Full wwPDB X-ray Structure Validation Report ⓘ

Jul 25, 2022 – 02:03 pm BST

PDB ID	:	7BMF
Title	:	Crystal structure of RecJCdc45 from Methanothermobacter thermoautotrofi-cus 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:

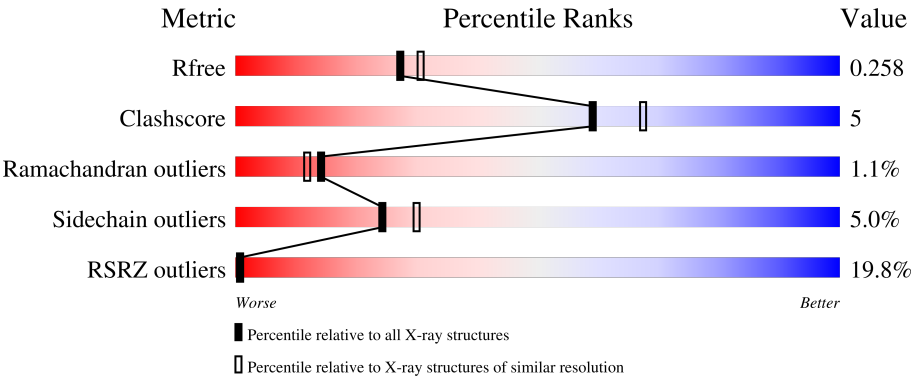
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance (i)

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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 <=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	16% 83% 11%
1	B	464	22% 83% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PEG	A	510	-	-	-	X

2 Entry composition (i)

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			

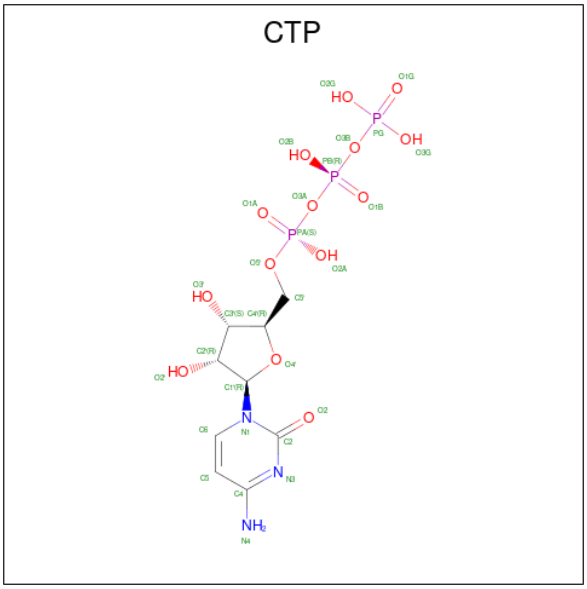
There are 14 discrepancies between the modelled and reference sequences:

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 (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

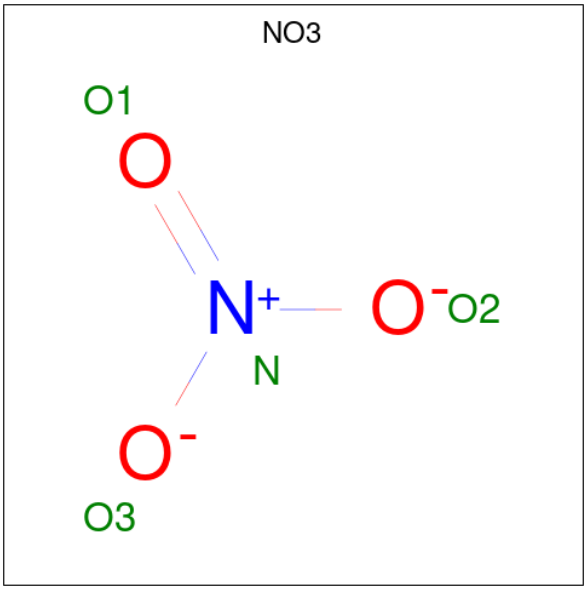
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		

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



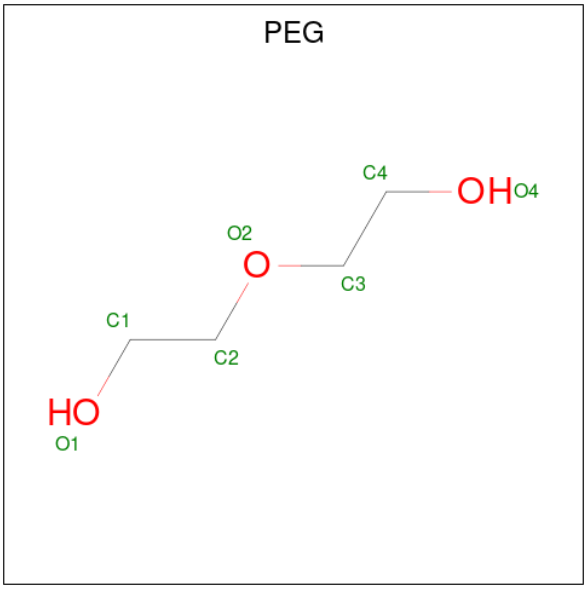
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			21	9	3	8	1		
3	B	1	Total	C	N	O	P	0	0
			21	9	3	8	1		

- Molecule 4 is NITRATE ION (three-letter code: 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 (three-letter code: 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.

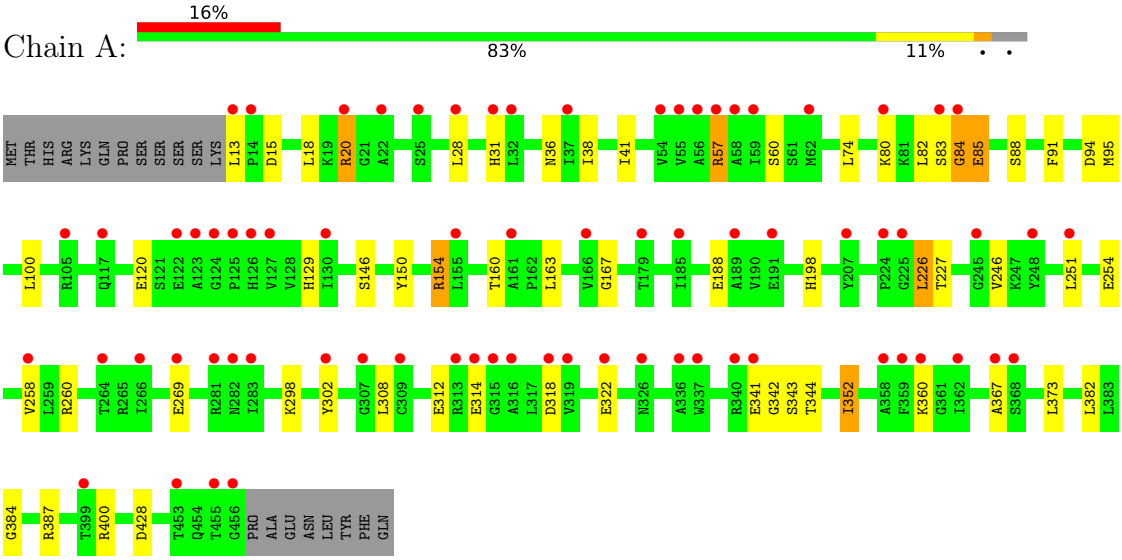
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	112	Total O 112 112	0	0
6	B	94	Total O 94 94	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

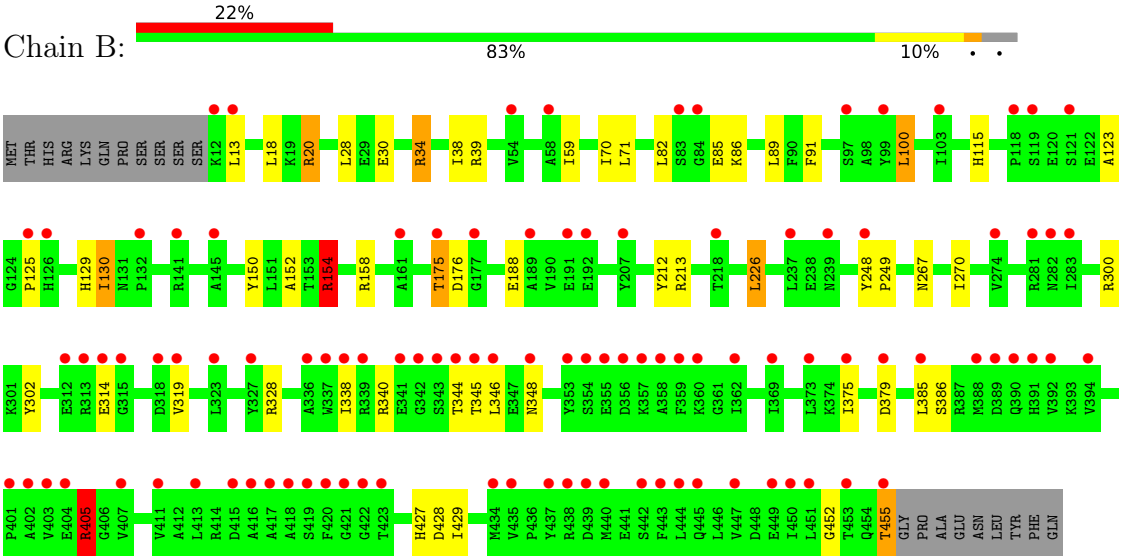
• Molecule 1: Conserved protein

Chain A:



• Molecule 1: Conserved protein

Chain B:



4 Data and refinement statistics (i)

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 48.23 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.7 (42.21-2.20) 96.8 (48.23-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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	2131 reflections (5.05%)	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)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.81	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, MN, CTP, 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	0.78	0/3367	0.92	5/4564 (0.1%)
1	B	0.78	0/3231	0.89	5/4392 (0.1%)
All	All	0.78	0/6598	0.90	10/8956 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	428	ASP	CB-CG-OD1	7.57	125.11	118.30
1	B	226	LEU	CB-CG-CD2	7.07	123.02	111.00
1	B	226	LEU	CB-CG-CD1	6.94	122.79	111.00
1	B	39	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	226	LEU	CB-CG-CD1	5.62	120.56	111.00
1	A	154	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	94	ASP	CB-CG-OD1	5.50	123.25	118.30
1	B	405	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	154	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	B	154	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3310	0	3213	29	0
1	B	3181	0	2998	32	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	6	0
All	All	6799	0	6280	60	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 (60) 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:HE1	1.75	0.68
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: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
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:HE2	1.84	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:ARG:NH2	6:B:608:HOH:O	2.43	0.51
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:B:455:THR:C	6:B:602:HOH:O	2.49	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:85:GLU:O	1:B:86:LYS:CB	2.60	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:B:338:ILE:HG22	1:B:375:ILE:HG21	1.98	0.46
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:A:74:LEU:HD13	1:A:95:MET:HE3	1.99	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: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
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: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:115:HIS:CE1	1:B:427:HIS:CE1	3.08	0.41
1:A:83:SER:C	1:A:84:GLY:O	2.59	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: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 (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	442/464 (95%)	421 (95%)	16 (4%)	5 (1%)	14	12
1	B	442/464 (95%)	416 (94%)	21 (5%)	5 (1%)	14	12
All	All	884/928 (95%)	837 (95%)	37 (4%)	10 (1%)	14	12

All (10) Ramachandran outliers are listed below:

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	339/379 (89%)	320 (94%)	19 (6%)	21	25
1	B	303/379 (80%)	290 (96%)	13 (4%)	29	36
All	All	642/758 (85%)	610 (95%)	32 (5%)	24	30

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	20	ARG
1	A	57	ARG
1	A	60	SER
1	A	80	LYS
1	A	82	LEU
1	A	91	PHE
1	A	100	LEU
1	A	120	GLU
1	A	226	LEU
1	A	269	GLU
1	A	298	LYS
1	A	302	TYR
1	A	308	LEU
1	A	318	ASP
1	A	322	GLU
1	A	344	THR
1	A	352	ILE
1	A	387	ARG
1	B	20	ARG
1	B	34	ARG
1	B	82	LEU
1	B	91	PHE
1	B	100	LEU
1	B	130	ILE
1	B	226	LEU
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	182	ASN
1	A	198	HIS
1	A	239	ASN
1	B	31	HIS
1	B	182	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	239	ASN
1	B	348	ASN
1	B	350	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	B	504	-	1,3,3	0.37	0	0,3,3	-	-
3	CTP	A	503	2	22,22,30	0.99	0	33,33,47	1.37	5 (15%)
4	NO3	A	504	-	1,3,3	0.07	0	0,3,3	-	-
5	PEG	A	509	-	6,6,6	0.89	0	5,5,5	2.02	2 (40%)
5	PEG	A	510	-	6,6,6	0.51	0	5,5,5	0.75	0
4	NO3	A	507	-	1,3,3	0.21	0	0,3,3	-	-
4	NO3	B	505	-	1,3,3	0.31	0	0,3,3	-	-
5	PEG	B	506	-	6,6,6	0.59	0	5,5,5	0.51	0
3	CTP	B	503	2	22,22,30	1.23	1 (4%)	33,33,47	1.03	1 (3%)
4	NO3	A	505	-	1,3,3	0.21	0	0,3,3	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PEG	B	507	-	6,6,6	0.80	0	5,5,5	1.13	0
5	PEG	A	508	-	3,3,6	0.36	0	2,2,5	0.32	0
4	NO3	A	506	-	1,3,3	0.46	0	0,3,3	-	-

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	A	503	2	-	0/10/26/38	0/2/2/2
5	PEG	A	509	-	-	2/4/4/4	-
5	PEG	A	510	-	-	1/4/4/4	-
5	PEG	B	506	-	-	2/4/4/4	-
3	CTP	B	503	2	-	0/10/26/38	0/2/2/2
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	2.88	1.66	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	503	CTP	C3'-C2'-C1'	3.60	108.27	101.43
5	A	509	PEG	C3-O2-C2	3.26	127.43	113.29
3	A	503	CTP	C1'-N1-C2	2.66	124.35	118.42
3	A	503	CTP	O2-C2-N3	-2.54	118.19	122.33
3	A	503	CTP	C5-C4-N4	-2.31	116.94	120.57
3	B	503	CTP	O2A-PA-O1A	2.25	119.48	110.68
3	A	503	CTP	C5'-C4'-C3'	-2.14	107.16	115.18
5	A	509	PEG	O4-C4-C3	2.10	124.02	111.81

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	510	PEG	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	507	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

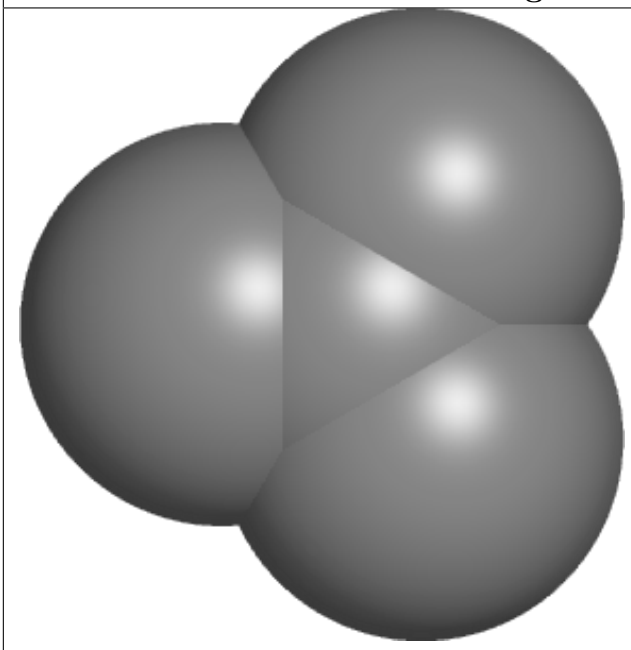
There are no ring outliers.

