



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2021 – 01:19 PM BST

PDB ID : 7NNY  
Title : Crystal structure of Mycobacterium tuberculosis ArgF in complex with naphthalen-1-ol.  
Authors : Mendes, V.; Gupta, P.; Burgess, A.; Sebastian-Perez, V.; Cattermole, E.; Meghir, C.; Blundell, T.L.  
Deposited on : 2021-02-25  
Resolution : 1.57 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

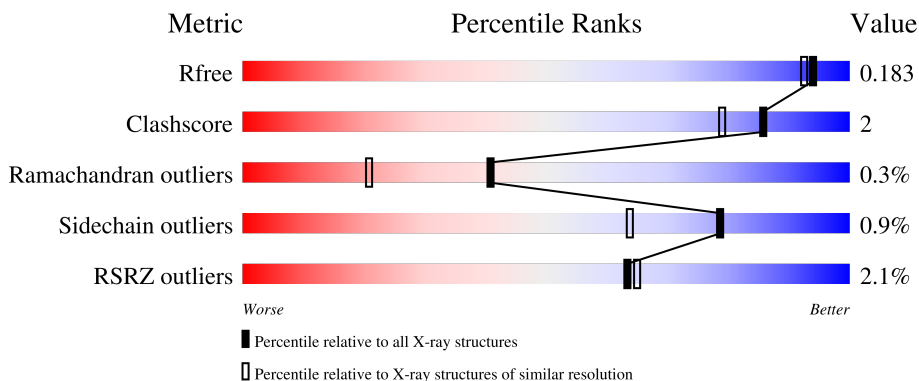
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.20  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.20

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

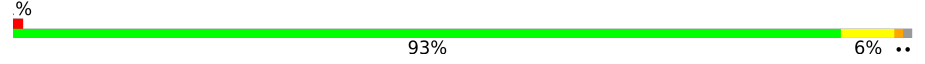
The reported resolution of this entry is 1.57 Å.

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.



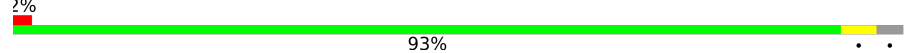
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	309	 2% 96%
1	B	309	 4% 91% 5%
1	C	309	 0% 93% 6%
1	D	309	 2% 92%
1	E	309	 2% 91% 6%

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Mol	Chain	Length	Quality of chain
1	F	309	 2% 93%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15623 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 Ornithine carbamoyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	308	Total 2328	C 1450	N 423	O 449	S 6	0	0	0
1	B	297	Total 2241	C 1402	N 406	O 428	S 5	0	0	0
1	C	307	Total 2316	C 1444	N 422	O 445	S 5	0	0	0
1	D	298	Total 2249	C 1407	N 407	O 430	S 5	0	0	0
1	E	300	Total 2273	C 1420	N 415	O 433	S 5	0	0	0
1	F	299	Total 2257	C 1410	N 410	O 432	S 5	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

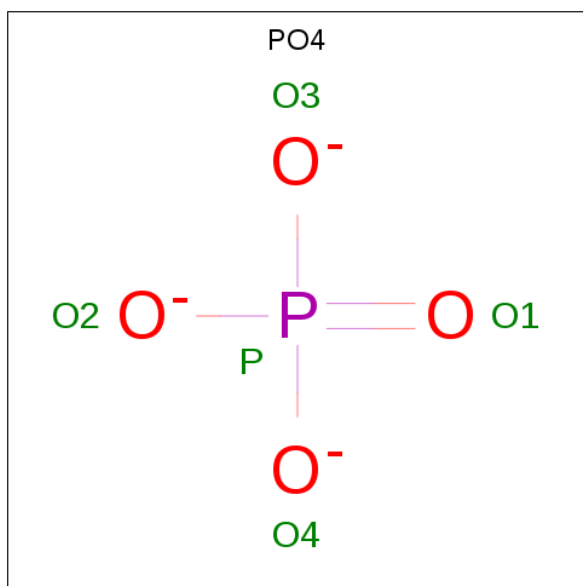
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P9WIT9
A	0	SER	-	expression tag	UNP P9WIT9
A	1	VAL	-	expression tag	UNP P9WIT9
B	-1	GLY	-	expression tag	UNP P9WIT9
B	0	SER	-	expression tag	UNP P9WIT9
B	1	VAL	-	expression tag	UNP P9WIT9
C	-1	GLY	-	expression tag	UNP P9WIT9
C	0	SER	-	expression tag	UNP P9WIT9
C	1	VAL	-	expression tag	UNP P9WIT9
D	-1	GLY	-	expression tag	UNP P9WIT9
D	0	SER	-	expression tag	UNP P9WIT9
D	1	VAL	-	expression tag	UNP P9WIT9
E	-1	GLY	-	expression tag	UNP P9WIT9
E	0	SER	-	expression tag	UNP P9WIT9
E	1	VAL	-	expression tag	UNP P9WIT9
F	-1	GLY	-	expression tag	UNP P9WIT9
F	0	SER	-	expression tag	UNP P9WIT9

