



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 09:46 PM BST

PDB ID : 5OLK
Title : Crystal structure of the ATP-cone-containing NrdB from *Leeuwenhoekiella blandensis*
Authors : Hasan, M.; Grinberg, A.R.; Sjoberg, B.M.; Logan, D.T.
Deposited on : 2017-07-28
Resolution : 2.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

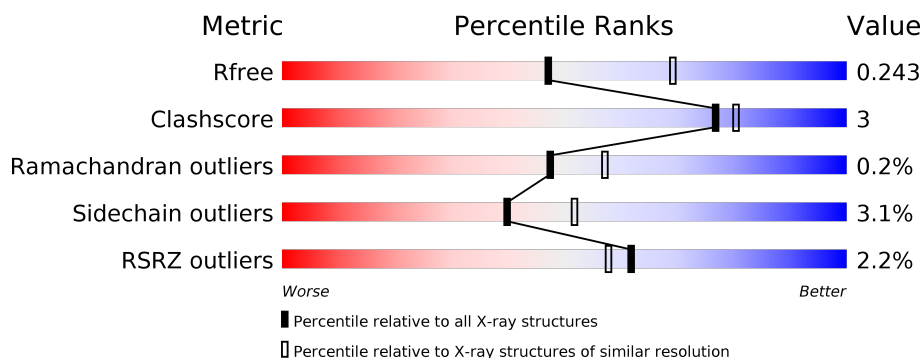
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	430	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 83%, yellow 7%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 83% 7% • 8% </div> </div>
1	B	430	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, green 78%, yellow 13%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 78% 13% 9% </div> </div>
1	C	430	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, green 82%, yellow 9%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 82% 9% • 8% </div> </div>
1	D	430	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, green 84%, yellow 6%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 84% 6% • 9% </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13380 atoms, of which 48 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.

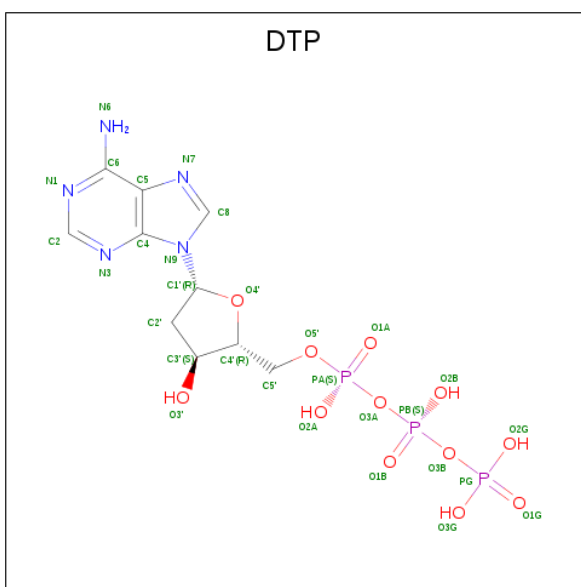
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase, beta subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			3240	2081	533	616	10			
1	B	392	Total	C	N	O	S	0	0	0
			3218	2065	531	612	10			
1	C	394	Total	C	N	O	S	0	0	0
			3235	2076	533	616	10			
1	D	393	Total	C	N	O	S	0	0	0
			3226	2071	532	613	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A3XHF9
A	-1	SER	-	expression tag	UNP A3XHF9
A	0	HIS	-	expression tag	UNP A3XHF9
B	-2	GLY	-	expression tag	UNP A3XHF9
B	-1	SER	-	expression tag	UNP A3XHF9
B	0	HIS	-	expression tag	UNP A3XHF9
C	-2	GLY	-	expression tag	UNP A3XHF9
C	-1	SER	-	expression tag	UNP A3XHF9
C	0	HIS	-	expression tag	UNP A3XHF9
D	-2	GLY	-	expression tag	UNP A3XHF9
D	-1	SER	-	expression tag	UNP A3XHF9
D	0	HIS	-	expression tag	UNP A3XHF9

- Molecule 2 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 30	C 10	N 5	O 12	P 3	0	0
2	A	1	Total 30	C 10	N 5	O 12	P 3	0	0
2	B	1	Total 30	C 10	N 5	O 12	P 3	0	0
2	B	1	Total 30	C 10	N 5	O 12	P 3	0	0
2	C	1	Total 30	C 10	N 5	O 12	P 3	0	0
2	C	1	Total 30	C 10	N 5	O 12	P 3	0	0
2	D	1	Total 30	C 10	N 5	O 12	P 3	0	0
2	D	1	Total 30	C 10	N 5	O 12	P 3	0	0

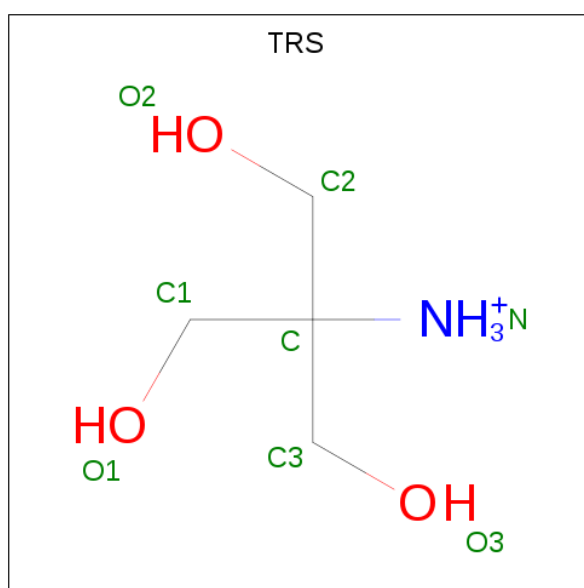
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by author).

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

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			20	4	12	1	3		
5	B	1	Total	C	H	N	O	0	0
			20	4	12	1	3		
5	C	1	Total	C	H	N	O	0	0
			20	4	12	1	3		
5	D	1	Total	C	H	N	O	0	0
			20	4	12	1	3		

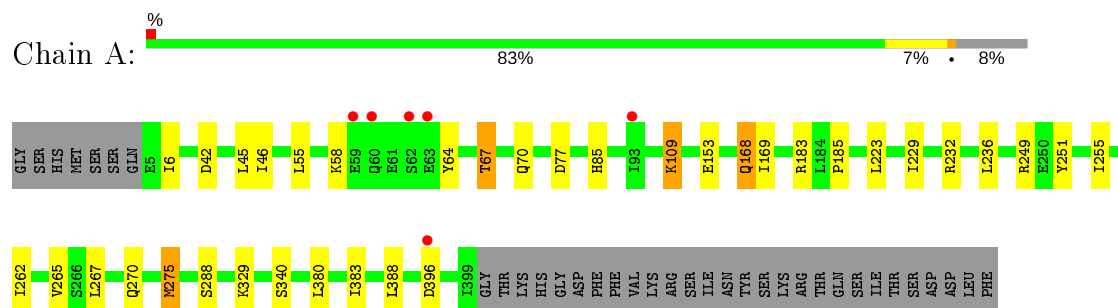
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	33	Total 33	O 33	0	0
6	B	31	Total 31	O 31	0	0
6	C	33	Total 33	O 33	0	0
6	D	32	Total 32	O 32	0	0

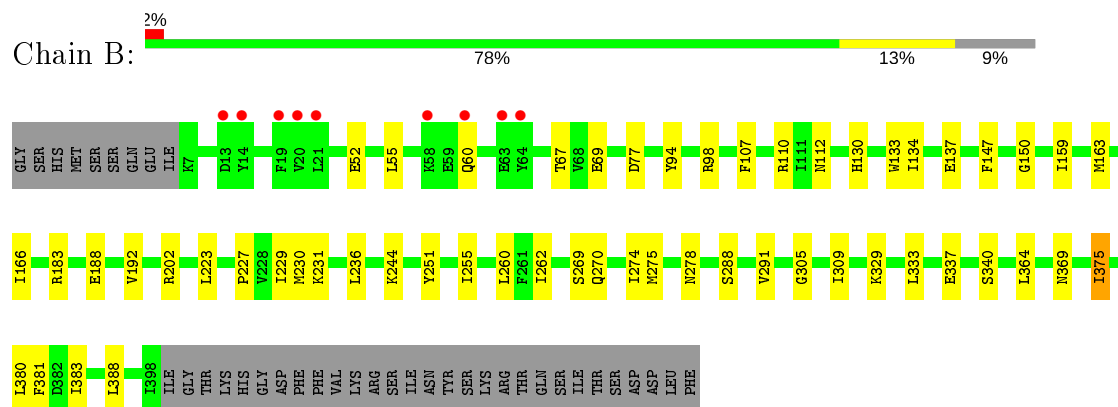
3 Residue-property plots [i](#)

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.

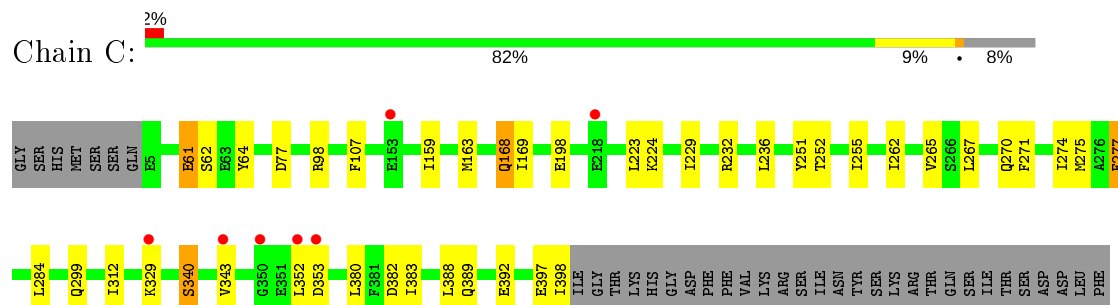
- Molecule 1: Ribonucleoside-diphosphate reductase, beta subunit 1



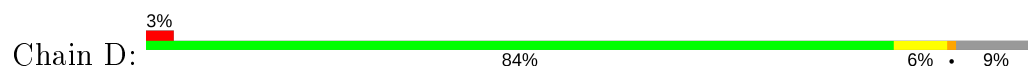
- Molecule 1: Ribonucleoside-diphosphate reductase, beta subunit 1

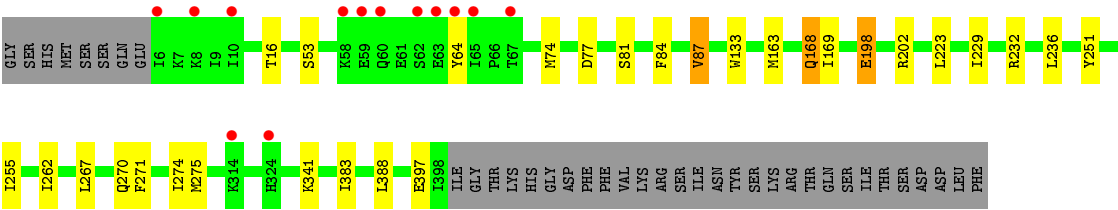


- Molecule 1: Ribonucleoside-diphosphate reductase, beta subunit 1



- Molecule 1: Ribonucleoside-diphosphate reductase, beta subunit 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	74.00Å 90.54Å 90.95Å 110.78° 98.99° 114.11°	Depositor
Resolution (Å)	44.70 – 2.45 44.74 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.8 (44.70-2.45) 97.8 (44.74-2.45)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.45Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.205 , 0.238 0.212 , 0.243	Depositor DCC
R_{free} test set	3353 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	52.6	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13380	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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: TRS, DTP, MG, MN

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	0.51	0/3308	0.65	0/4460
1	B	0.50	0/3286	0.64	0/4430
1	C	0.49	0/3303	0.65	0/4453
1	D	0.51	0/3294	0.64	0/4441
All	All	0.50	0/13191	0.65	0/17784

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3240	0	3205	13	0
1	B	3218	0	3181	29	0
1	C	3235	0	3198	22	0
1	D	3226	0	3192	17	0
2	A	60	0	24	0	0
2	B	60	0	24	0	0
2	C	60	0	24	0	0
2	D	60	0	24	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	8	12	12	0	0
5	B	8	12	12	3	0
5	C	8	12	12	1	0
5	D	8	12	12	0	0
6	A	33	0	0	0	0
6	B	31	0	0	1	0
6	C	33	0	0	0	0
6	D	32	0	0	0	0
All	All	13332	48	12920	78	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 3.

