	UNP Q9UDR5
B	19	GLY	-	expression tag	UNP Q9UDR5
B	20	SER	-	expression tag	UNP Q9UDR5
C	19	GLY	-	expression tag	UNP Q9UDR5
C	20	SER	-	expression tag	UNP Q9UDR5
D	19	GLY	-	expression tag	UNP Q9UDR5
D	20	SER	-	expression tag	UNP Q9UDR5

- Molecule 2 is 1-ETHYL-PYRROLIDINE-2,5-DIONE (three-letter code: NEN) (formula: $C_6H_9NO_2$) (labeled as "Ligand of Interest" by depositor).

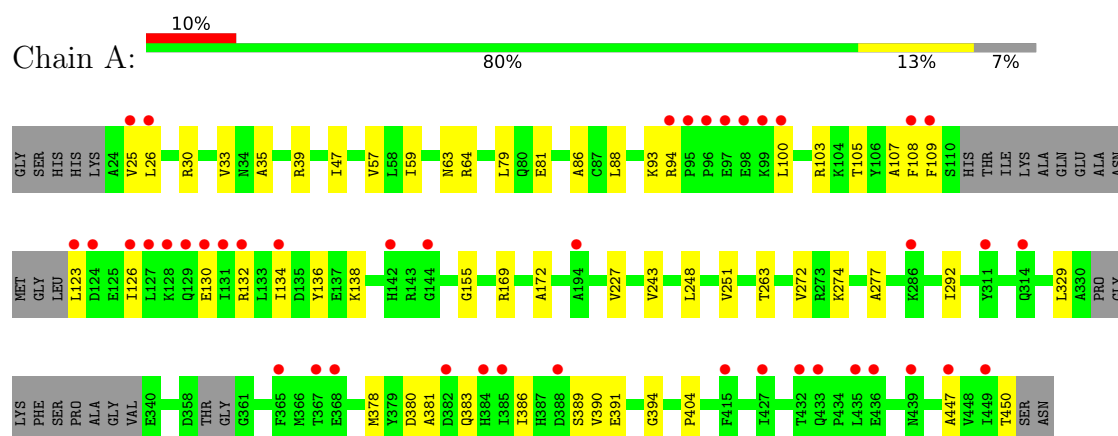


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	6	1	2		
2	B	1	Total	C	N	O	0	0
			9	6	1	2		
2	C	1	Total	C	N	O	0	0
			9	6	1	2		
2	D	1	Total	C	N	O	0	0
			9	6	1	2		

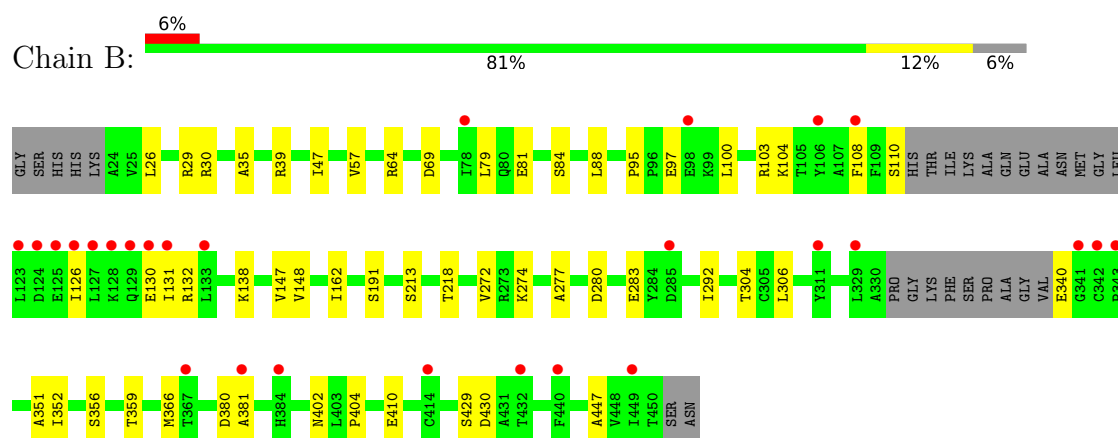
3 Residue-property plots [i](#)

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.

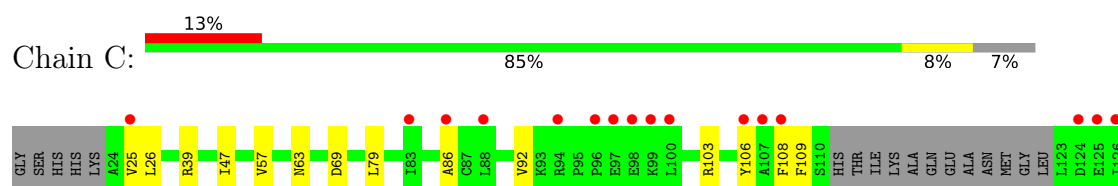
- Molecule 1: Alpha-aminoadipic semialdehyde synthase, mitochondrial