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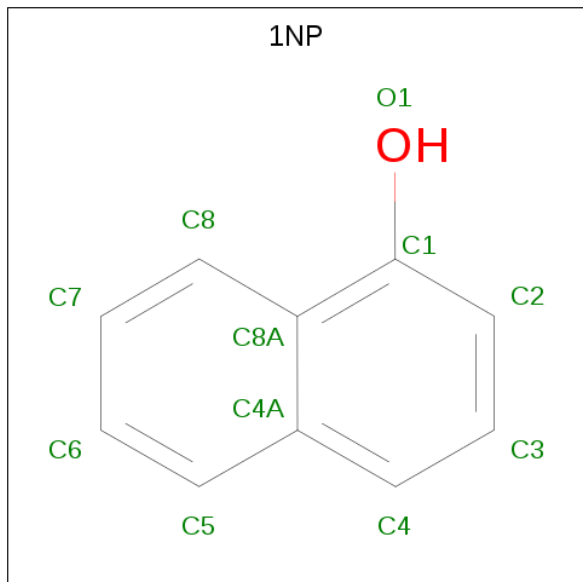
Chain	Residue	Modelled	Actual	Comment	Reference
F	1	VAL	-	expression tag	UNP P9WIT9

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	C	1	5	4	1	0	0
2	C	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	E	1	5	4	1	0	0
2	E	1	5	4	1	0	0
2	E	1	5	4	1	0	0

- Molecule 3 is 1-NAPHTHOL (three-letter code: 1NP) (formula: C<sub>10</sub>H<sub>8</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 11 10 1	0	0
3	A	1	Total C O 11 10 1	0	0
3	A	1	Total C O 11 10 1	0	0
3	B	1	Total C O 11 10 1	0	0
3	C	1	Total C O 11 10 1	0	0
3	C	1	Total C O 11 10 1	0	0
3	D	1	Total C O 11 10 1	0	0
3	D	1	Total C O 11 10 1	0	0
3	E	1	Total C O 11 10 1	0	0
3	E	1	Total C O 11 10 1	0	0
3	F	1	Total C O 11 10 1	0	0
3	F	1	Total C O 11 10 1	0	0

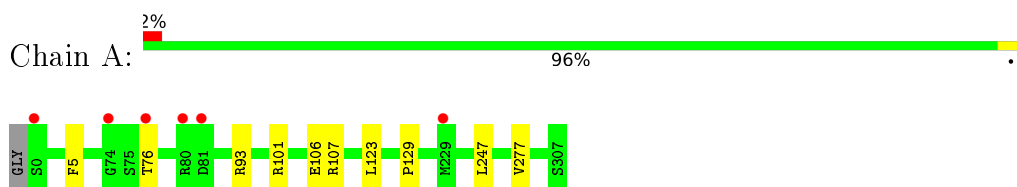
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	361	Total O 361 361	0	0
4	B	264	Total O 264 264	0	0
4	C	292	Total O 292 292	0	0
4	D	274	Total O 274 274	0	0
4	E	300	Total O 300 300	0	0
4	F	281	Total O 281 281	0	0

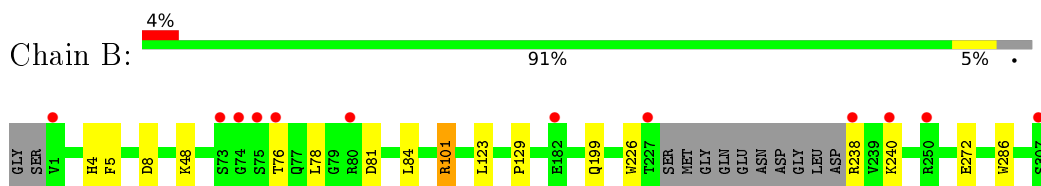
### 3 Residue-property plots [i](#)

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.

