



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:46 PM UTC

PDB ID : 7BMF / pdb_00007bmf
Title : Crystal structure of RecJCdc45 from Methanothermobacter thermoautotrophicus in complex with dCTP
Authors : De March, M.; Onesti, S.
Deposited on : 2021-01-20
Resolution : 2.20 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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)	:	2.49

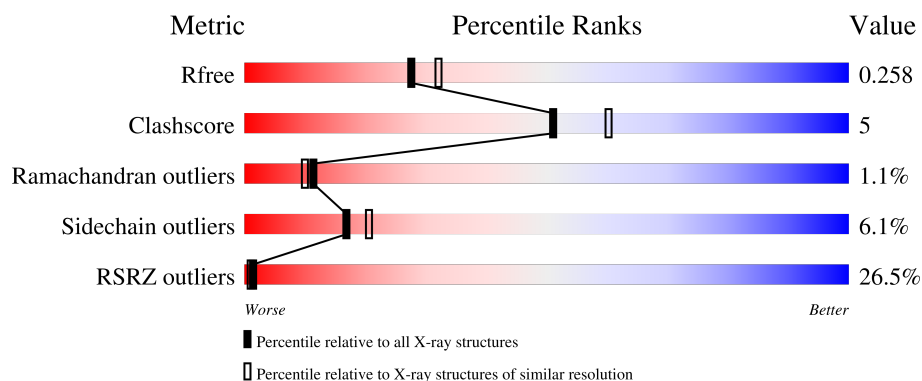
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	464	
1	B	464	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6799 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 Conserved protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3310	2083	570	644	13			
1	B	444	Total	C	N	O	S	0	0	0
			3181	2001	555	614	11			

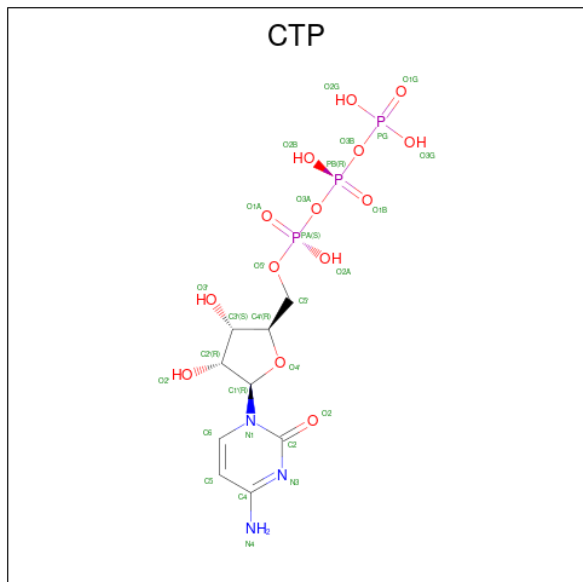
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	458	ALA	-	expression tag	UNP O27473
A	459	GLU	-	expression tag	UNP O27473
A	460	ASN	-	expression tag	UNP O27473
A	461	LEU	-	expression tag	UNP O27473
A	462	TYR	-	expression tag	UNP O27473
A	463	PHE	-	expression tag	UNP O27473
A	464	GLN	-	expression tag	UNP O27473
B	458	ALA	-	expression tag	UNP O27473
B	459	GLU	-	expression tag	UNP O27473
B	460	ASN	-	expression tag	UNP O27473
B	461	LEU	-	expression tag	UNP O27473
B	462	TYR	-	expression tag	UNP O27473
B	463	PHE	-	expression tag	UNP O27473
B	464	GLN	-	expression tag	UNP O27473

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

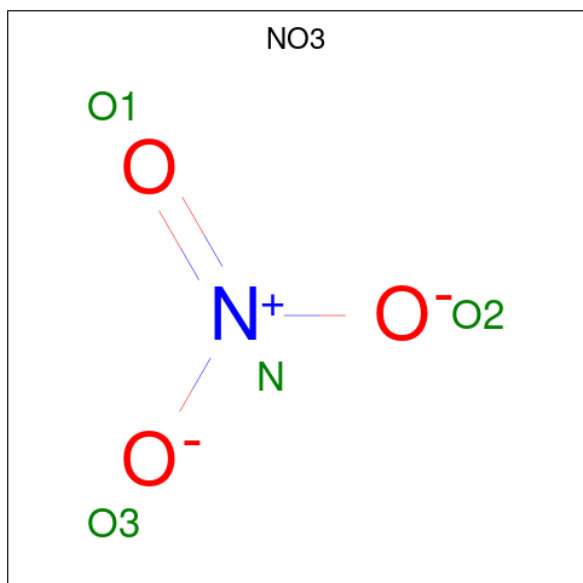
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		

- Molecule 3 is CYTIDINE-5'-TRIPHOSPHATE (CCD ID: CTP) (formula: $C_9H_{16}N_3O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



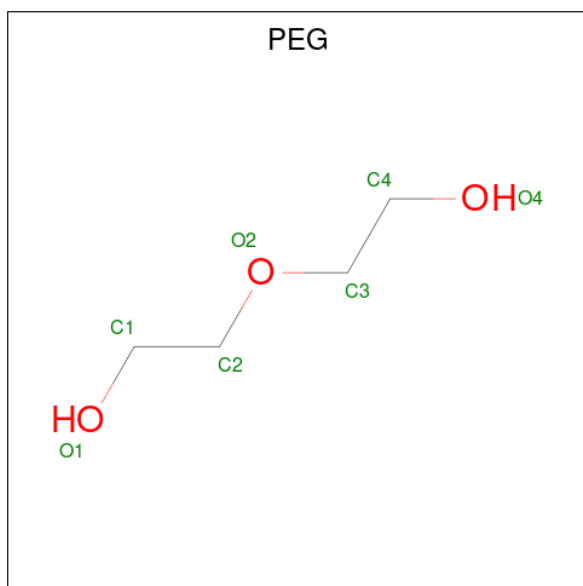
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			21	9	3	8	1		
3	B	1	Total	C	N	O	P	0	0
			21	9	3	8	1		

- Molecule 4 is NITRATE ION (CCD ID: NO3) (formula: NO_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total N O 4 1 3	0	0
4	A	1	Total N O 4 1 3	0	0
4	A	1	Total N O 4 1 3	0	0
4	A	1	Total N O 4 1 3	0	0
4	B	1	Total N O 4 1 3	0	0
4	B	1	Total N O 4 1 3	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0

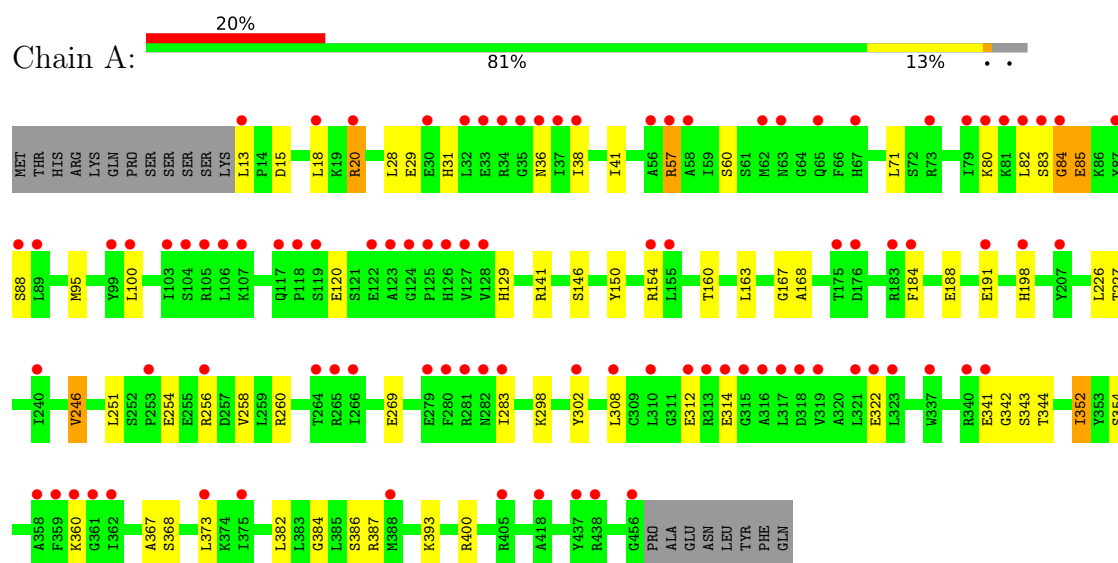
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	112	Total 112	O 112	0	0
6	B	94	Total 94	O 94	0	0

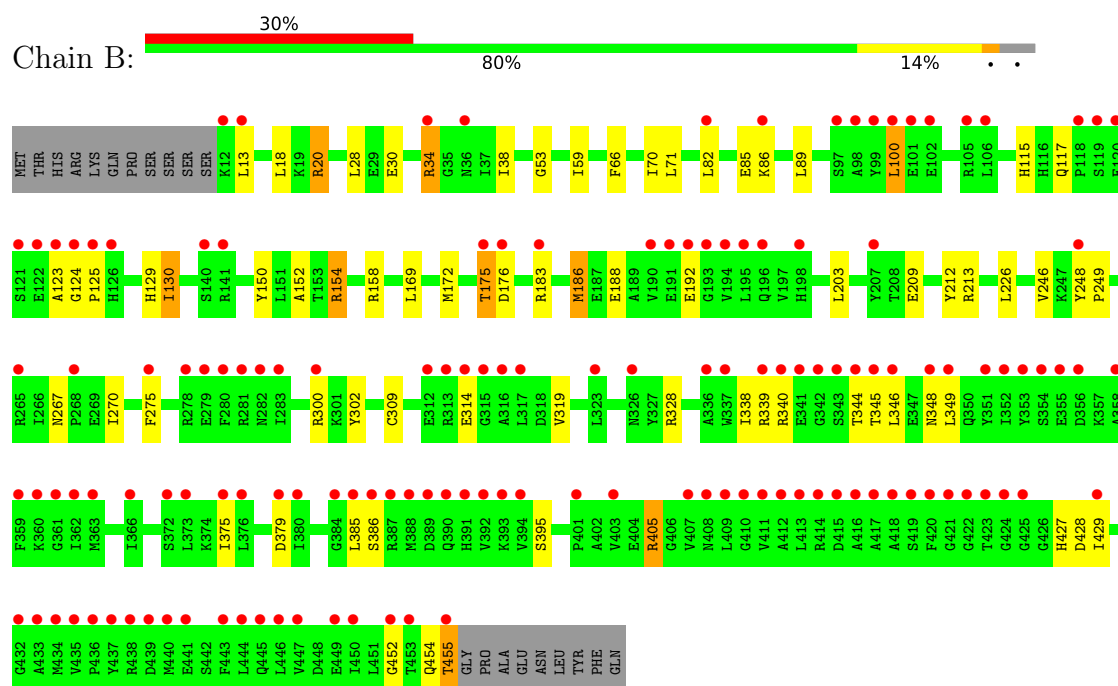
3 Residue-property plots

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: Conserved protein



• Molecule 1: Conserved protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.75Å 53.88Å 86.72Å 79.86° 82.77° 63.98°	Depositor
Resolution (Å)	42.21 – 2.20 42.21 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.7 (42.21-2.20) 96.8 (42.21-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.254 , 0.299 0.263 , 0.258	Depositor DCC
R_{free} test set	2145 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	5.8	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	6799	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% 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: CTP, PEG, MN, NO3

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	1.08	3/3367 (0.1%)	1.13	2/4564 (0.0%)
1	B	1.13	3/3231 (0.1%)	1.14	10/4392 (0.2%)
All	All	1.10	6/6598 (0.1%)	1.14	12/8956 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	395	SER	CA-C	-6.13	1.45	1.52
1	A	168	ALA	N-CA	5.77	1.53	1.46
1	A	393	LYS	C-O	-5.54	1.17	1.24
1	B	66	PHE	C-O	-5.37	1.17	1.23
1	B	203	LEU	C-O	-5.16	1.17	1.23
1	A	368	SER	C-O	-5.13	1.18	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	124	GLY	CA-C-N	10.52	132.99	119.84
1	B	124	GLY	C-N-CA	10.52	132.99	119.84
1	A	302	TYR	N-CA-C	-7.00	100.12	110.48
1	B	117	GLN	CA-C-N	6.65	128.16	119.84
1	B	117	GLN	C-N-CA	6.65	128.16	119.84
1	B	209	GLU	CA-C-N	-6.21	113.38	119.78
1	B	209	GLU	C-N-CA	-6.21	113.38	119.78
1	B	454	GLN	N-CA-C	5.54	119.30	112.54
1	A	354	SER	N-CA-C	5.33	117.36	108.99
1	B	192	GLU	N-CA-C	5.24	118.83	112.23
1	B	53	GLY	N-CA-C	5.11	118.82	112.64
1	B	309	CYS	N-CA-C	5.07	116.81	111.28

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	A	3310	0	3213	30	0
1	B	3181	0	2998	38	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	21	0	12	0	0
3	B	21	0	12	0	0
4	A	16	0	0	0	0
4	B	8	0	0	0	0
5	A	18	0	25	3	0
5	B	14	0	20	0	0
6	A	112	0	0	5	0
6	B	94	0	0	7	0
All	All	6799	0	6280	67	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 5.