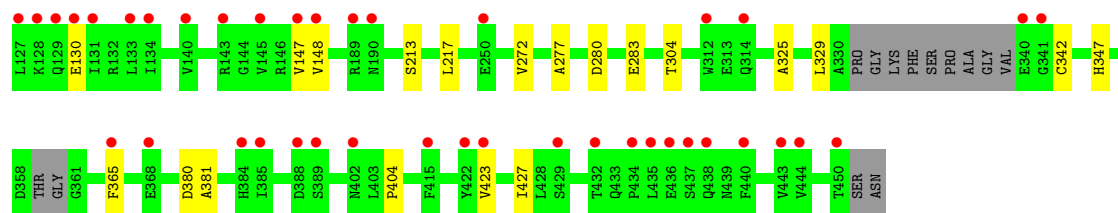


- Molecule 1: Alpha-aminoadipic semialdehyde synthase, mitochondrial

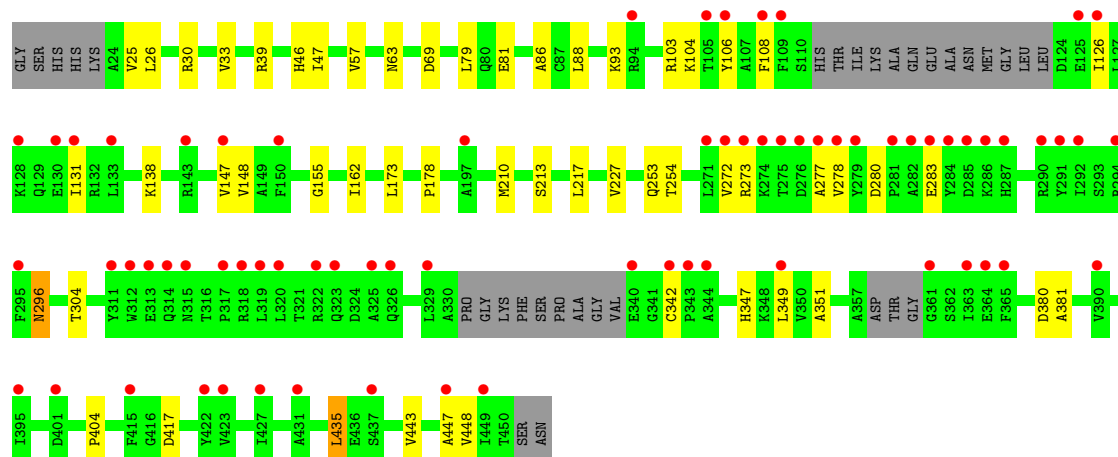
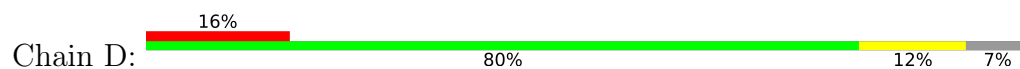


- Molecule 1: Alpha-aminoadipic semialdehyde synthase, mitochondrial





● Molecule 1: Alpha-aminoadipic semialdehyde synthase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.10Å 155.96Å 78.35Å 90.00° 100.20° 90.00°	Depositor
Resolution (Å)	47.49 – 2.45 47.49 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.49-2.45) 99.9 (47.49-2.45)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.234 , 0.258 0.234 , 0.258	Depositor DCC
R_{free} test set	3248 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	54.1	Xtriage
Anisotropy	0.728	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12739	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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: NEN

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	0.24	0/3246	0.44	0/4400
1	B	0.24	0/3258	0.42	0/4418
1	C	0.24	0/3246	0.42	0/4400
1	D	0.24	0/3230	0.42	0/4378
All	All	0.24	0/12980	0.43	0/17596

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	A	3177	0	3145	28	0
1	B	3188	0	3156	29	0
1	C	3177	0	3145	19	0
1	D	3161	0	3130	27	0
2	A	9	0	8	0	0
2	B	9	0	8	0	0
2	C	9	0	8	0	0
2	D	9	0	7	0	0
All	All	12739	0	12607	100	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 4.