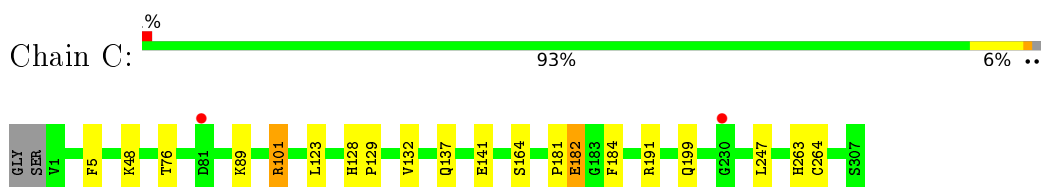
- Molecule 1: Ornithine carbamoyltransferase



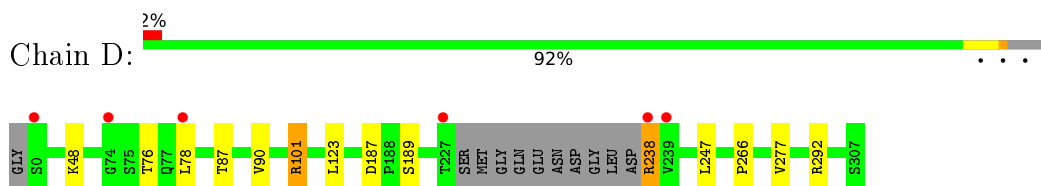
- Molecule 1: Ornithine carbamoyltransferase



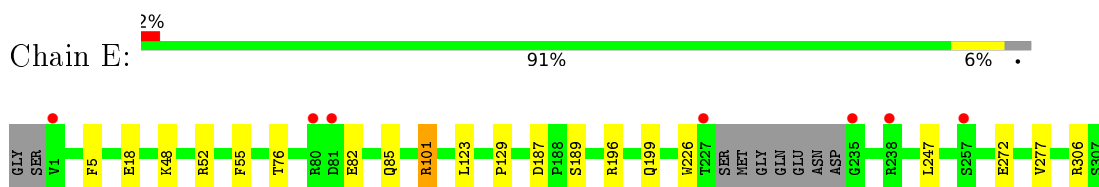
- Molecule 1: Ornithine carbamoyltransferase



- Molecule 1: Ornithine carbamoyltransferase

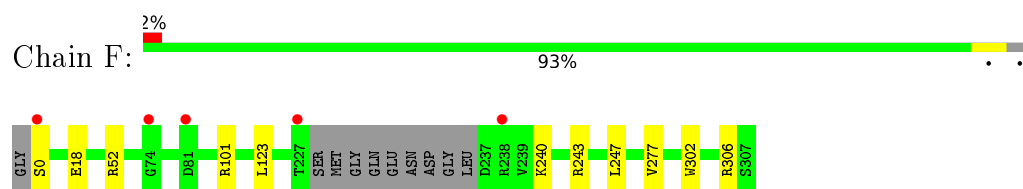


- Molecule 1: Ornithine carbamoyltransferase



- Molecule 1: Ornithine carbamoyltransferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.95Å 143.78Å 97.28Å 90.00° 117.60° 90.00°	Depositor
Resolution (Å)	48.97 – 1.57 86.21 – 1.57	Depositor EDS
% Data completeness (in resolution range)	94.5 (48.97-1.57) 94.6 (86.21-1.57)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 1.57Å)	Xtrriage
Refinement program	PHENIX 1.18.2	Depositor
R, $R_{free}$	0.166 , 0.184 0.167 , 0.183	Depositor DCC
$R_{free}$ test set	14816 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.7	Xtrriage
Anisotropy	0.129	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	15623	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1NP, PO4

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	0.42	0/2369	0.64	0/3223
1	B	0.39	0/2281	0.63	0/3106
1	C	0.38	0/2357	0.62	0/3208
1	D	0.37	0/2289	0.62	0/3116
1	E	0.41	0/2313	0.64	0/3147
1	F	0.38	0/2297	0.60	0/3128
All	All	0.39	0/13906	0.62	0/18928

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	2328	0	2304	6	0
1	B	2241	0	2222	15	0
1	C	2316	0	2290	12	0
1	D	2249	0	2231	9	0
1	E	2273	0	2262	12	0
1	F	2257	0	2230	6	0
2	A	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
2	C	10	0	0	1	0
2	D	10	0	0	0	0
2	E	15	0	0	0	0
3	A	33	0	21	2	0
3	B	11	0	7	1	0
3	C	22	0	14	2	0
3	D	22	0	14	3	0
3	E	22	0	14	1	0
3	F	22	0	14	1	0
4	A	361	0	0	3	0
4	B	264	0	0	4	0
4	C	292	0	0	3	0
4	D	274	0	0	1	0
4	E	300	0	0	3	0
4	F	281	0	0	1	0
All	All	15623	0	13623	59	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 2.