All (67) 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:A:41:ILE:HG22	1:A:95:MET:CE	2.02	0.89
1:A:57:ARG:NH2	6:A:601:HOH:O	2.16	0.77
1:A:41:ILE:HG22	1:A:95:MET:HE2	1.73	0.70
1:B:30:GLU:OE1	6:B:601:HOH:O	2.14	0.65
1:B:130:ILE:HD12	1:B:152:ALA:HB2	1.81	0.62
5:A:509:PEG:H41	1:B:70:ILE:O	1.99	0.62
1:B:348:ASN:ND2	6:B:605:HOH:O	2.34	0.60
1:B:186:MET:HE1	6:B:657:HOH:O	2.01	0.60
1:B:20:ARG:HD3	1:B:129:HIS:O	2.01	0.59
1:B:130:ILE:CD1	1:B:152:ALA:HB2	2.33	0.58
1:A:84:GLY:O	1:A:85:GLU:O	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:MET:HE2	1:B:275:PHE:CE1	2.39	0.57
1:B:28:LEU:HD11	1:B:59:ILE:HD11	1.85	0.57
1:A:198:HIS:HD2	6:A:610:HOH:O	1.86	0.57
1:A:13:LEU:HD23	1:A:18:LEU:HD21	1.88	0.55
1:A:41:ILE:HG22	1:A:95:MET:HE1	1.87	0.55
1:B:455:THR:C	6:B:602:HOH:O	2.49	0.55
1:A:367:ALA:HB1	1:A:382:LEU:HD23	1.90	0.53
1:A:400:ARG:HD3	6:A:699:HOH:O	2.07	0.53
1:B:452:GLY:O	6:B:602:HOH:O	2.19	0.53
5:A:509:PEG:H41	1:B:71:LEU:HD23	1.91	0.53
1:B:248:TYR:HB3	1:B:249:PRO:HD3	1.91	0.53
1:A:154:ARG:HD2	1:A:188:GLU:OE1	2.09	0.52
1:B:158:ARG:HD2	6:B:662:HOH:O	2.09	0.52
1:B:428:ASP:OD1	1:B:429:ILE:N	2.43	0.51
1:B:328:ARG:NH2	6:B:608:HOH:O	2.43	0.51
1:A:71:LEU:HD12	1:A:95:MET:HE1	1.93	0.50
5:A:509:PEG:C4	1:B:70:ILE:O	2.59	0.50
1:B:28:LEU:HD11	1:B:59:ILE:CD1	2.39	0.50
1:A:20:ARG:HD3	1:A:129:HIS:O	2.12	0.49
1:B:175:THR:OG1	1:B:176:ASP:N	2.45	0.48
1:B:100:LEU:HG	1:B:123:ALA:HB2	1.96	0.48
1:B:30:GLU:OE2	1:B:34:ARG:NH2	2.47	0.47
1:B:405:ARG:O	1:B:455:THR:HG22	2.14	0.47
1:B:345:THR:HG22	1:B:346:LEU:O	2.14	0.47
1:A:246:VAL:CG2	1:A:251:LEU:HD23	2.45	0.46
1:B:212:TYR:CE1	1:B:213:ARG:HG2	2.50	0.46
1:B:13:LEU:HD23	1:B:18:LEU:HD21	1.96	0.46
1:A:28:LEU:CD1	1:A:38:ILE:HD13	2.45	0.46
1:A:83:SER:C	1:A:84:GLY:O	2.59	0.46
1:B:338:ILE:HG22	1:B:375:ILE:HG21	1.98	0.46
1:B:85:GLU:O	1:B:86:LYS:CB	2.60	0.45
1:A:146:SER:OG	1:A:167:GLY:HA3	2.17	0.45
1:B:154:ARG:HD2	1:B:188:GLU:OE1	2.18	0.44
1:A:260:ARG:NH2	6:A:608:HOH:O	2.51	0.43
1:B:300:ARG:HA	1:B:302:TYR:CE1	2.53	0.43
1:A:160:THR:O	1:A:163:LEU:HB2	2.19	0.43
1:A:341:GLU:HG2	1:B:319:VAL:HG21	2.00	0.43
1:A:36:ASN:ND2	1:A:88:SER:OG	2.52	0.43
1:B:169:LEU:O	1:B:172:MET:HE2	2.19	0.43
1:A:343:SER:HA	1:A:352:ILE:HD12	2.00	0.43
1:A:227:THR:HB	1:A:373:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ILE:HG22	1:A:384:GLY:HA2	2.01	0.42
1:B:38:ILE:HD12	1:B:89:LEU:HD23	2.02	0.42
1:B:186:MET:HE2	1:B:275:PHE:CZ	2.55	0.42
1:A:13:LEU:CD2	1:A:18:LEU:HD21	2.48	0.42
1:A:36:ASN:ND2	6:A:602:HOH:O	2.36	0.41
1:B:267:ASN:O	1:B:270:ILE:HG22	2.20	0.41
1:B:349:LEU:HD12	1:B:349:LEU:C	2.45	0.41
1:B:115:HIS:CE1	1:B:427:HIS:CE1	3.08	0.41
1:A:184:PHE:CD2	1:A:184:PHE:C	2.98	0.41
1:A:254:GLU:O	1:A:258:VAL:HG23	2.21	0.41
1:B:150:TYR:CZ	1:B:154:ARG:HG3	2.55	0.41
1:B:172:MET:HE2	1:B:172:MET:HA	2.02	0.40
1:A:150:TYR:O	1:A:154:ARG:N	2.54	0.40
1:A:342:GLY:O	1:A:352:ILE:HD11	2.22	0.40
1:A:31:HIS:O	1:A:36:ASN:OD1	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	442/464 (95%)	421 (95%)	16 (4%)	5 (1%)	11	10
1	B	442/464 (95%)	416 (94%)	21 (5%)	5 (1%)	11	10
All	All	884/928 (95%)	837 (95%)	37 (4%)	10 (1%)	11	10

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	GLU
1	A	360	LYS
1	B	314	GLU

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Mol	Chain	Res	Type
1	B	340	ARG
1	A	314	GLU
1	B	125	PRO
1	B	175	THR
1	A	84	GLY
1	A	312	GLU
1	B	154	ARG

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	339/379 (89%)	316 (93%)	23 (7%)	14	17
1	B	303/379 (80%)	287 (95%)	16 (5%)	20	26
All	All	642/758 (85%)	603 (94%)	39 (6%)	17	20

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	20	ARG
1	A	29	GLU
1	A	57	ARG
1	A	60	SER
1	A	80	LYS
1	A	82	LEU
1	A	100	LEU
1	A	120	GLU
1	A	141	ARG
1	A	191	GLU
1	A	226	LEU
1	A	246	VAL
1	A	256	ARG
1	A	269	GLU
1	A	283	ILE

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Mol	Chain	Res	Type
1	A	298	LYS
1	A	308	LEU
1	A	322	GLU
1	A	344	THR
1	A	352	ILE
1	A	386	SER
1	A	387	ARG
1	B	20	ARG
1	B	34	ARG
1	B	82	LEU
1	B	100	LEU
1	B	130	ILE
1	B	183	ARG
1	B	186	MET
1	B	226	LEU
1	B	246	VAL
1	B	339	ARG
1	B	344	THR
1	B	379	ASP
1	B	385	LEU
1	B	386	SER
1	B	405	ARG
1	B	455	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	198	HIS
1	A	239	ASN
1	A	348	ASN
1	B	31	HIS
1	B	239	ASN
1	B	348	ASN
1	B	350	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 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	$\# Z > 2$
4	NO3	A	507	-	1,3,3	0.25	0	0,3,3	-	-
3	CTP	B	503	2	22,22,30	1.25	1 (4%)	32,33,47	1.04	1 (3%)
4	NO3	A	504	-	1,3,3	0.01	0	0,3,3	-	-
5	PEG	B	506	-	6,6,6	0.60	0	5,5,5	0.50	0
4	NO3	A	505	-	1,3,3	0.25	0	0,3,3	-	-
4	NO3	B	505	-	1,3,3	0.23	0	0,3,3	-	-
5	PEG	A	509	-	6,6,6	0.90	0	5,5,5	2.01	2 (40%)
3	CTP	A	503	2	22,22,30	1.00	0	32,33,47	1.38	5 (15%)
5	PEG	A	510	-	6,6,6	0.52	0	5,5,5	0.75	0
4	NO3	B	504	-	1,3,3	0.40	0	0,3,3	-	-
5	PEG	B	507	-	6,6,6	0.81	0	5,5,5	1.12	0
4	NO3	A	506	-	1,3,3	0.49	0	0,3,3	-	-
5	PEG	A	508	-	3,3,6	0.33	0	2,2,5	0.36	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	CTP	B	503	2	-	0/10/26/38	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	B	506	-	-	2/4/4/4	-
5	PEG	A	509	-	-	2/4/4/4	-
3	CTP	A	503	2	-	0/10/26/38	0/2/2/2
5	PEG	A	510	-	-	1/4/4/4	-
5	PEG	B	507	-	-	2/4/4/4	-
5	PEG	A	508	-	-	1/1/1/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	CTP	PA-O3A	3.00	1.66	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	503	CTP	C3'-C2'-C1'	3.60	108.27	101.46
5	A	509	PEG	C3-O2-C2	3.24	127.43	113.26
3	A	503	CTP	C1'-N1-C2	2.68	124.35	118.44
3	A	503	CTP	O2-C2-N3	-2.62	118.19	122.33
3	A	503	CTP	C5'-C4'-C3'	-2.24	107.16	115.21
3	B	503	CTP	O2A-PA-O1A	2.22	119.48	110.83
3	A	503	CTP	C5-C4-N4	-2.11	116.94	120.63
5	A	509	PEG	O4-C4-C3	2.07	124.02	111.82

There are no chirality outliers.

All (8) torsion outliers are listed below:

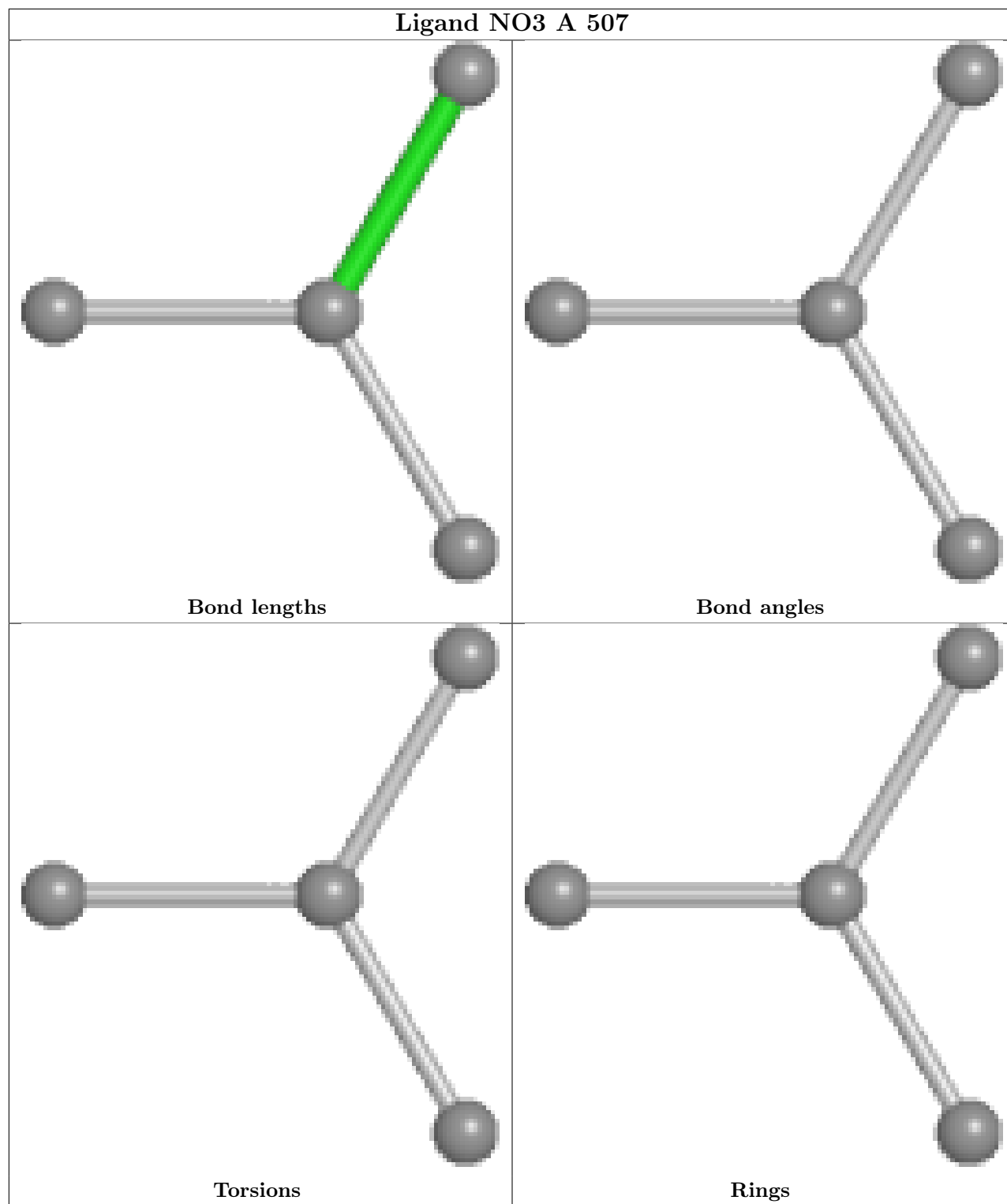
Mol	Chain	Res	Type	Atoms
5	B	507	PEG	O1-C1-C2-O2
5	A	510	PEG	O1-C1-C2-O2
5	A	508	PEG	O2-C3-C4-O4
5	B	506	PEG	O1-C1-C2-O2
5	A	509	PEG	O1-C1-C2-O2
5	B	507	PEG	C4-C3-O2-C2
5	A	509	PEG	C1-C2-O2-C3
5	B	506	PEG	O2-C3-C4-O4

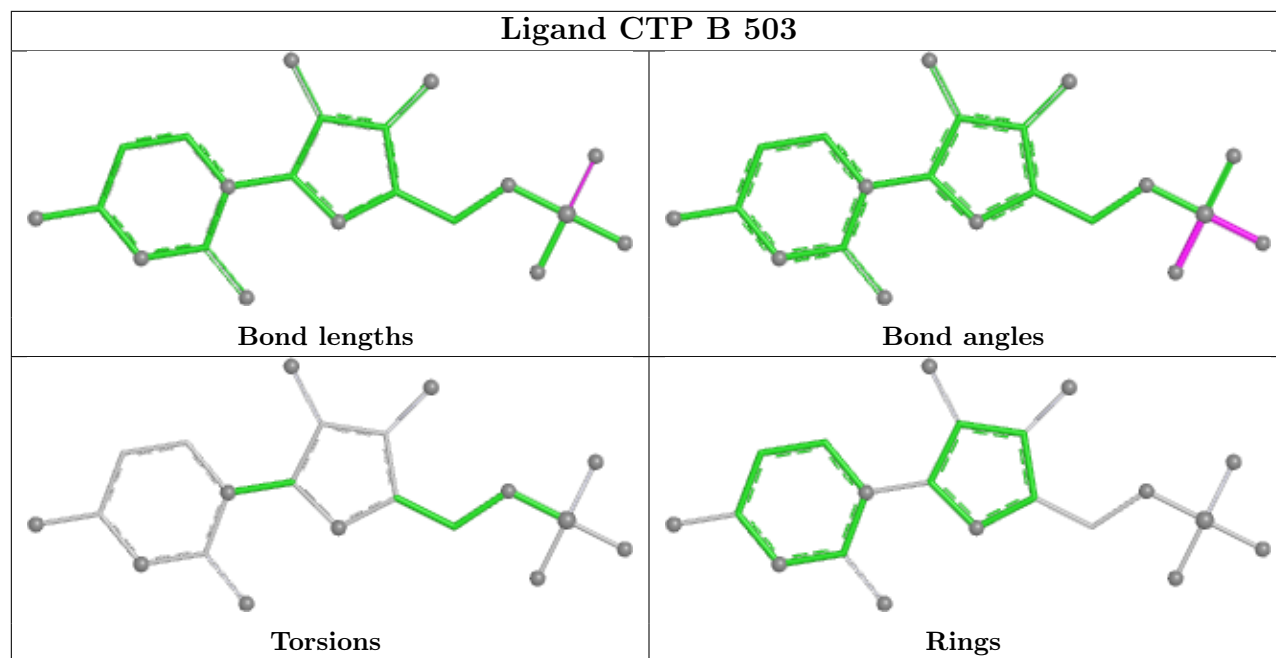
There are no ring outliers.