1 monomer is involved in 3 short contacts:

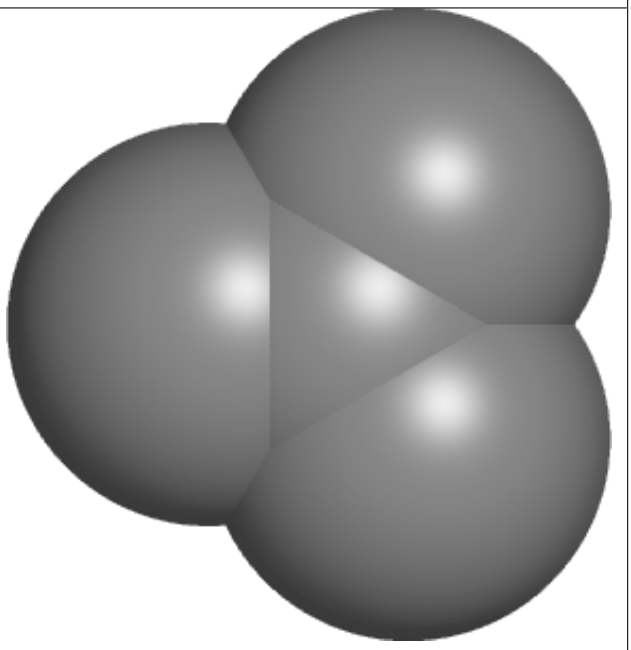
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	509	PEG	3	0

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 then 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.

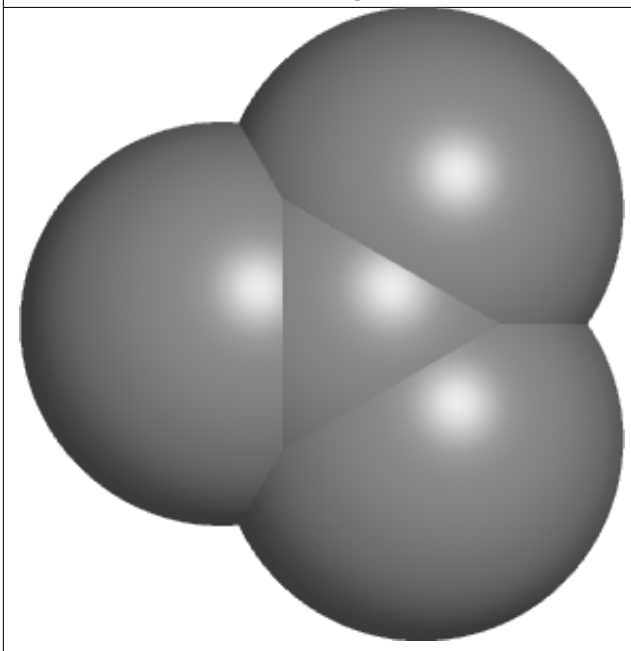
Ligand NO3 B 504



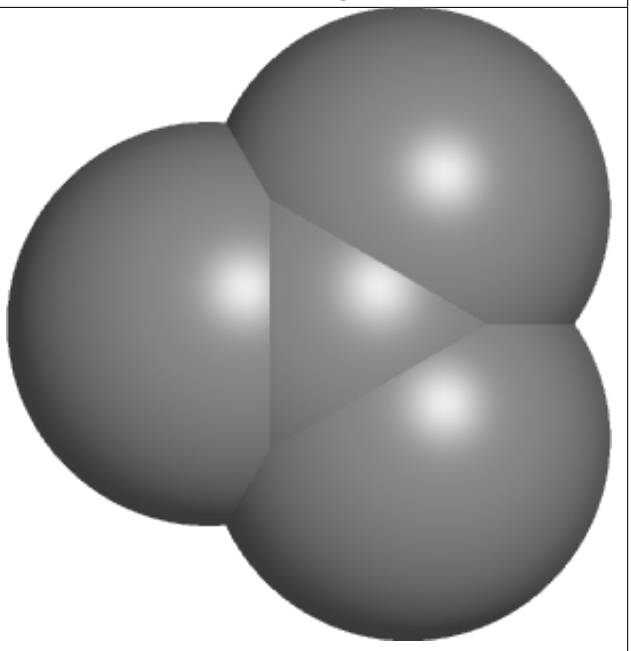
Bond lengths



Bond angles

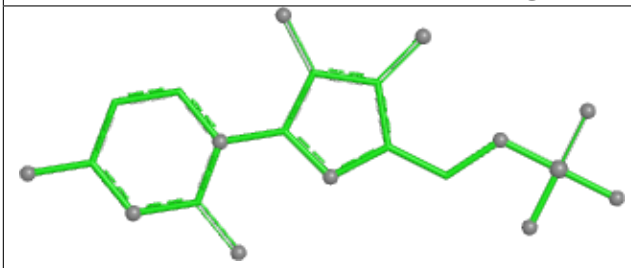


Torsions

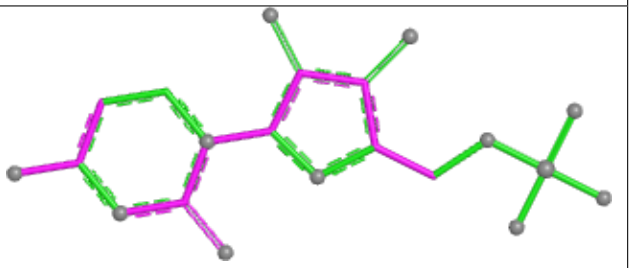


Rings

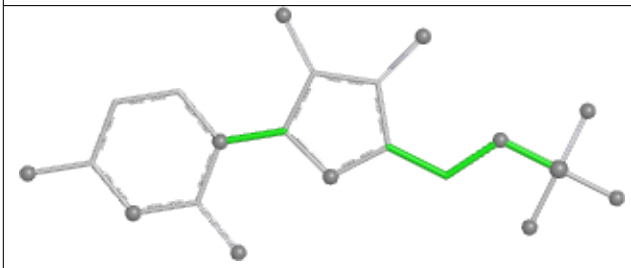
Ligand CTP A 503



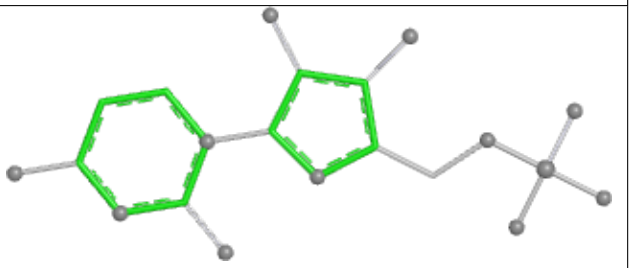
Bond lengths



Bond angles

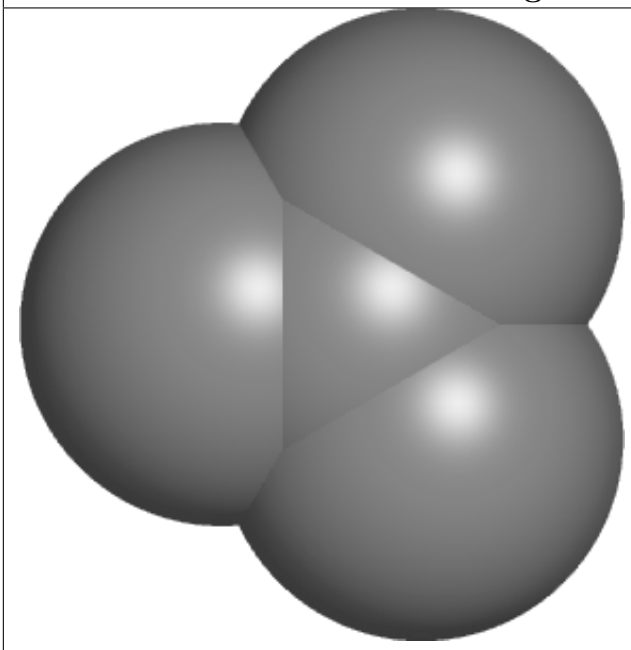


Torsions

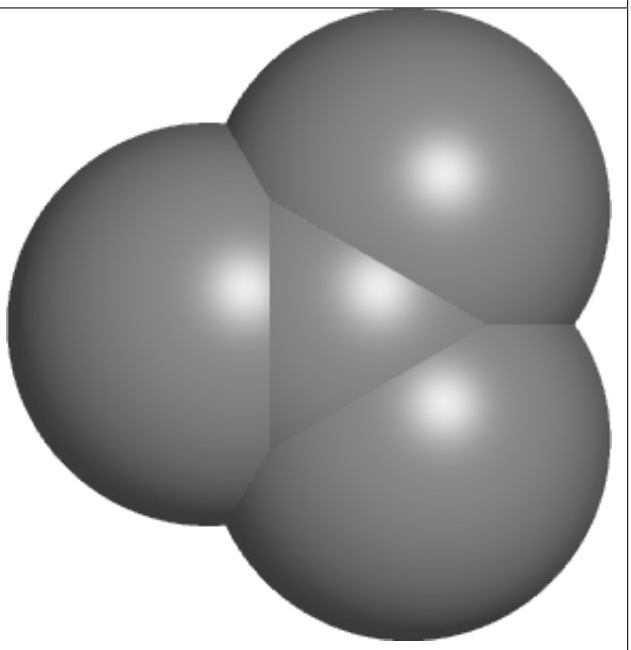


Rings

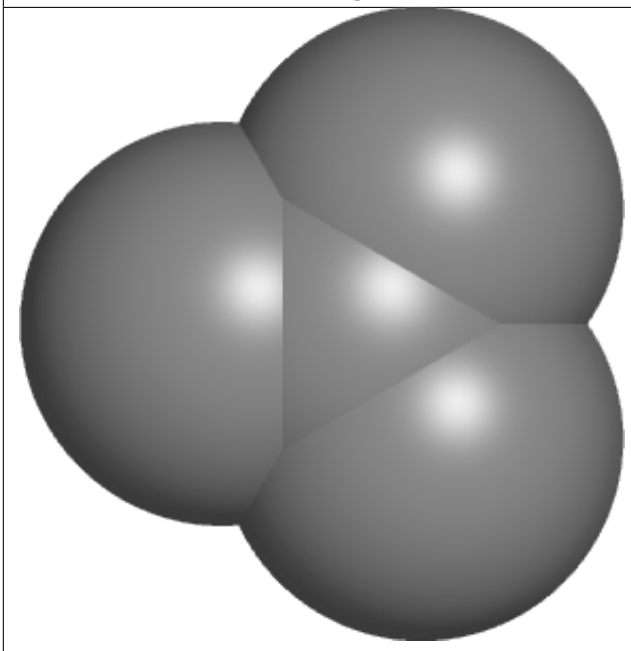
Ligand NO3 A 504



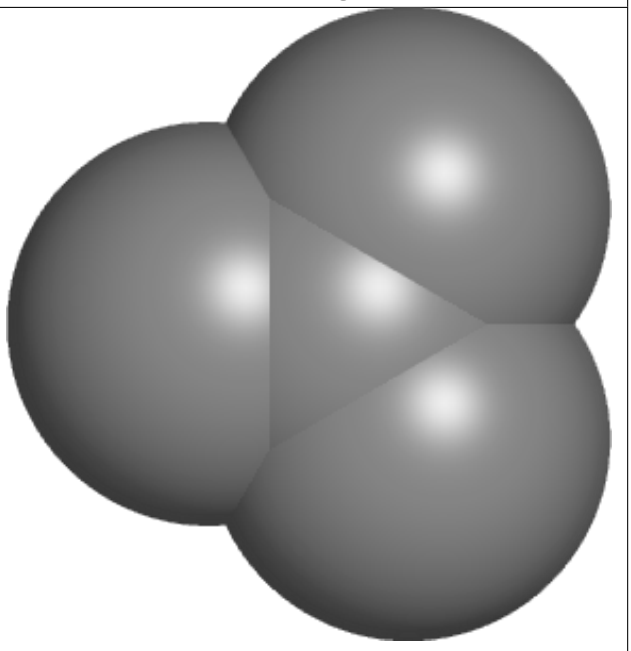
Bond lengths



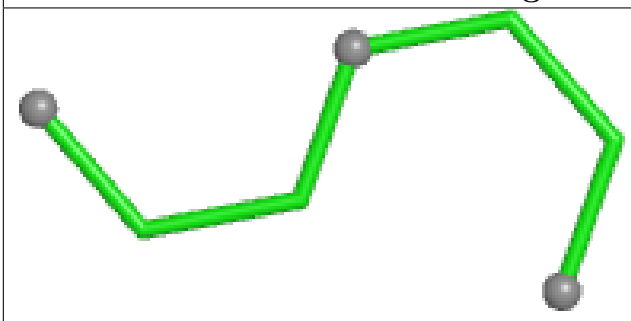
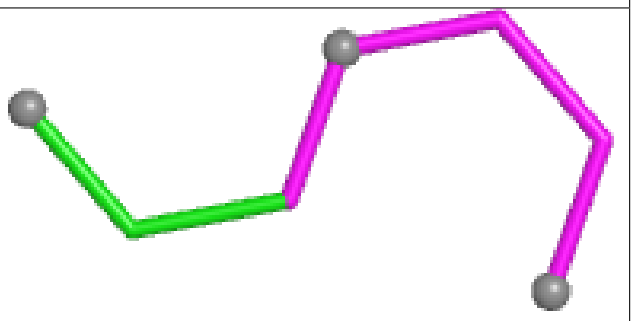
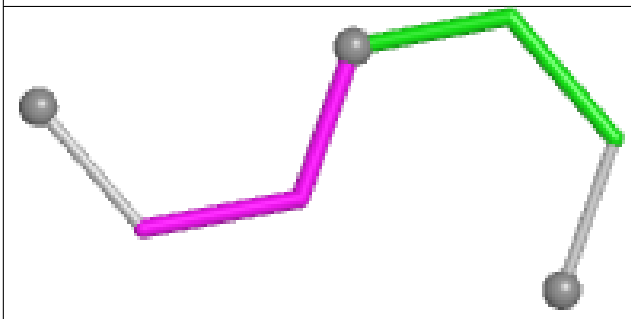
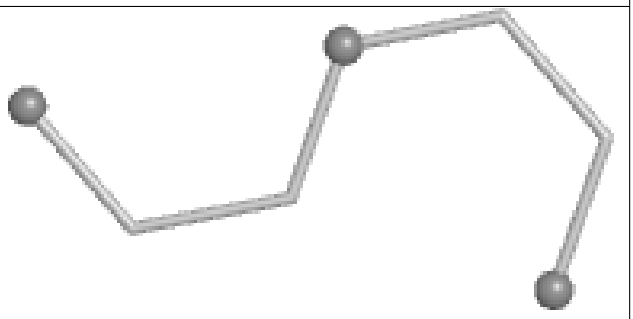
Bond angles