All (59) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:LEU:HD11	1:D:87:THR:HG21	1.61	0.82
1:D:247:LEU:HD22	1:D:277:VAL:HG11	1.66	0.77
1:E:247:LEU:HD22	1:E:277:VAL:HG11	1.70	0.74
1:D:76:THR:O	3:D:604:1NP:H2	1.89	0.72
1:A:247:LEU:HD22	1:A:277:VAL:HG11	1.73	0.69
1:E:199:GLN:NE2	4:E:601:HOH:O	2.31	0.63
2:A:602:PO4:O3	3:A:603:1NP:H3	1.99	0.61
1:B:240:LYS:NZ	4:B:701:HOH:O	2.38	0.57
1:C:191:ARG:NH1	4:C:701:HOH:O	2.39	0.56
1:A:76:THR:O	3:A:603:1NP:H2	2.07	0.55
1:B:78:LEU:HD21	1:B:84:LEU:HD13	1.90	0.53
1:B:78:LEU:CD2	1:B:84:LEU:HD13	2.38	0.53
1:A:93:ARG:NH2	4:A:702:HOH:O	2.40	0.53
1:F:247:LEU:HD22	1:F:277:VAL:HG11	1.90	0.53
1:E:196:ARG:NH2	4:E:602:HOH:O	2.43	0.51
1:B:226:TRP:CZ2	1:B:272:GLU:HA	2.45	0.51
1:B:286:TRP:CD1	1:C:89:LYS:HE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:602:PO4:O4	3:C:604:1NP:H3	2.10	0.51
1:E:196:ARG:HG3	4:E:748:HOH:O	2.10	0.50
1:D:292:ARG:NH2	4:D:702:HOH:O	2.40	0.49
1:B:286:TRP:CG	1:C:89:LYS:HE2	2.47	0.49
1:C:5:PHE:CE2	1:C:129:PRO:HB2	2.47	0.49
1:C:76:THR:O	3:C:604:1NP:H2	2.12	0.49
1:F:240:LYS:HA	1:F:243:ARG:HG3	1.94	0.48
1:A:93:ARG:NE	4:A:702:HOH:O	2.44	0.48
1:E:48:LYS:O	1:E:101:ARG:HD2	2.14	0.47
1:B:4:HIS:HB3	4:B:886:HOH:O	2.13	0.47
1:B:78:LEU:HD21	1:B:84:LEU:CD1	2.44	0.47
1:C:48:LYS:O	1:C:101:ARG:HD2	2.15	0.47
1:E:226:TRP:CZ2	1:E:272:GLU:HA	2.49	0.47
4:A:759:HOH:O	1:B:81:ASP:HB2	2.15	0.47
1:D:187:ASP:OD2	1:D:189:SER:HB3	2.15	0.47
1:D:238:ARG:HD3	1:D:238:ARG:HA	1.70	0.47
3:D:604:1NP:H4	1:F:52:ARG:CZ	2.46	0.46
1:E:76:THR:O	3:E:505:1NP:H2	2.16	0.46
1:D:48:LYS:O	1:D:101:ARG:HD2	2.15	0.46
1:F:0:SER:HA	4:F:710:HOH:O	2.17	0.45
1:B:48:LYS:O	1:B:101:ARG:HD2	2.18	0.44
1:E:18:GLU:OE1	1:E:306:ARG:NH2	2.51	0.43
1:A:5:PHE:CE2	1:A:129:PRO:HB2	2.53	0.43
1:C:181:PRO:HG2	1:C:184:PHE:CD1	2.53	0.43
1:B:199:GLN:NE2	4:B:706:HOH:O	2.50	0.43
1:B:238:ARG:CB	4:B:701:HOH:O	2.66	0.43
1:C:132:VAL:HG21	1:C:164:SER:HB3	2.01	0.43
1:A:106:GLU:HG2	1:A:107:ARG:N	2.33	0.43
1:E:187:ASP:OD1	1:E:189:SER:HB3	2.19	0.42
1:B:5:PHE:CE2	1:B:129:PRO:HB2	2.55	0.42
1:D:90:VAL:HG11	3:D:603:1NP:C8A	2.50	0.42
1:C:263:HIS:ND1	1:C:264:CYS:O	2.51	0.42
1:B:76:THR:HG22	3:B:602:1NP:H2	2.01	0.42
1:F:18:GLU:OE1	1:F:306:ARG:NH2	2.54	0.41
1:D:266:PRO:HB3	1:E:82:GLU:HB2	2.01	0.41
1:C:182:GLU:HG3	4:C:885:HOH:O	2.20	0.41
1:E:52:ARG:HG3	3:F:402:1NP:H7	2.02	0.41
1:C:137:GLN:O	1:C:141:GLU:HG3	2.21	0.41
1:C:199:GLN:NE2	4:C:709:HOH:O	2.53	0.41
1:F:302:TRP:O	1:F:306:ARG:HG2	2.19	0.41
1:B:78:LEU:C	1:B:78:LEU:HD23	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:PHE:CE2	1:E:129:PRO:HB2	2.56	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	306/309 (99%)	300 (98%)	5 (2%)	1 (0%)	41 21
1	B	293/309 (95%)	285 (97%)	7 (2%)	1 (0%)	41 21
1	C	305/309 (99%)	300 (98%)	4 (1%)	1 (0%)	41 21
1	D	294/309 (95%)	288 (98%)	5 (2%)	1 (0%)	41 21
1	E	296/309 (96%)	287 (97%)	8 (3%)	1 (0%)	41 21
1	F	295/309 (96%)	286 (97%)	8 (3%)	1 (0%)	41 21
All	All	1789/1854 (96%)	1746 (98%)	37 (2%)	6 (0%)	41 21