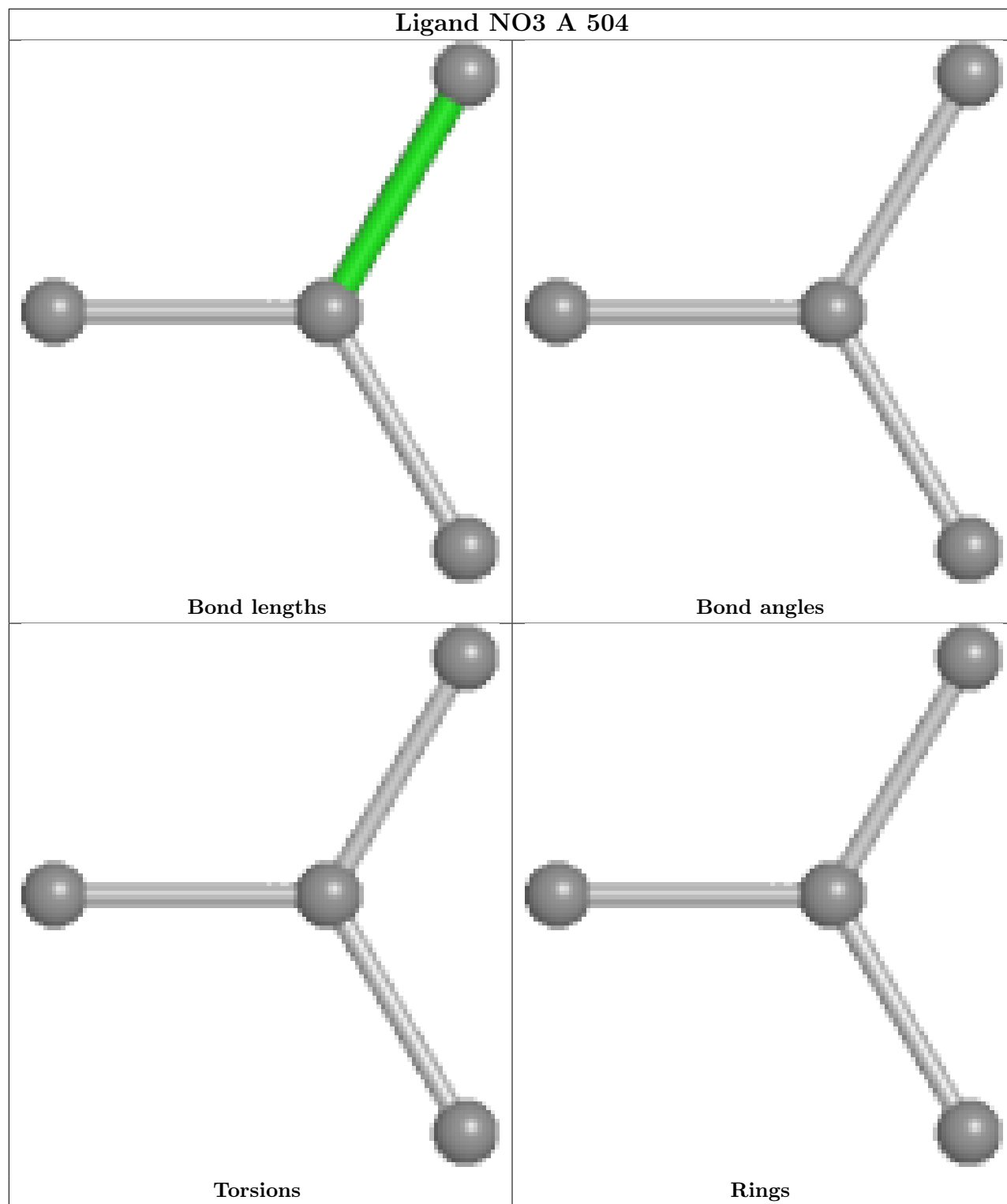
1 monomer is involved in 3 short contacts:

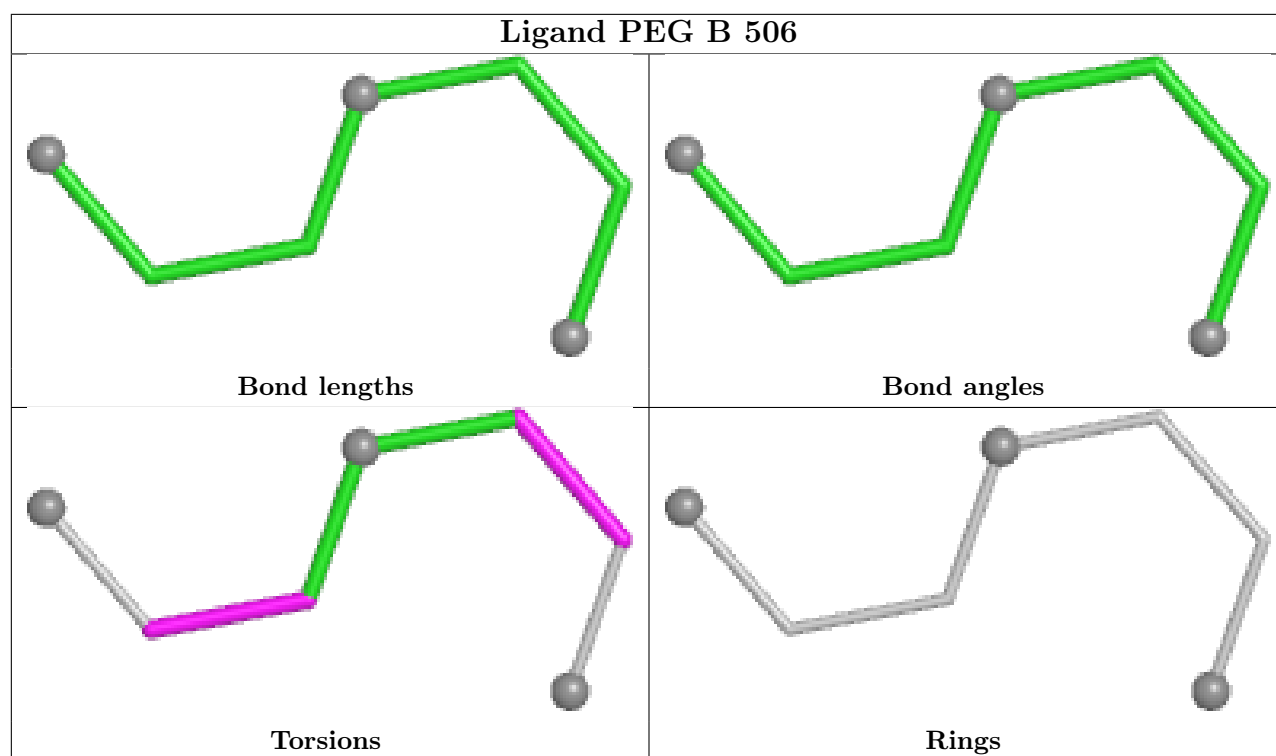
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	509	PEG	3	0

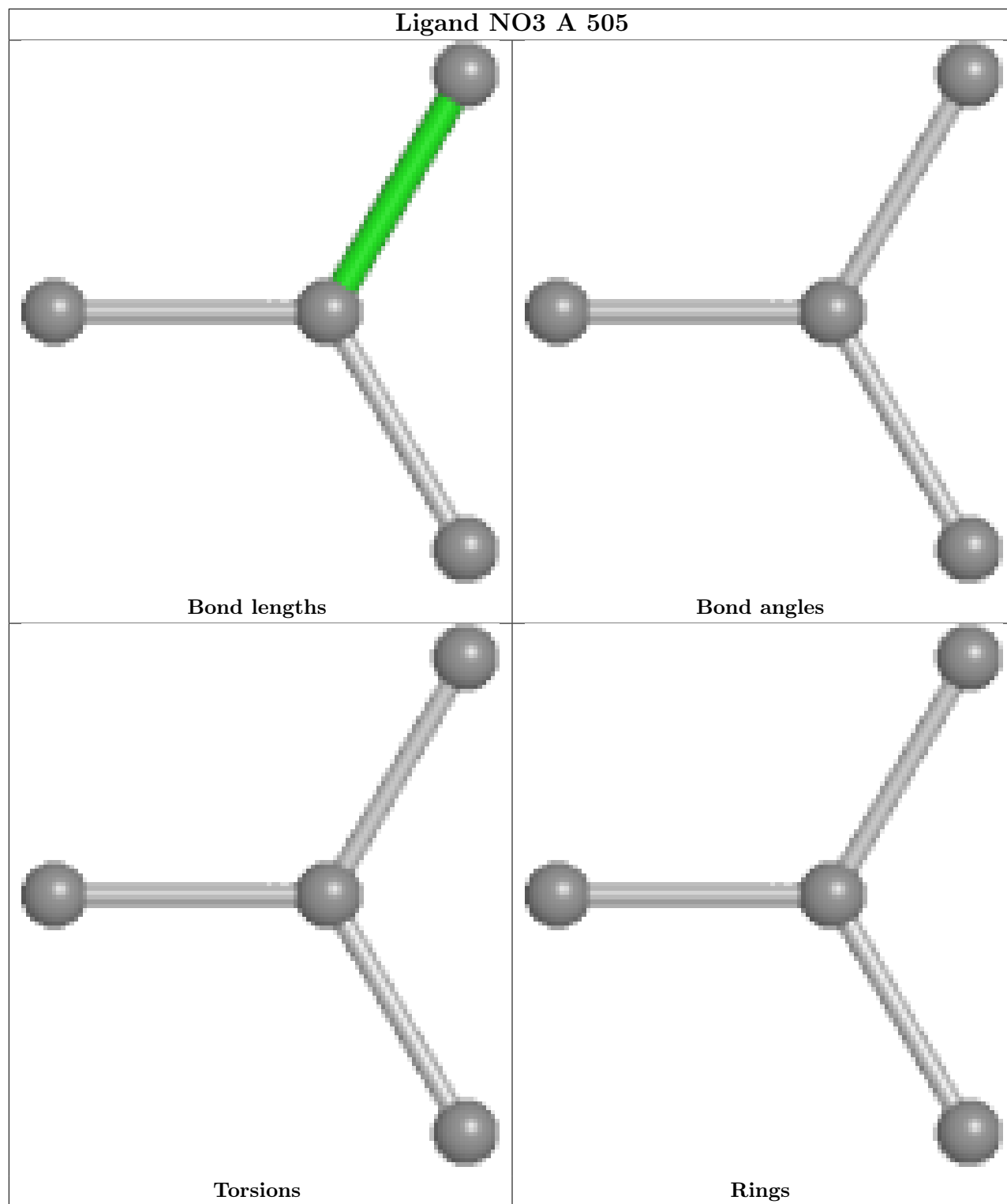
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