All (100) 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:B:103:ARG:NH1	1:B:130:GLU:OE2	2.24	0.69
1:B:132:ARG:NH1	1:B:429:SER:OG	2.27	0.68
1:A:30:ARG:NH2	1:A:81:GLU:OE2	2.28	0.66
1:A:33:VAL:HG11	1:A:93:LYS:HG3	1.78	0.66
1:D:147:VAL:HG13	1:D:148:VAL:HG23	1.78	0.65
1:A:103:ARG:NH2	1:A:130:GLU:OE1	2.33	0.62
1:C:63:ASN:ND2	1:D:213:SER:OG	2.34	0.60
1:A:169:ARG:NH1	1:A:390:VAL:O	2.33	0.60
1:B:132:ARG:NH2	1:B:430:ASP:O	2.34	0.60
1:A:63:ASN:ND2	1:B:213:SER:OG	2.35	0.59
1:B:97:GLU:HA	1:B:100:LEU:HD12	1.84	0.58
1:D:253:GLN:HG3	1:D:254:THR:HG23	1.87	0.57
1:C:147:VAL:HG13	1:C:148:VAL:HG23	1.86	0.57
1:C:380:ASP:OD1	1:C:381:ALA:N	2.38	0.56
1:D:138:LYS:HB3	1:D:447:ALA:HA	1.88	0.55
1:C:26:LEU:HB2	1:C:427:ILE:HD12	1.88	0.55
1:D:47:ILE:HD12	1:D:57:VAL:HG11	1.88	0.55
1:D:69:ASP:HB3	1:D:79:LEU:HD11	1.90	0.54
1:A:272:VAL:HB	1:A:277:ALA:HA	1.91	0.53
1:A:274:LYS:HG2	1:A:292:ILE:HG23	1.90	0.53
1:A:26:LEU:HD13	1:A:88:LEU:HD23	1.90	0.52
1:B:272:VAL:HB	1:B:277:ALA:HA	1.91	0.52
1:C:47:ILE:HD12	1:C:57:VAL:HG11	1.91	0.52
1:A:47:ILE:HD12	1:A:57:VAL:HG11	1.92	0.52
1:D:296:ASN:N	1:D:296:ASN:OD1	2.43	0.52
1:C:25:VAL:HB	1:C:86:ALA:HA	1.91	0.51
1:B:47:ILE:HD12	1:B:57:VAL:HG11	1.92	0.51
1:B:340:GLU:N	1:B:340:GLU:OE2	2.44	0.51
1:B:356:SER:OG	1:B:359:THR:OG1	2.27	0.50
1:C:213:SER:OG	1:D:63:ASN:ND2	2.41	0.50
1:A:105:THR:HG23	1:A:132:ARG:HB3	1.94	0.50
1:A:126:ILE:HG21	1:A:450:THR:HB	1.94	0.50
1:A:138:LYS:HB2	1:A:447:ALA:HA	1.94	0.50
1:B:306:LEU:HB3	1:B:352:ILE:HG23	1.92	0.50
1:D:380:ASP:OD1	1:D:381:ALA:N	2.43	0.50
1:B:126:ILE:HG23	1:B:131:ILE:HB	1.95	0.49
1:B:274:LYS:HG2	1:B:292:ILE:HG23	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:ASP:HB3	1:C:79:LEU:HD11	1.95	0.49
1:A:123:LEU:N	1:A:126:ILE:HG12	2.28	0.49
1:D:46:HIS:NE2	1:D:417:ASP:OD1	2.42	0.49
1:A:380:ASP:OD1	1:A:381:ALA:N	2.46	0.48
1:D:26:LEU:HD13	1:D:88:LEU:HD23	1.96	0.48
1:D:33:VAL:HG11	1:D:93:LYS:HB2	1.96	0.48
1:D:39:ARG:HH11	1:D:404:PRO:HB2	1.79	0.48
1:D:106:TYR:HB3	1:D:108:PHE:CZ	2.48	0.48
1:D:25:VAL:HB	1:D:86:ALA:HA	1.95	0.48
1:B:29:ARG:CZ	1:B:95:PRO:HB3	2.43	0.47
1:D:126:ILE:HG23	1:D:131:ILE:HD11	1.97	0.47
1:B:35:ALA:HA	1:B:64:ARG:HH11	1.78	0.47
1:A:94:ARG:HB3	1:A:108:PHE:CD1	2.50	0.47
1:B:280:ASP:HB3	1:B:283:GLU:HB3	1.96	0.46
1:C:103:ARG:HG2	1:C:130:GLU:HG3	1.97	0.46
1:D:162:ILE:HD11	1:D:351:ALA:HB1	1.97	0.46
1:A:109:PHE:CE1	1:A:136:TYR:HB2	2.51	0.46
1:D:347:HIS:HD2	1:D:349:LEU:O	1.99	0.46
1:D:272:VAL:HB	1:D:277:ALA:HA	1.98	0.46
1:B:84:SER:HA	1:B:104:LYS:NZ	2.31	0.46
1:B:380:ASP:OD1	1:B:381:ALA:N	2.47	0.46
1:C:106:TYR:HB3	1:C:108:PHE:CE2	2.50	0.45
1:C:280:ASP:HB3	1:C:283:GLU:HB3	1.97	0.45
1:B:30:ARG:NH2	1:B:81:GLU:OE1	2.48	0.45
1:C:39:ARG:HH11	1:C:404:PRO:HB2	1.81	0.45
1:A:35:ALA:HA	1:A:64:ARG:HH11	1.81	0.45
1:A:329:LEU:HD21	1:A:394:GLY:HA2	1.99	0.45
1:B:147:VAL:HG23	1:B:148:VAL:HG23	1.99	0.45
1:A:378:MET:HG3	1:A:389:SER:O	2.17	0.44
1:B:191:SER:OG	1:B:410:GLU:OE2	2.33	0.44
1:D:435:LEU:HD11	1:D:448:VAL:HG11	1.99	0.44
1:C:423:VAL:O	1:C:427:ILE:HG12	2.16	0.44
1:B:162:ILE:HD11	1:B:351:ALA:HB1	1.99	0.44
1:A:25:VAL:HB	1:A:86:ALA:HA	2.00	0.44
1:A:389:SER:O	1:A:389:SER:OG	2.33	0.44
1:B:69:ASP:HB3	1:B:79:LEU:HD11	2.00	0.43
1:C:213:SER:HB3	1:C:342:CYS:HB2	2.00	0.43
1:B:218:THR:O	1:B:304:THR:OG1	2.31	0.43
1:A:243:VAL:HG11	1:A:251:VAL:HG21	2.01	0.43
1:C:329:LEU:HD22	1:C:347:HIS:CD2	2.54	0.43
1:A:59:ILE:O	1:A:79:LEU:HA	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:PHE:HE1	1:B:110:SER:HB2	1.83	0.42
1:C:92:VAL:O	1:C:109:PHE:HB2	2.19	0.42
1:C:272:VAL:HB	1:C:277:ALA:HA	2.02	0.42
1:B:138:LYS:HB2	1:B:447:ALA:HA	2.01	0.41
1:C:325:ALA:HB2	1:C:365:PHE:CE1	2.55	0.41
1:D:178:PRO:HD2	1:D:210:MET:SD	2.60	0.41
1:D:273:ARG:HB2	1:D:278:VAL:O	2.19	0.41
1:D:103:ARG:O	1:D:104:LYS:HD3	2.20	0.41
1:B:39:ARG:HH11	1:B:404:PRO:HB2	1.85	0.41
1:D:30:ARG:NH2	1:D:81:GLU:OE1	2.53	0.41
1:A:107:ALA:HA	1:A:134:ILE:O	2.21	0.40
1:A:155:GLY:HA3	1:A:227:VAL:O	2.20	0.40
1:B:26:LEU:HD13	1:B:88:LEU:HD23	2.03	0.40
1:D:217:LEU:HD22	1:D:304:THR:HG21	2.02	0.40
1:A:172:ALA:HB1	1:A:391:GLU:HG2	2.03	0.40
1:A:248:LEU:HD11	1:A:263:THR:HG21	2.02	0.40
1:B:366:MET:HE2	1:B:366:MET:HB2	1.89	0.40
1:C:217:LEU:HD22	1:C:304:THR:HG21	2.02	0.40
1:D:280:ASP:HB3	1:D:283:GLU:HB3	2.03	0.40
1:A:39:ARG:HH11	1:A:404:PRO:HB2	1.87	0.40
1:B:79:LEU:HD23	1:B:79:LEU:HA	1.99	0.40
1:D:155:GLY:HA3	1:D:227:VAL:O	2.21	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	A	396/434 (91%)	387 (98%)	9 (2%)	0	100	100
1	B	400/434 (92%)	393 (98%)	7 (2%)	0	100	100
1	C	396/434 (91%)	384 (97%)	12 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	394/434 (91%)	383 (97%)	11 (3%)	0	100	100
All	All	1586/1736 (91%)	1547 (98%)	39 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	345/367 (94%)	342 (99%)	3 (1%)	78	86
1	B	346/367 (94%)	345 (100%)	1 (0%)	92	95
1	C	345/367 (94%)	345 (100%)	0	100	100
1	D	343/367 (94%)	338 (98%)	5 (2%)	65	76
All	All	1379/1468 (94%)	1370 (99%)	9 (1%)	84	90

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	LEU
1	A	383	GLN
1	A	386	ILE
1	B	402	ASN
1	D	173	LEU
1	D	296	ASN
1	D	342	CYS
1	D	435	LEU
1	D	443	VAL

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	NEN	A	501	1	9,9,9	1.05	1 (11%)	12,12,12	1.02	1 (8%)
2	NEN	D	501	1	9,9,9	1.00	1 (11%)	12,12,12	1.51	2 (16%)
2	NEN	B	501	1	9,9,9	1.03	1 (11%)	12,12,12	1.36	1 (8%)
2	NEN	C	501	1	9,9,9	1.02	1 (11%)	12,12,12	1.38	1 (8%)

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	NEN	A	501	1	-	0/2/15/15	0/1/1/1
2	NEN	D	501	1	-	0/2/15/15	0/1/1/1
2	NEN	B	501	1	-	0/2/15/15	0/1/1/1
2	NEN	C	501	1	-	0/2/15/15	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NEN	C3-N1	2.19	1.42	1.38
2	A	501	NEN	C3-N1	2.18	1.42	1.38
2	C	501	NEN	C3-N1	2.09	1.42	1.38
2	D	501	NEN	C3-N1	2.03	1.42	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	NEN	C3-N1-C2	-4.15	111.06	112.96
2	B	501	NEN	C3-N1-C2	-3.80	111.22	112.96
2	C	501	NEN	C3-N1-C2	-3.79	111.22	112.96
2	A	501	NEN	C3-N1-C2	-2.77	111.69	112.96
2	D	501	NEN	C5-N1-C2	2.05	125.26	122.59