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	LEU
1	B	123	LEU
1	C	123	LEU
1	D	123	LEU
1	E	123	LEU
1	F	123	LEU

### 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	242/243 (100%)	241 (100%)	1 (0%)	91	84
1	B	232/243 (96%)	230 (99%)	2 (1%)	78	64
1	C	239/243 (98%)	235 (98%)	4 (2%)	60	36
1	D	233/243 (96%)	231 (99%)	2 (1%)	78	64
1	E	236/243 (97%)	233 (99%)	3 (1%)	69	48
1	F	233/243 (96%)	232 (100%)	1 (0%)	91	84
All	All	1415/1458 (97%)	1402 (99%)	13 (1%)	78	64

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	ARG
1	B	8	ASP
1	B	101	ARG
1	C	101	ARG
1	C	128	HIS
1	C	182	GLU
1	C	247	LEU
1	D	101	ARG
1	D	238	ARG
1	E	55	PHE
1	E	85	GLN
1	E	101	ARG
1	F	101	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	296	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](#)

23 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PO4	E	502	-	4,4,4	0.81	0	6,6,6	0.32	0
2	PO4	A	601	-	4,4,4	1.01	0	6,6,6	0.65	0
3	1NP	C	603	-	12,12,12	1.15	2 (16%)	16,16,16	1.74	5 (31%)
3	1NP	D	603	-	12,12,12	1.11	1 (8%)	16,16,16	1.66	5 (31%)
3	1NP	F	401	-	12,12,12	1.09	0	16,16,16	1.46	3 (18%)
2	PO4	A	602	-	4,4,4	0.93	0	6,6,6	0.52	0
2	PO4	E	503	-	4,4,4	0.78	0	6,6,6	0.70	0
3	1NP	E	505	-	12,12,12	1.08	0	16,16,16	1.60	5 (31%)
2	PO4	C	601	-	4,4,4	1.03	0	6,6,6	0.61	0
3	1NP	A	604	-	12,12,12	1.09	0	16,16,16	1.69	6 (37%)
2	PO4	D	602	-	4,4,4	0.77	0	6,6,6	0.55	0
3	1NP	F	402	-	12,12,12	1.09	0	16,16,16	1.72	6 (37%)
2	PO4	A	606	-	4,4,4	0.76	0	6,6,6	0.41	0
3	1NP	B	602	-	12,12,12	1.10	0	16,16,16	1.68	5 (31%)
3	1NP	A	605	-	12,12,12	1.11	0	16,16,16	1.85	7 (43%)
2	PO4	C	602	-	4,4,4	0.92	0	6,6,6	0.56	0
2	PO4	E	501	-	4,4,4	0.88	0	6,6,6	0.75	0
3	1NP	D	604	-	12,12,12	1.08	0	16,16,16	1.79	6 (37%)
3	1NP	A	603	-	12,12,12	1.07	0	16,16,16	1.66	4 (25%)
2	PO4	B	601	-	4,4,4	0.84	0	6,6,6	0.48	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	1NP	E	504	-	12,12,12	1.10	1 (8%)	16,16,16	1.98	6 (37%)
2	PO4	D	601	-	4,4,4	1.14	0	6,6,6	0.73	0
3	1NP	C	604	-	12,12,12	1.08	0	16,16,16	1.65	6 (37%)