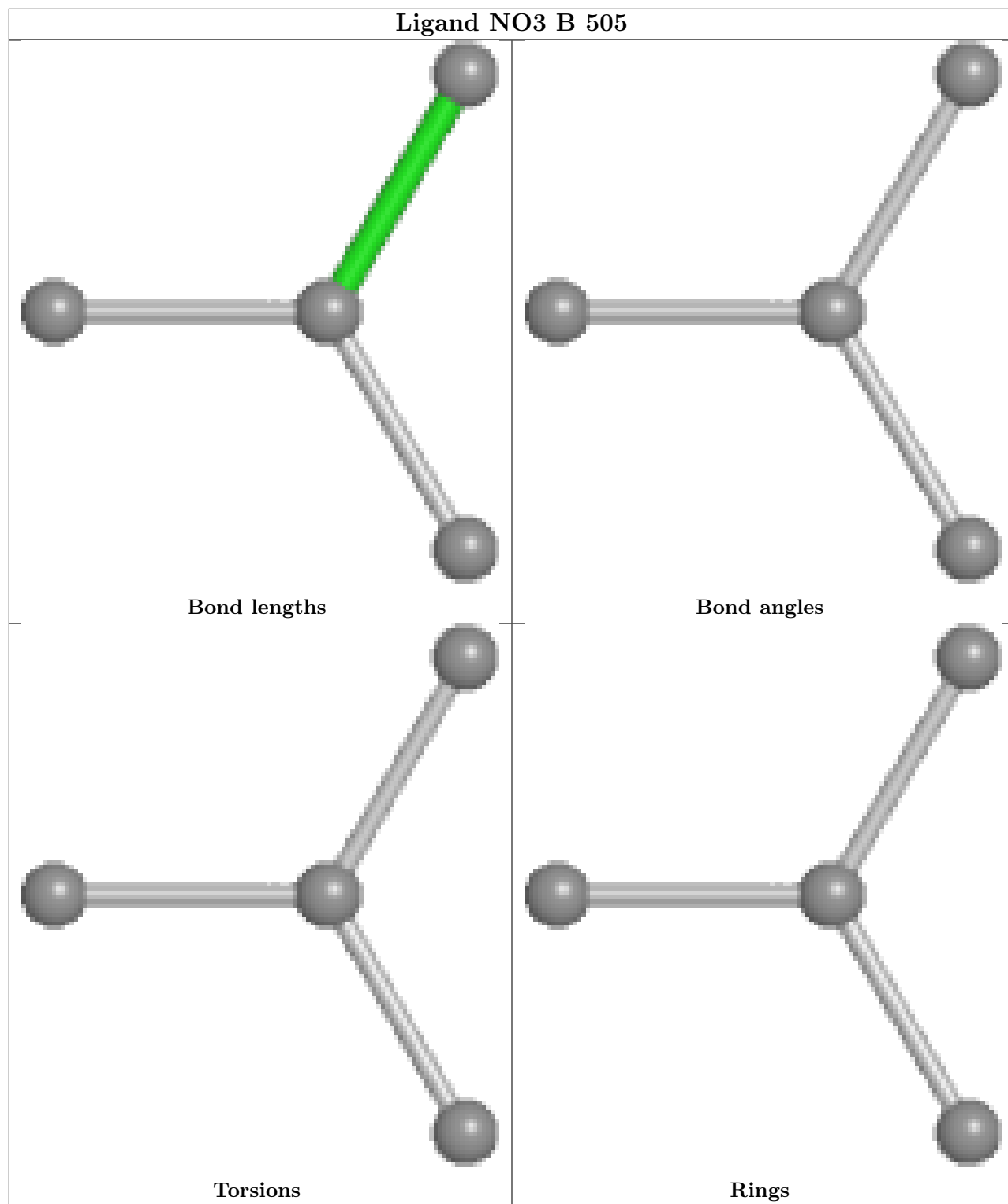


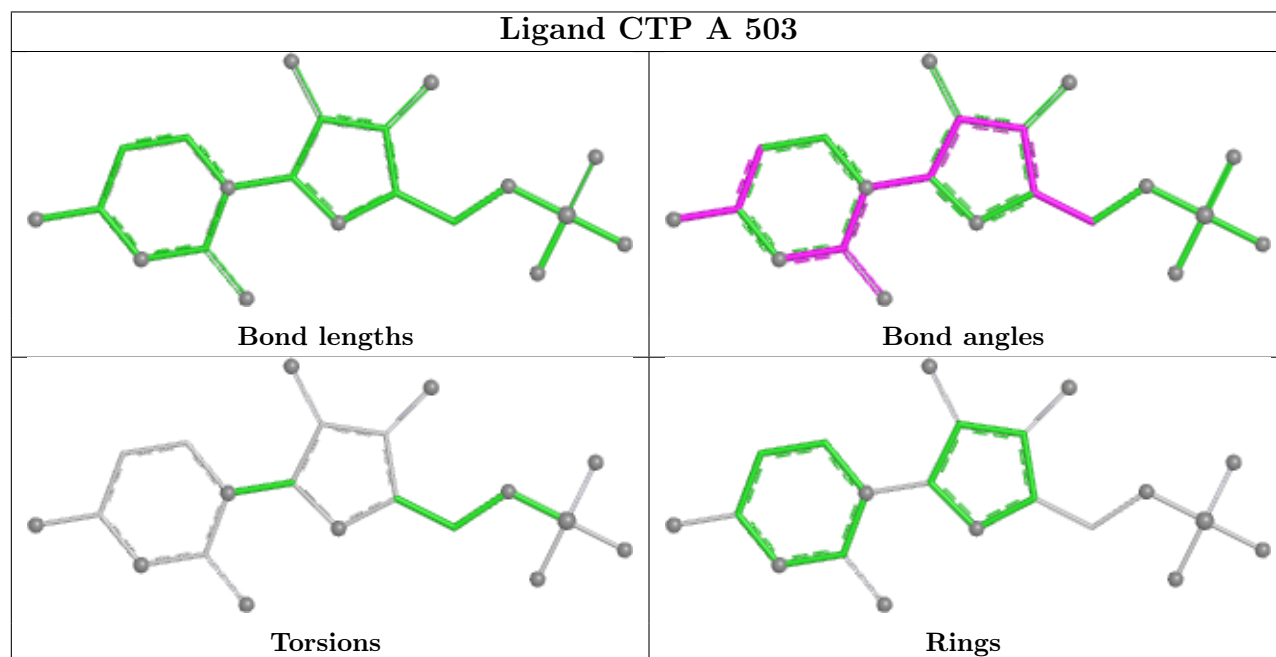
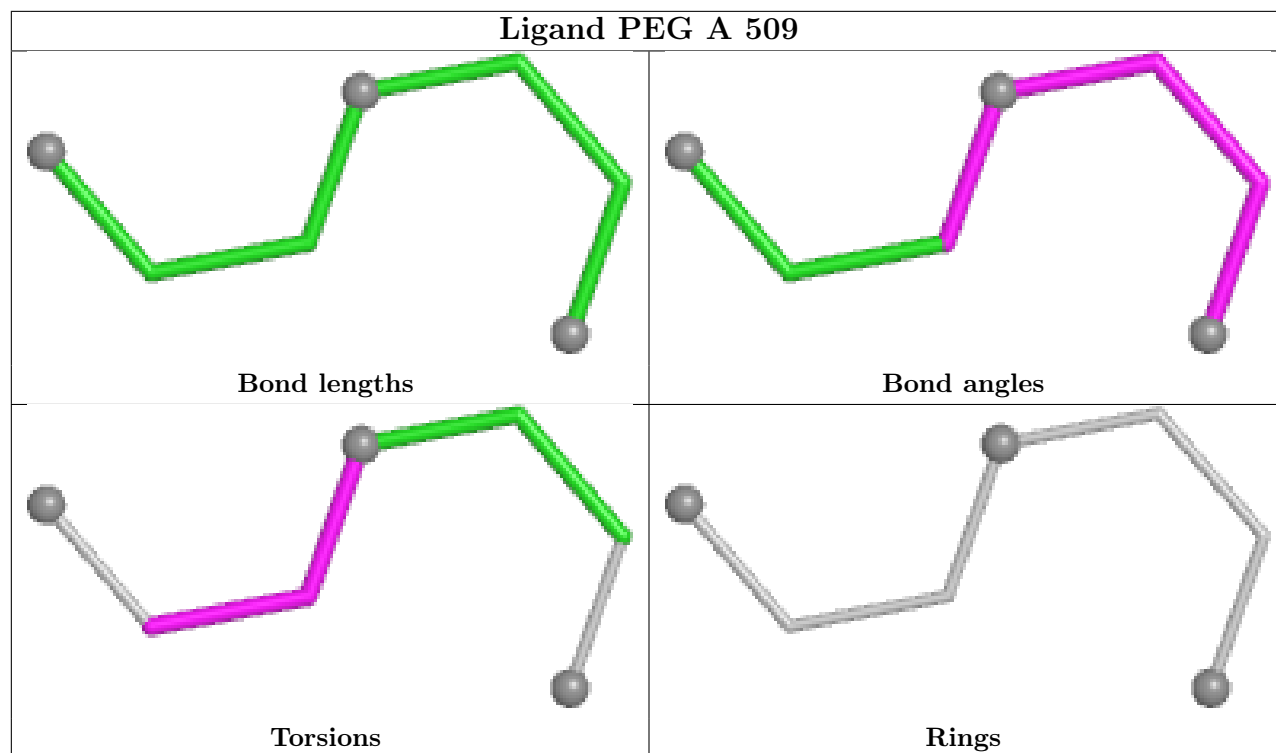