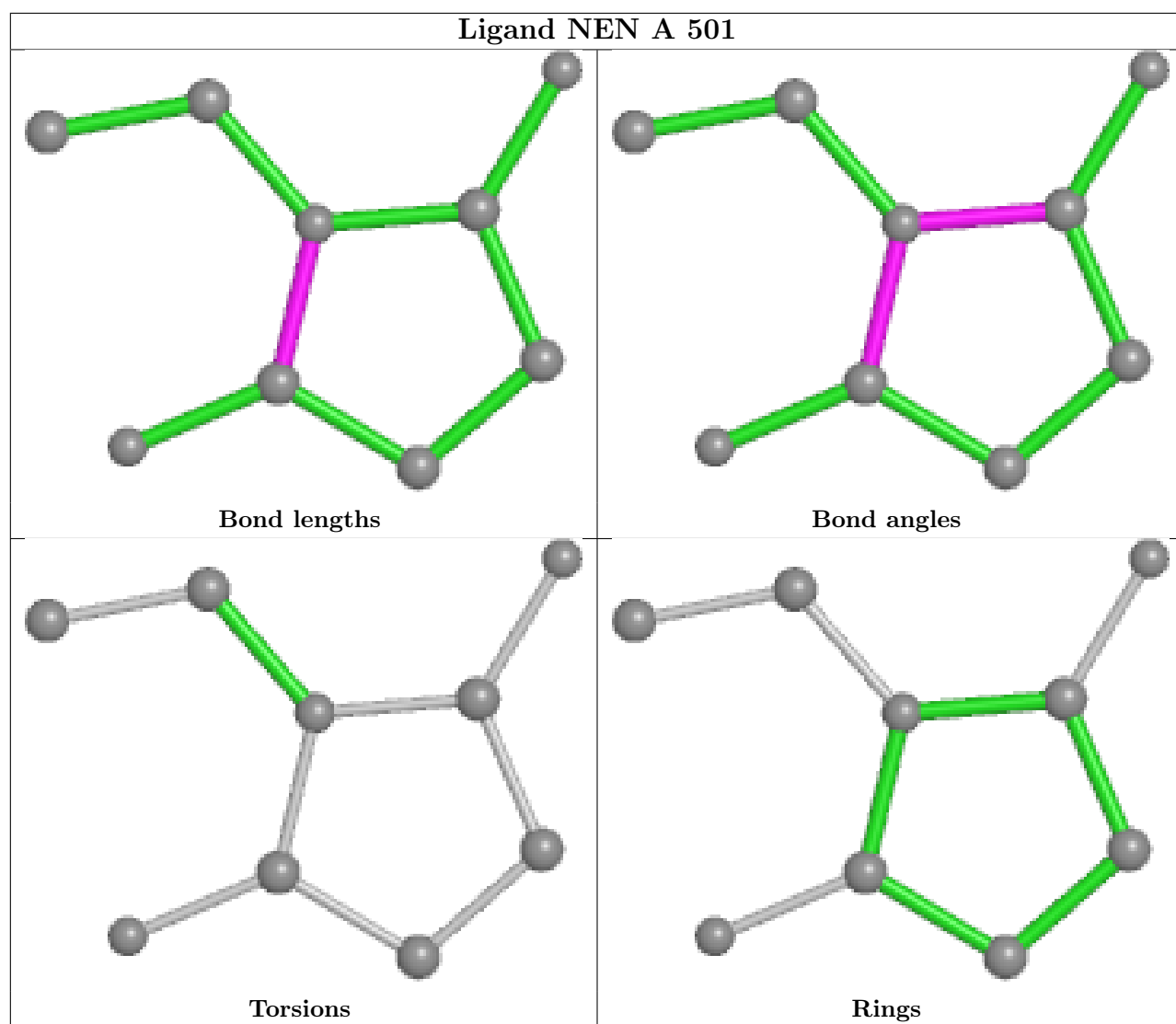
There are no chirality outliers.

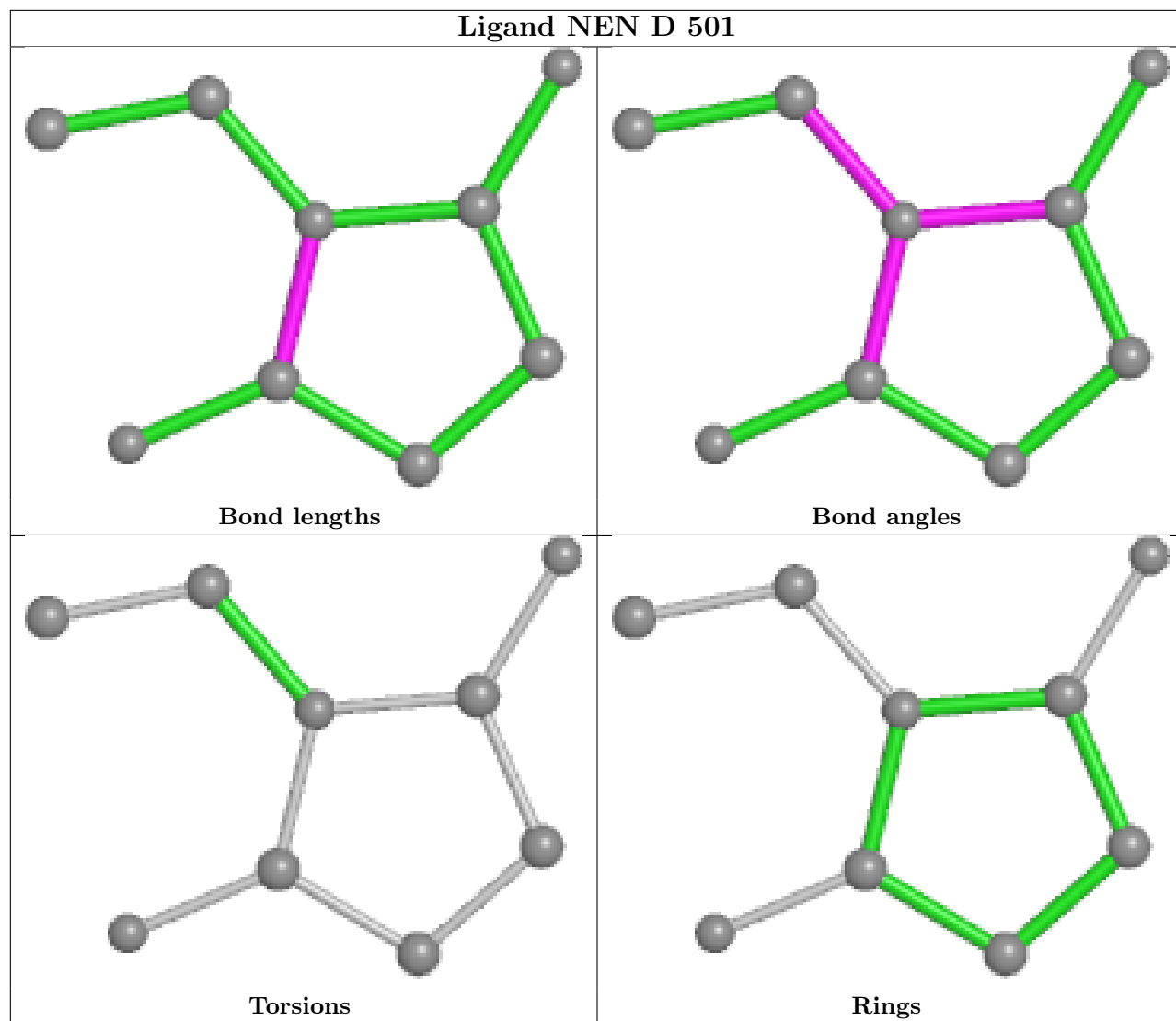
There are no torsion outliers.