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	1NP	D	603	-	-	-	0/2/2/2
3	1NP	F	401	-	-	-	0/2/2/2
3	1NP	B	602	-	-	-	0/2/2/2
3	1NP	E	504	-	-	-	0/2/2/2
3	1NP	A	605	-	-	-	0/2/2/2
3	1NP	E	505	-	-	-	0/2/2/2
3	1NP	C	604	-	-	-	0/2/2/2
3	1NP	A	604	-	-	-	0/2/2/2
3	1NP	C	603	-	-	-	0/2/2/2
3	1NP	D	604	-	-	-	0/2/2/2
3	1NP	F	402	-	-	-	0/2/2/2
3	1NP	A	603	-	-	-	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	603	1NP	C1-C8A	2.09	1.46	1.42
3	D	603	1NP	C1-C8A	2.08	1.46	1.42
3	E	504	1NP	C3-C2	2.04	1.43	1.38
3	C	603	1NP	C3-C2	2.02	1.43	1.38

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	504	1NP	C6-C5-C4A	3.24	125.51	120.44
3	E	504	1NP	C5-C4A-C8A	-3.11	115.03	119.12
3	E	504	1NP	C7-C8-C8A	3.01	125.07	120.89
3	D	604	1NP	C6-C5-C4A	3.00	125.13	120.44
3	F	402	1NP	C2-C1-C8A	2.97	123.97	120.91
3	D	604	1NP	C7-C8-C8A	2.94	124.97	120.89
3	A	605	1NP	C7-C8-C8A	2.94	124.97	120.89
3	A	604	1NP	C7-C8-C8A	2.92	124.94	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	605	1NP	C6-C5-C4A	2.86	124.92	120.44
3	A	605	1NP	C2-C1-C8A	2.83	123.82	120.91
3	C	603	1NP	C6-C5-C4A	2.81	124.84	120.44
3	D	603	1NP	C7-C8-C8A	2.68	124.61	120.89
3	C	604	1NP	C6-C5-C4A	2.67	124.62	120.44
3	C	603	1NP	C7-C8-C8A	2.67	124.60	120.89
3	A	603	1NP	C7-C8-C8A	2.62	124.53	120.89
3	D	603	1NP	C6-C5-C4A	2.59	124.50	120.44
3	E	504	1NP	O1-C1-C8A	-2.59	113.07	116.31
3	F	401	1NP	C7-C8-C8A	2.58	124.47	120.89
3	C	603	1NP	C8-C8A-C1	2.56	125.73	122.21
3	A	603	1NP	C6-C5-C4A	2.55	124.43	120.44
3	B	602	1NP	C2-C1-C8A	2.50	123.48	120.91
3	D	604	1NP	C8-C8A-C1	2.48	125.62	122.21
3	F	402	1NP	C3-C4-C4A	2.48	124.32	120.44
3	E	505	1NP	C6-C5-C4A	2.48	124.32	120.44
3	B	602	1NP	C6-C5-C4A	2.47	124.30	120.44
3	E	505	1NP	C7-C8-C8A	2.46	124.31	120.89
3	C	604	1NP	C7-C8-C8A	2.45	124.29	120.89
3	F	401	1NP	C6-C5-C4A	2.45	124.27	120.44
3	A	605	1NP	C5-C4A-C8A	-2.45	115.90	119.12
3	E	505	1NP	C8-C8A-C1	2.43	125.55	122.21
3	A	603	1NP	C5-C4A-C8A	-2.43	115.92	119.12
3	F	402	1NP	C3-C2-C1	-2.41	117.24	120.28
3	C	603	1NP	C2-C1-C8A	2.40	123.38	120.91
3	A	604	1NP	C2-C1-C8A	2.39	123.36	120.91
3	B	602	1NP	C7-C8-C8A	2.35	124.15	120.89
3	D	603	1NP	C8-C8A-C1	2.34	125.43	122.21
3	D	604	1NP	C3-C4-C4A	2.34	124.10	120.44
3	E	504	1NP	C2-C1-C8A	2.33	123.30	120.91
3	E	505	1NP	C3-C4-C4A	2.30	124.04	120.44
3	B	602	1NP	C3-C4-C4A	2.30	124.04	120.44
3	D	603	1NP	C2-C1-C8A	2.29	123.27	120.91
3	F	402	1NP	C7-C8-C8A	2.27	124.04	120.89
3	F	401	1NP	C5-C4A-C8A	-2.23	116.19	119.12
3	A	604	1NP	C6-C5-C4A	2.23	123.92	120.44
3	F	402	1NP	C4-C4A-C8A	-2.22	116.20	119.12
3	D	604	1NP	C5-C4A-C8A	-2.22	116.20	119.12
3	C	604	1NP	C3-C4-C4A	2.22	123.91	120.44
3	A	603	1NP	C2-C1-C8A	2.22	123.19	120.91
3	B	602	1NP	C5-C4A-C8A	-2.21	116.21	119.12
3	E	504	1NP	C6-C7-C8	-2.16	117.42	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	604	1NP	C5-C4A-C8A	-2.14	116.30	119.12
3	C	604	1NP	C2-C1-C8A	2.14	123.11	120.91
3	E	505	1NP	C2-C1-C8A	2.14	123.11	120.91
3	C	604	1NP	C8-C8A-C1	2.12	125.12	122.21
3	D	603	1NP	C3-C4-C4A	2.10	123.72	120.44
3	C	603	1NP	C3-C4-C4A	2.09	123.71	120.44
3	A	604	1NP	C3-C4-C4A	2.09	123.71	120.44
3	A	605	1NP	C6-C7-C8	-2.08	117.52	120.44
3	A	604	1NP	C6-C7-C8	-2.08	117.52	120.44
3	A	605	1NP	C3-C2-C1	-2.07	117.67	120.28
3	A	604	1NP	C5-C4A-C8A	-2.06	116.41	119.12
3	D	604	1NP	C2-C1-C8A	2.06	123.03	120.91
3	F	402	1NP	C6-C5-C4A	2.05	123.65	120.44
3	A	605	1NP	C8-C8A-C1	2.05	125.02	122.21