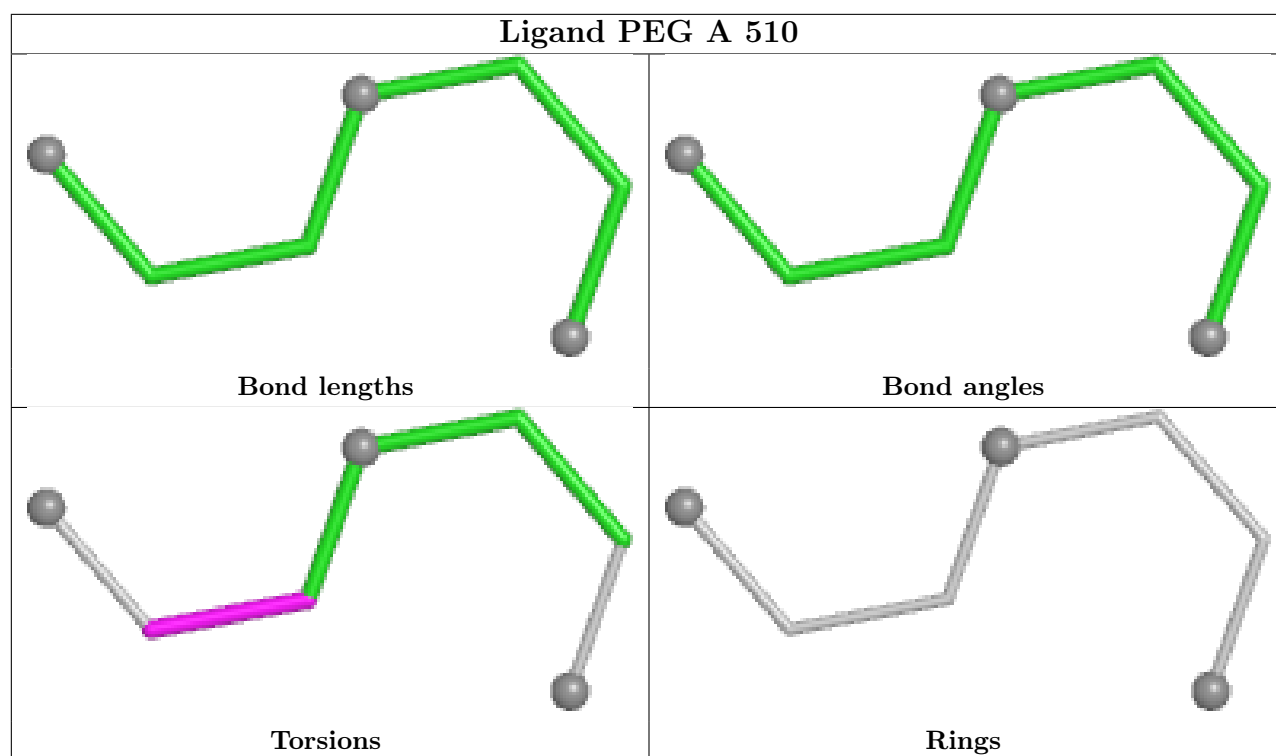


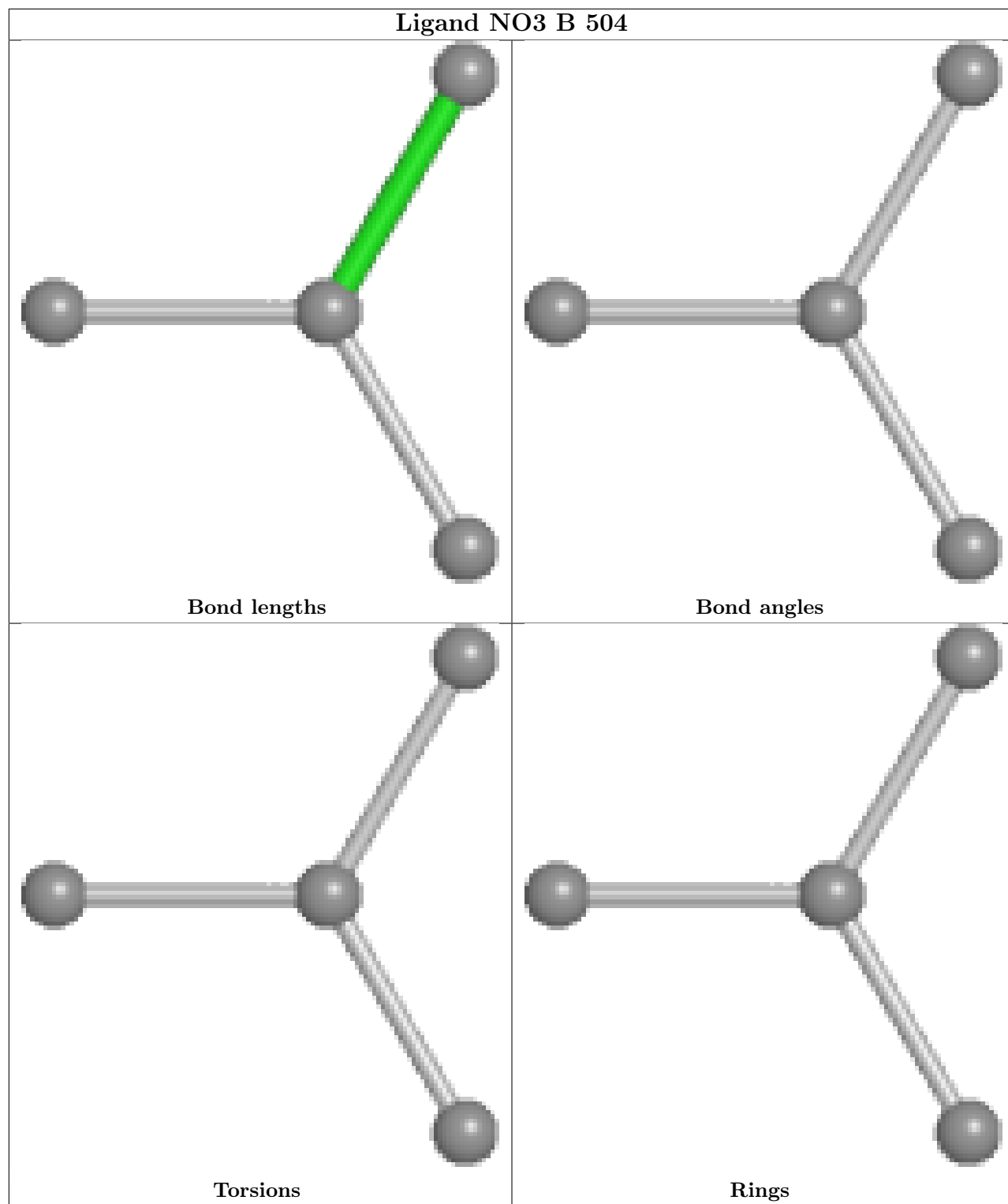


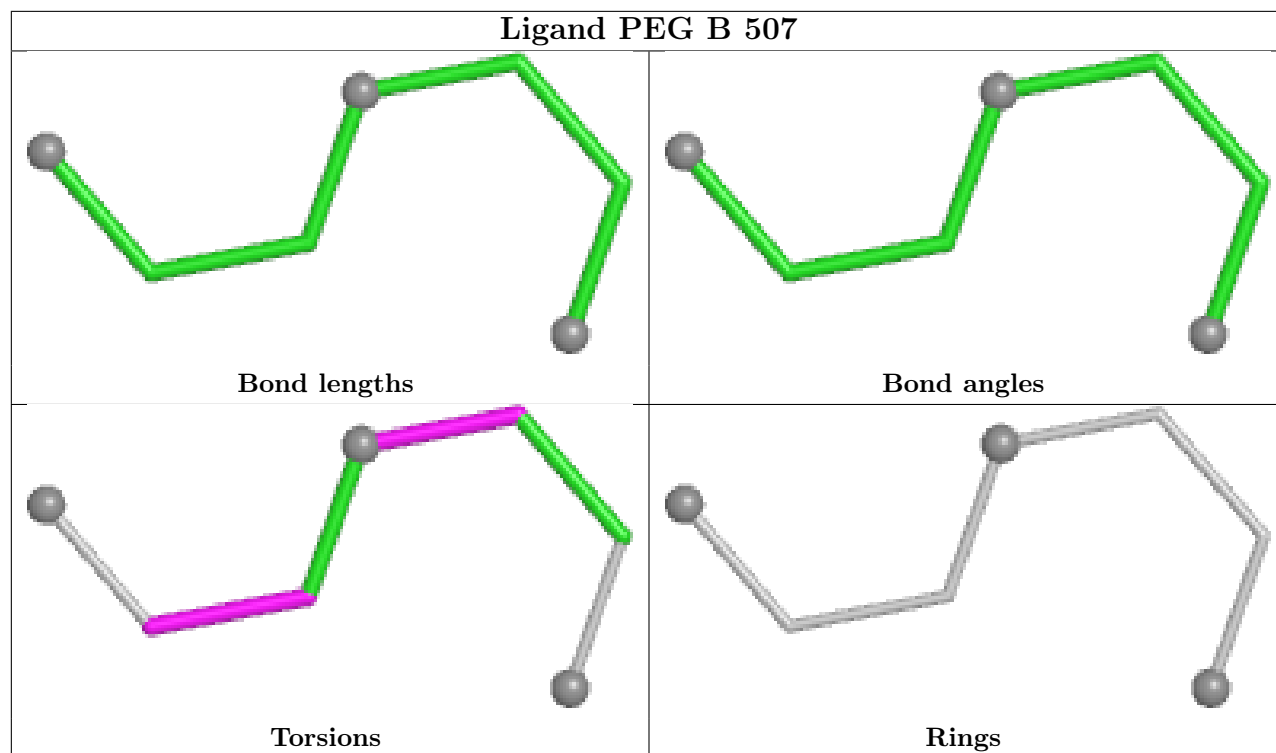


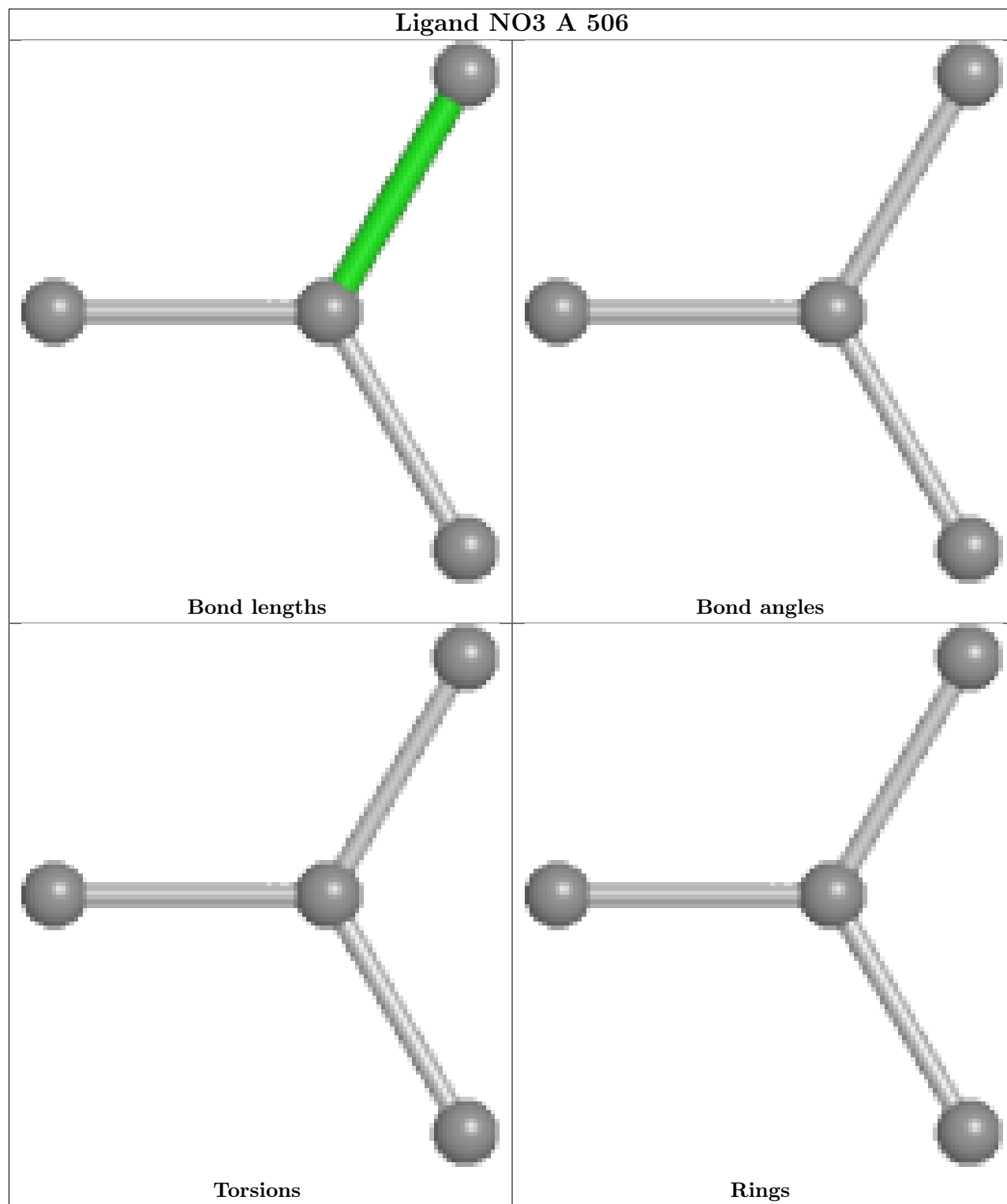


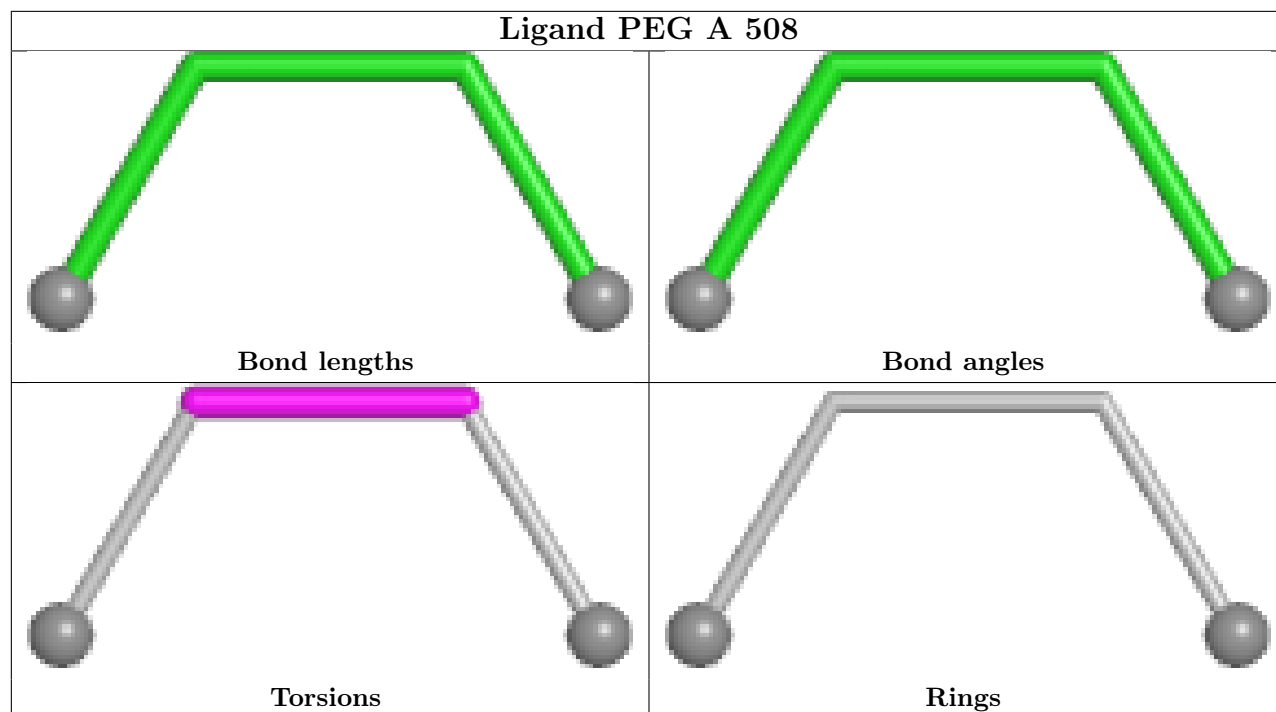












5.7 Other polymers [i](#)

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

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	444/464 (95%)	1.29	95 (21%) 2 2	15, 28, 51, 86	0
1	B	444/464 (95%)	1.64	140 (31%) 1 1	14, 30, 64, 82	0
All	All	888/928 (95%)	1.46	235 (26%) 1 1	14, 29, 57, 86	0

All (235) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	119	SER	7.8
1	B	358	ALA	7.7
1	B	439	ASP	6.9
1	B	359	PHE	6.5
1	B	423	THR	6.0
1	B	438	ARG	6.0
1	B	422	GLY	5.7
1	B	418	ALA	5.2
1	B	421	GLY	5.2
1	B	417	ALA	5.0
1	B	388	MET	4.9
1	B	435	VAL	4.9
1	B	341	GLU	4.9
1	B	314	GLU	4.8
1	B	118	PRO	4.8
1	B	440	MET	4.7
1	B	437	TYR	4.7
1	B	391	HIS	4.7
1	B	387	ARG	4.7
1	B	282	ASN	4.7
1	B	392	VAL	4.6
1	A	314	GLU	4.6
1	B	362	ILE	4.4
1	B	339	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	416	ALA	4.4
1	A	282	ASN	4.4
1	B	354	SER	4.3
1	B	175	THR	4.3
1	B	125	PRO	4.2
1	B	436	PRO	4.2
1	A	315	GLY	4.2
1	B	355	GLU	4.2
1	B	207	TYR	4.2
1	A	313	ARG	4.2
1	B	340	ARG	4.1
1	A	456	GLY	4.1
1	B	356	ASP	4.1
1	B	419	SER	4.1
1	A	123	ALA	4.0
1	B	390	GLN	4.0
1	B	360	LYS	4.0
1	B	446	LEU	4.0
1	A	107	LYS	4.0
1	B	126	HIS	3.9
1	B	123	ALA	3.9
1	B	315	GLY	3.9
1	B	415	ASP	3.9
1	B	313	ARG	3.9
1	B	312	GLU	3.8
1	B	434	MET	3.7
1	B	283	ILE	3.7
1	B	124	GLY	3.7
1	B	361	GLY	3.7
1	B	413	LEU	3.7
1	B	420	PHE	3.7
1	B	375	ILE	3.7
1	A	87	TYR	3.6
1	A	62	MET	3.6
1	B	389	ASP	3.6
1	B	407	VAL	3.6
1	A	312	GLU	3.5
1	B	386	SER	3.5
1	B	278	ARG	3.5
1	A	125	PRO	3.5
1	B	433	ALA	3.4
1	A	375	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	411	VAL	3.4
1	B	121	SER	3.4
1	A	317	LEU	3.4
1	B	353	TYR	3.4
1	A	316	ALA	3.4
1	B	449	GLU	3.4
1	A	106	LEU	3.3
1	B	352	ILE	3.3
1	B	281	ARG	3.3
1	B	337	TRP	3.3
1	B	97	SER	3.3
1	A	176	ASP	3.3
1	B	366	ILE	3.3
1	A	280	PHE	3.3
1	B	120	GLU	3.2
1	A	283	ILE	3.2
1	B	190	VAL	3.2
1	B	447	VAL	3.2
1	A	341	GLU	3.2
1	B	323	LEU	3.2
1	B	412	ALA	3.1
1	A	13	LEU	3.1
1	A	80	LYS	3.1
1	B	345	THR	3.1
1	A	126	HIS	3.1
1	A	265	ARG	3.1
1	B	342	GLY	3.0
1	A	266	ILE	3.0
1	A	318	ASP	3.0
1	B	445	GLN	3.0
1	B	316	ALA	2.9
1	B	12	LYS	2.9
1	B	380	ILE	2.9
1	B	349	LEU	2.9
1	B	444	LEU	2.9
1	A	362	ILE	2.9
1	B	122	GLU	2.9
1	A	358	ALA	2.9
1	A	84	GLY	2.9
1	A	88	SER	2.8
1	B	105	ARG	2.8
1	B	351	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	32	LEU	2.8
1	B	13	LEU	2.8
1	B	385	LEU	2.8
1	B	443	PHE	2.8
1	A	319	VAL	2.8
1	B	176	ASP	2.8
1	A	359	PHE	2.8
1	B	280	PHE	2.8
1	B	403	VAL	2.8
1	A	57	ARG	2.8
1	B	36	ASN	2.8
1	B	344	THR	2.7
1	B	141	ARG	2.7
1	B	191	GLU	2.7
1	A	122	GLU	2.7
1	A	322	GLU	2.7
1	B	414	ARG	2.7
1	A	63	ASN	2.6
1	A	83	SER	2.6
1	A	302	TYR	2.6
1	B	394	VAL	2.6
1	B	441	GLU	2.6
1	B	450	ILE	2.6
1	A	308	LEU	2.5
1	B	194	VAL	2.5
1	B	372	SER	2.5
1	A	154	ARG	2.5
1	B	300	ARG	2.5
1	B	376	LEU	2.5
1	B	425	GLY	2.5
1	A	38	ILE	2.5
1	A	191	GLU	2.5
1	A	82	LEU	2.5
1	B	379	ASP	2.5
1	A	33	GLU	2.4
1	A	119	SER	2.4
1	A	18	LEU	2.4
1	B	106	LEU	2.4
1	B	393	LYS	2.4
1	A	36	ASN	2.4
1	A	56	ALA	2.4
1	A	253	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	98	ALA	2.4
1	B	452	GLY	2.4
1	A	321	LEU	2.4
1	A	99	TYR	2.4
1	B	265	ARG	2.4
1	B	343	SER	2.4
1	B	34	ARG	2.4
1	A	30	GLU	2.4
1	B	102	GLU	2.4
1	A	118	PRO	2.4
1	B	410	GLY	2.4
1	B	453	THR	2.4
1	A	37	ILE	2.4
1	A	155	LEU	2.4
1	B	317	LEU	2.4
1	B	432	GLY	2.3
1	A	198	HIS	2.3
1	B	192	GLU	2.3
1	B	193	GLY	2.3
1	B	336	ALA	2.3
1	A	256	ARG	2.3
1	A	100	LEU	2.3
1	B	409	LEU	2.3
1	B	424	GLY	2.3
1	A	281	ARG	2.3
1	A	67	HIS	2.3
1	A	127	VAL	2.3
1	A	184	PHE	2.3
1	B	100	LEU	2.3
1	B	348	ASN	2.3
1	B	99	TYR	2.3
1	A	264	THR	2.3
1	A	103	ILE	2.3
1	B	346	LEU	2.2
1	A	20	ARG	2.2
1	A	124	GLY	2.2
1	A	388	MET	2.2
1	A	175	THR	2.2
1	A	207	TYR	2.2
1	A	279	GLU	2.2
1	B	279	GLU	2.2
1	B	455	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	140	SER	2.2
1	A	240	ILE	2.2
1	A	437	TYR	2.2
1	A	337	TRP	2.2
1	B	82	LEU	2.2
1	B	408	ASN	2.2
1	A	360	LYS	2.2
1	A	79	ILE	2.2
1	A	323	LEU	2.2
1	A	340	ARG	2.2
1	A	405	ARG	2.2
1	B	195	LEU	2.2
1	B	101	GLU	2.2
1	A	35	GLY	2.2
1	A	65	GLN	2.2
1	A	361	GLY	2.2
1	A	105	ARG	2.1
1	A	89	LEU	2.1
1	B	275	PHE	2.1
1	A	34	ARG	2.1
1	B	183	ARG	2.1
1	A	183	ARG	2.1
1	A	438	ARG	2.1
1	A	418	ALA	2.1
1	B	248	TYR	2.1
1	A	117	GLN	2.1
1	B	268	PRO	2.1
1	B	384	GLY	2.1
1	B	363	MET	2.1
1	A	128	VAL	2.1
1	A	310	LEU	2.0
1	A	373	LEU	2.0
1	B	429	ILE	2.0
1	B	401	PRO	2.0
1	A	81	LYS	2.0
1	A	104	SER	2.0
1	A	58	ALA	2.0
1	B	196	GLN	2.0
1	B	198	HIS	2.0
1	B	326	ASN	2.0
1	B	373	LEU	2.0
1	A	73	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	86	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