All (78) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:PHE:O	5:B:1006:TRS:H21	1.63	0.97
1:D:84:PHE:HB3	1:D:87:VAL:HG13	1.62	0.82
1:B:107:PHE:O	5:B:1006:TRS:C2	2.31	0.78
1:D:271:PHE:O	1:D:275:MET:HG2	1.83	0.77
1:C:252:THR:HG22	1:C:312:ILE:HD13	1.66	0.76
1:A:67:THR:HG22	1:A:70:GLN:H	1.51	0.75
1:B:236:LEU:HD23	1:B:262:ILE:HD12	1.67	0.75
1:A:236:LEU:HD23	1:A:262:ILE:HD12	1.69	0.74
1:B:110:ARG:HD2	1:B:112:ASN:O	1.88	0.73
1:B:260:LEU:HD11	1:B:375:ILE:HG12	1.70	0.73
1:C:340:SER:O	1:C:343:VAL:HG22	1.88	0.72
1:D:236:LEU:HD23	1:D:262:ILE:HD12	1.70	0.72
1:C:236:LEU:HD23	1:C:262:ILE:HD12	1.70	0.72
1:B:305:GLY:O	1:B:309:ILE:HD12	1.92	0.70
1:C:198:GLU:HG3	1:D:198:GLU:HG2	1.77	0.66
1:B:67:THR:HG22	1:B:69:GLU:H	1.59	0.66
1:C:271:PHE:O	1:C:275:MET:HG2	1.98	0.63
1:B:369:ASN:HD21	1:B:381:PHE:H	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:LYS:HG2	1:C:380:LEU:HD13	1.83	0.60
1:B:269:SER:HB3	1:B:364:LEU:HD21	1.84	0.60
1:A:109:LYS:HD2	1:A:185:PRO:HB2	1.84	0.59
1:B:163:MET:HE3	1:B:274:ILE:HG13	1.86	0.57
1:C:252:THR:HG21	1:C:312:ILE:HG21	1.89	0.54
1:D:251:TYR:CE2	1:D:255:ILE:HD11	2.43	0.54
1:A:275:MET:HE1	1:A:288:SER:O	2.07	0.54
1:B:251:TYR:CE2	1:B:255:ILE:HD11	2.42	0.54
1:A:251:TYR:CE2	1:A:255:ILE:HD11	2.43	0.53
1:C:251:TYR:CE2	1:C:255:ILE:HD11	2.43	0.53
1:A:168:GLN:OE1	1:A:232:ARG:HD3	2.09	0.53
1:C:168:GLN:HG2	1:C:232:ARG:HH11	1.74	0.52
1:D:383:ILE:HG21	1:D:388:LEU:HD22	1.92	0.52
1:D:53:SER:HB2	1:D:74:MET:CE	2.40	0.52
1:A:383:ILE:HG21	1:A:388:LEU:HD22	1.92	0.52
1:A:329:LYS:HG3	1:A:380:LEU:HD21	1.92	0.51
1:D:168:GLN:HG2	1:D:232:ARG:HH11	1.75	0.51
1:C:163:MET:HA	1:C:163:MET:HE2	1.92	0.51
1:D:163:MET:HA	1:D:163:MET:HE2	1.93	0.50
1:B:163:MET:HE1	1:B:166:ILE:HD12	1.92	0.50
1:C:383:ILE:HG21	1:C:388:LEU:HD22	1.92	0.50
1:B:383:ILE:HG21	1:B:388:LEU:HD22	1.92	0.50
1:C:299:GLN:HG2	1:C:398:ILE:HD13	1.93	0.50
1:B:52:GLU:HA	1:B:55:LEU:HD12	1.94	0.50
1:B:147:PHE:HZ	1:B:159:ILE:HG21	1.77	0.50
1:A:6:ILE:HG12	1:A:55:LEU:HD23	1.93	0.50
1:B:107:PHE:O	5:B:1006:TRS:H12	2.12	0.50
1:B:227:PRO:O	1:B:231:LYS:HG2	2.13	0.49
1:B:134:ILE:O	1:B:137:GLU:HG2	2.14	0.47
1:D:163:MET:HE3	1:D:274:ILE:HD11	1.97	0.46
1:D:133:TRP:O	1:D:202:ARG:HD2	2.15	0.46
1:B:278:ASN:HB2	1:B:288:SER:OG	2.16	0.46
1:D:53:SER:HB2	1:D:74:MET:HE1	1.98	0.46
1:B:130:HIS:HB2	6:B:1125:HOH:O	2.14	0.45
1:B:227:PRO:HA	1:B:230:MET:CE	2.46	0.45
1:C:163:MET:HE3	1:C:274:ILE:HD11	1.97	0.45
1:C:163:MET:HE3	1:C:274:ILE:CD1	2.46	0.45
1:D:163:MET:HE3	1:D:274:ILE:CD1	2.47	0.45
1:C:159:ILE:HD11	1:C:277:PHE:CD2	2.52	0.45
1:C:198:GLU:CG	1:D:198:GLU:HG2	2.46	0.44
1:B:133:TRP:O	1:B:202:ARG:HD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:PHE:HB3	5:C:1006:TRS:H31	2.00	0.43
1:B:275:MET:HE2	1:B:291:VAL:HG12	2.01	0.43
1:A:169:ILE:HB	1:A:267:LEU:HD21	2.00	0.43
1:C:61:GLU:HB3	1:C:64:TYR:HB2	2.01	0.43
1:A:85:HIS:HE1	1:D:81:SER:OG	2.01	0.43
1:C:389:GLN:HA	1:C:392:GLU:HG2	2.00	0.42
1:B:188:GLU:O	1:B:192:VAL:HG23	2.19	0.42
1:A:42:ASP:O	1:A:46:ILE:HG12	2.19	0.42
1:C:169:ILE:HD11	1:C:236:LEU:CD1	2.50	0.42
1:B:329:LYS:HG2	1:B:380:LEU:HD13	2.03	0.41
1:B:227:PRO:HA	1:B:230:MET:HE3	2.03	0.41
1:C:169:ILE:HB	1:C:267:LEU:HD21	2.02	0.41
1:D:169:ILE:HB	1:D:267:LEU:HD21	2.03	0.41
1:A:223:LEU:HG	1:A:229:ILE:HG13	2.03	0.41
1:B:333:LEU:O	1:B:337:GLU:HG2	2.21	0.41
1:B:94:TYR:O	1:B:98:ARG:HG2	2.20	0.40
1:C:223:LEU:HG	1:C:229:ILE:HG13	2.03	0.40
1:B:223:LEU:HG	1:B:229:ILE:HG13	2.04	0.40
1:D:223:LEU:HG	1:D:229:ILE:HG13	2.03	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	393/430 (91%)	385 (98%)	7 (2%)	1 (0%)	41	49
1	B	390/430 (91%)	383 (98%)	6 (2%)	1 (0%)	41	49
1	C	392/430 (91%)	380 (97%)	11 (3%)	1 (0%)	41	49
1	D	391/430 (91%)	382 (98%)	9 (2%)	0	100	100
All	All	1566/1720 (91%)	1530 (98%)	33 (2%)	3 (0%)	47	57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	LYS
1	C	62	SER
1	B	150	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	354/387 (92%)	340 (96%)	14 (4%)	31	41
1	B	352/387 (91%)	345 (98%)	7 (2%)	55	67
1	C	354/387 (92%)	340 (96%)	14 (4%)	31	41
1	D	353/387 (91%)	344 (98%)	9 (2%)	47	60
All	All	1413/1548 (91%)	1369 (97%)	44 (3%)	40	52

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	64	TYR
1	A	67	THR
1	A	77	ASP
1	A	109	LYS
1	A	153	GLU
1	A	168	GLN
1	A	183	ARG
1	A	249	ARG
1	A	265	VAL
1	A	270	GLN
1	A	275	MET
1	A	340	SER
1	A	396	ASP
1	B	60	GLN
1	B	77	ASP
1	B	183	ARG

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Mol	Chain	Res	Type
1	B	244	LYS
1	B	270	GLN
1	B	340	SER
1	B	375	ILE
1	C	61	GLU
1	C	77	ASP
1	C	98	ARG
1	C	168	GLN
1	C	224	LYS
1	C	265	VAL
1	C	270	GLN
1	C	277	PHE
1	C	284	LEU
1	C	340	SER
1	C	352	LEU
1	C	353	ASP
1	C	382	ASP
1	C	397	GLU
1	D	16	THR
1	D	64	TYR
1	D	77	ASP
1	D	87	VAL
1	D	168	GLN
1	D	198	GLU
1	D	270	GLN
1	D	341	LYS
1	D	397	GLU

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

Mol	Chain	Res	Type
1	A	85	HIS
1	A	217	ASN
1	B	57	ASN
1	B	85	HIS
1	B	145	GLN
1	B	325	ASN
1	B	369	ASN
1	C	122	ASN
1	C	289	ASN
1	C	334	ASN
1	D	85	HIS

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Mol	Chain	Res	Type
1	D	122	ASN
1	D	217	ASN
1	D	361	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 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
2	DTP	A	1001	3	26,32,32	1.45	4 (15%)	30,50,50	0.83	1 (3%)
2	DTP	D	1001	3	26,32,32	1.43	5 (19%)	30,50,50	0.82	0
2	DTP	B	1001	3	26,32,32	1.45	4 (15%)	30,50,50	0.73	0
2	DTP	B	1002	3	26,32,32	1.48	3 (11%)	30,50,50	0.79	0
2	DTP	D	1002	3	26,32,32	1.40	4 (15%)	30,50,50	0.91	2 (6%)
5	TRS	D	1006	-	7,7,7	0.23	0	9,9,9	0.29	0
5	TRS	A	1006	-	7,7,7	0.28	0	9,9,9	0.29	0
5	TRS	C	1006	-	7,7,7	0.28	0	9,9,9	0.24	0
5	TRS	B	1006	-	7,7,7	0.25	0	9,9,9	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DTP	C	1002	3	26,32,32	1.46	3 (11%)	30,50,50	0.78	0
2	DTP	A	1002	3	26,32,32	1.66	4 (15%)	30,50,50	0.65	0
2	DTP	C	1001	3	26,32,32	1.48	6 (23%)	30,50,50	0.79	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DTP	A	1001	3	-	2/18/34/34	0/3/3/3
2	DTP	D	1001	3	-	2/18/34/34	0/3/3/3
2	DTP	B	1001	3	-	2/18/34/34	0/3/3/3
2	DTP	B	1002	3	-	1/18/34/34	0/3/3/3
2	DTP	D	1002	3	-	2/18/34/34	0/3/3/3
5	TRS	D	1006	-	-	3/9/9/9	-
5	TRS	A	1006	-	-	3/9/9/9	-
5	TRS	C	1006	-	-	4/9/9/9	-
5	TRS	B	1006	-	-	3/9/9/9	-
2	DTP	C	1002	3	-	2/18/34/34	0/3/3/3
2	DTP	A	1002	3	-	1/18/34/34	0/3/3/3
2	DTP	C	1001	3	-	2/18/34/34	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1002	DTP	C2-N3	4.41	1.39	1.32
2	A	1002	DTP	C4-N3	4.12	1.41	1.35
2	D	1002	DTP	C4-N3	3.93	1.41	1.35
2	A	1002	DTP	C2-N3	3.49	1.37	1.32
2	D	1001	DTP	C4-N3	3.36	1.40	1.35
2	C	1001	DTP	C4-N3	3.35	1.40	1.35
2	C	1002	DTP	C4-N3	3.29	1.40	1.35
2	A	1001	DTP	C4-N3	3.25	1.40	1.35
2	A	1001	DTP	PG-O1G	3.24	1.61	1.50
2	B	1001	DTP	C4-N3	3.23	1.40	1.35
2	B	1002	DTP	C4-N3	3.22	1.40	1.35
2	A	1001	DTP	C2-N3	3.16	1.37	1.32
2	D	1001	DTP	C2-N3	3.15	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	DTP	C2-N3	3.03	1.37	1.32
2	B	1001	DTP	C2-N3	3.01	1.37	1.32
2	C	1002	DTP	O3'-C3'	-2.95	1.37	1.43
2	A	1002	DTP	C2-N1	2.72	1.39	1.33
2	A	1002	DTP	PG-O1G	2.69	1.59	1.50
2	B	1001	DTP	C2-N1	2.66	1.38	1.33
2	C	1001	DTP	C2-N1	2.61	1.38	1.33
2	D	1002	DTP	C2-N3	2.50	1.36	1.32
2	C	1002	DTP	C2-N3	2.48	1.36	1.32
2	D	1002	DTP	C2-N1	2.48	1.38	1.33
2	D	1001	DTP	PG-O1G	2.42	1.58	1.50
2	B	1002	DTP	C2-N1	2.41	1.38	1.33
2	D	1002	DTP	O3'-C3'	-2.34	1.38	1.43
2	D	1001	DTP	C2-N1	2.33	1.38	1.33
2	A	1001	DTP	C2-N1	2.19	1.38	1.33
2	D	1001	DTP	C5'-C4'	2.18	1.58	1.51
2	C	1001	DTP	C5'-C4'	2.15	1.58	1.51
2	C	1001	DTP	PA-O1A	2.13	1.58	1.50
2	B	1001	DTP	C5'-C4'	2.05	1.58	1.51
2	C	1001	DTP	PG-O2G	2.02	1.62	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1002	DTP	O3G-PG-O3B	3.32	115.76	104.64
2	A	1001	DTP	O3G-PG-O3B	2.32	112.40	104.64
2	D	1002	DTP	C4-C5-N7	2.02	111.50	109.40