There are no chirality outliers.

There are no torsion outliers.

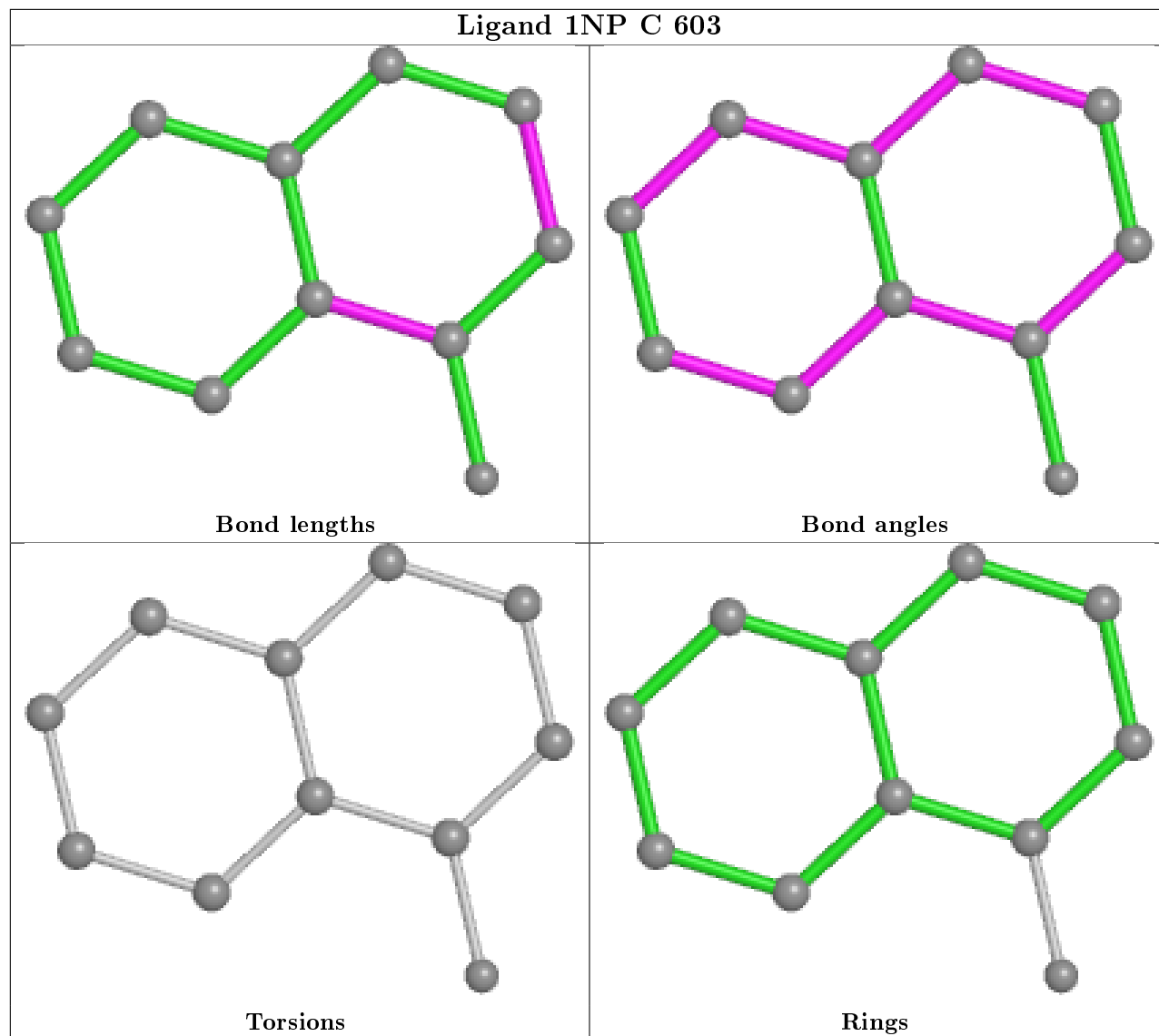
There are no ring outliers.