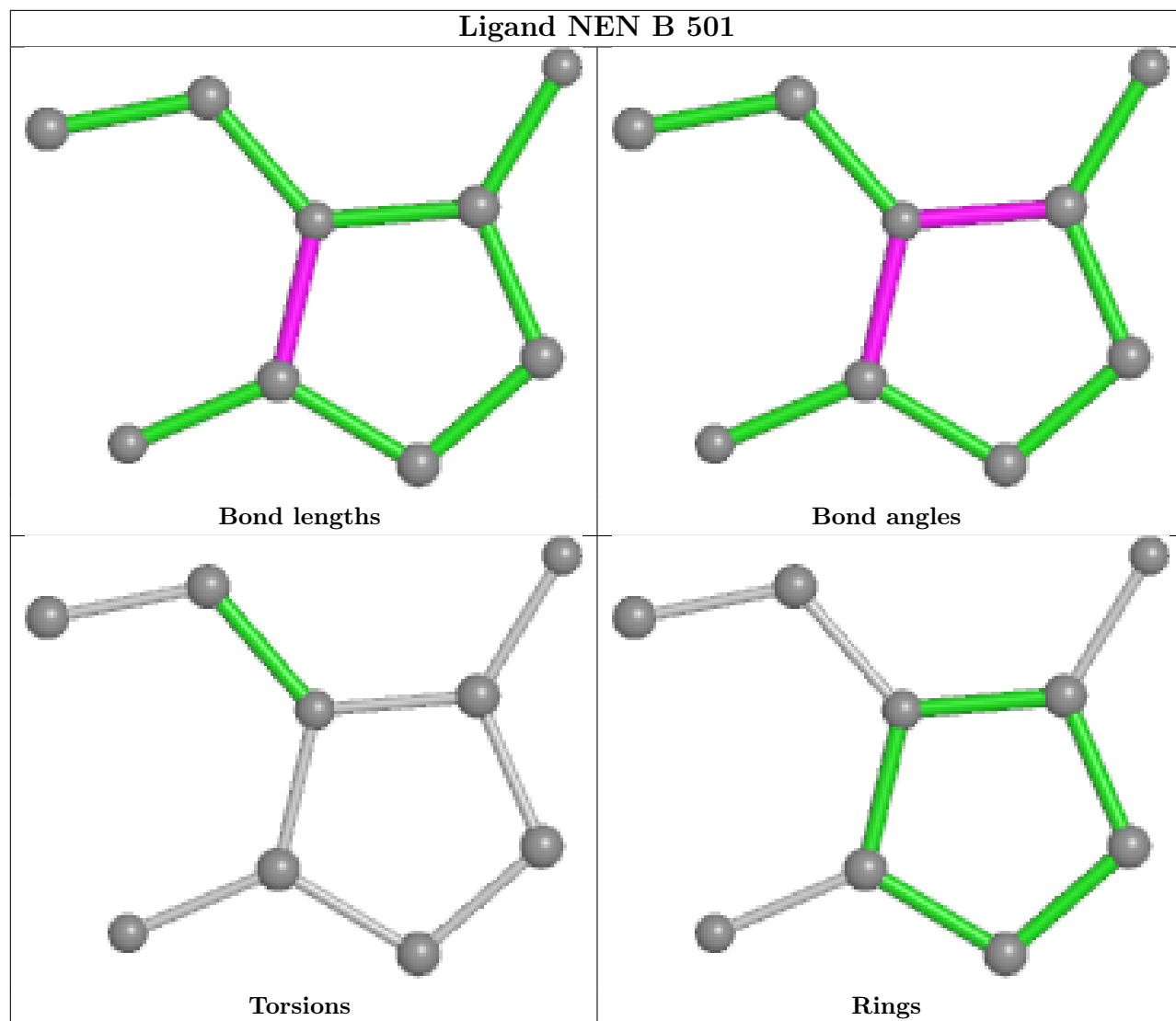
There are no ring outliers.