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1006	TRS	C2-C-C1-O1
5	B	1006	TRS	C3-C-C1-O1
5	B	1006	TRS	N-C-C1-O1
5	D	1006	TRS	C2-C-C1-O1
2	C	1001	DTP	PB-O3B-PG-O1G
2	B	1001	DTP	PB-O3B-PG-O1G
5	D	1006	TRS	N-C-C1-O1
5	C	1006	TRS	N-C-C1-O1
5	A	1006	TRS	N-C-C3-O3
2	C	1002	DTP	PB-O3B-PG-O1G

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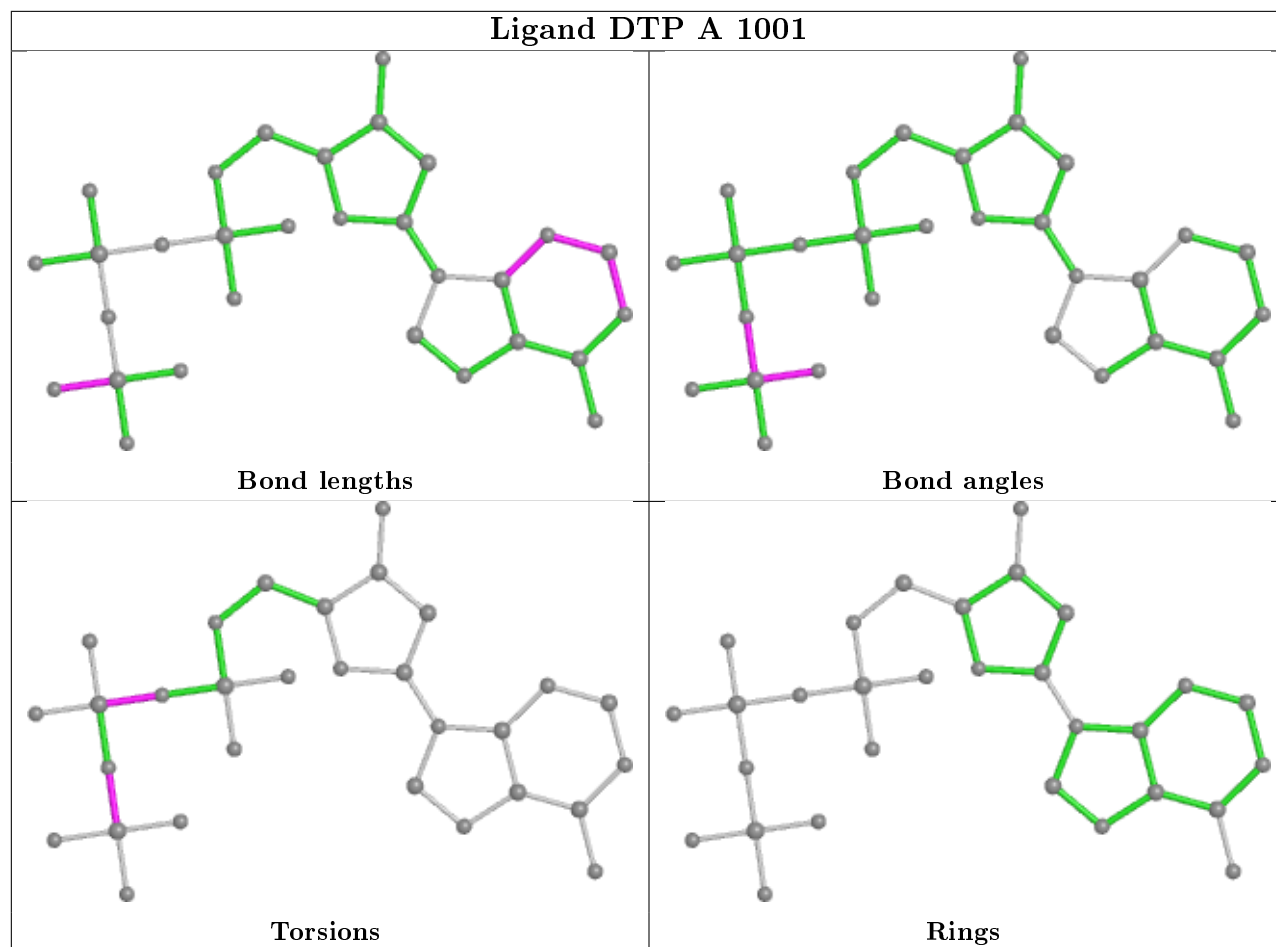
Mol	Chain	Res	Type	Atoms
2	C	1002	DTP	PA-O3A-PB-O2B
2	C	1001	DTP	PA-O3A-PB-O2B
2	D	1001	DTP	PA-O3A-PB-O2B
2	A	1002	DTP	PA-O3A-PB-O2B
2	A	1001	DTP	PA-O3A-PB-O2B
5	D	1006	TRS	C3-C-C1-O1
5	C	1006	TRS	C1-C-C3-O3
5	C	1006	TRS	C2-C-C3-O3
5	A	1006	TRS	C1-C-C3-O3
5	A	1006	TRS	C2-C-C3-O3
2	D	1002	DTP	PA-O3A-PB-O1B
2	B	1002	DTP	PA-O3A-PB-O1B
2	D	1001	DTP	PB-O3B-PG-O3G
2	A	1001	DTP	PB-O3B-PG-O2G
5	C	1006	TRS	N-C-C3-O3
2	D	1002	DTP	PA-O3A-PB-O2B
2	B	1001	DTP	PA-O3A-PB-O1B

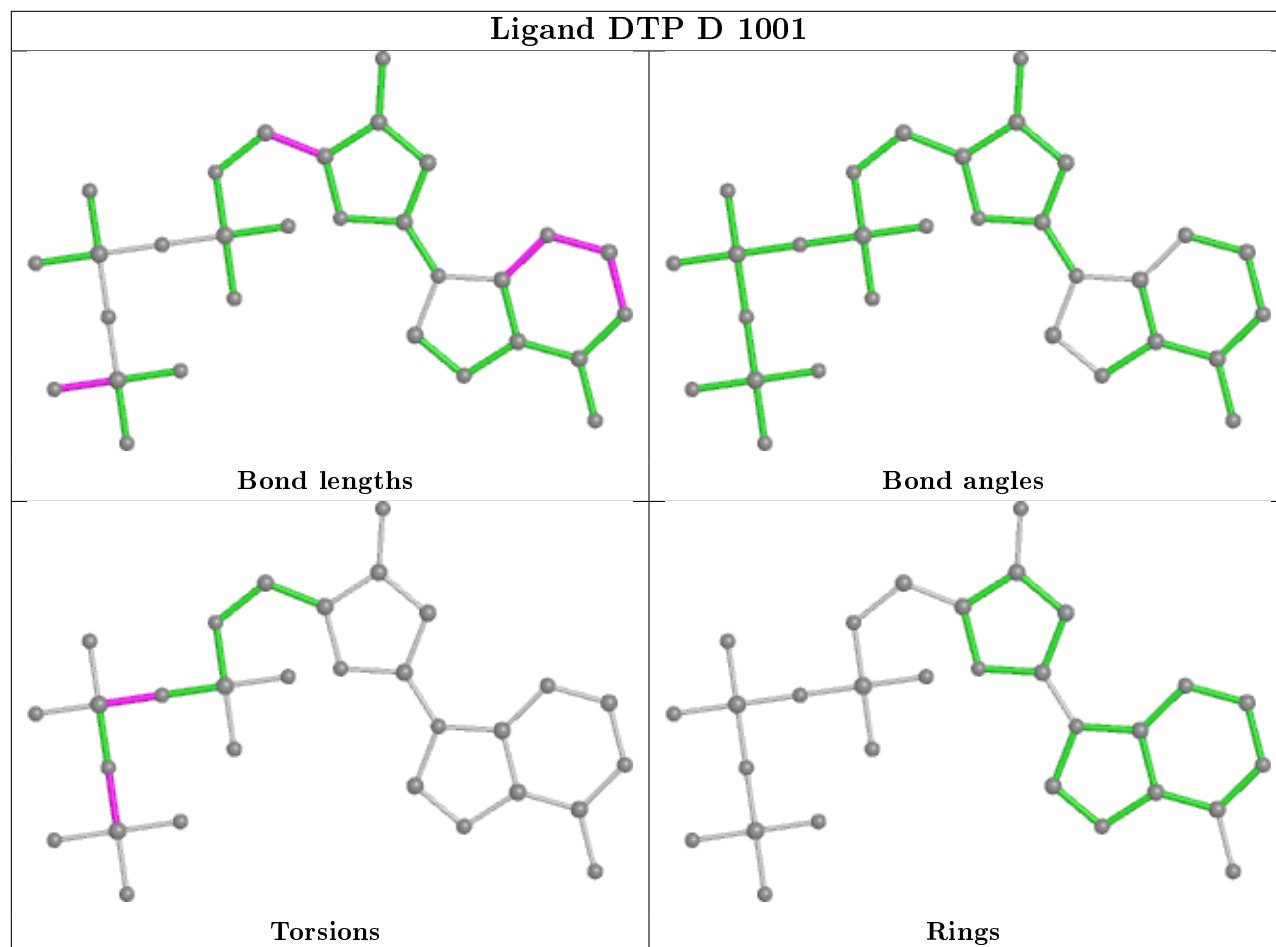
There are no ring outliers.

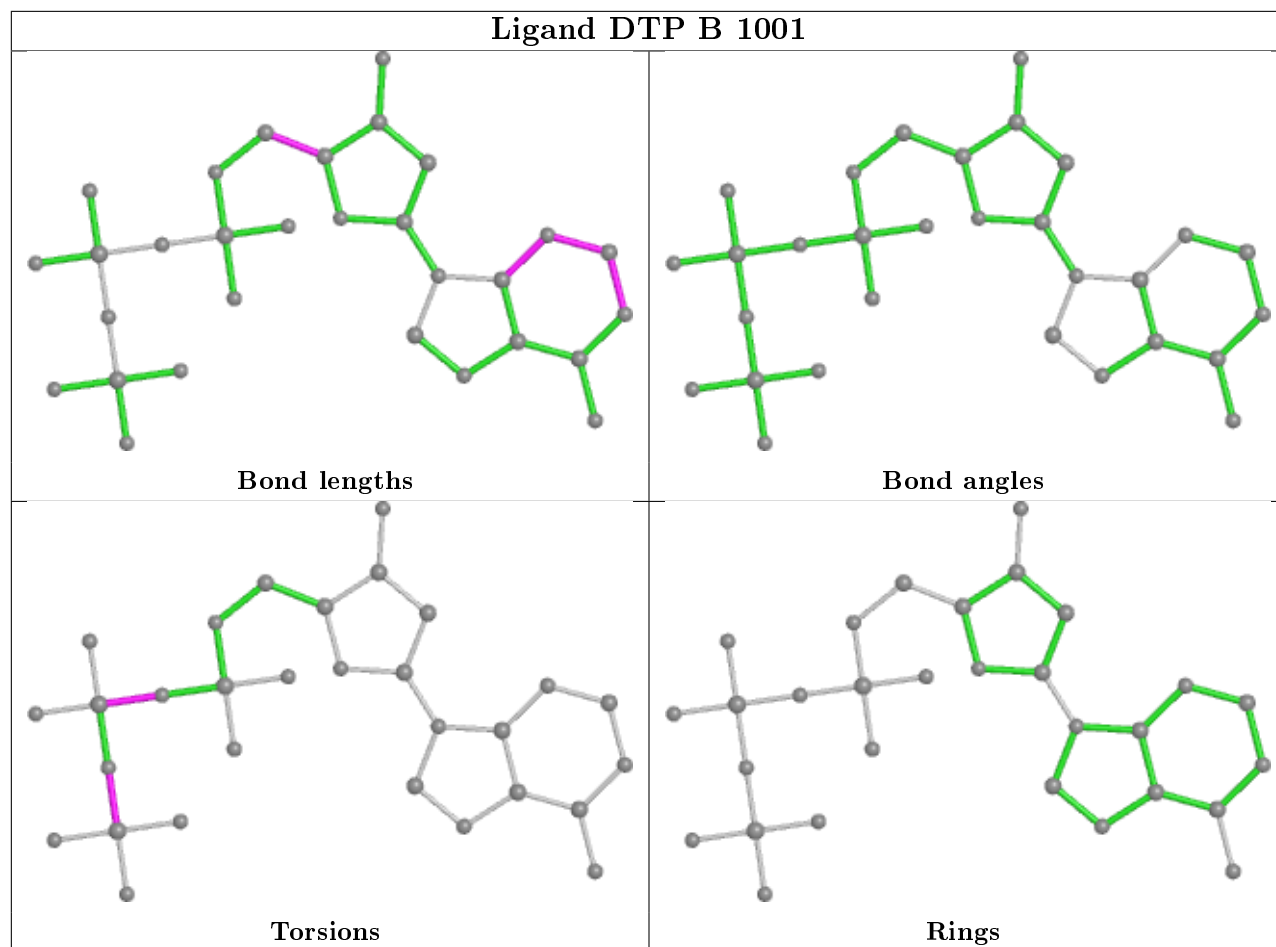
2 monomers are involved in 4 short contacts:

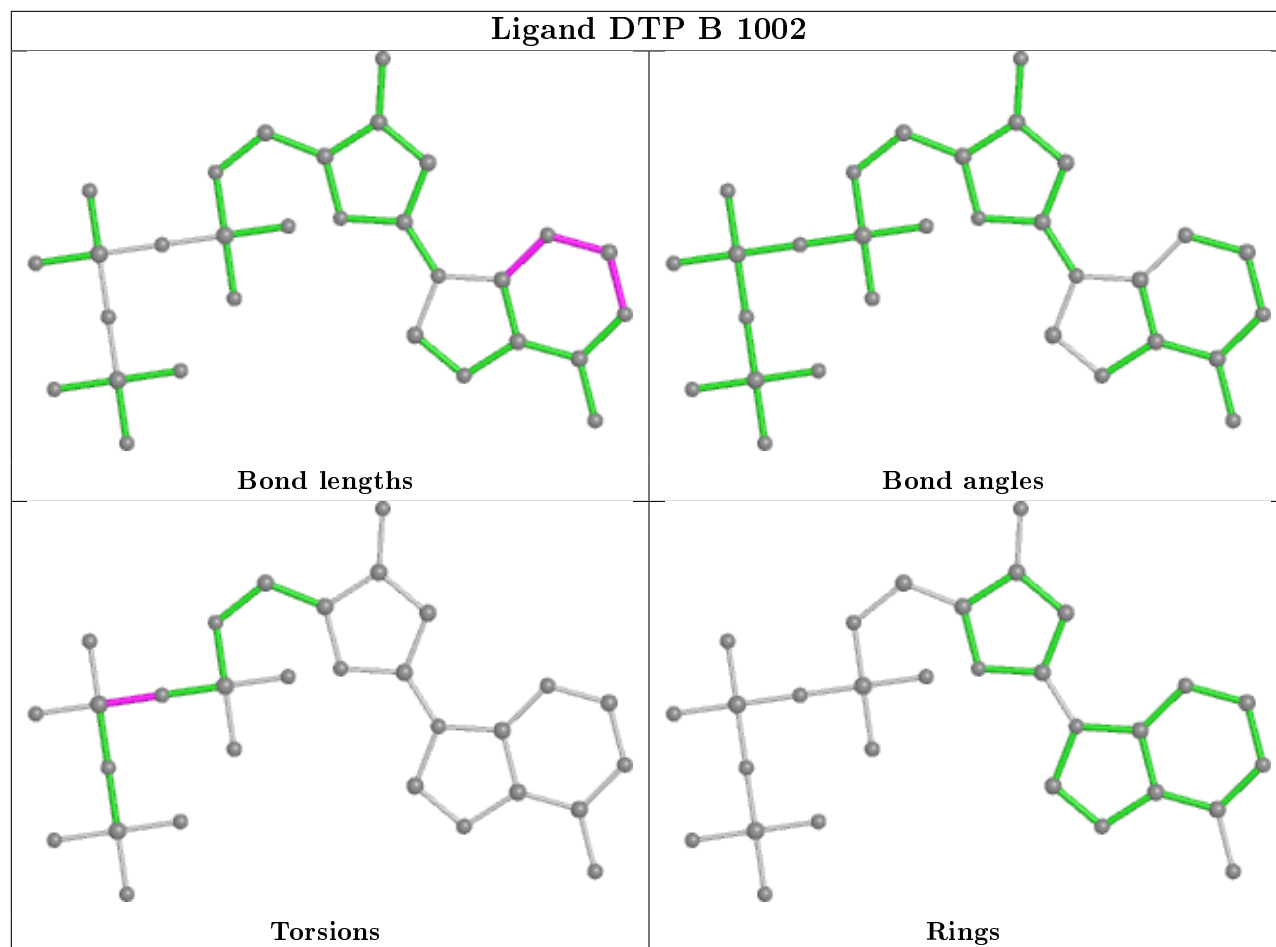
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1006	TRS	1	0
5	B	1006	TRS	3	0

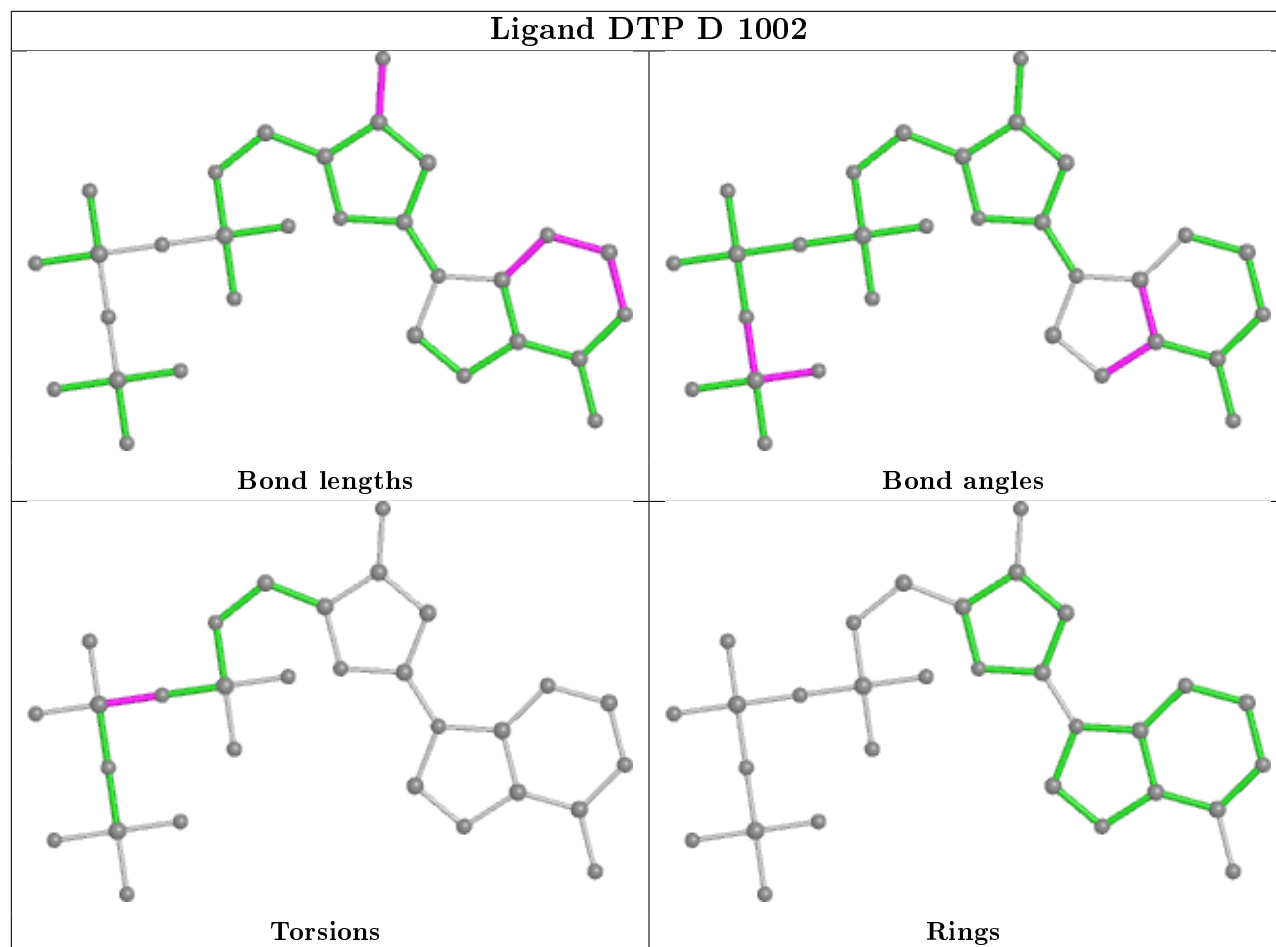
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