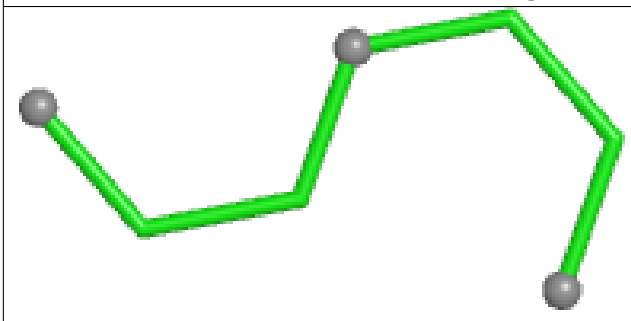
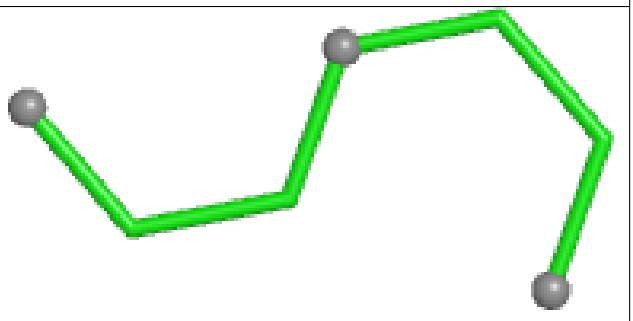
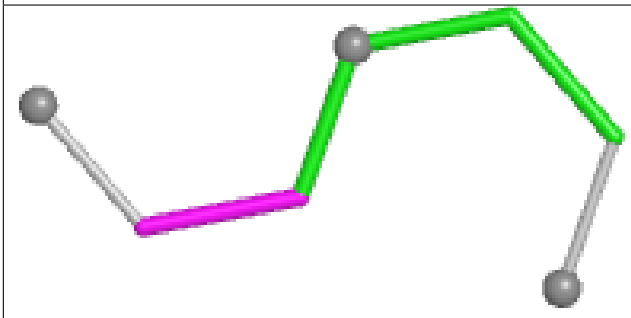
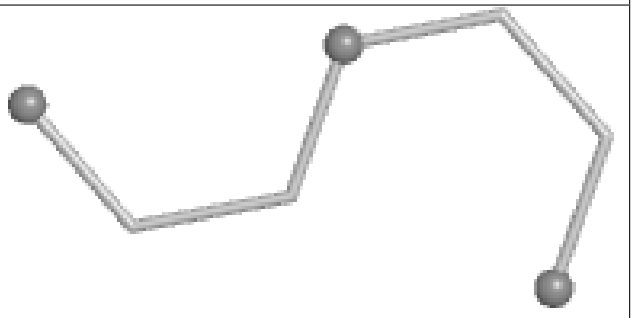


Torsions

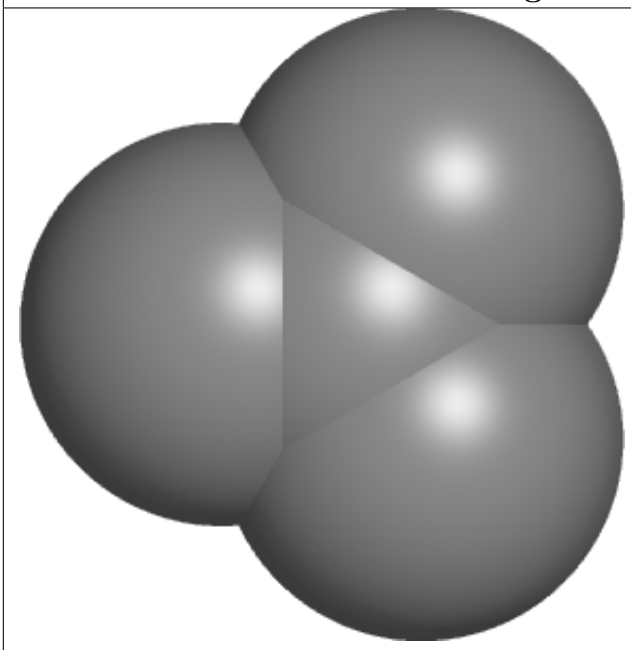


Rings

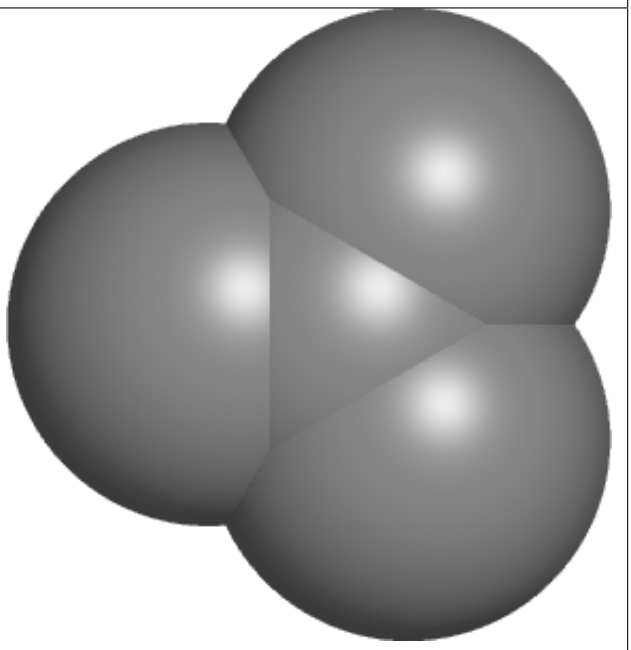
Ligand PEG A 509	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PEG A 510	
 Bond lengths	 Bond angles
 Torsions	 Rings