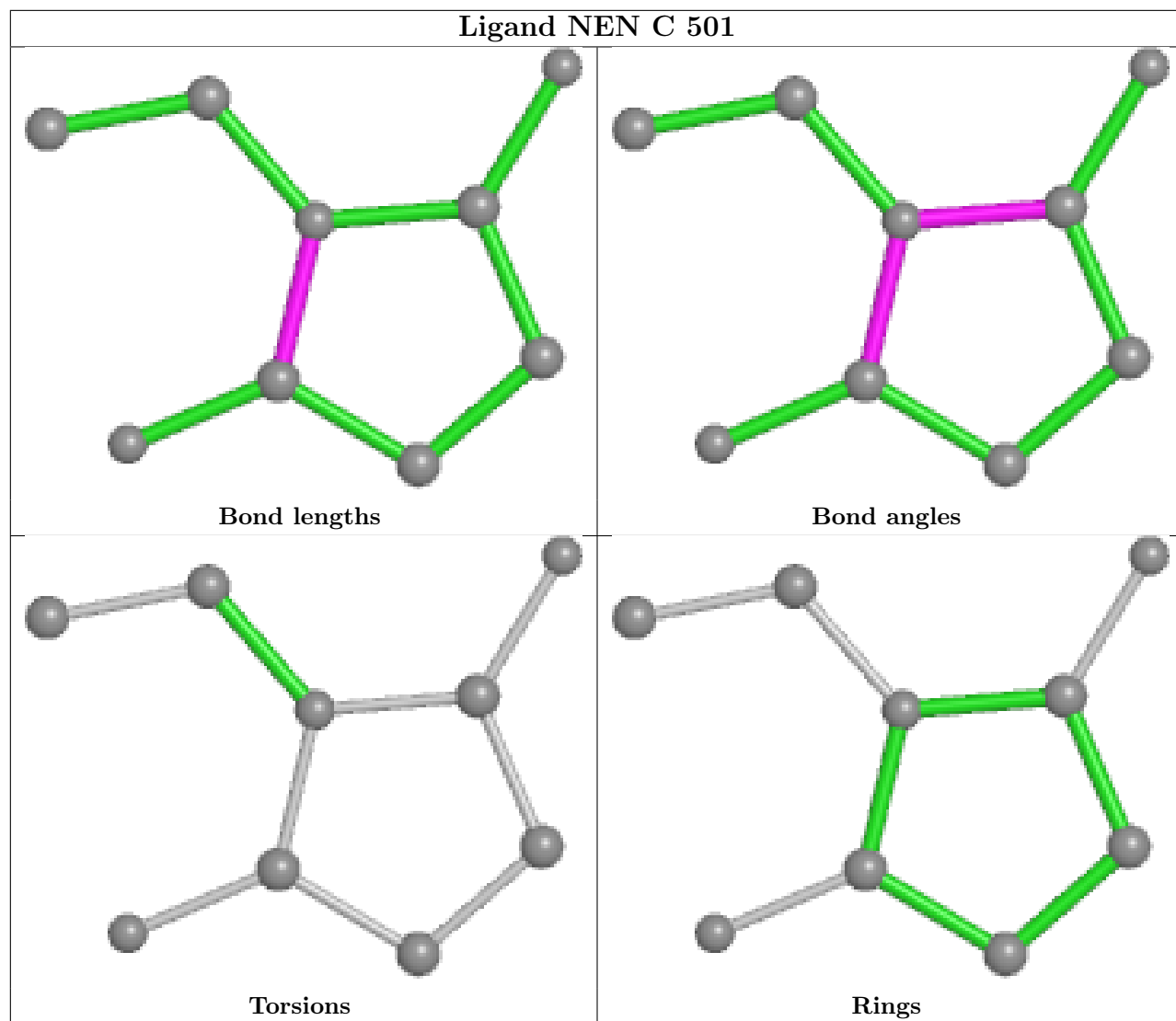
No monomer is involved in short contacts.

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	404/434 (93%)	0.72	43 (10%) 6 4	44, 74, 132, 182	0
1	B	406/434 (93%)	0.60	27 (6%) 17 14	48, 70, 121, 186	0
1	C	404/434 (93%)	0.90	56 (13%) 2 1	44, 80, 138, 204	0
1	D	402/434 (92%)	1.05	70 (17%) 1 1	43, 91, 158, 222	0
All	All	1616/1736 (93%)	0.82	196 (12%) 4 2	43, 78, 141, 222	0

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	127	LEU	9.5
1	C	96	PRO	9.0
1	B	123	LEU	8.5
1	D	126	ILE	7.4
1	D	282	ALA	7.3
1	D	125	GLU	6.6
1	D	276	ASP	6.6
1	C	108	PHE	6.4
1	C	128	LYS	6.4
1	A	128	LYS	6.4
1	C	124	ASP	6.2
1	B	311	TYR	6.0
1	D	311	TYR	5.9
1	D	272	VAL	5.8
1	B	125	GLU	5.7
1	A	123	LEU	5.5
1	D	108	PHE	5.4
1	A	126	ILE	5.2
1	C	106	TYR	5.1
1	B	127	LEU	5.1
1	C	143	ARG	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	311	TYR	4.8
1	D	320	LEU	4.7
1	C	140	VAL	4.7
1	D	343	PRO	4.6
1	D	283	GLU	4.6
1	D	325	ALA	4.5
1	C	125	GLU	4.5
1	D	314	GLN	4.4
1	D	342	CYS	4.4
1	A	142	HIS	4.3
1	C	340	GLU	4.3
1	A	95	PRO	4.2
1	D	273	ARG	4.2
1	D	315	ASN	4.2
1	D	133	LEU	4.2
1	D	286	LYS	4.2
1	D	294	ARG	4.1
1	C	435	LEU	4.0
1	C	94	ARG	4.0
1	C	312	TRP	4.0
1	C	134	ILE	4.0
1	D	278	VAL	4.0
1	A	124	ASP	3.9
1	B	133	LEU	3.7
1	A	388	ASP	3.7
1	D	106	TYR	3.6
1	D	365	PHE	3.6
1	D	319	LEU	3.6
1	A	26	LEU	3.6
1	A	134	ILE	3.6
1	D	317	PRO	3.6
1	C	145	VAL	3.6
1	B	126	ILE	3.5
1	D	295	PHE	3.5
1	D	415	PHE	3.5
1	D	274	LYS	3.5
1	A	427	ILE	3.5
1	D	128	LYS	3.5
1	A	98	GLU	3.5
1	D	329	LEU	3.5
1	C	129	GLN	3.5
1	A	314	GLN	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	124	ASP	3.4
1	C	440	PHE	3.4
1	D	312	TRP	3.4
1	D	313	GLU	3.4
1	C	25	VAL	3.4
1	C	147	VAL	3.3
1	D	131	ILE	3.3
1	A	384	HIS	3.3
1	D	292	ILE	3.3
1	D	281	PRO	3.2
1	D	364	GLU	3.2
1	A	368	GLU	3.2
1	C	131	ILE	3.2
1	C	130	GLU	3.2
1	D	318	ARG	3.2
1	A	132	ARG	3.1
1	B	128	LYS	3.1
1	D	322	ARG	3.1
1	A	99	LYS	3.1
1	C	429	SER	3.1
1	C	368	GLU	3.1
1	A	96	PRO	3.1
1	A	131	ILE	3.1
1	D	363	ILE	3.1
1	C	443	VAL	3.0
1	D	390	VAL	3.0
1	D	361	GLY	3.0
1	C	450	THR	3.0
1	D	427	ILE	2.9
1	C	384	HIS	2.9
1	D	109	PHE	2.9
1	A	144	GLY	2.9
1	C	127	LEU	2.9
1	B	341	GLY	2.9
1	D	285	ASP	2.9
1	C	133	LEU	2.9
1	C	415	PHE	2.9
1	A	94	ARG	2.9
1	A	432	THR	2.9
1	C	388	ASP	2.9
1	D	94	ARG	2.9
1	D	143	ARG	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	130	GLU	2.8
1	A	129	GLN	2.8
1	C	107	ALA	2.8
1	A	382	ASP	2.8
1	C	83	ILE	2.8
1	D	326	GLN	2.8
1	A	433	GLN	2.8
1	A	100	LEU	2.8
1	C	389	SER	2.7
1	B	285	ASP	2.7
1	C	423	VAL	2.7
1	D	401	ASP	2.7
1	B	108	PHE	2.7
1	C	126	ILE	2.7
1	A	436	GLU	2.6
1	D	290	ARG	2.6
1	D	431	ALA	2.6
1	A	108	PHE	2.6
1	D	150	PHE	2.6
1	C	422	TYR	2.6
1	A	439	ASN	2.6
1	D	447	ALA	2.6
1	C	314	GLN	2.6
1	B	106	TYR	2.6
1	B	414	CYS	2.5
1	C	432	THR	2.5
1	D	147	VAL	2.5
1	C	97	GLU	2.5
1	A	415	PHE	2.5
1	B	432	THR	2.5
1	D	449	ILE	2.5
1	A	286	LYS	2.5
1	A	367	THR	2.5
1	A	365	PHE	2.5
1	D	291	TYR	2.5
1	B	343	PRO	2.5
1	B	98	GLU	2.5
1	D	323	GLN	2.4
1	A	447	ALA	2.4
1	D	437	SER	2.4
1	C	385	ILE	2.4
1	D	277	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	367	THR	2.4
1	C	86	ALA	2.3
1	D	275	THR	2.3
1	B	342	CYS	2.3
1	D	344	ALA	2.3
1	A	435	LEU	2.3
1	A	97	GLU	2.3
1	B	440	PHE	2.3
1	B	130	GLU	2.3
1	D	271	LEU	2.3
1	C	99	LYS	2.3
1	B	131	ILE	2.3
1	A	109	PHE	2.3
1	C	88	LEU	2.3
1	C	434	PRO	2.2
1	D	197	ALA	2.2
1	C	444	VAL	2.2
1	B	129	GLN	2.2
1	D	130	GLU	2.2
1	B	449	ILE	2.2
1	C	98	GLU	2.2
1	B	329	LEU	2.2
1	D	423	VAL	2.2
1	A	194	ALA	2.2
1	C	365	PHE	2.2
1	A	449	ILE	2.1
1	C	341	GLY	2.1
1	D	284	TYR	2.1
1	C	438	GLN	2.1
1	D	422	TYR	2.1
1	A	385	ILE	2.1
1	D	395	ILE	2.1
1	D	287	HIS	2.1
1	A	25	VAL	2.1
1	C	437	SER	2.1
1	C	402	ASN	2.1
1	C	250	GLU	2.1
1	B	384	HIS	2.1
1	B	381	ALA	2.1
1	D	105	THR	2.1
1	B	78	ILE	2.0
1	C	148	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	190	ASN	2.0
1	C	100	LEU	2.0
1	C	189	ARG	2.0
1	D	349	LEU	2.0
1	C	436	GLU	2.0
1	D	279	TYR	2.0
1	D	340	GLU	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 [i](#)