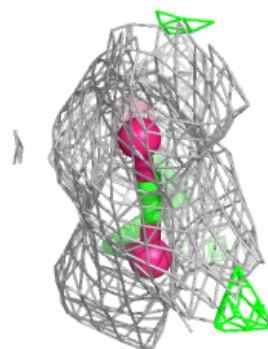
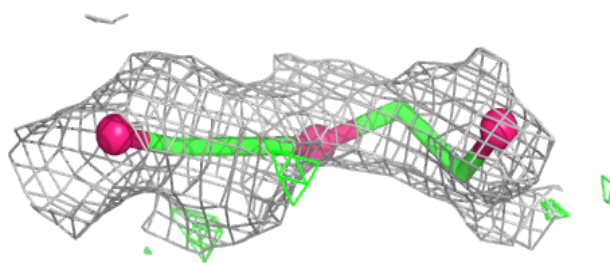
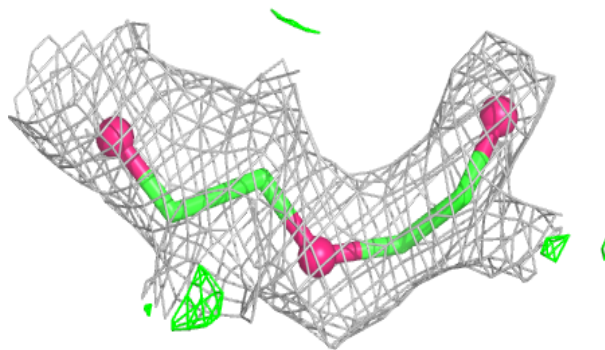
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PEG	A	510	7/7	0.66	0.23	48,52,55,58	0
4	NO3	B	505	4/4	0.72	0.24	42,46,46,54	0
5	PEG	A	509	7/7	0.73	0.30	45,46,50,53	0
4	NO3	B	504	4/4	0.75	0.22	38,44,45,49	0
4	NO3	A	504	4/4	0.75	0.16	29,32,37,38	0
5	PEG	A	508	4/7	0.76	0.20	48,49,51,58	0
4	NO3	A	506	4/4	0.77	0.20	50,53,56,58	0
4	NO3	A	505	4/4	0.77	0.21	50,50,52,55	0
5	PEG	B	506	7/7	0.78	0.25	37,46,57,57	0
5	PEG	B	507	7/7	0.84	0.19	24,31,37,39	0
4	NO3	A	507	4/4	0.86	0.15	33,37,38,39	0
3	CTP	B	503	21/29	0.91	0.13	17,32,38,49	0
3	CTP	A	503	21/29	0.93	0.10	17,23,27,36	0
2	MN	B	502	1/1	0.98	0.03	22,22,22,22	0
2	MN	A	501	1/1	0.98	0.03	24,24,24,24	0
2	MN	A	502	1/1	0.99	0.02	17,17,17,17	0
2	MN	B	501	1/1	0.99	0.02	17,17,17,17	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.

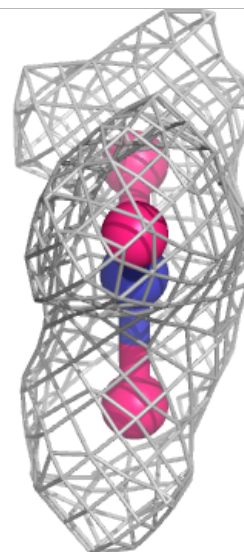
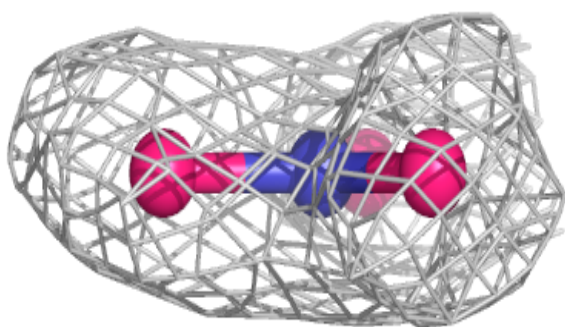
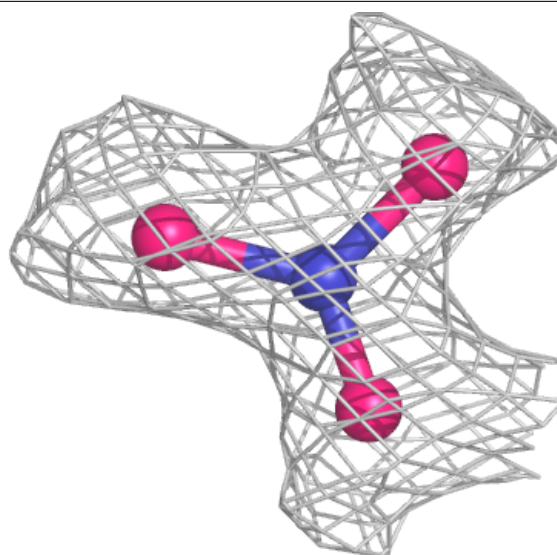
Electron density around PEG A 510:

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



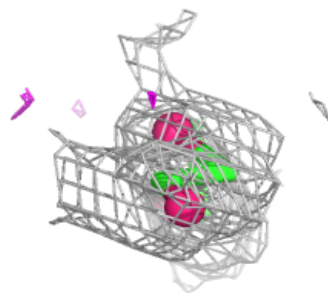
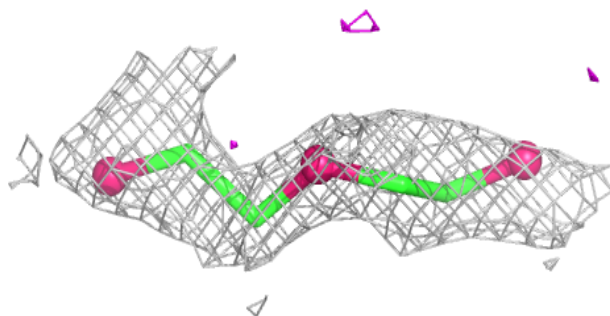
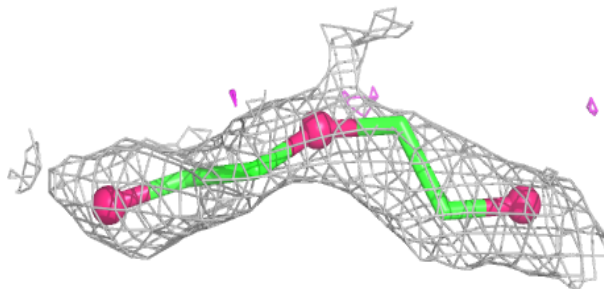
Electron density around NO3 B 505:

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



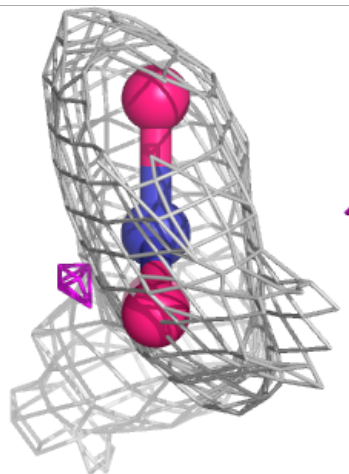
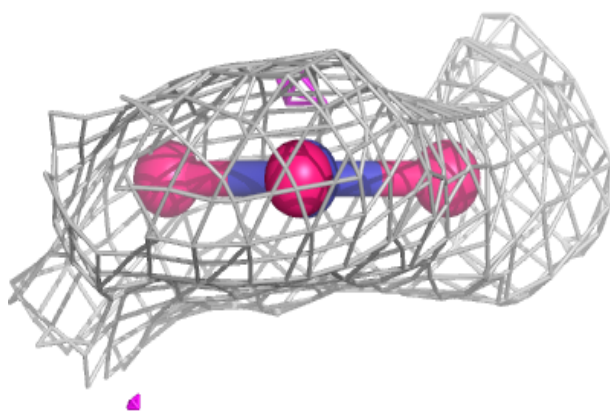
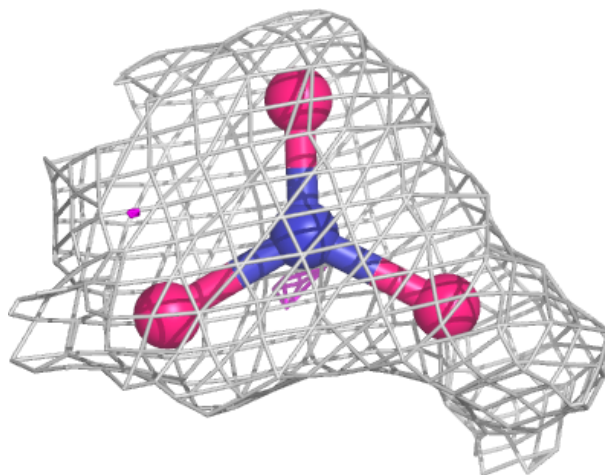
Electron density around PEG A 509:

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



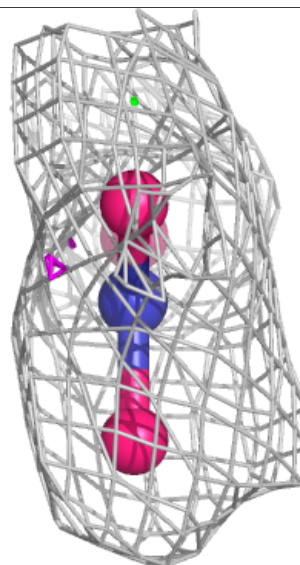
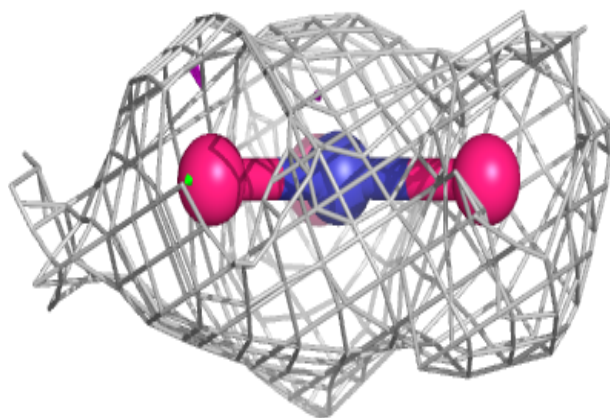
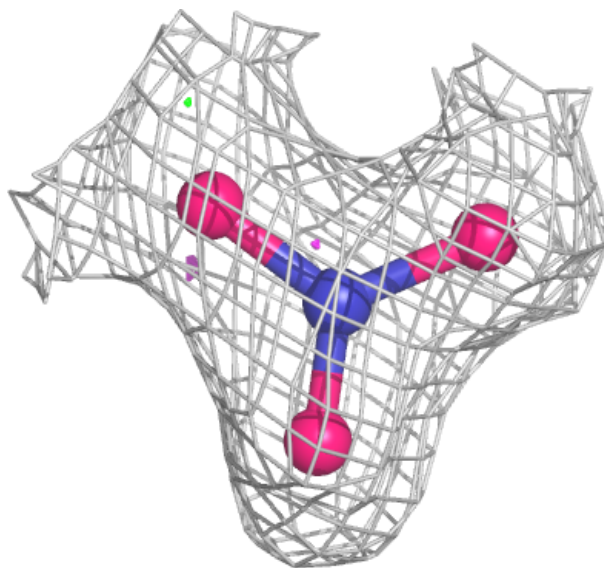
Electron density around NO3 B 504:

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



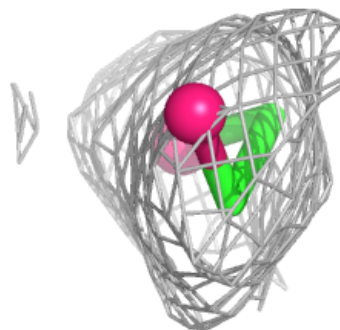
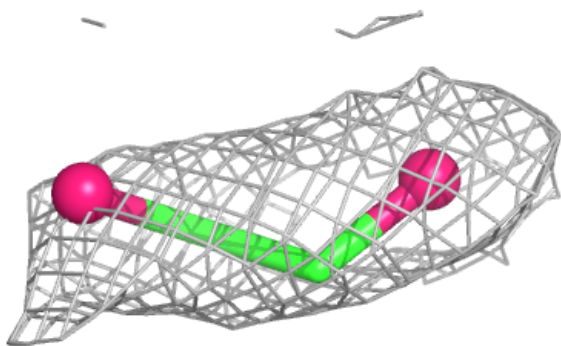
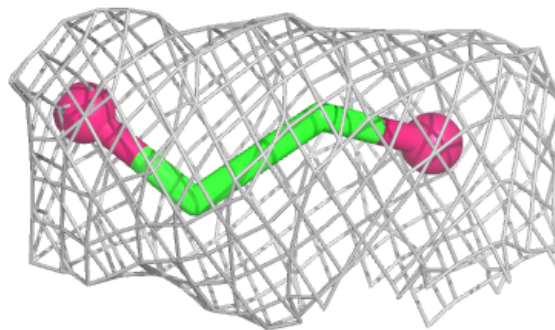
Electron density around NO3 A 504:

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



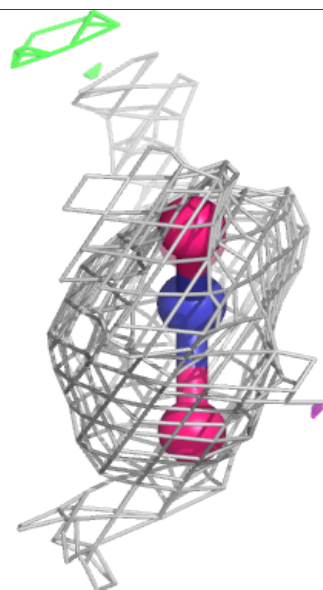
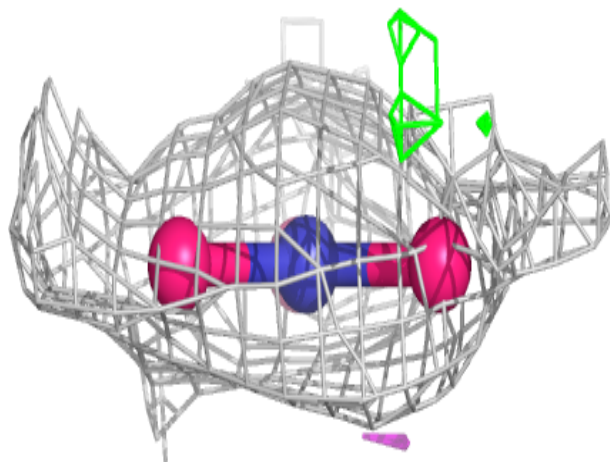
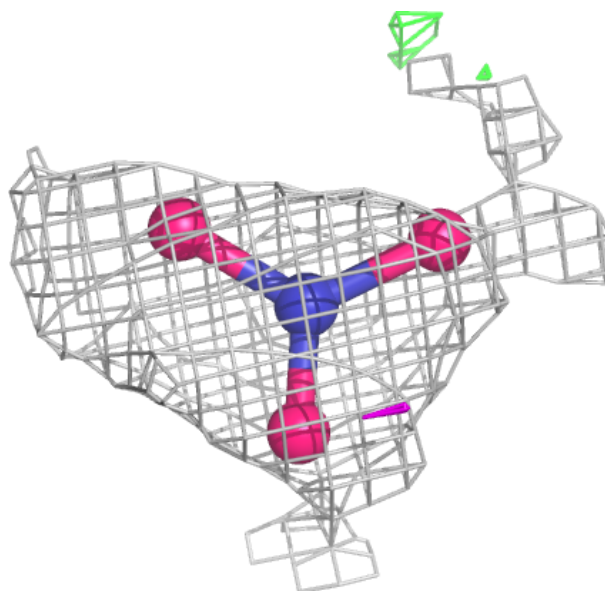
Electron density around PEG A 508:

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



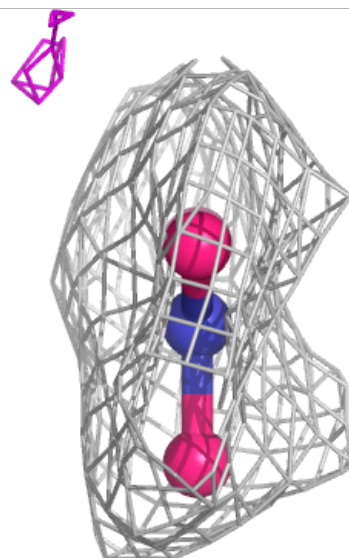
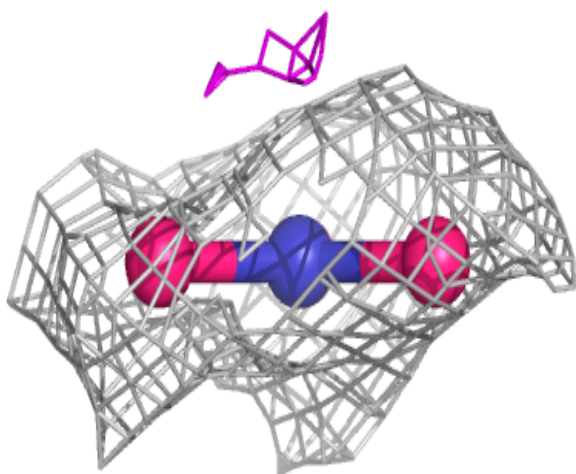
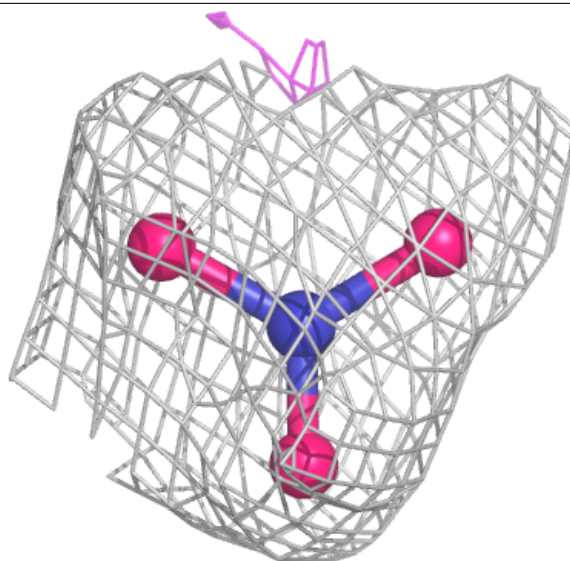
Electron density around NO3 A 506:

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



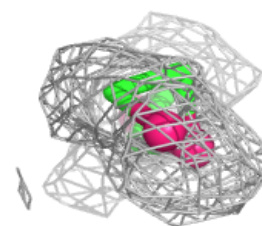
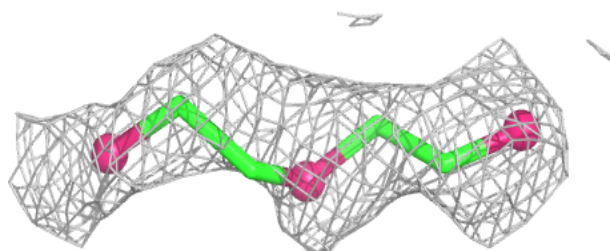
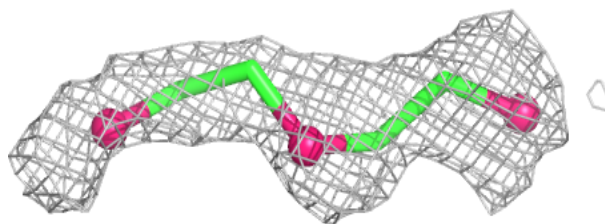
Electron density around NO3 A 505:

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

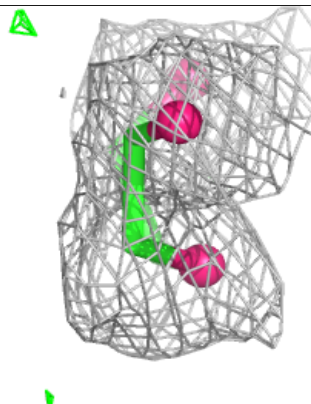
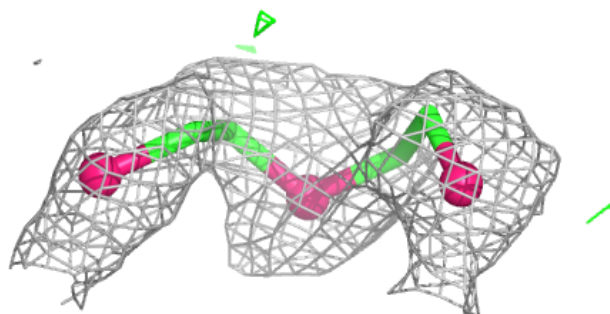
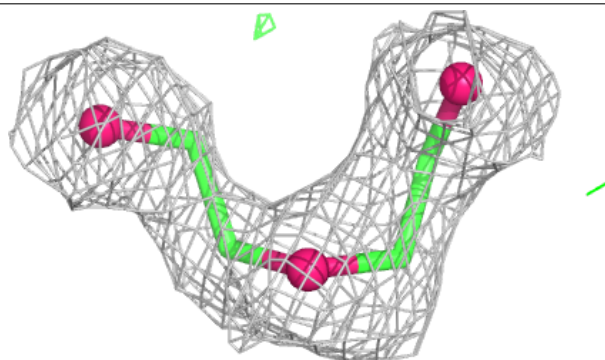


Electron density around PEG B 506:

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

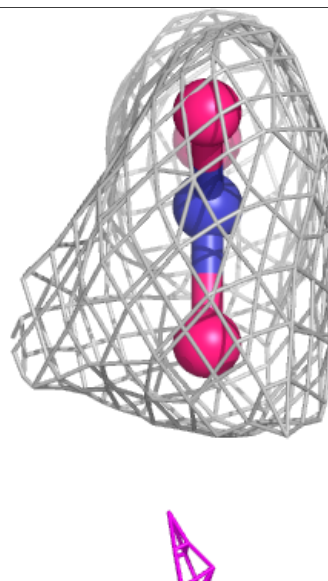
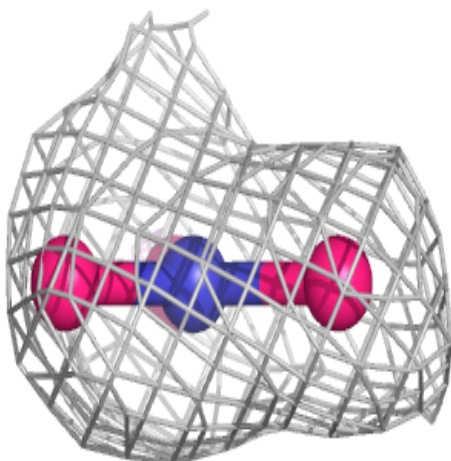
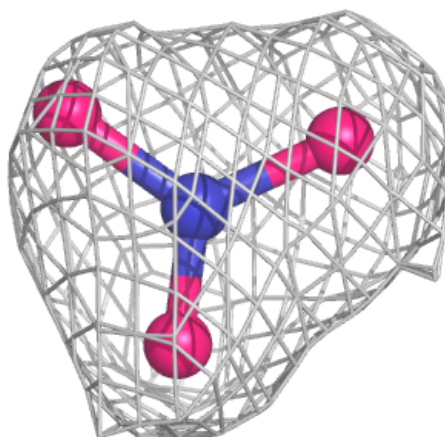
**Electron density around PEG B 507:**

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



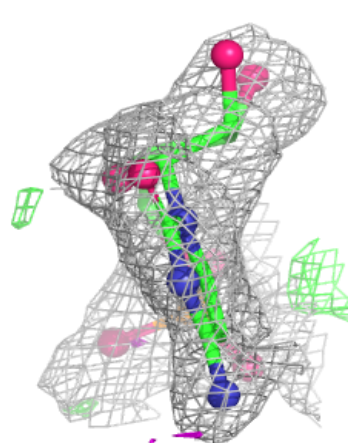
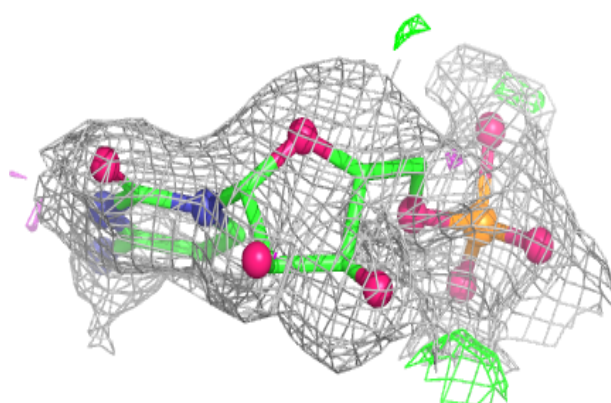
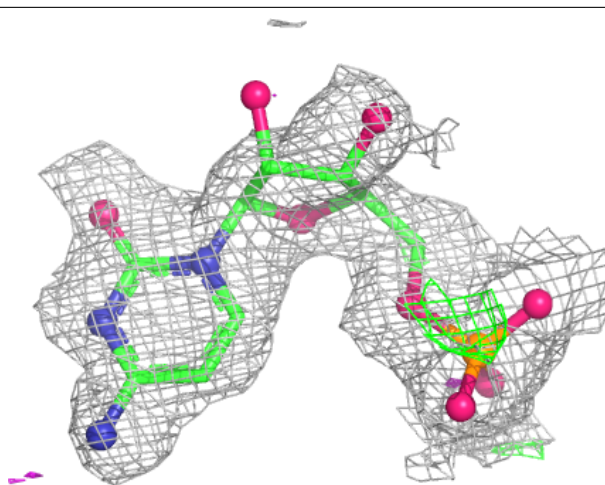
Electron density around NO3 A 507:

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



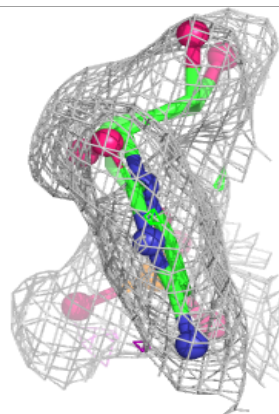
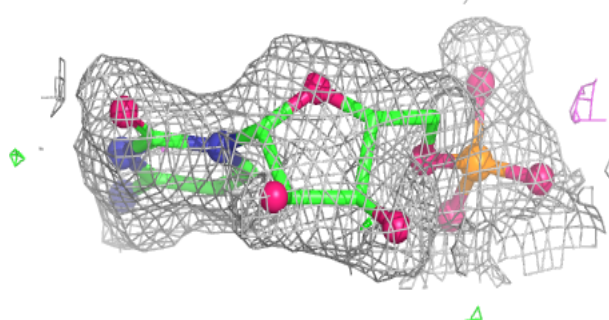
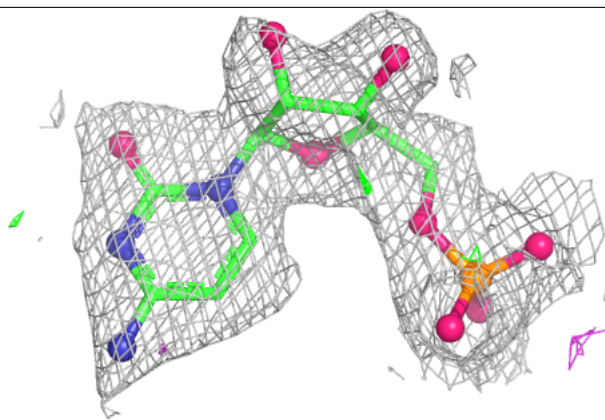
Electron density around CTP B 503:

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



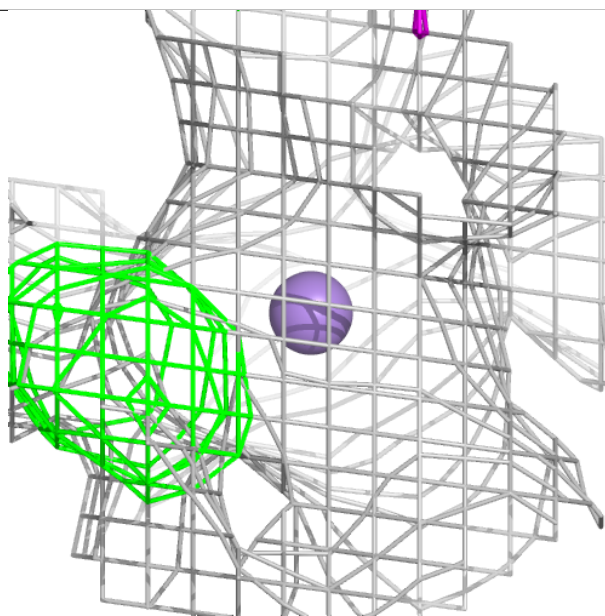
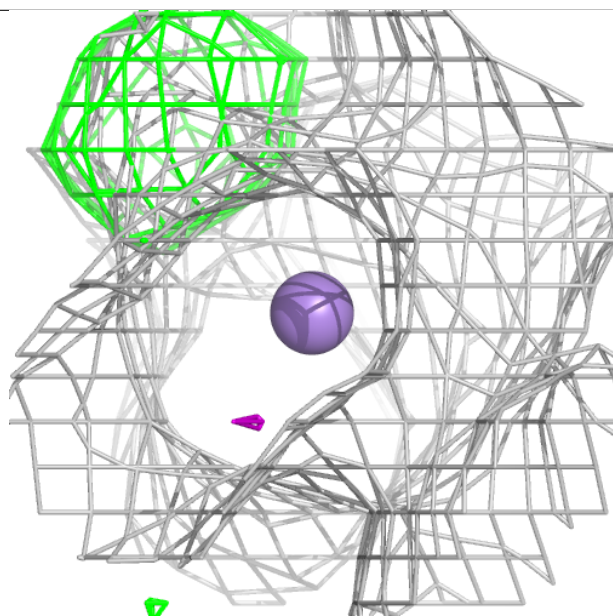
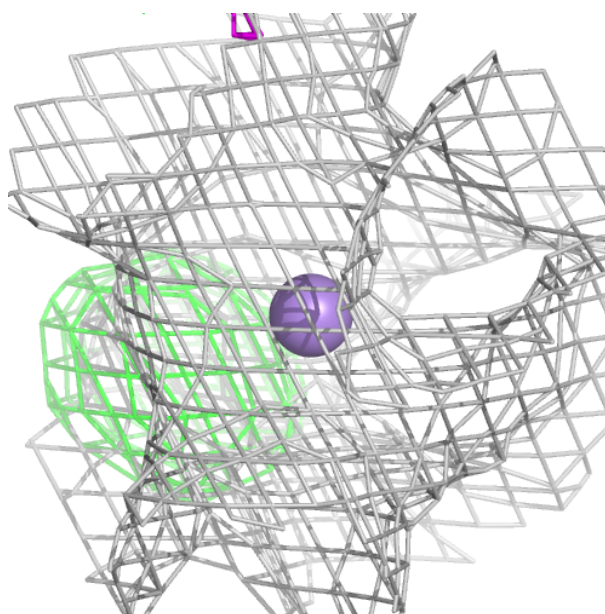
Electron density around CTP A 503:

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



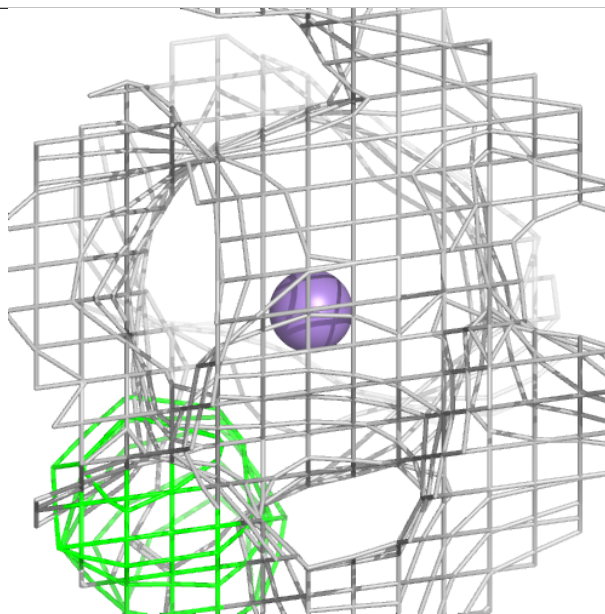
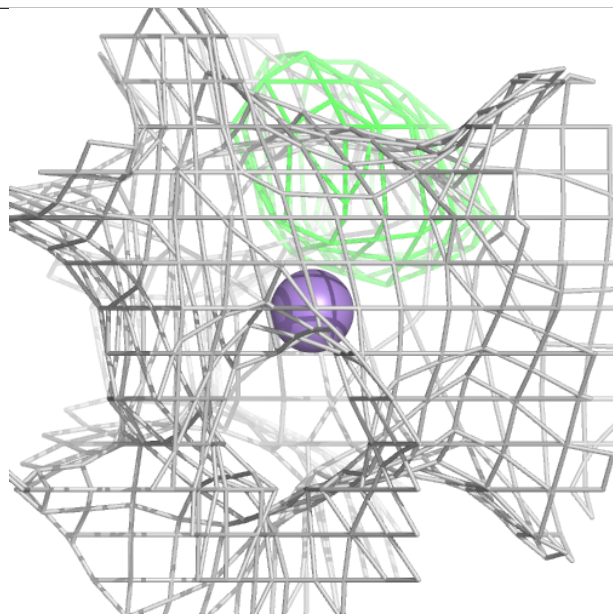
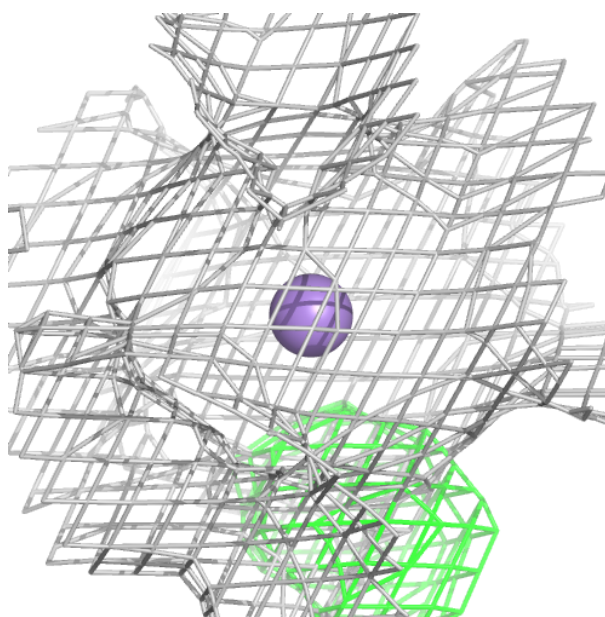
Electron density around MN B 502:

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



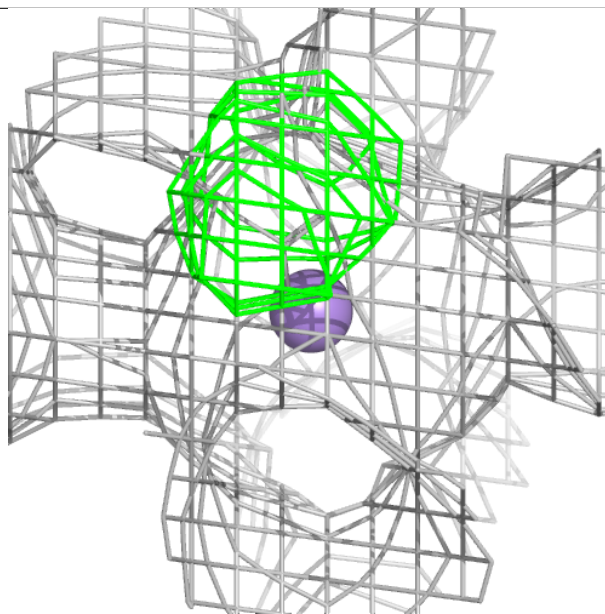
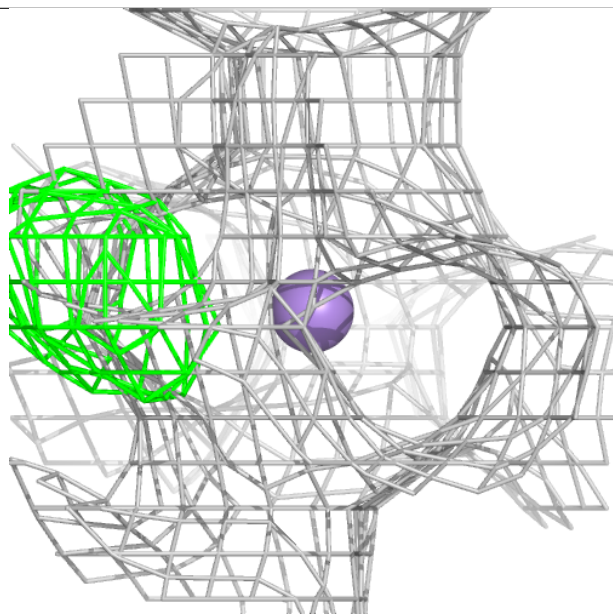
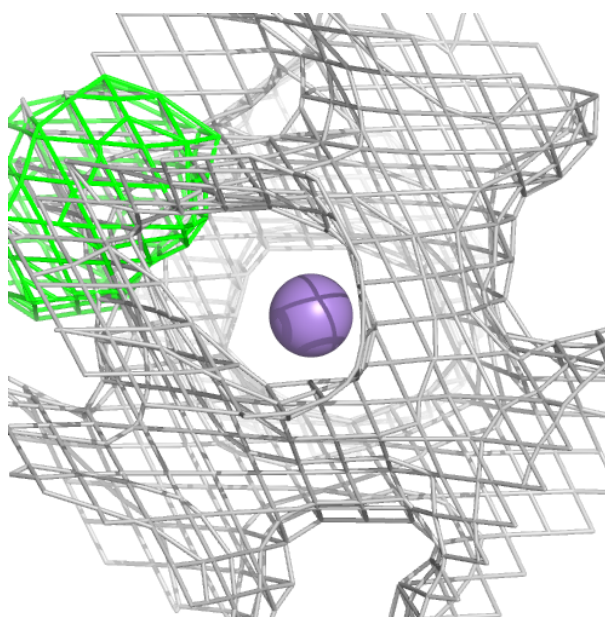
Electron density around MN A 501:

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



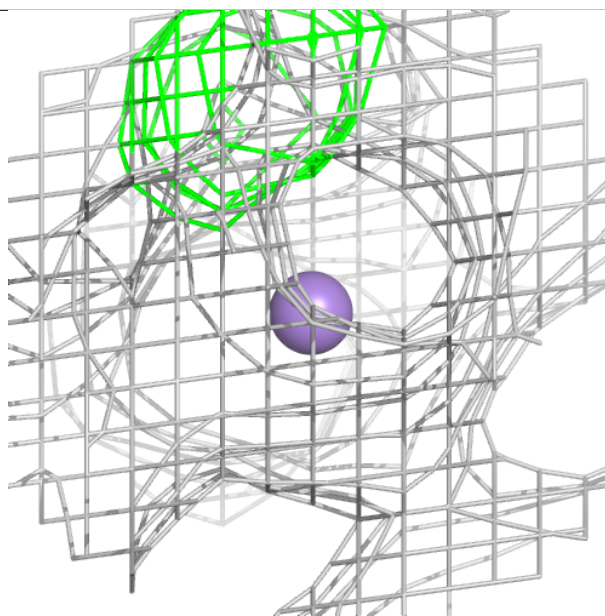
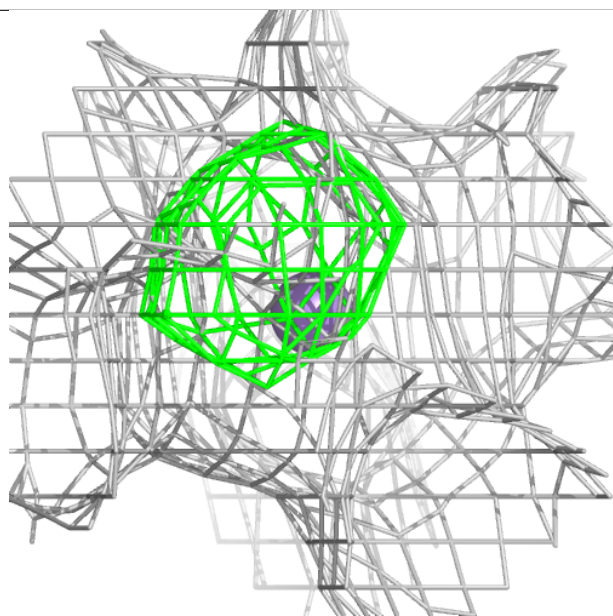
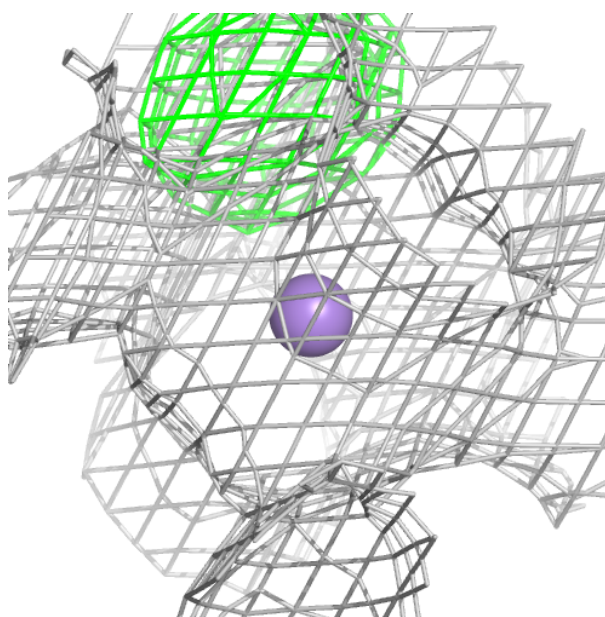
Electron density around MN A 502:

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



Electron density around MN B 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.