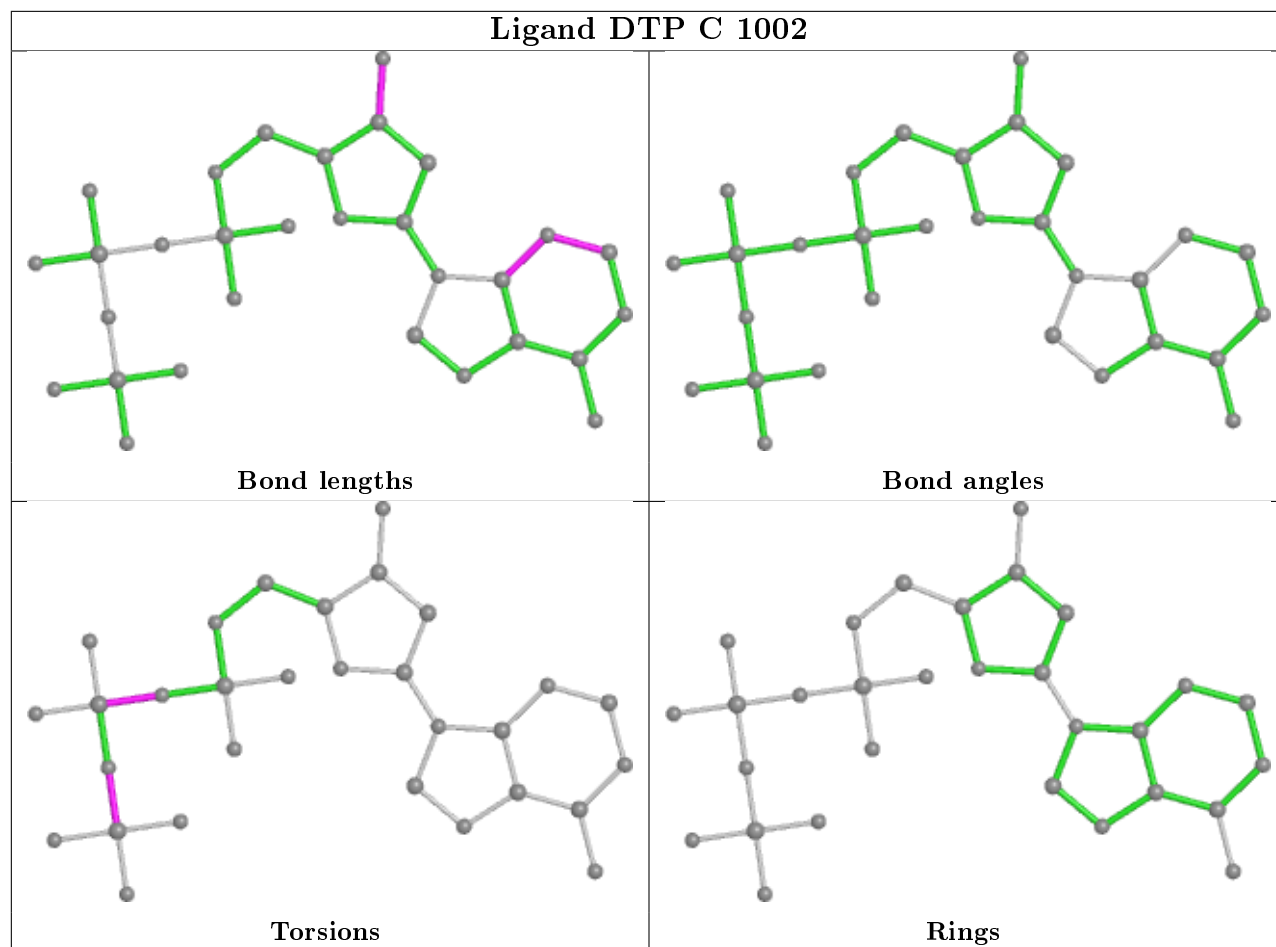


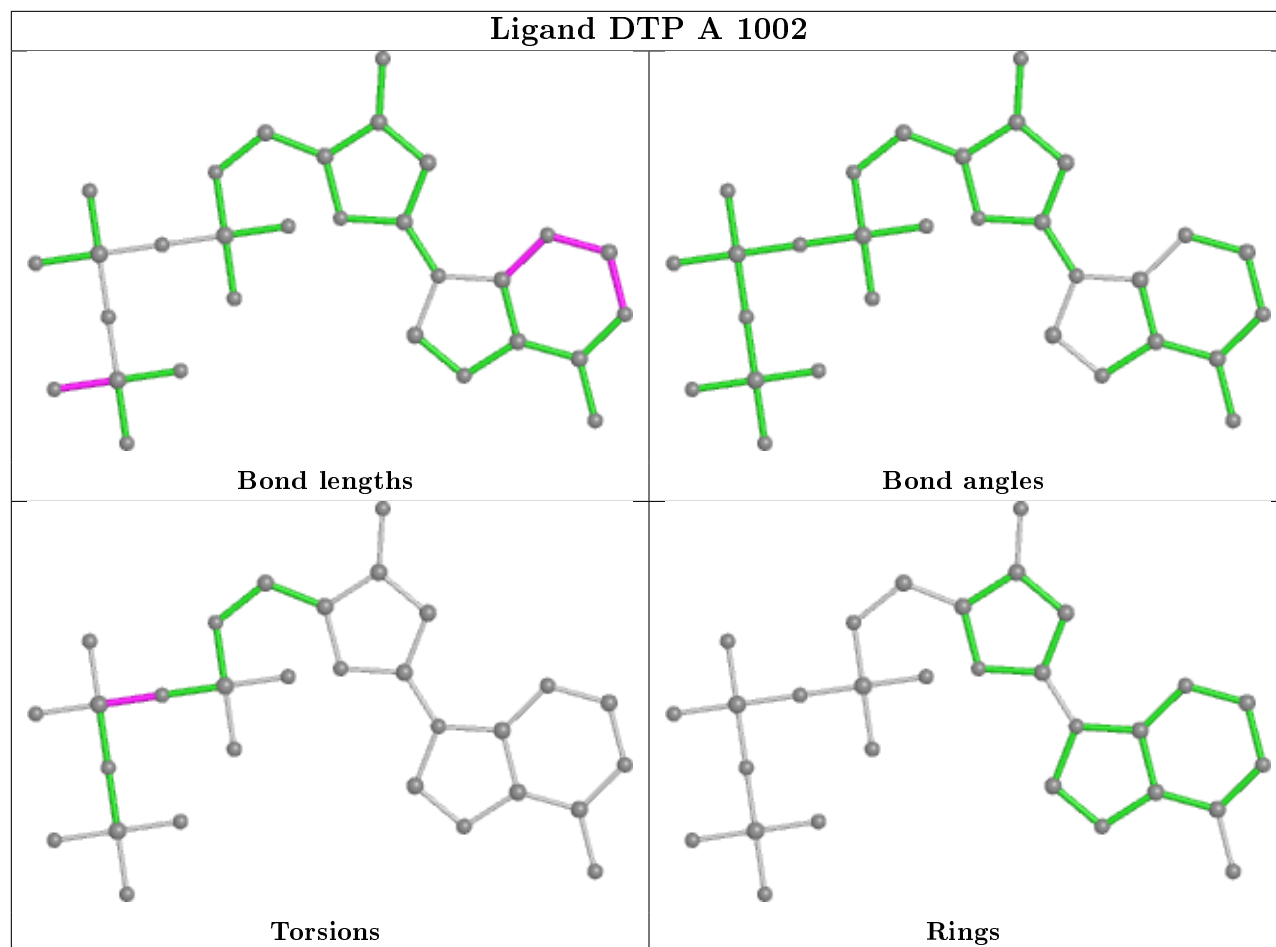


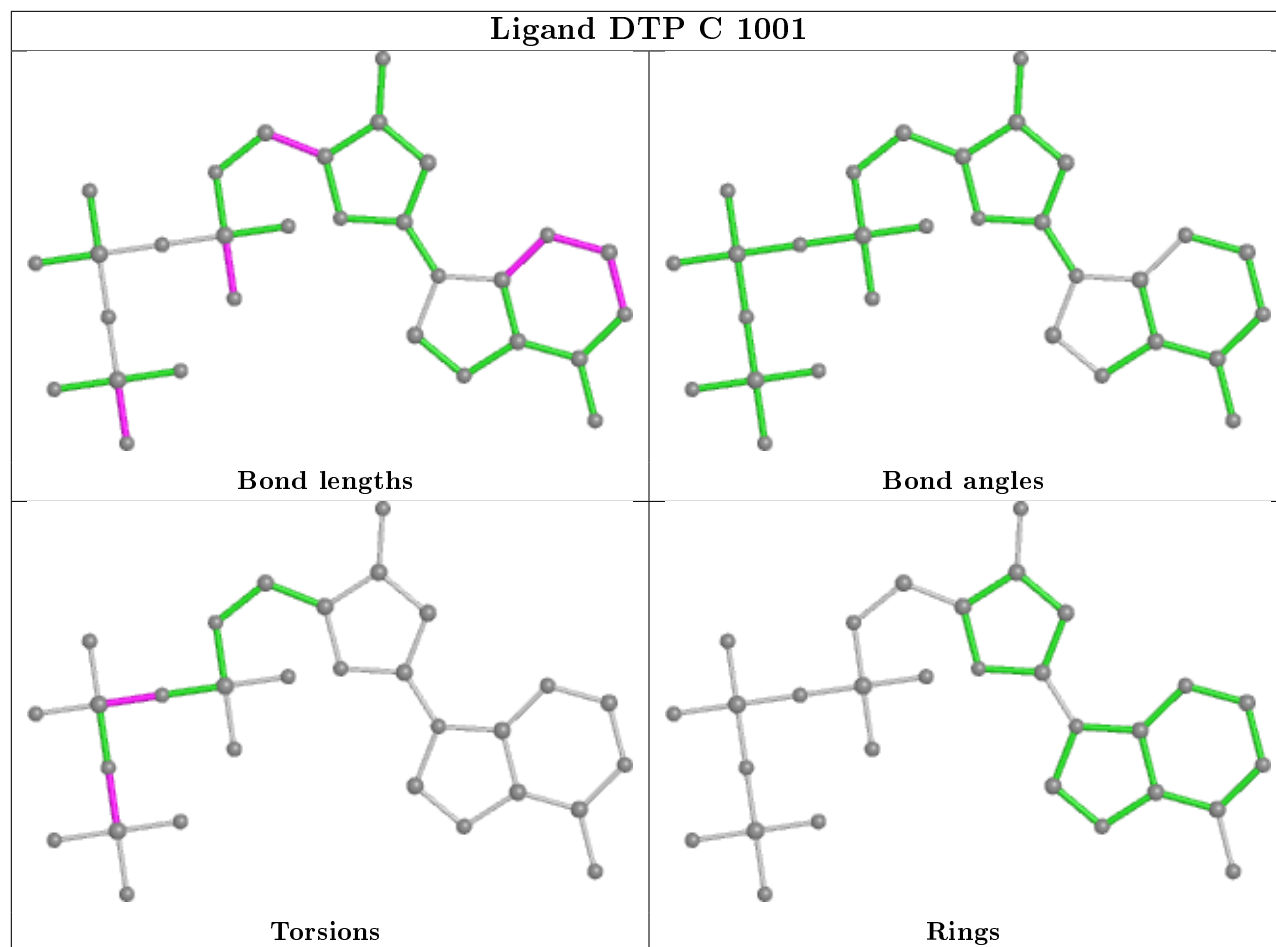












5.7 Other polymers [i](#)

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	395/430 (91%)	-0.15	6 (1%) 73 71	40, 61, 87, 118	0
1	B	392/430 (91%)	-0.06	9 (2%) 60 56	40, 65, 98, 115	0
1	C	394/430 (91%)	-0.05	7 (1%) 68 65	40, 66, 95, 114	0
1	D	393/430 (91%)	-0.09	13 (3%) 46 43	40, 63, 90, 127	0
All	All	1574/1720 (91%)	-0.09	35 (2%) 62 58	40, 64, 93, 127	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	59	GLU	6.6
1	D	64	TYR	4.7
1	A	60	GLN	4.3
1	D	62	SER	4.2
1	D	65	ILE	4.2
1	B	58	LYS	4.1
1	D	60	GLN	3.9
1	B	64	TYR	3.5
1	D	8	LYS	3.1
1	B	19	PHE	3.1
1	B	13	ASP	3.0
1	B	63	GLU	2.9
1	A	396	ASP	2.9
1	C	352	LEU	2.9
1	D	59	GLU	2.9
1	C	153	GLU	2.8
1	C	218	GLU	2.8
1	B	60	GLN	2.8
1	B	14	TYR	2.6
1	C	329	LYS	2.4
1	B	21	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	353	ASP	2.3
1	C	350	GLY	2.2
1	D	314	LYS	2.2
1	D	63	GLU	2.2
1	D	67	THR	2.2
1	A	63	GLU	2.1
1	A	93	ILE	2.1
1	D	6	ILE	2.1
1	D	10	ILE	2.1
1	A	62	SER	2.1
1	C	343	VAL	2.1
1	B	20	VAL	2.0
1	D	324	HIS	2.0
1	D	58	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 monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	TRS	D	1006	8/8	0.77	0.16	88,92,94,94	0
5	TRS	B	1006	8/8	0.78	0.15	67,74,77,77	0
5	TRS	A	1006	8/8	0.78	0.19	66,79,83,83	0
5	TRS	C	1006	8/8	0.88	0.14	56,64,71,71	0
2	DTP	B	1001	30/30	0.92	0.16	80,88,108,109	0
2	DTP	D	1002	30/30	0.94	0.13	53,62,95,97	0
3	MG	D	1003	1/1	0.94	0.11	52,52,52,52	0
2	DTP	D	1001	30/30	0.95	0.15	77,83,115,116	0
2	DTP	B	1002	30/30	0.95	0.12	61,66,81,85	0

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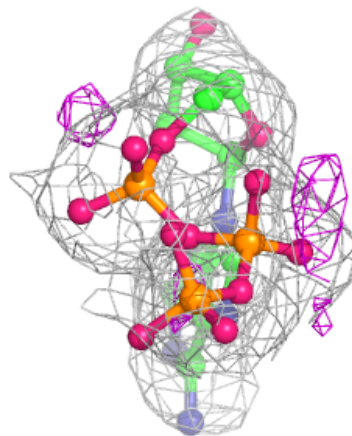
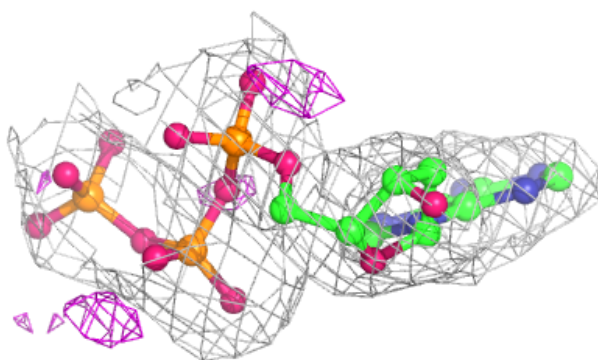
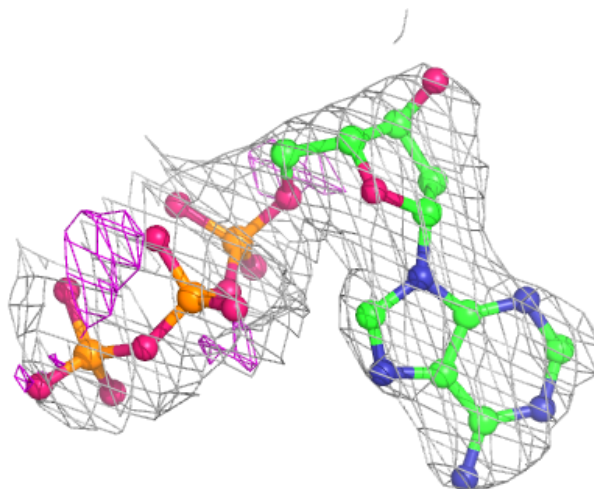
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	DTP	A	1002	30/30	0.95	0.12	52,59,84,85	0
2	DTP	A	1001	30/30	0.97	0.13	46,50,86,88	0
3	MG	A	1003	1/1	0.97	0.14	48,48,48,48	0
2	DTP	C	1001	30/30	0.97	0.13	34,48,81,85	0
2	DTP	C	1002	30/30	0.97	0.11	40,49,61,65	0
4	MN	C	1005	1/1	0.97	0.10	76,76,76,76	0
3	MG	B	1003	1/1	0.98	0.09	62,62,62,62	0
4	MN	C	1004	1/1	0.99	0.12	69,69,69,69	0
4	MN	A	1005	1/1	0.99	0.12	54,54,54,54	0
4	MN	B	1005	1/1	0.99	0.10	67,67,67,67	0
4	MN	B	1004	1/1	0.99	0.13	63,63,63,63	0
3	MG	C	1003	1/1	0.99	0.12	28,28,28,28	0
4	MN	A	1004	1/1	0.99	0.12	71,71,71,71	0
4	MN	D	1005	1/1	0.99	0.12	71,71,71,71	0
4	MN	D	1004	1/1	1.00	0.12	66,66,66,66	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.