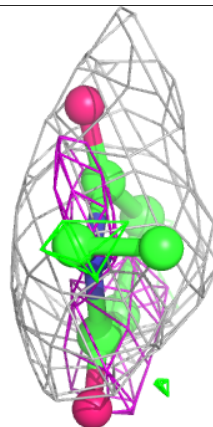
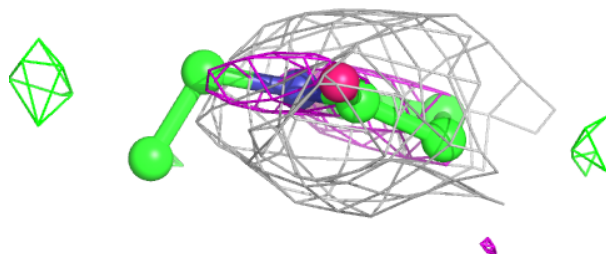
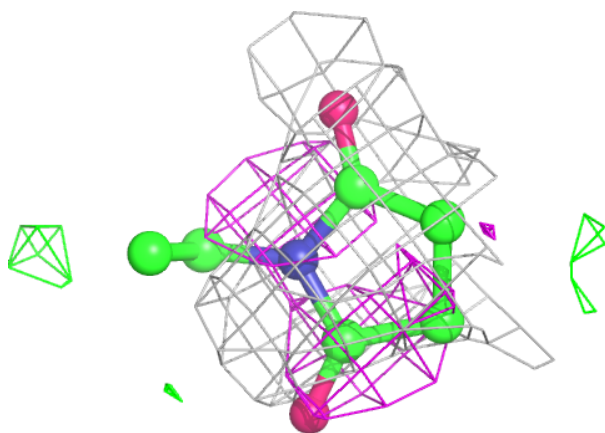
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NEN	C	501	9/9	0.76	0.34	70,76,79,79	0
2	NEN	D	501	9/9	0.77	0.37	71,76,77,77	0
2	NEN	A	501	9/9	0.80	0.33	65,71,72,73	0
2	NEN	B	501	9/9	0.83	0.28	62,67,70,70	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.

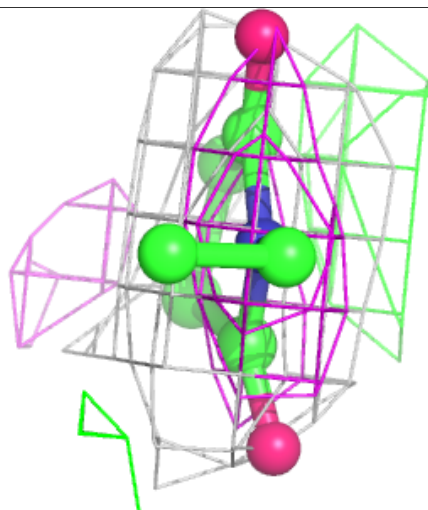
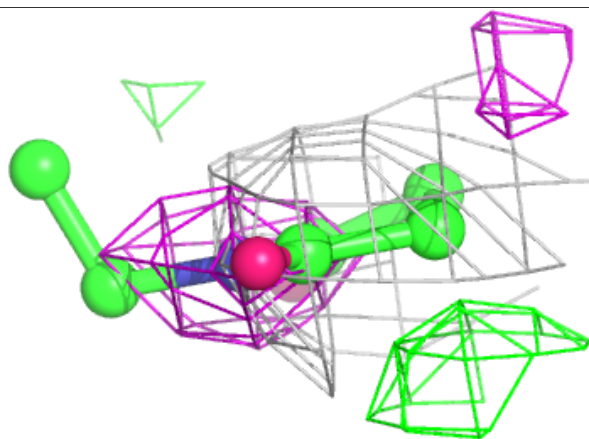
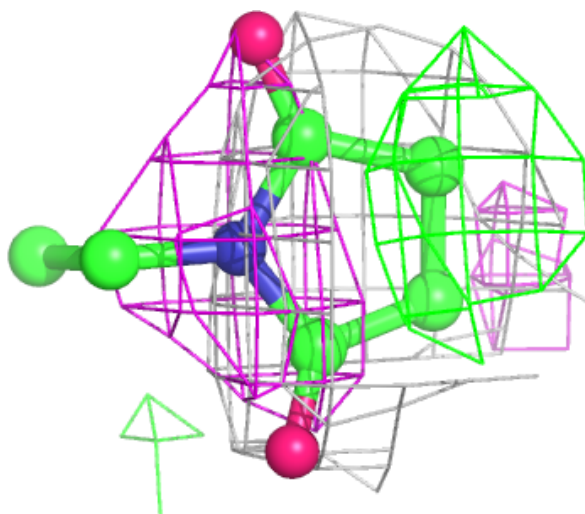
Electron density around NEN C 501:

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



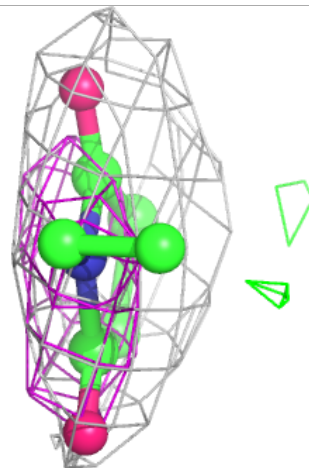
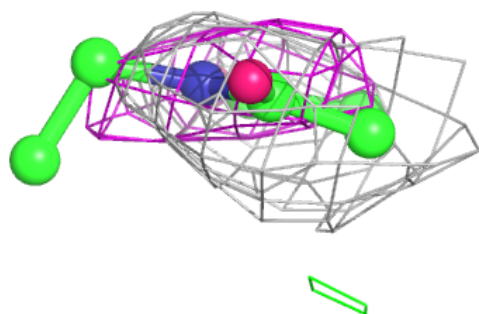
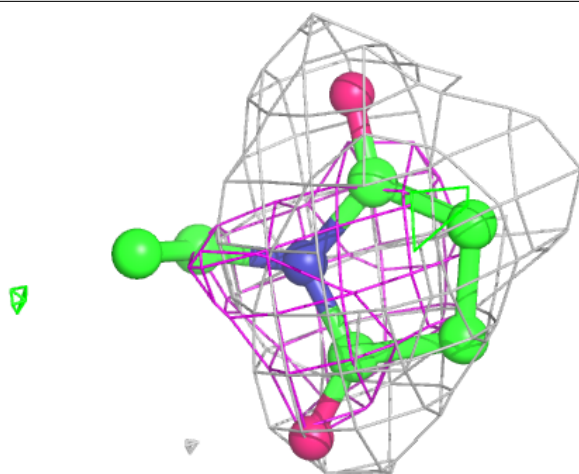
Electron density around NEN D 501:

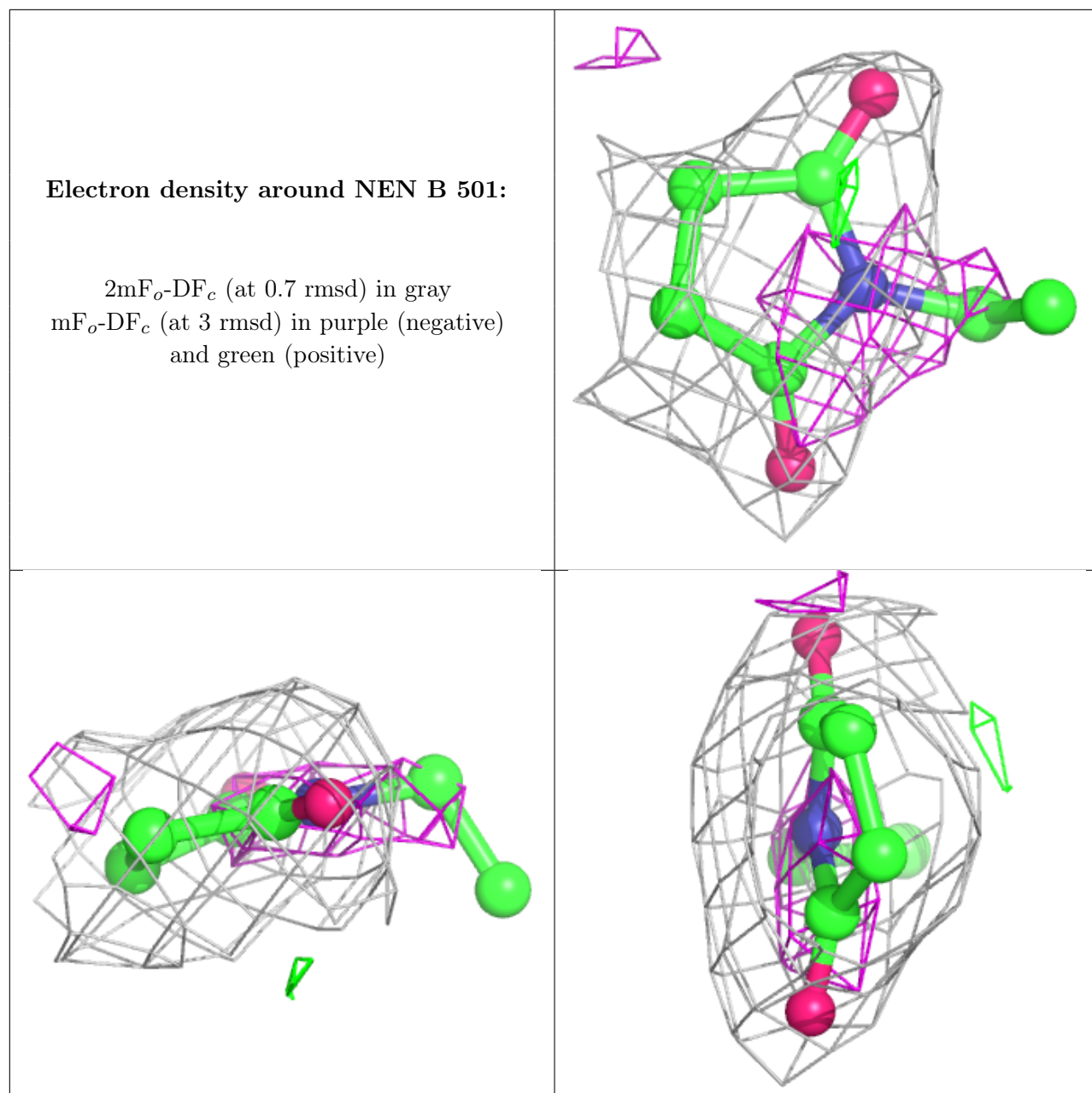
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NEN A 501:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.