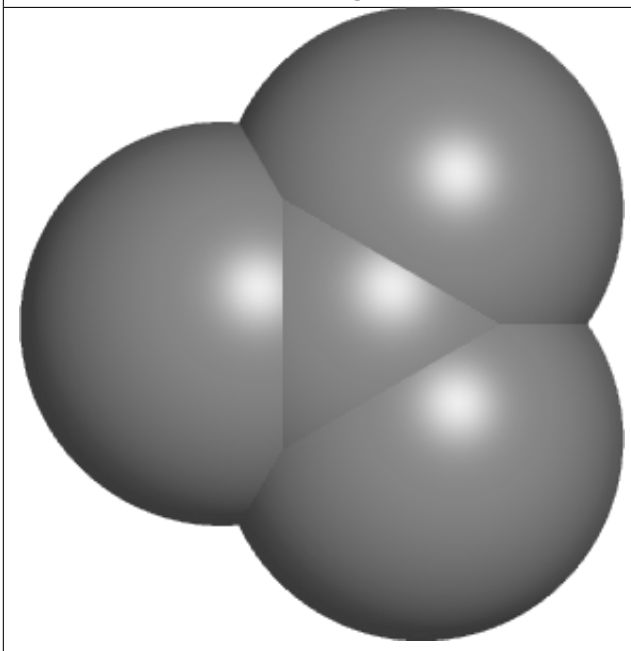
Ligand NO3 A 507



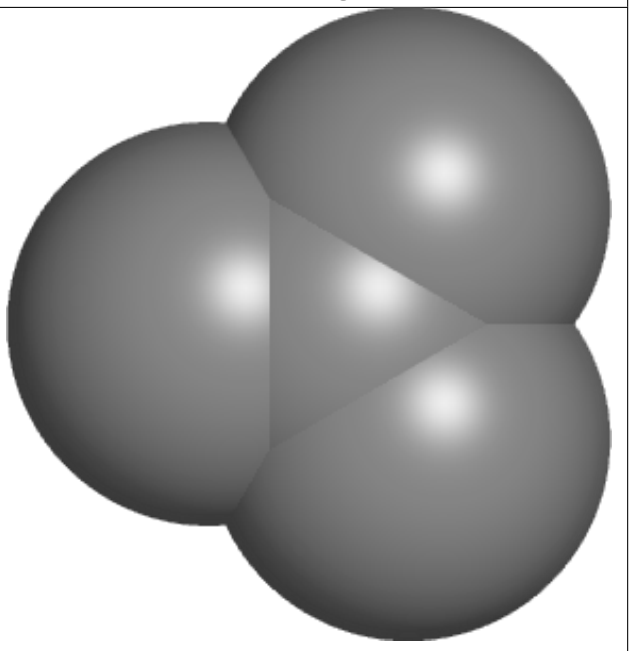
Bond lengths



Bond angles

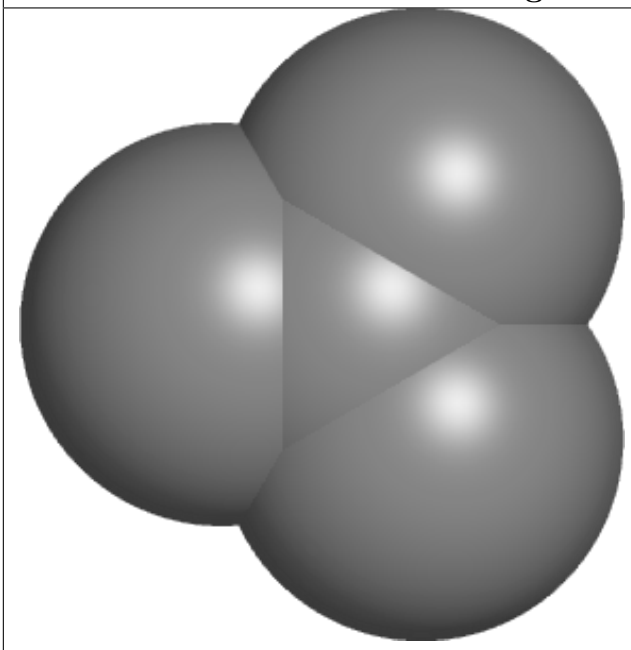


Torsions

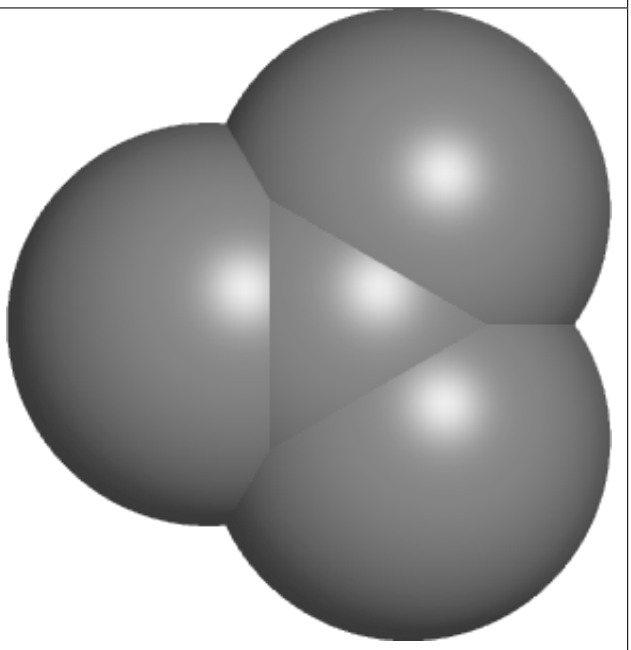


Rings

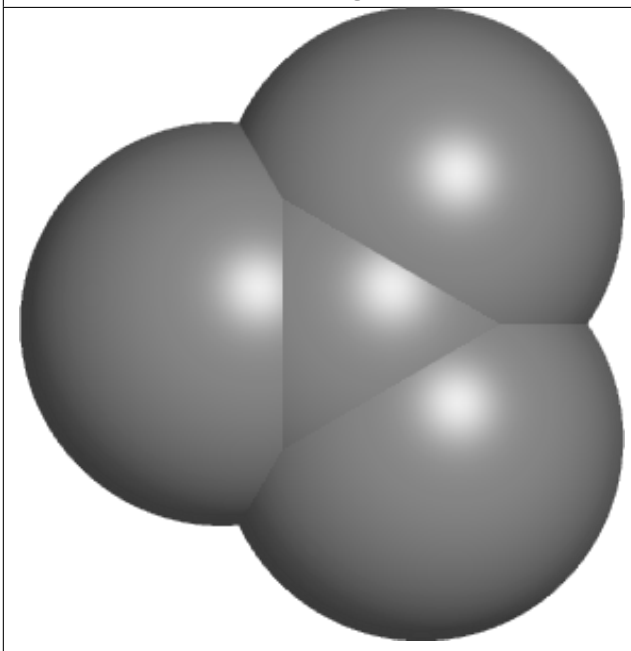
Ligand NO3 B 505



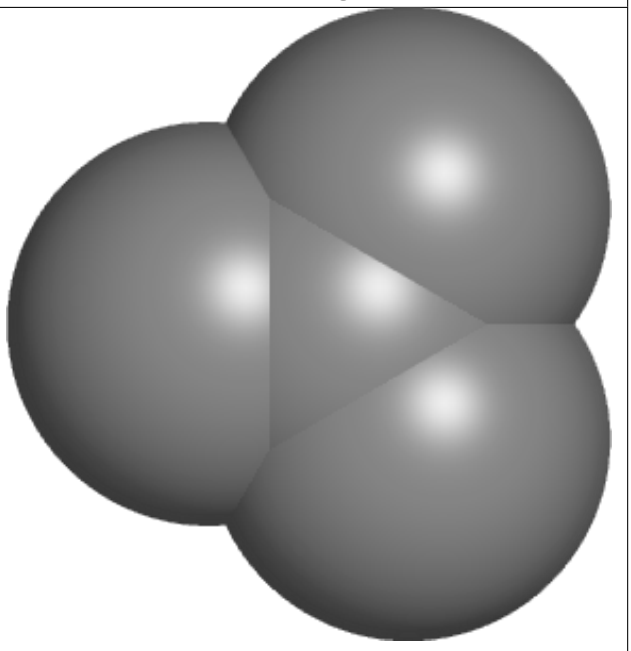
Bond lengths



Bond angles

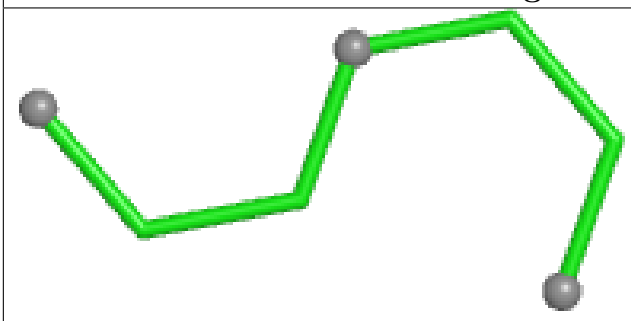


Torsions

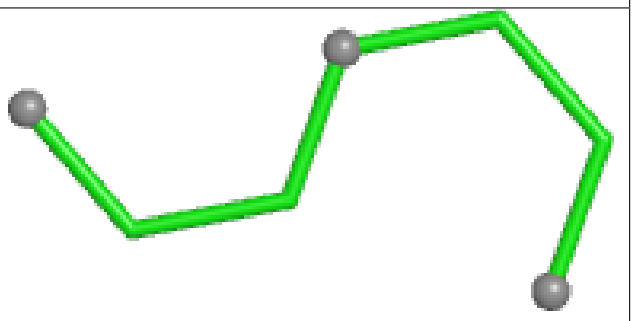


Rings

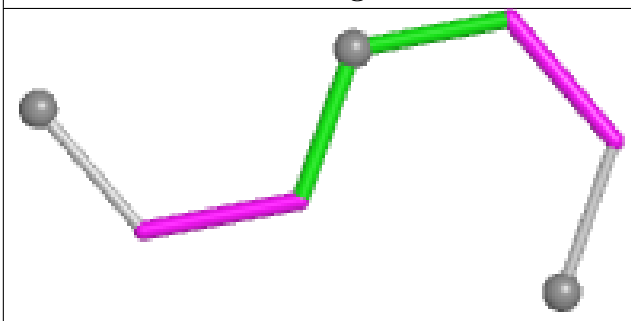
Ligand PEG B 506



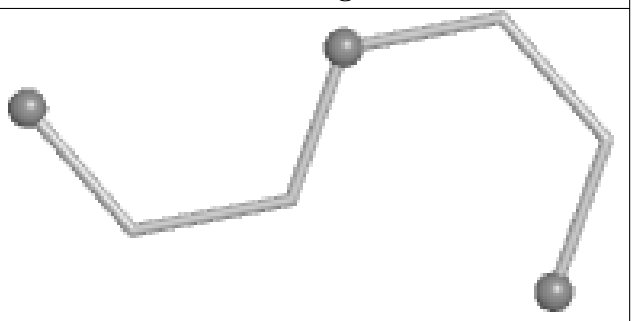
Bond lengths



Bond angles

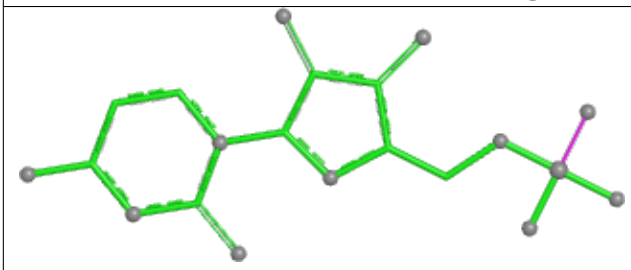


Torsions

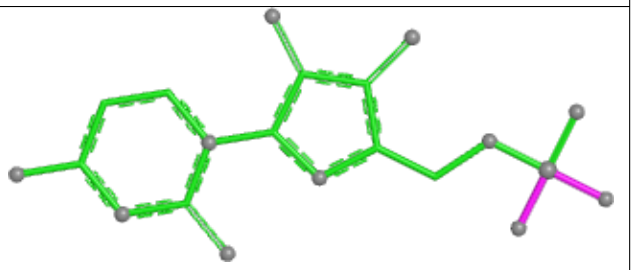


Rings

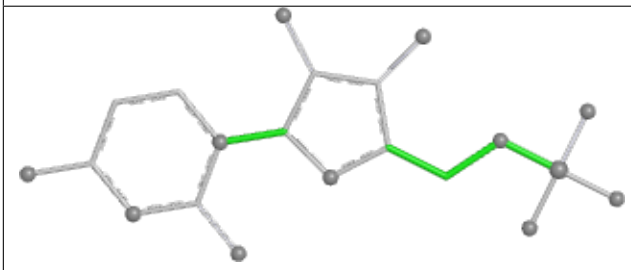
Ligand CTP B 503



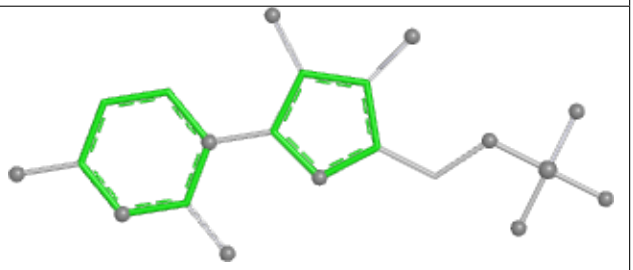
Bond lengths



Bond angles

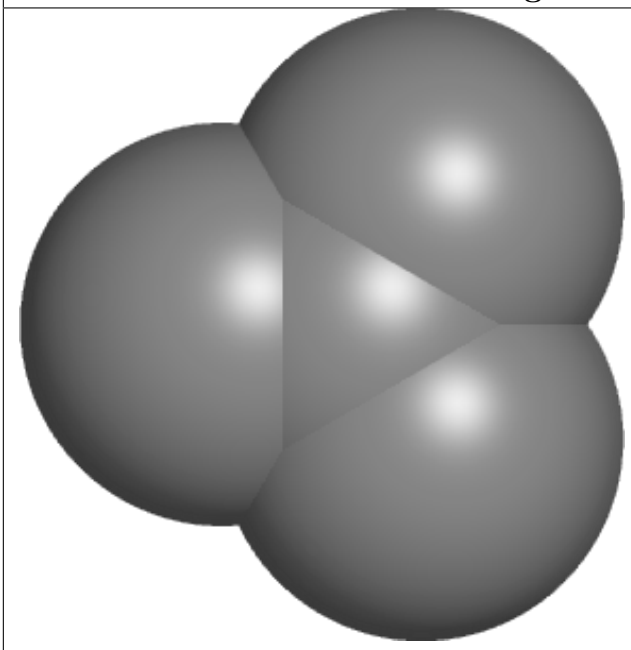


Torsions

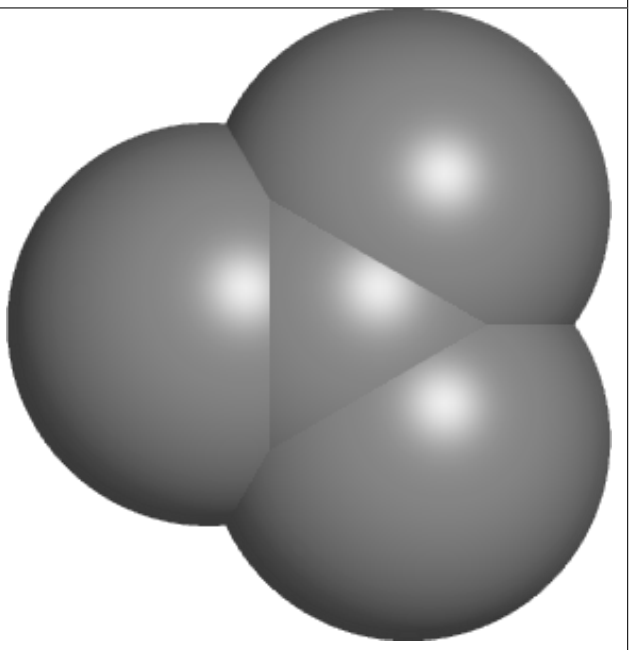


Rings

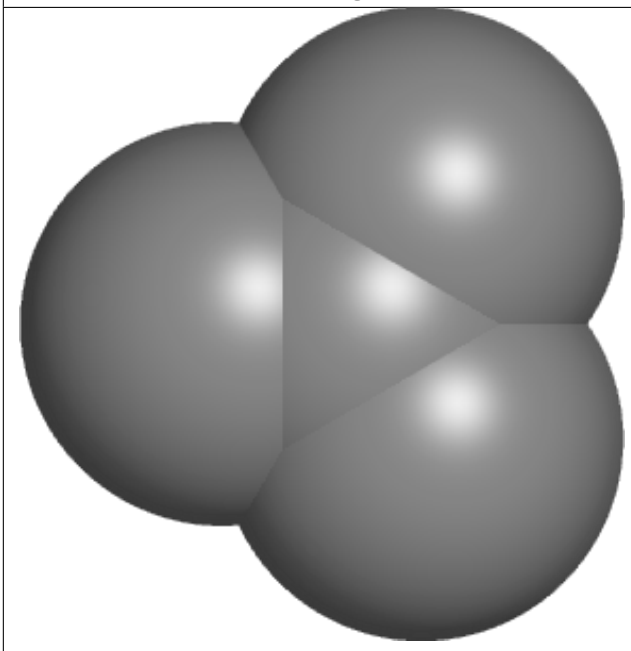
Ligand NO3 A 505



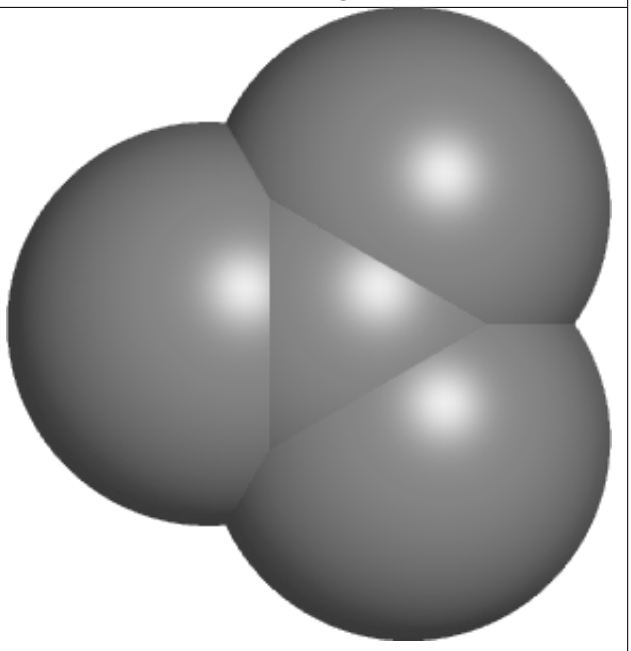
Bond lengths



Bond angles

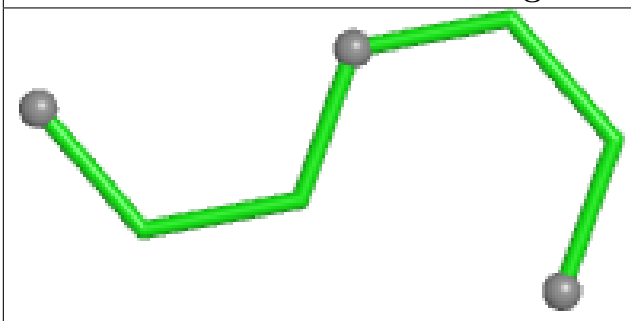


Torsions

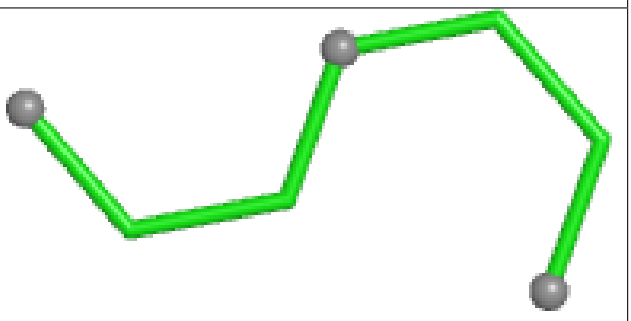


Rings

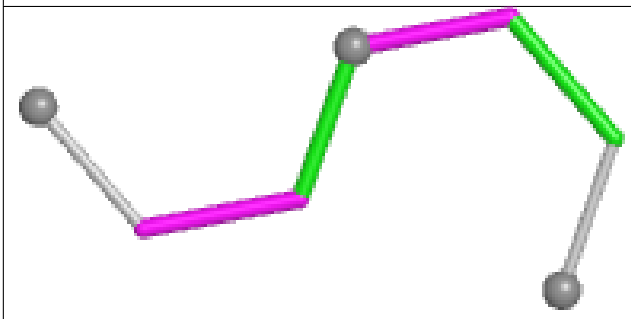
Ligand PEG B 507



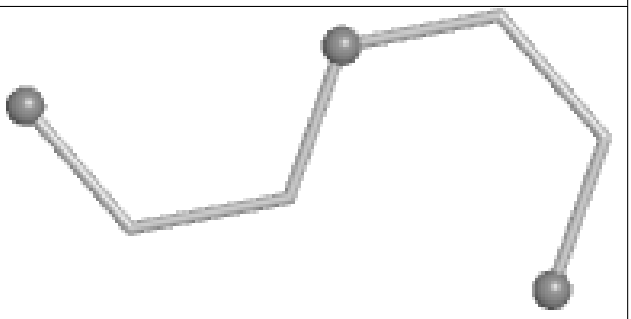
Bond lengths



Bond angles

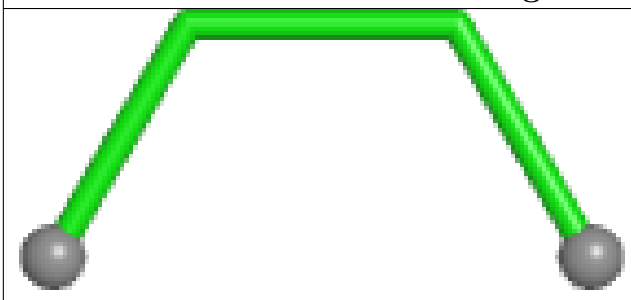


Torsions

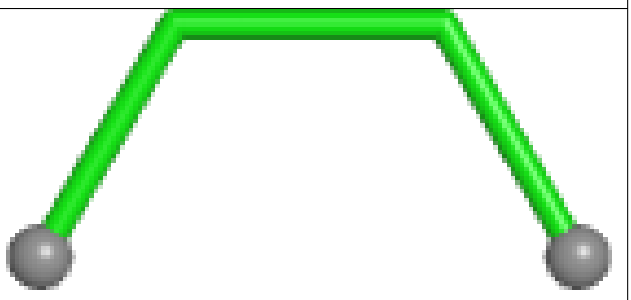


Rings

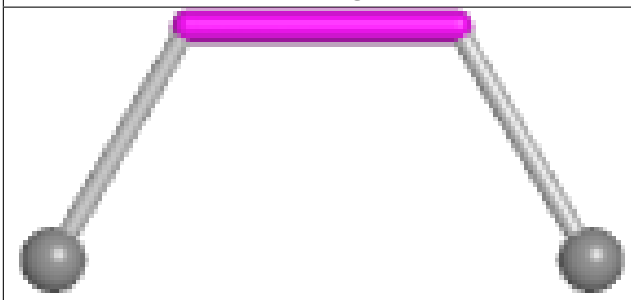
Ligand PEG A 508



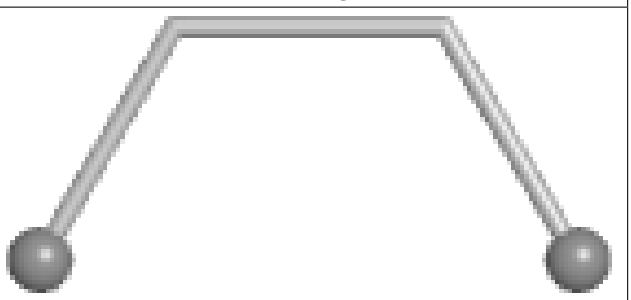
Bond lengths



Bond angles

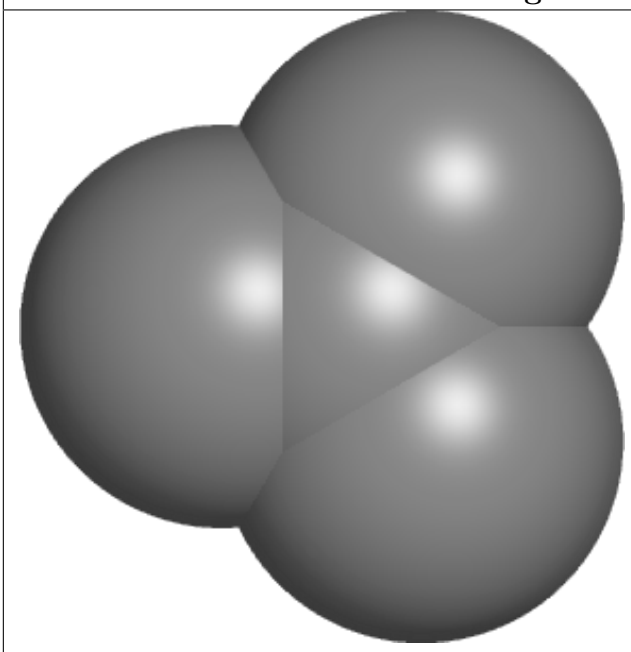


Torsions

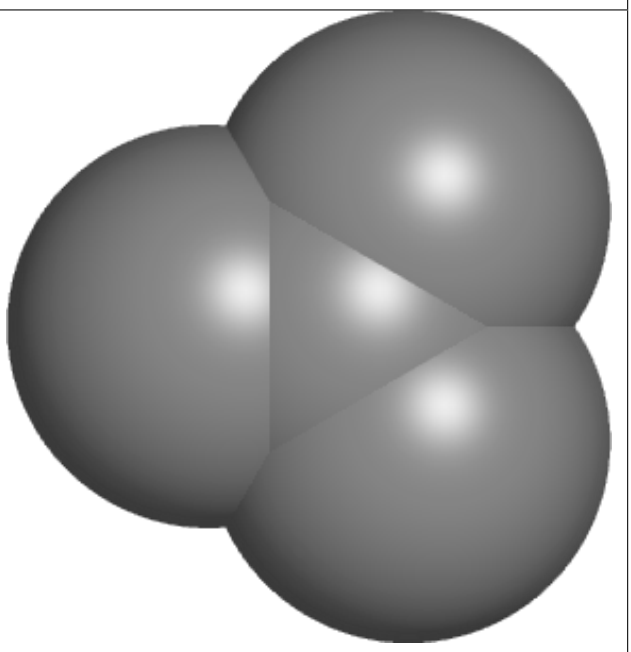


Rings

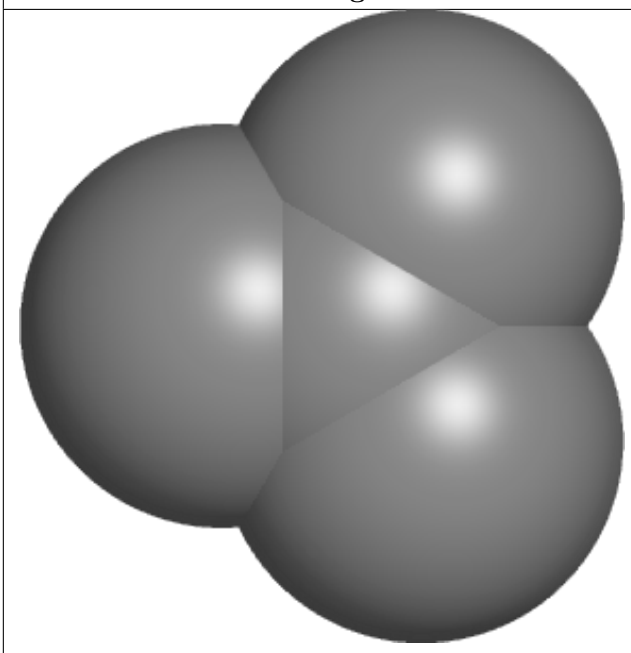
Ligand NO3 A 506



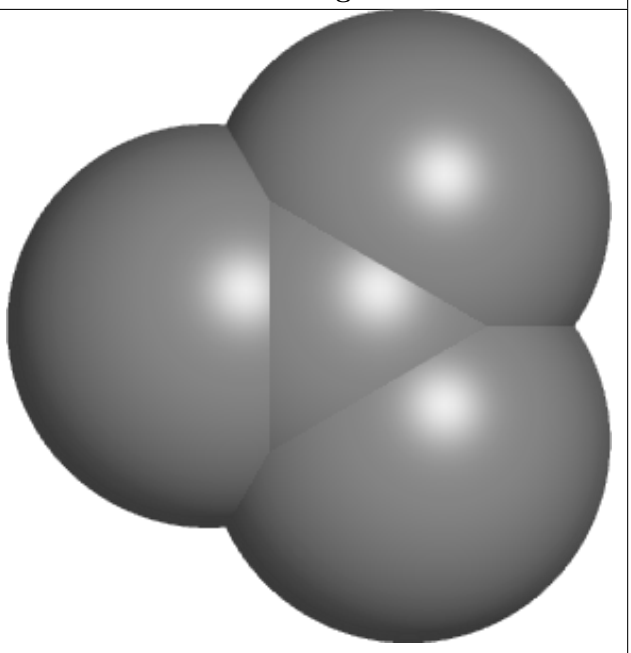
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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%)	1.25	73 (16%)	1	1	15, 28, 51, 86	0
1	B	444/464 (95%)	1.48	103 (23%)	0	0	14, 30, 64, 82	0
All	All	888/928 (95%)	1.36	176 (19%)	1	1	14, 29, 57, 86	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	282	ASN	7.7
1	A	126	HIS	7.2
1	A	316	ALA	7.1
1	B	438	ARG	6.9
1	A	315	GLY	6.7
1	B	391	HIS	6.2
1	B	358	ALA	6.1
1	B	337	TRP	6.0
1	B	119	SER	6.0
1	B	447	VAL	5.7
1	B	359	PHE	5.5
1	B	420	PHE	5.4
1	B	313	ARG	5.3
1	B	126	HIS	5.1
1	A	125	PRO	5.1
1	B	417	ALA	5.0
1	A	123	ALA	4.9
1	A	318	ASP	4.9
1	B	207	TYR	4.9
1	A	314	GLU	4.6
1	B	315	GLY	4.6
1	B	439	ASP	4.6
1	B	437	TYR	4.5
1	B	422	GLY	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	341	GLU	4.3
1	B	421	GLY	4.3
1	B	435	VAL	4.3
1	B	423	THR	4.2
1	B	314	GLU	4.2
1	B	440	MET	4.2
1	B	388	MET	4.0
1	B	434	MET	4.0
1	B	418	ALA	3.9
1	B	411	VAL	3.9
1	A	84	GLY	3.8
1	B	360	LYS	3.8
1	B	58	ALA	3.8
1	B	125	PRO	3.8
1	B	338	ILE	3.7
1	B	401	PRO	3.7
1	A	266	ILE	3.7
1	B	416	ALA	3.6
1	A	282	ASN	3.6
1	A	83	SER	3.6
1	B	175	THR	3.5
1	B	373	LEU	3.5
1	B	348	ASN	3.4
1	B	189	ALA	3.4
1	A	313	ARG	3.4
1	B	177	GLY	3.3
1	B	455	THR	3.3
1	B	319	VAL	3.3
1	A	37	ILE	3.2
1	B	336	ALA	3.2
1	B	281	ARG	3.2
1	B	379	ASP	3.1
1	A	322	GLU	3.1
1	B	283	ILE	3.1