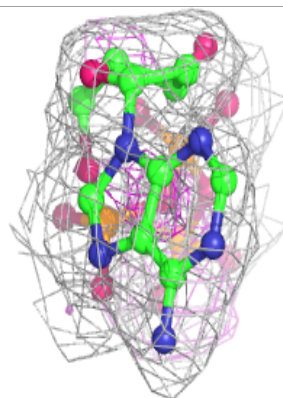
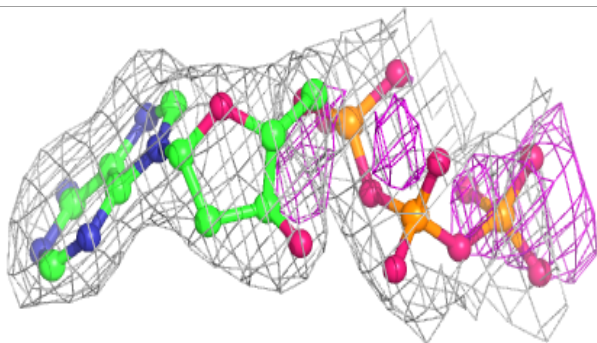
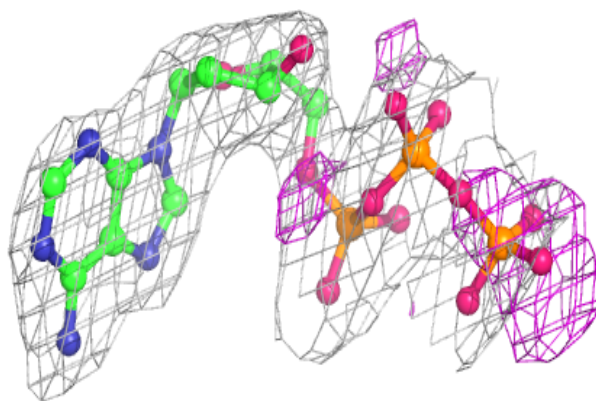
Electron density around DTP B 1001:

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



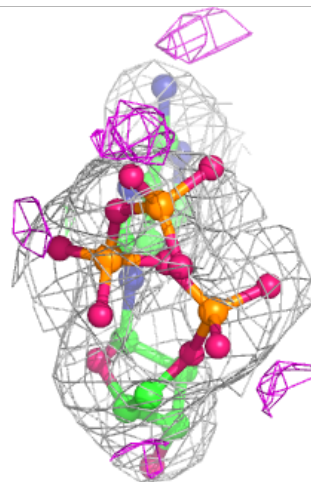
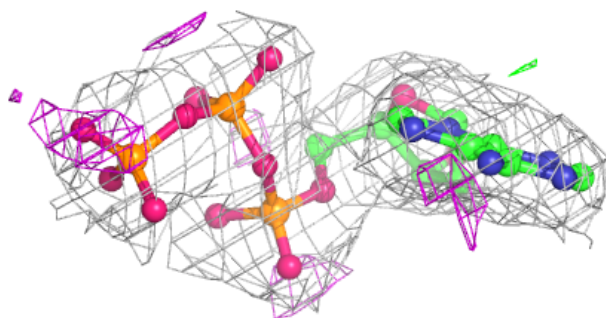
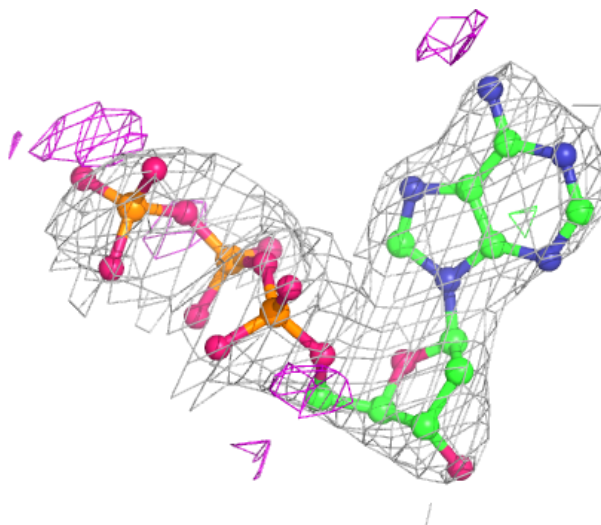
Electron density around DTP D 1002:

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



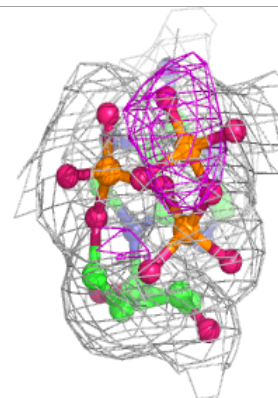
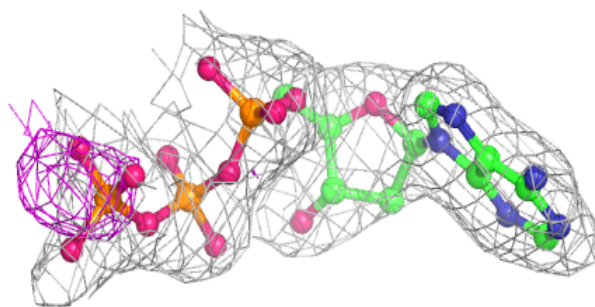
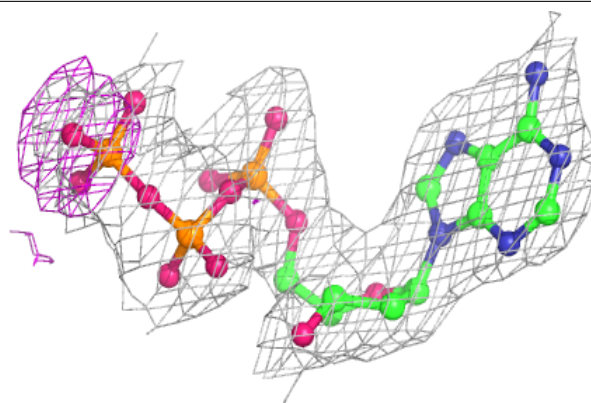
Electron density around DTP D 1001:

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

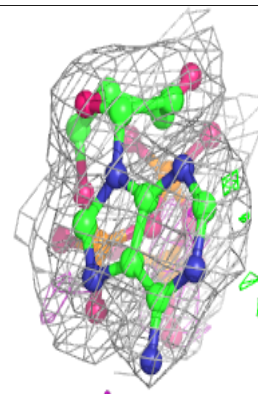
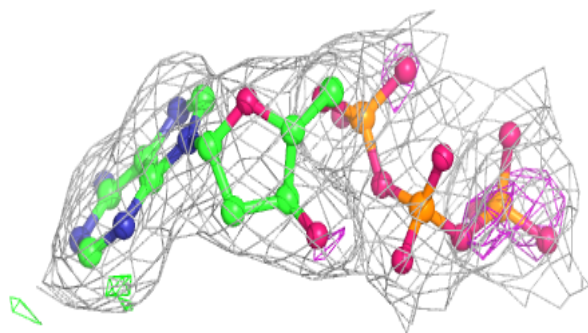
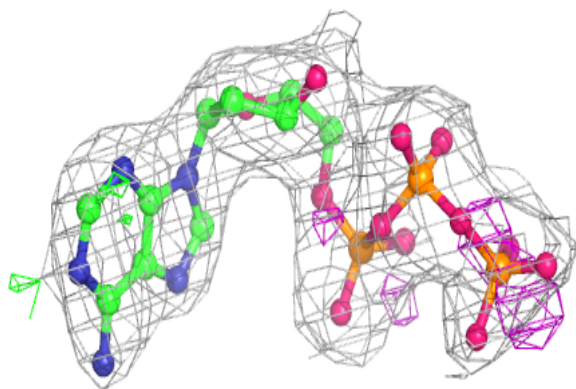


Electron density around DTP B 1002:

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

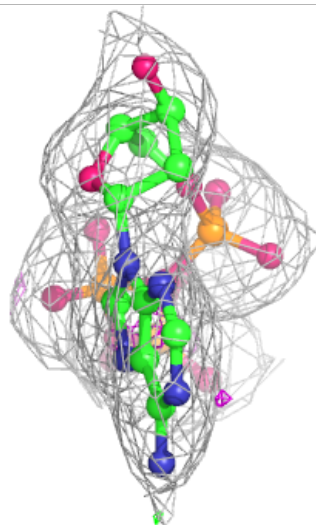
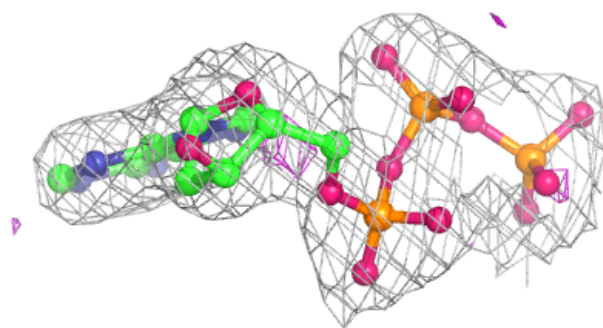
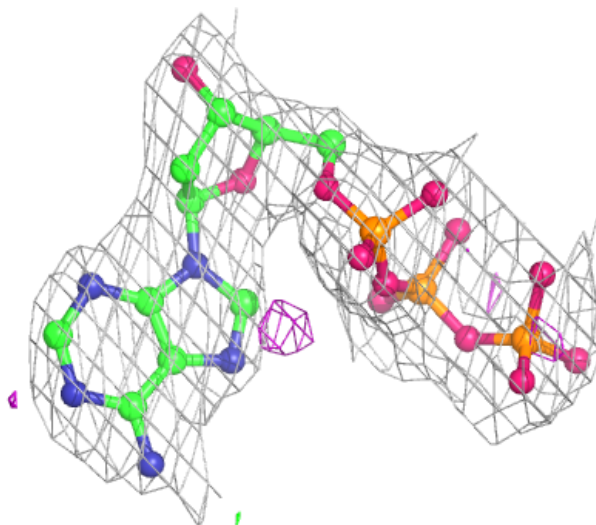
**Electron density around DTP A 1002:**

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



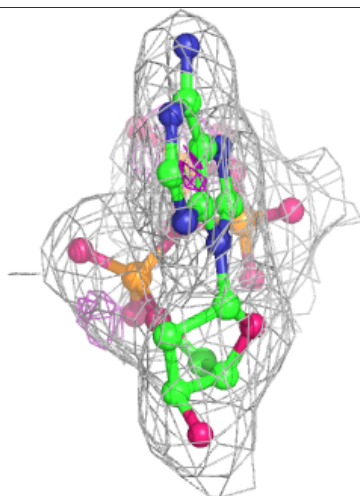
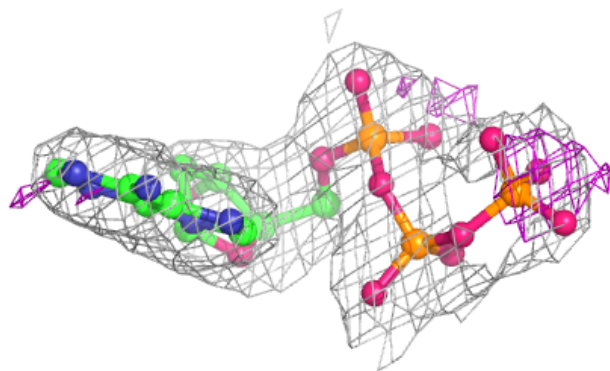
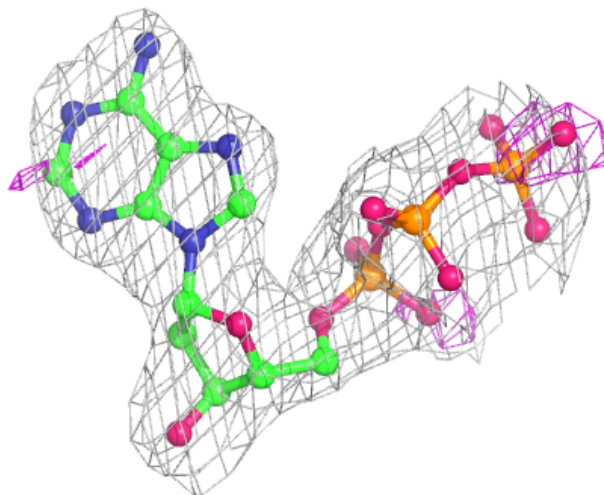
Electron density around DTP A 1001:

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



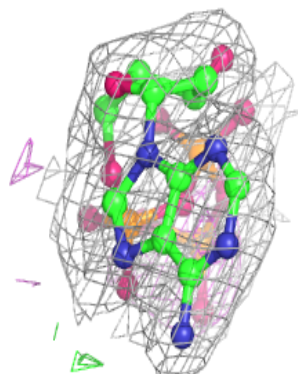
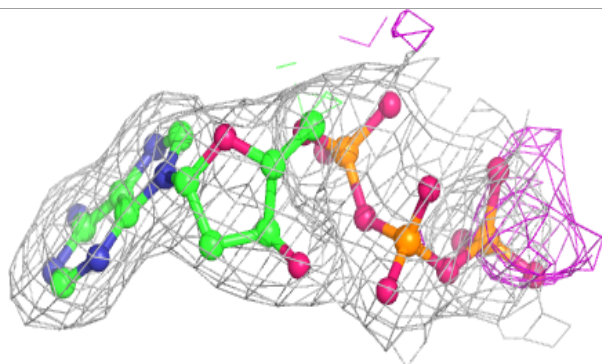
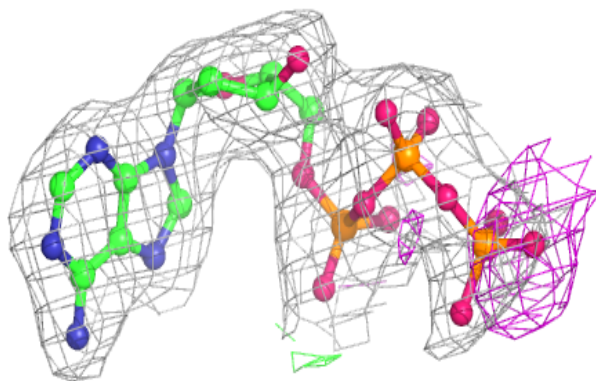
Electron density around DTP C 1001:

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



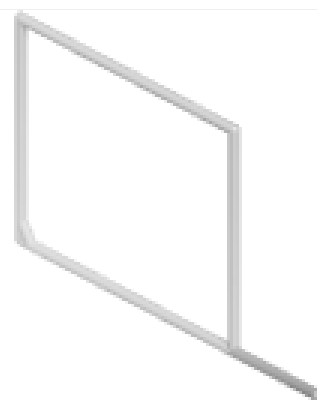
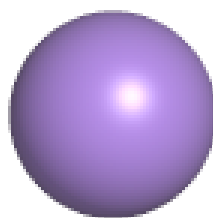
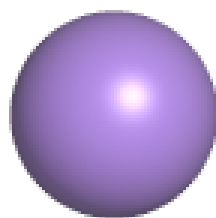
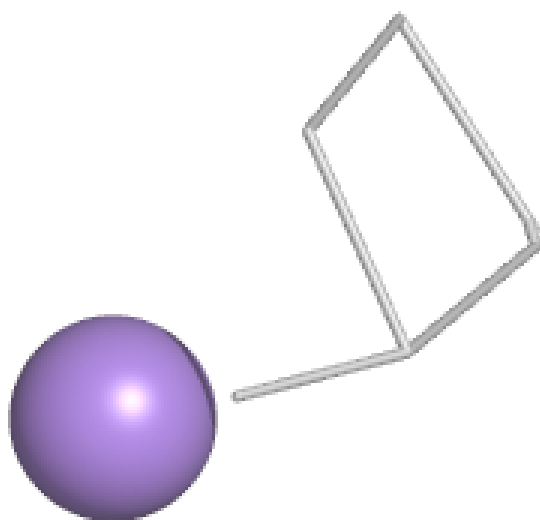
Electron density around DTP C 1002:

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



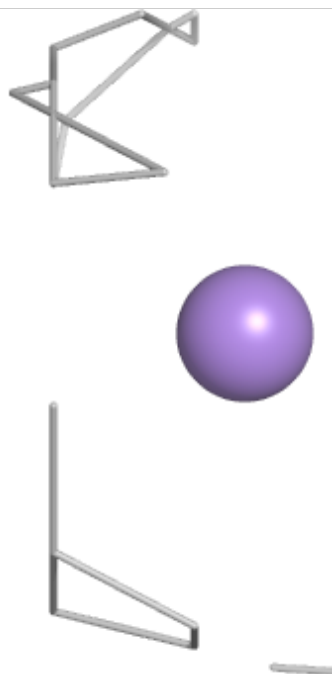
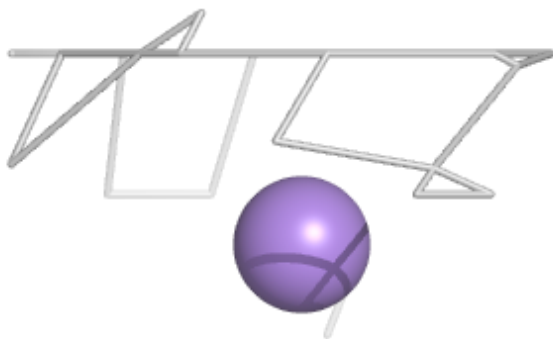
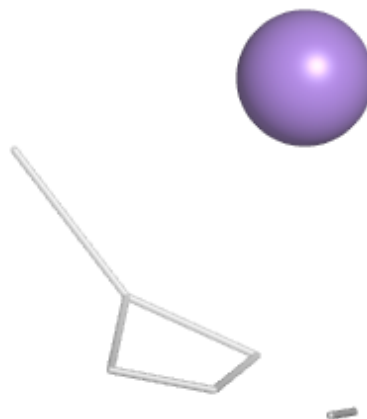
Electron density around MN C 1005:

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



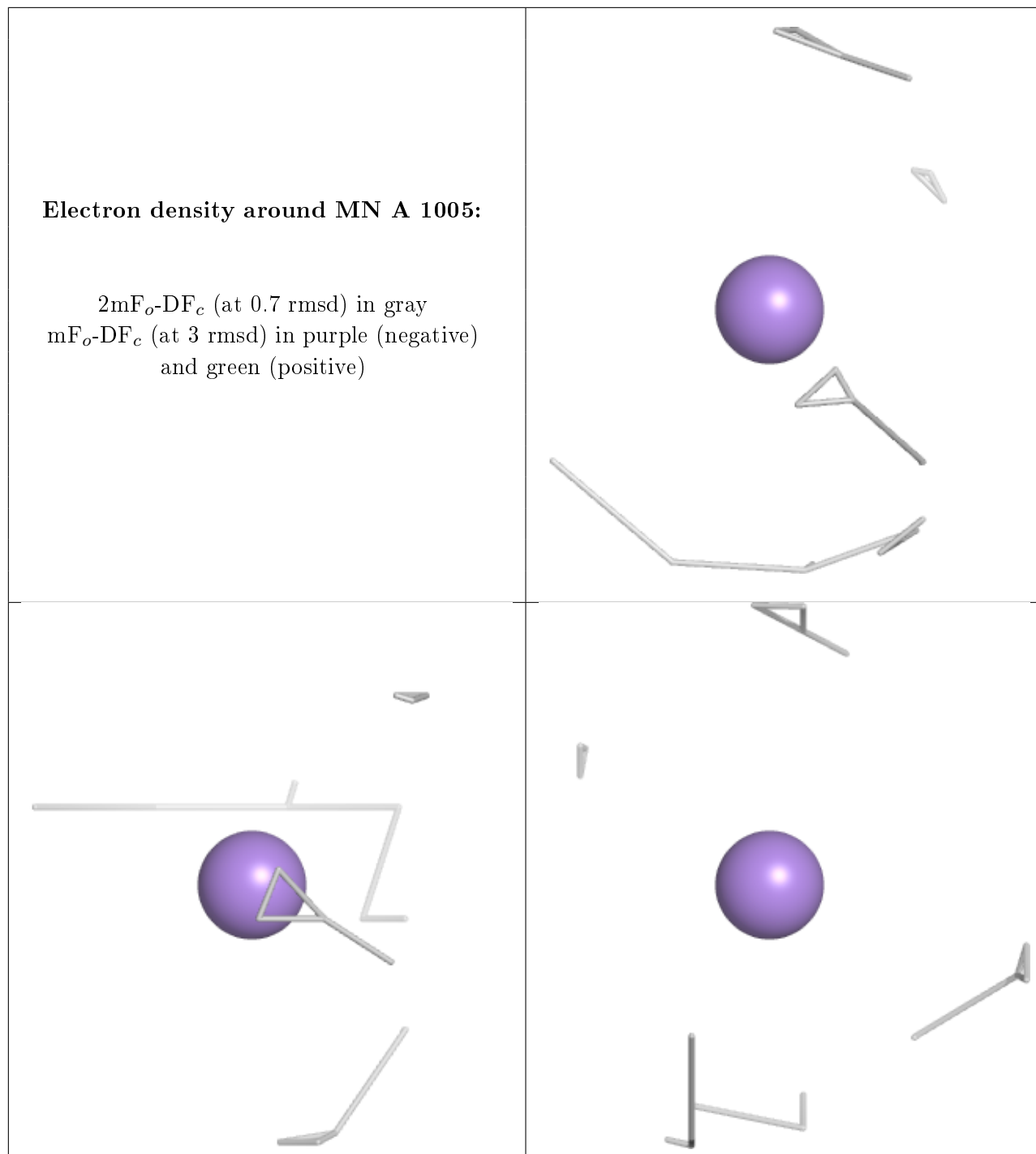
Electron density around MN C 1004:

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



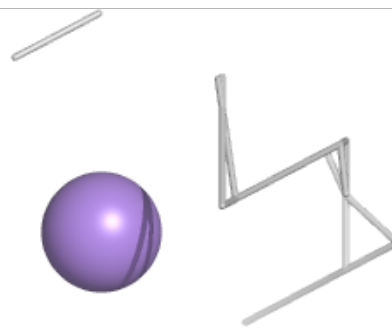
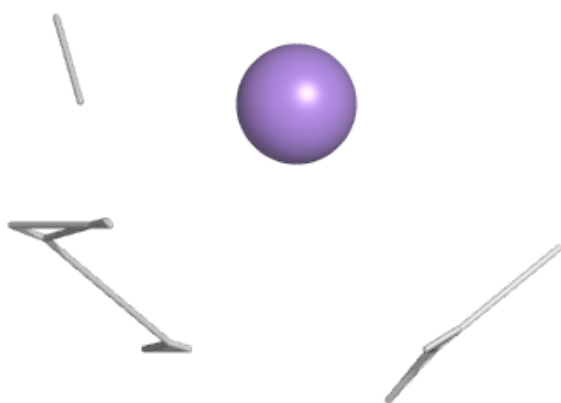
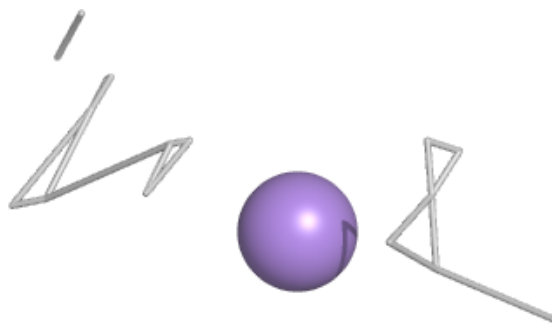
Electron density around MN A 1005:

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



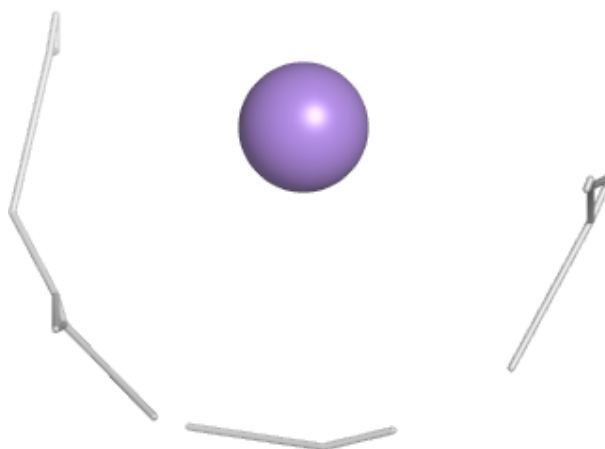
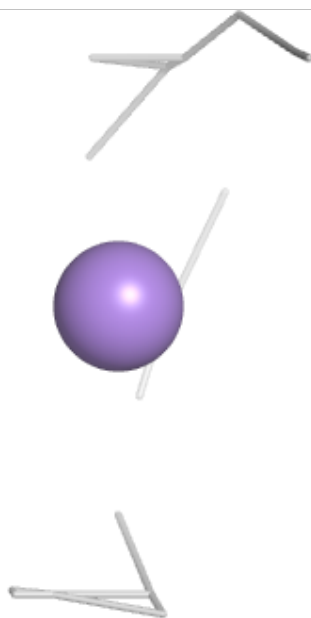
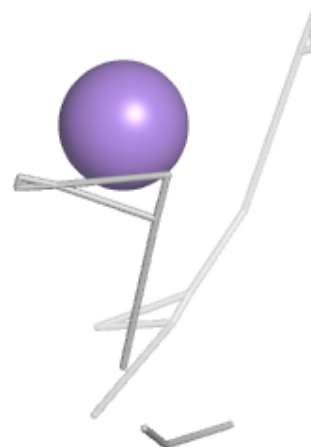
Electron density around MN B 1005:

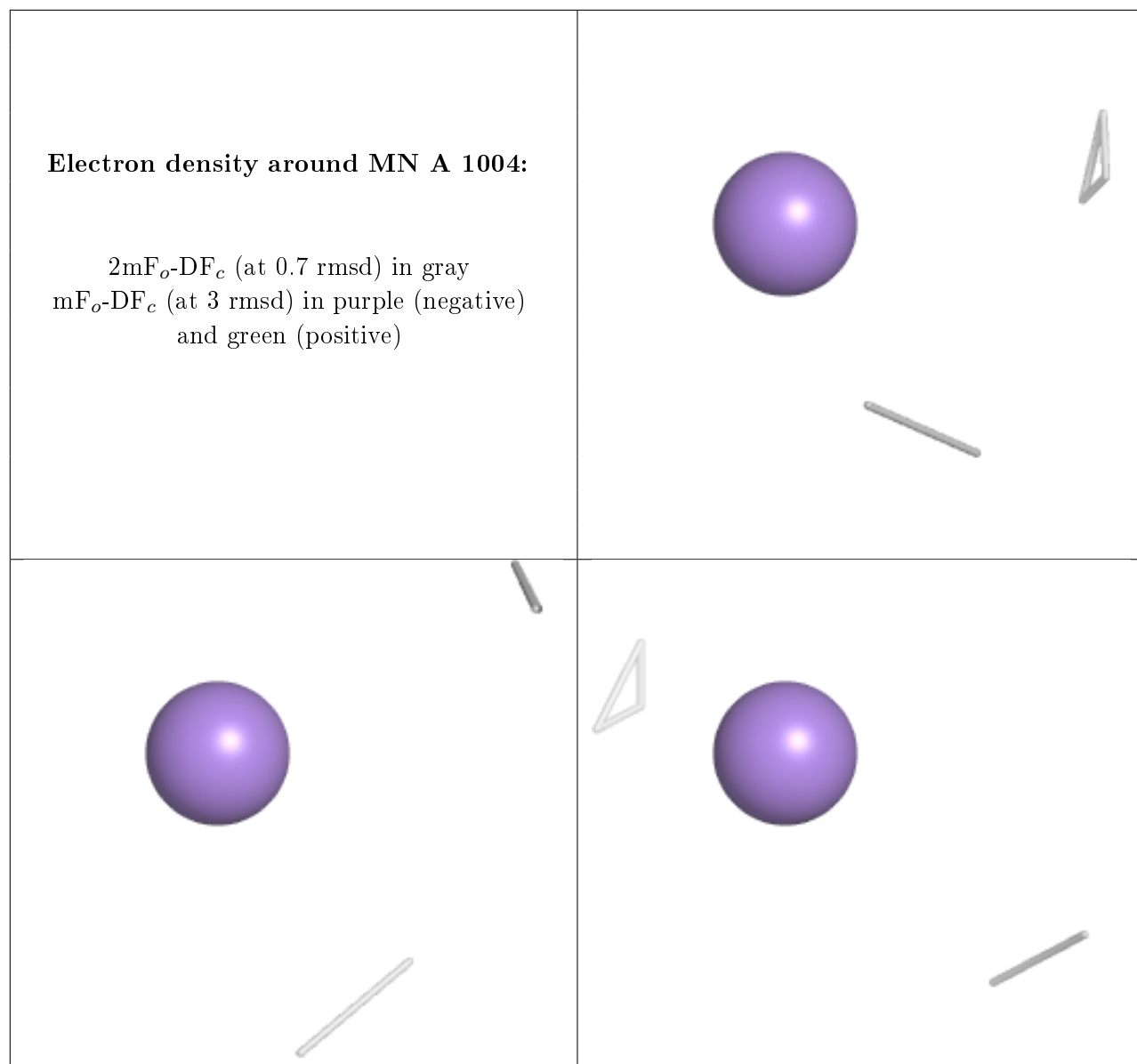
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MN B 1004:

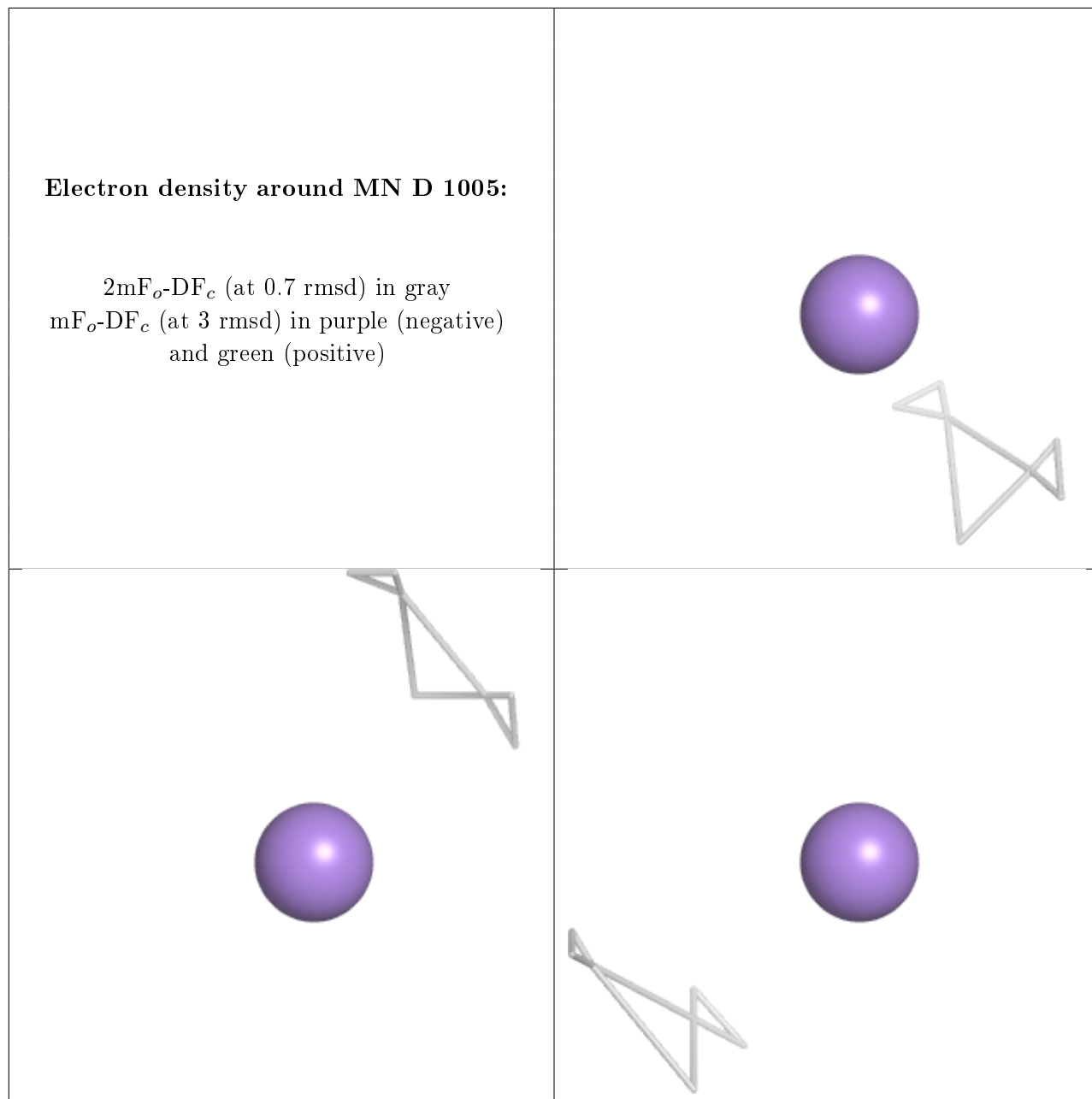
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

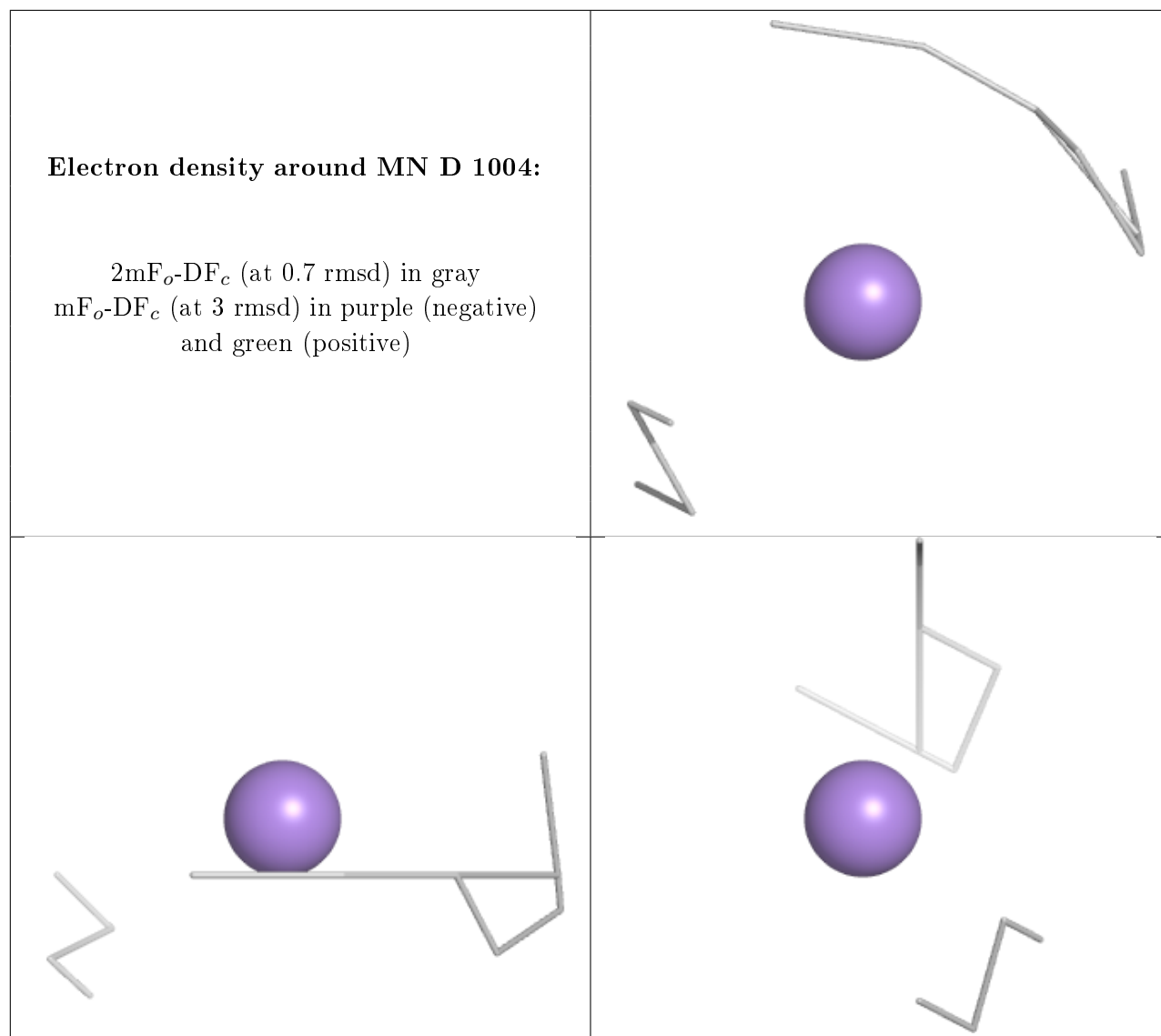




Electron density around MN D 1005:

$2mF_o-DF_c$ (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.