1	B	356	ASP	3.1
1	B	369	ILE	3.0
1	B	413	LEU	3.0
1	B	342	GLY	3.0
1	B	353	TYR	3.0
1	B	121	SER	3.0
1	B	84	GLY	3.0
1	B	392	VAL	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	360	LYS	2.9
1	A	20	ARG	2.9
1	B	118	PRO	2.9
1	B	312	GLU	2.8
1	B	354	SER	2.8
1	B	419	SER	2.8
1	B	390	GLN	2.8
1	B	346	LEU	2.8
1	B	344	THR	2.8
1	B	362	ILE	2.8
1	A	56	ALA	2.7
1	B	13	LEU	2.7
1	B	394	VAL	2.7
1	B	385	LEU	2.7
1	A	155	LEU	2.7
1	B	54	VAL	2.7
1	B	389	ASP	2.7
1	A	337	TRP	2.7
1	B	445	GLN	2.7
1	A	264	THR	2.7
1	A	127	VAL	2.6
1	A	14	PRO	2.6
1	A	319	VAL	2.6
1	A	225	GLY	2.6
1	A	281	ARG	2.6
1	B	248	TYR	2.6
1	A	55	VAL	2.6
1	A	105	ARG	2.5
1	A	13	LEU	2.5
1	A	341	GLU	2.5
1	A	185	ILE	2.5
1	B	442	SER	2.5
1	A	28	LEU	2.5
1	B	339	ARG	2.5
1	B	345	THR	2.5
1	B	161	ALA	2.4
1	A	22	ALA	2.4
1	B	449	GLU	2.4
1	A	122	GLU	2.4
1	A	367	ALA	2.4
1	A	189	ALA	2.4
1	B	12	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	269	GLU	2.3
1	B	239	ASN	2.3
1	B	443	PHE	2.3
1	A	456	GLY	2.3
1	A	25	SER	2.3
1	A	251	LEU	2.3
1	B	145	ALA	2.3
1	B	97	SER	2.3
1	A	248	TYR	2.3
1	A	62	MET	2.3
1	A	31	HIS	2.3
1	B	191	GLU	2.3
1	B	355	GLU	2.3
1	A	362	ILE	2.3
1	A	124	GLY	2.2
1	A	207	TYR	2.2
1	A	302	TYR	2.2
1	A	54	VAL	2.2
1	B	103	ILE	2.2
1	B	453	THR	2.2
1	B	318	ASP	2.2
1	B	357	LYS	2.2
1	B	375	ILE	2.2
1	B	402	ALA	2.2
1	A	224	PRO	2.2
1	A	359	PHE	2.2
1	A	57	ARG	2.2
1	B	141	ARG	2.2
1	B	343	SER	2.2
1	B	407	VAL	2.2
1	A	59	ILE	2.2
1	A	80	LYS	2.2
1	A	161	ALA	2.2
1	A	32	LEU	2.2
1	B	404	GLU	2.2
1	B	403	VAL	2.1
1	A	117	GLN	2.1
1	A	191	GLU	2.1
1	A	358	ALA	2.1
1	A	455	THR	2.1
1	B	415	ASP	2.1
1	A	336	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	444	LEU	2.1
1	B	451	LEU	2.1
1	B	327	TYR	2.1
1	A	309	CYS	2.1
1	A	399	THR	2.1
1	A	166	VAL	2.1
1	B	132	PRO	2.1
1	B	450	ILE	2.1
1	A	179	THR	2.1
1	A	307	GLY	2.1
1	B	83	SER	2.1
1	A	453	THR	2.0
1	A	58	ALA	2.0
1	A	258	VAL	2.0
1	B	274	VAL	2.0
1	A	340	ARG	2.0
1	A	130	ILE	2.0
1	B	323	LEU	2.0
1	A	326	ASN	2.0
1	B	99	TYR	2.0
1	A	283	ILE	2.0
1	B	192	GLU	2.0
1	B	237	LEU	2.0
1	A	245	GLY	2.0
1	A	368	SER	2.0
1	B	218	THR	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)

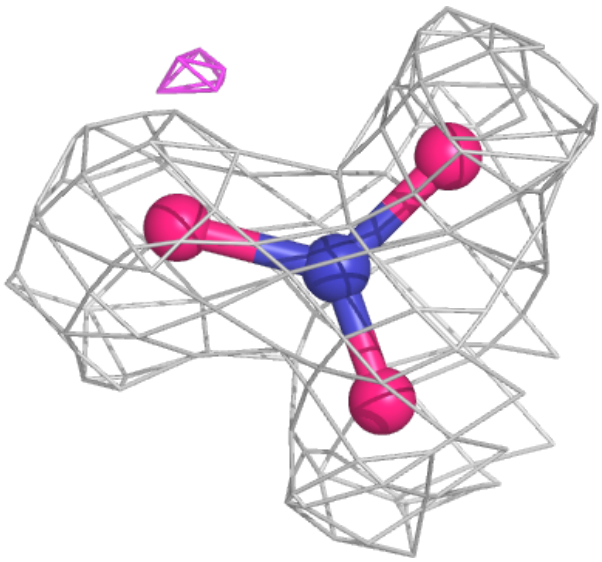
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

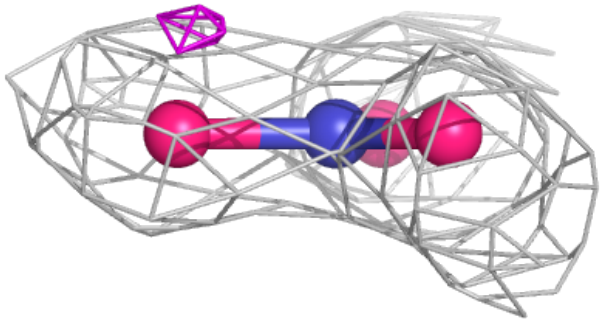
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NO3	B	505	4/4	0.50	0.25	42,46,46,54	0
5	PEG	A	510	7/7	0.52	0.41	48,52,55,58	0
4	NO3	A	505	4/4	0.63	0.21	50,50,52,55	0
5	PEG	B	506	7/7	0.65	0.28	37,46,57,57	0
5	PEG	A	509	7/7	0.67	0.33	45,46,50,53	0
4	NO3	B	504	4/4	0.70	0.27	38,44,45,49	0
5	PEG	B	507	7/7	0.70	0.32	24,31,37,39	0
4	NO3	A	506	4/4	0.77	0.27	50,53,56,58	0
5	PEG	A	508	4/7	0.81	0.19	48,49,51,58	0
3	CTP	A	503	21/29	0.85	0.21	17,23,27,36	0
4	NO3	A	504	4/4	0.86	0.18	29,32,37,38	0
3	CTP	B	503	21/29	0.88	0.22	17,32,38,49	0
4	NO3	A	507	4/4	0.91	0.17	33,37,38,39	0
2	MN	B	502	1/1	0.95	0.07	22,22,22,22	0
2	MN	A	501	1/1	0.95	0.13	24,24,24,24	0
2	MN	A	502	1/1	0.97	0.12	17,17,17,17	0
2	MN	B	501	1/1	0.99	0.09	17,17,17,17	0

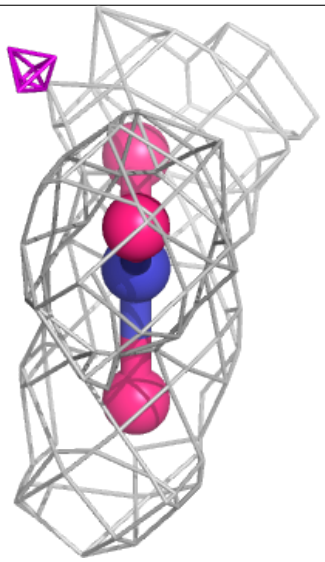
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

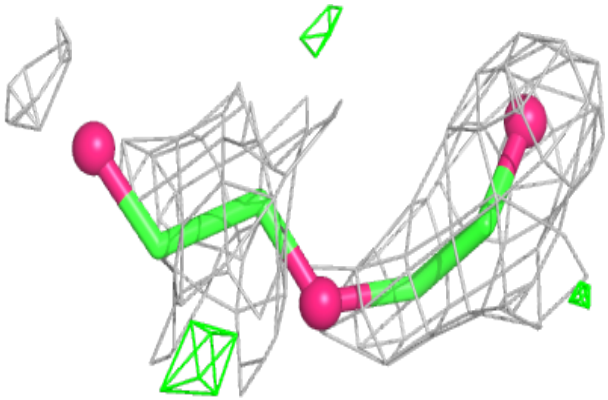


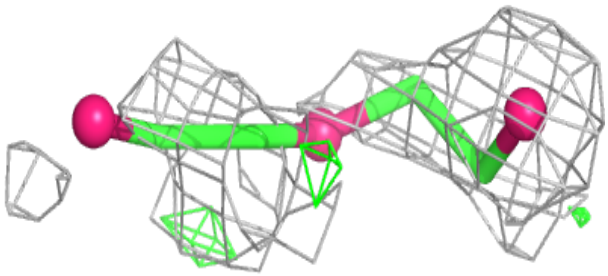


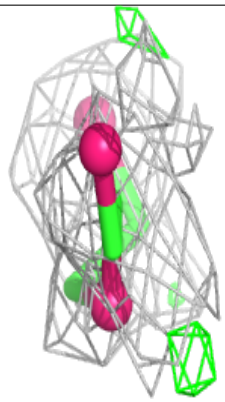


Electron density around PEG A 510:

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

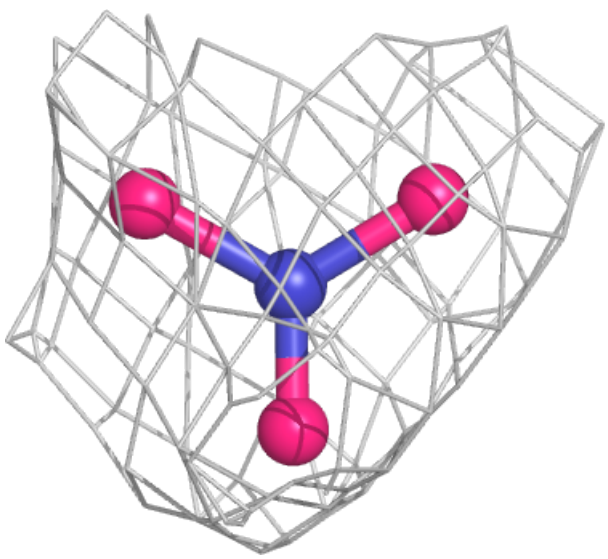


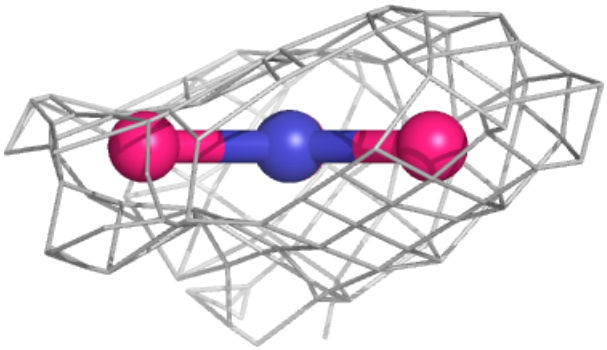


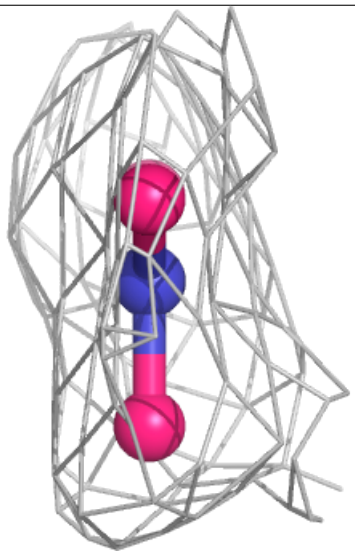


Electron density around NO3 A 505:

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

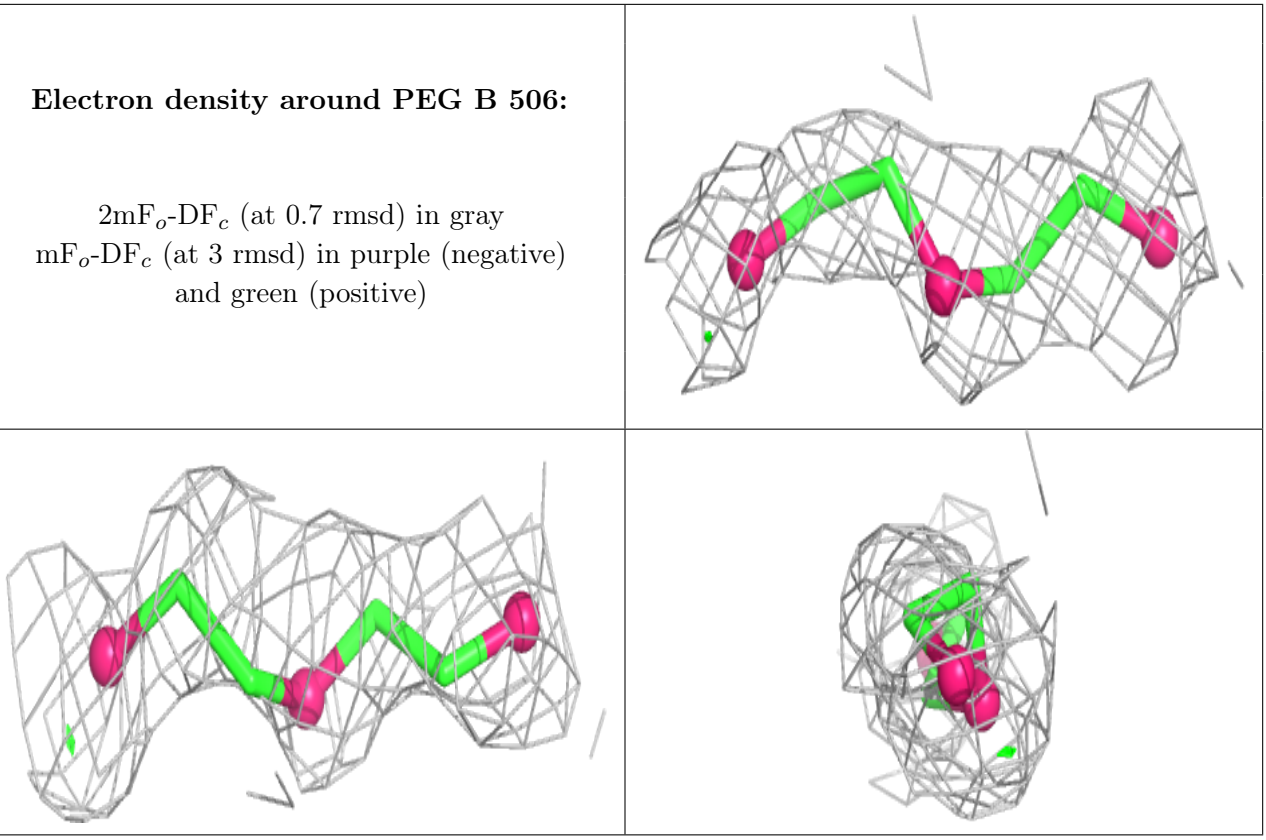






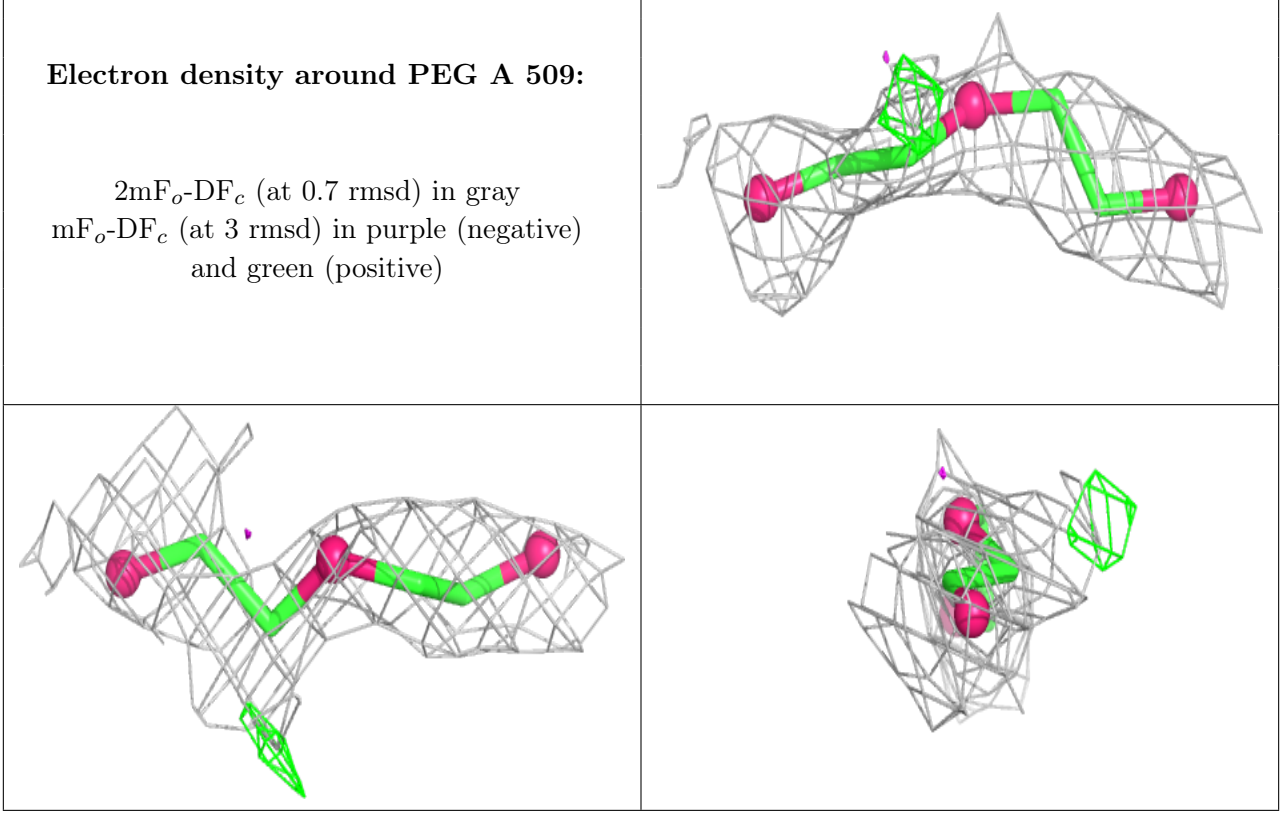
Electron density around PEG B 506:

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



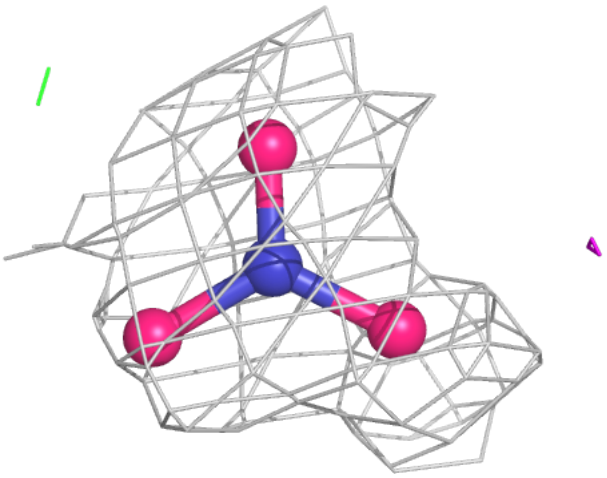
Electron density around PEG A 509:

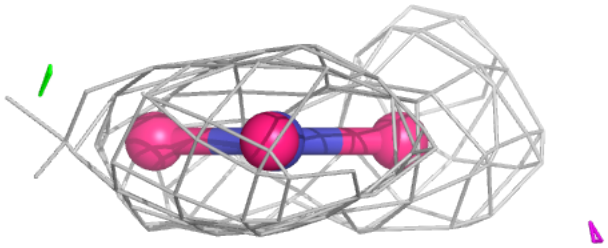
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

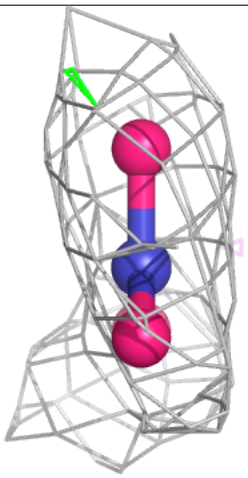


Electron density around NO3 B 504:

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

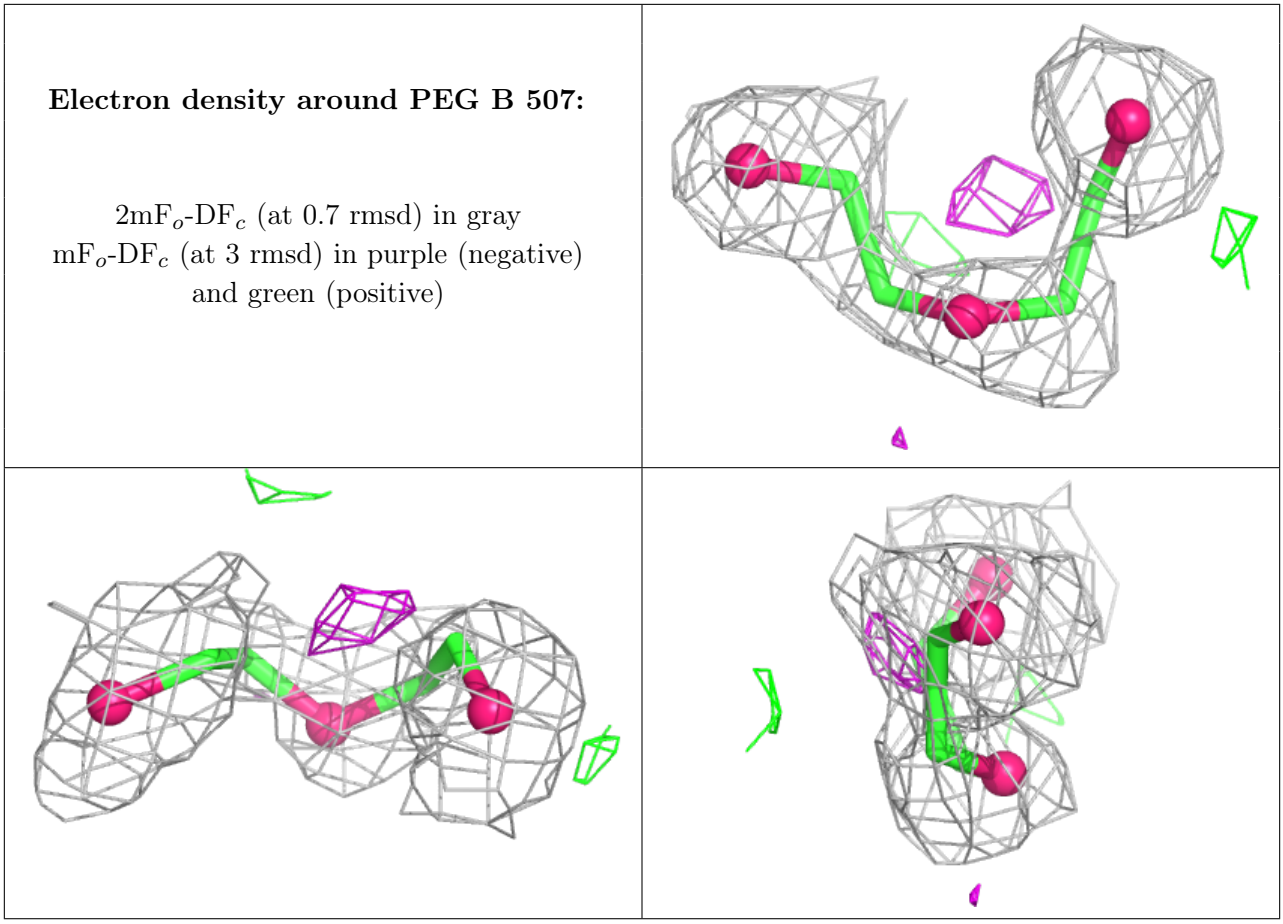






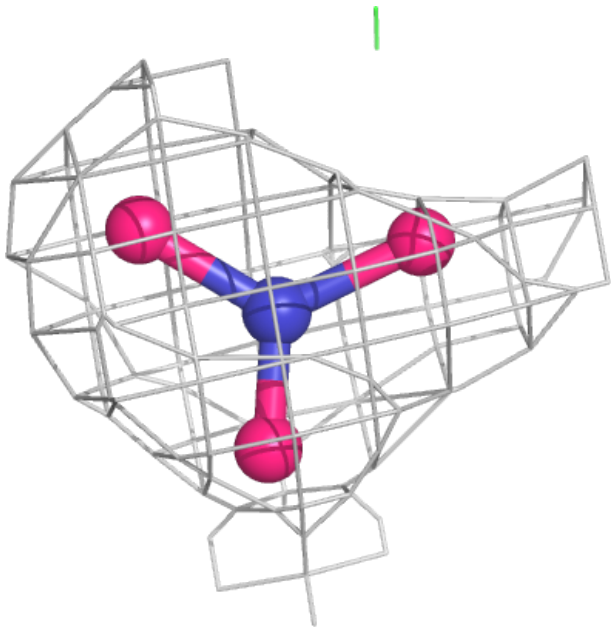
Electron density around PEG B 507:

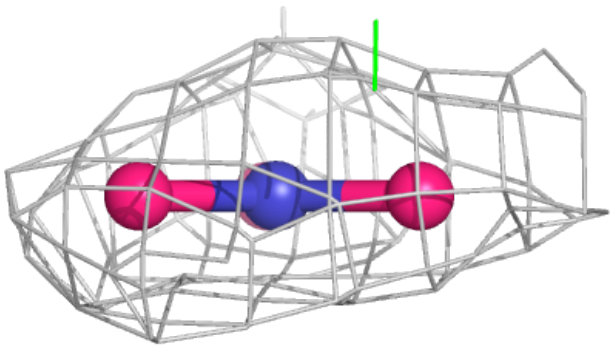
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

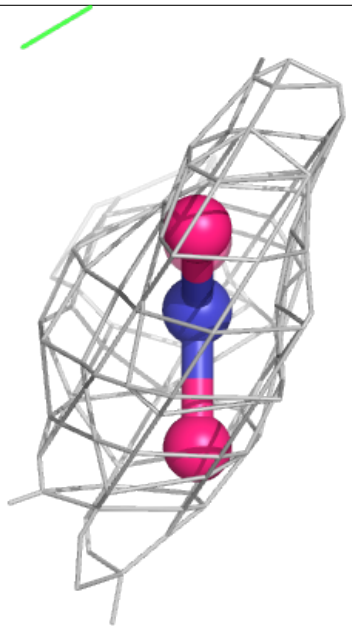


Electron density around NO3 A 506:

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

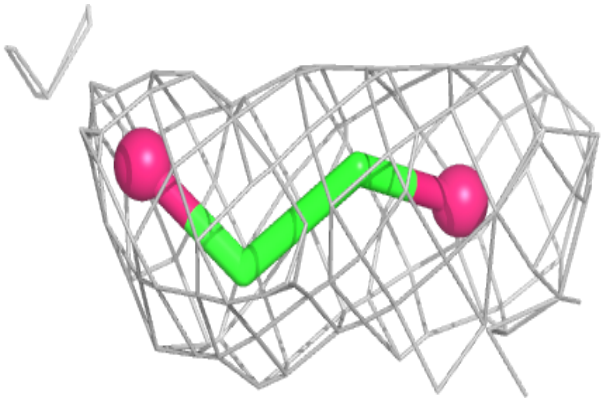


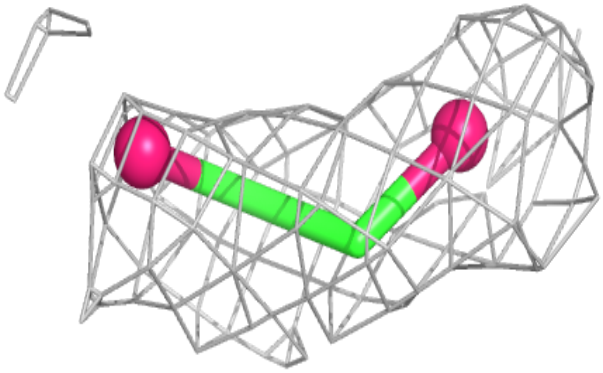


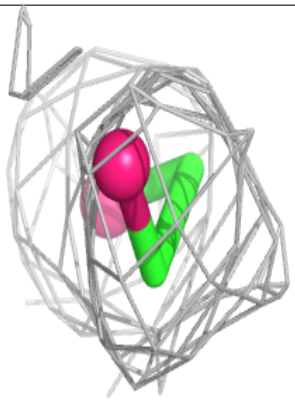


Electron density around PEG A 508:

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

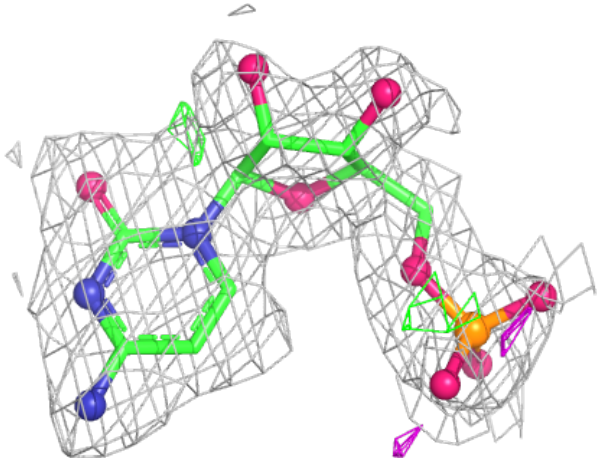


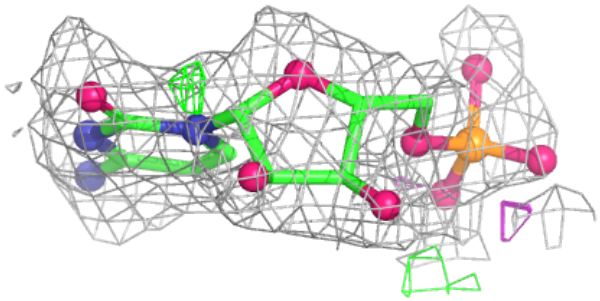


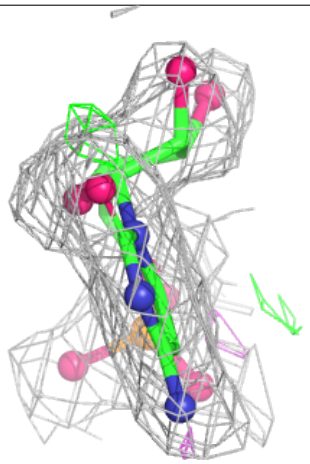


Electron density around CTP A 503:

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

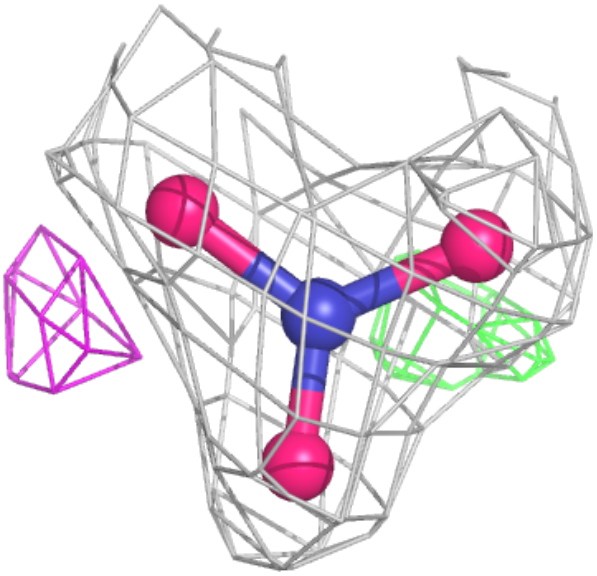


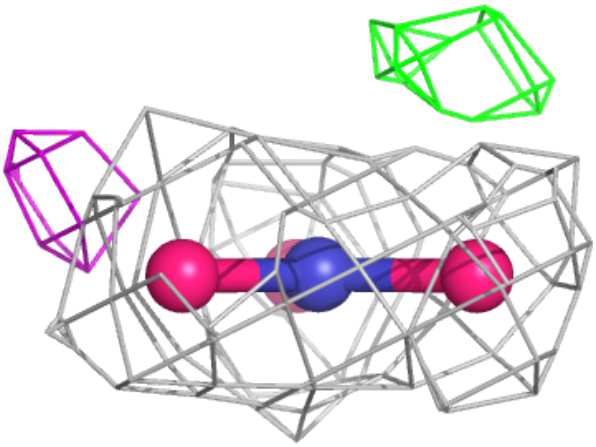


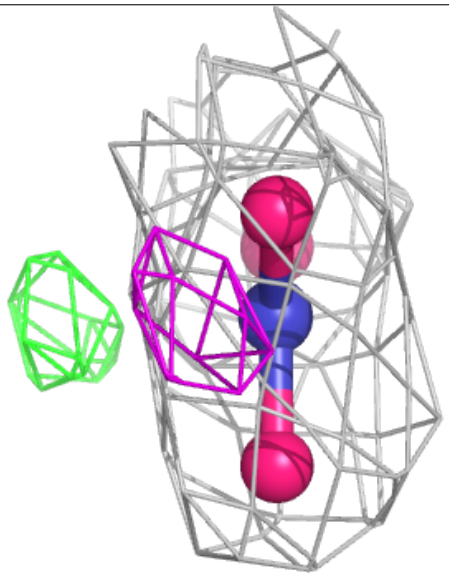


Electron density around NO3 A 504:

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

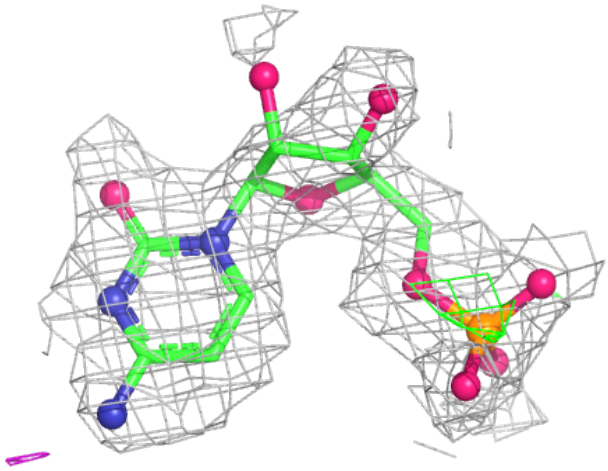


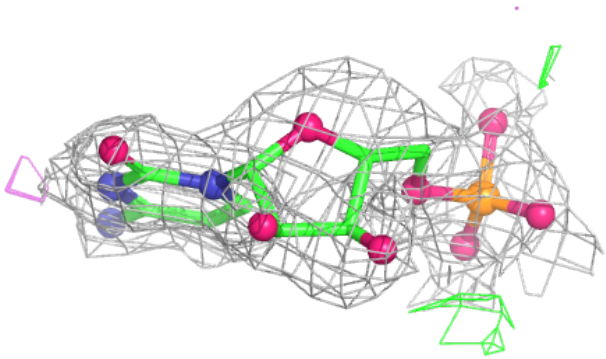


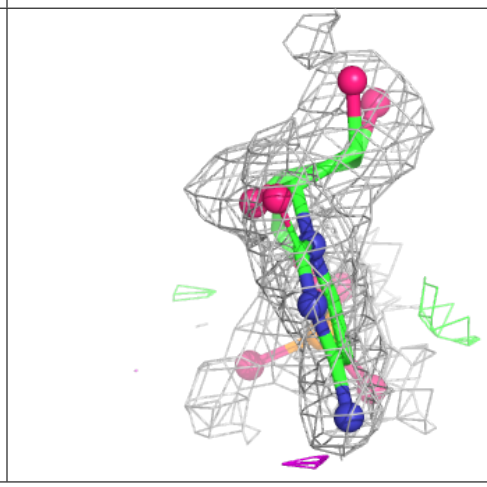


Electron density around CTP B 503:

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

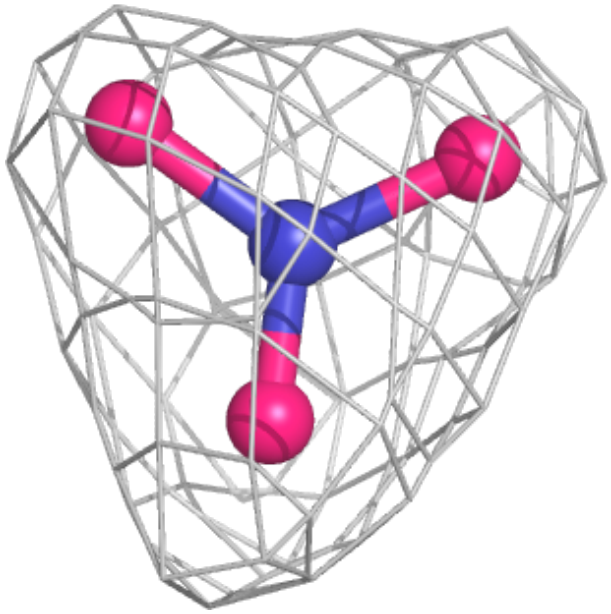


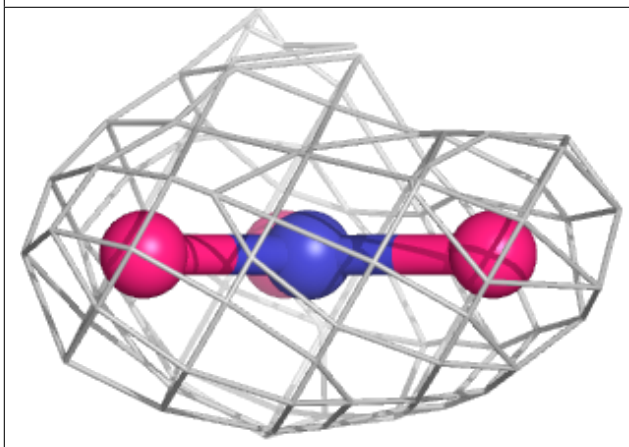


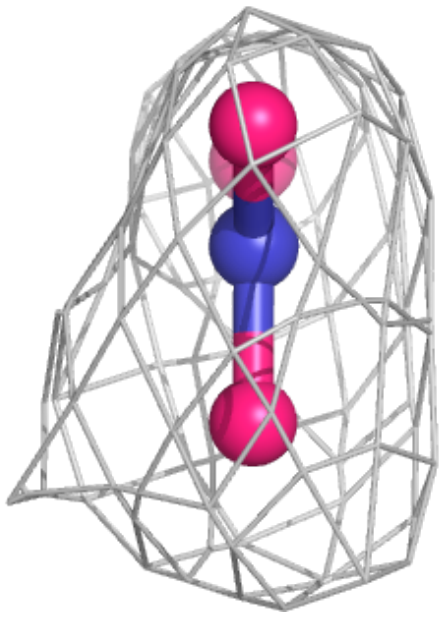


Electron density around NO3 A 507:

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

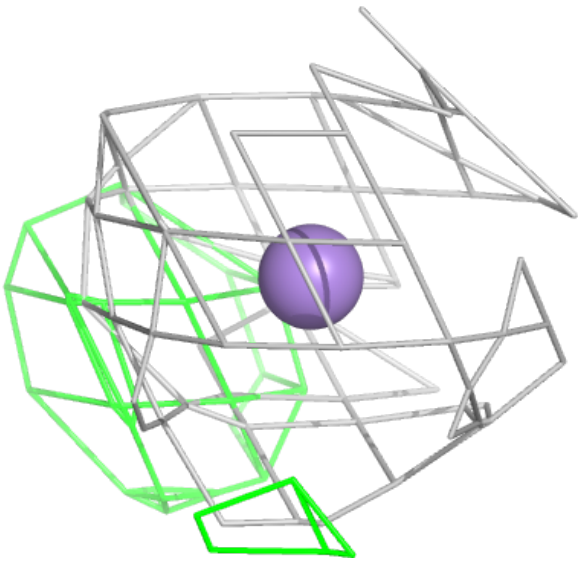


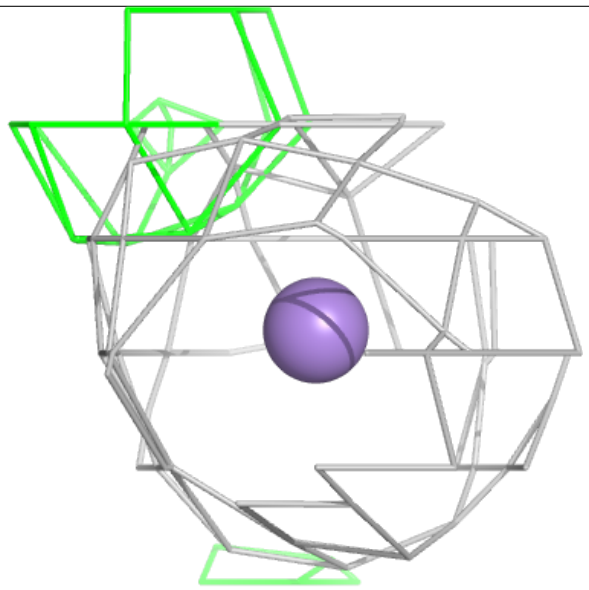


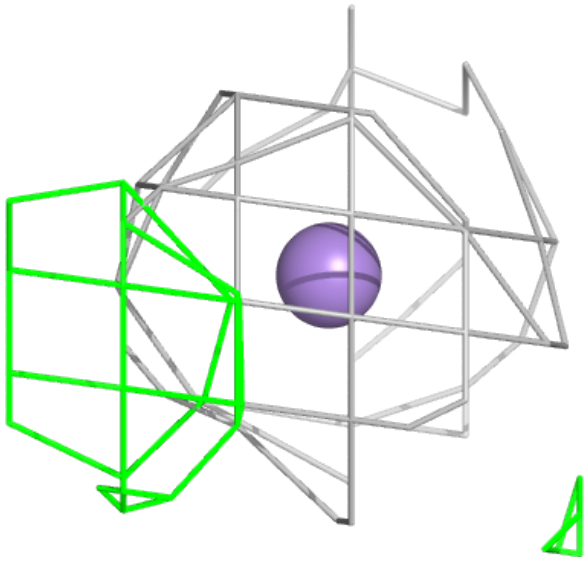


Electron density around MN B 502:

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

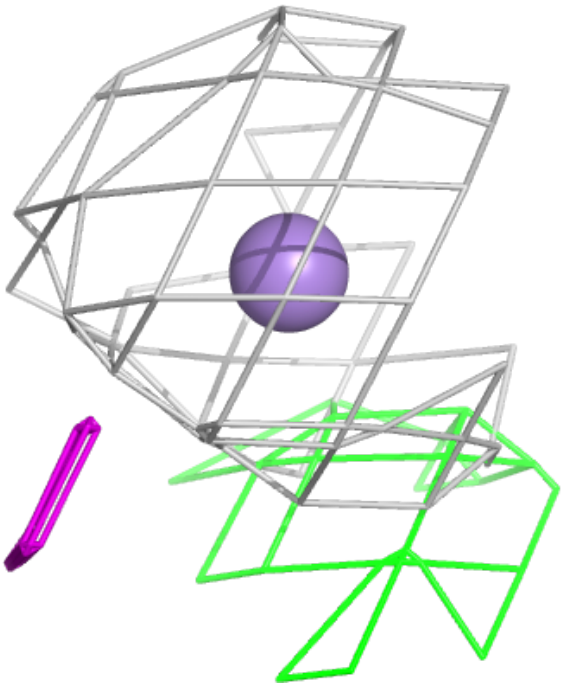


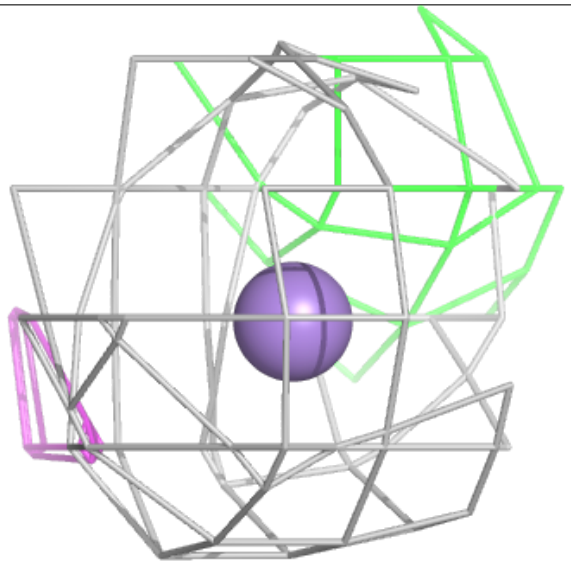


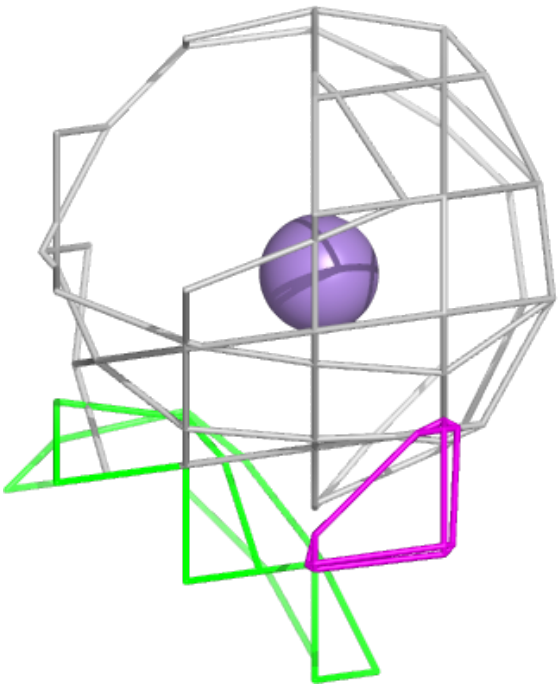


Electron density around MN A 501:

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

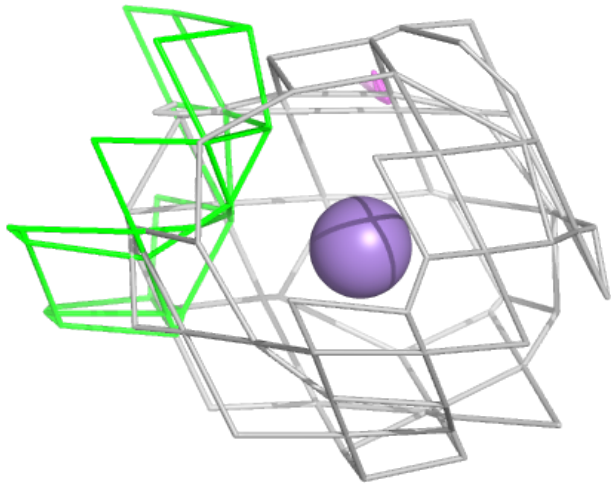


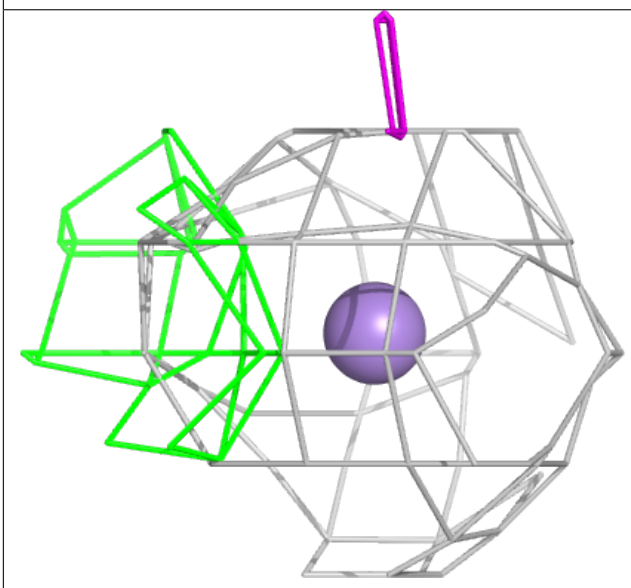


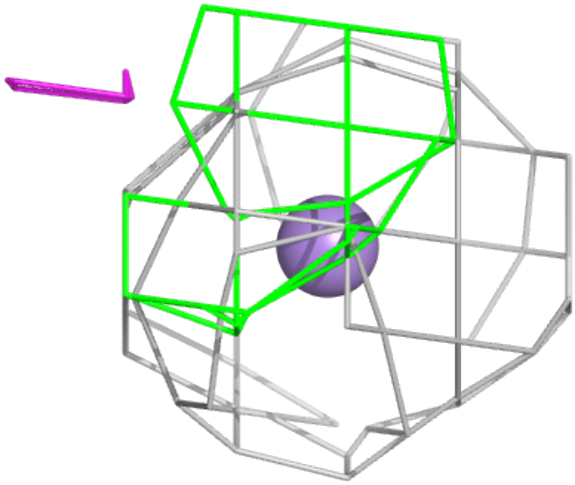


Electron density around MN A 502:

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

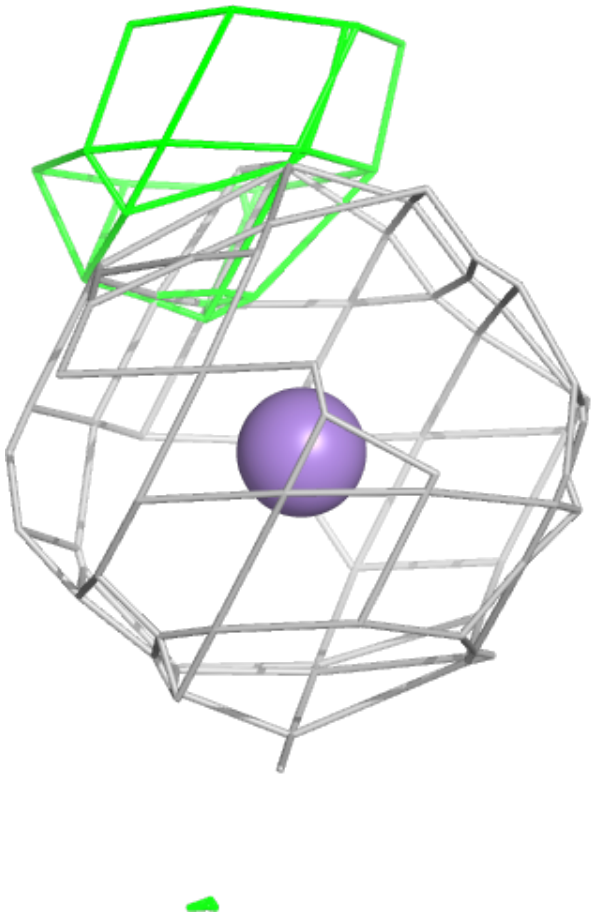


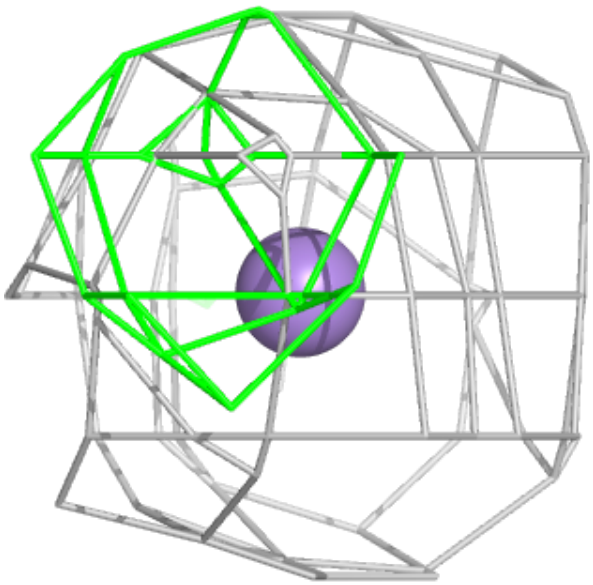


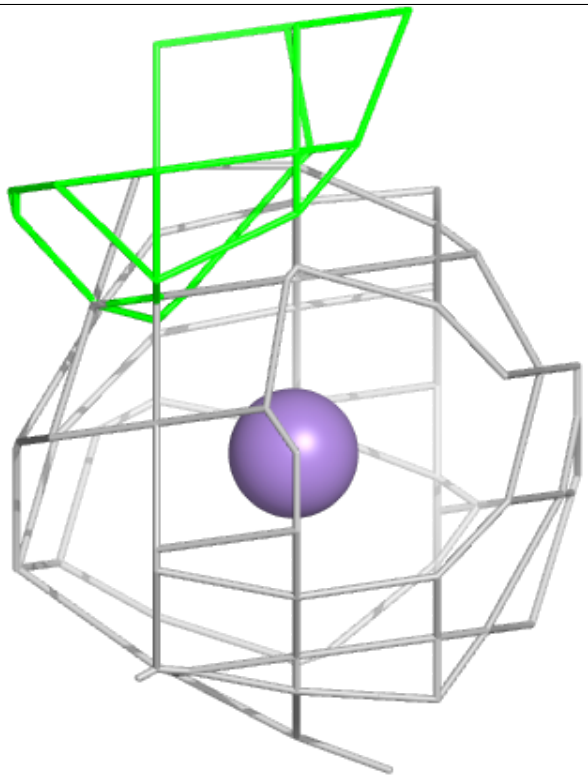


Electron density around MN B 501:

$2mF_o$-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 (i)

There are no such residues in this entry.