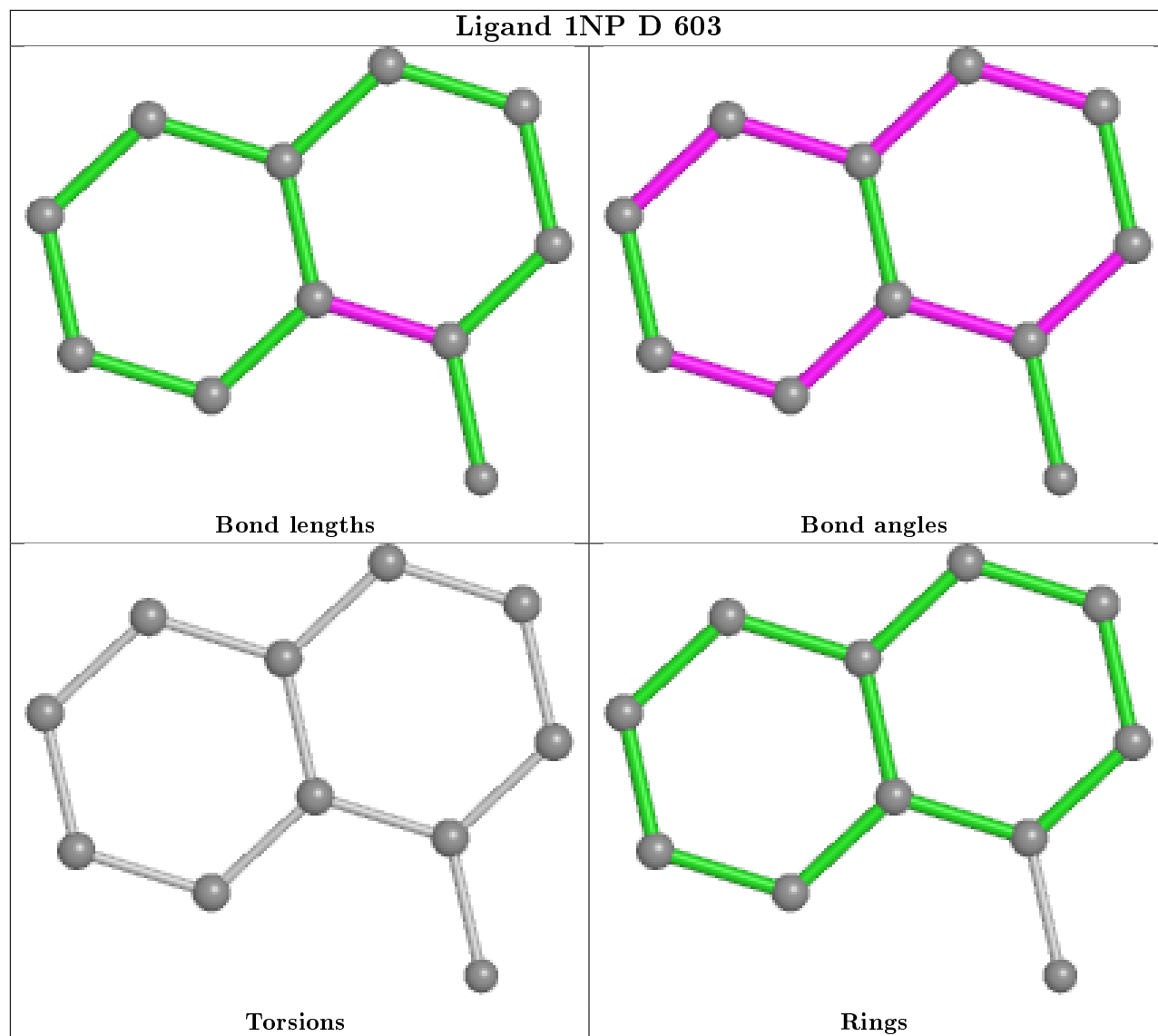
9 monomers are involved in 10 short contacts:

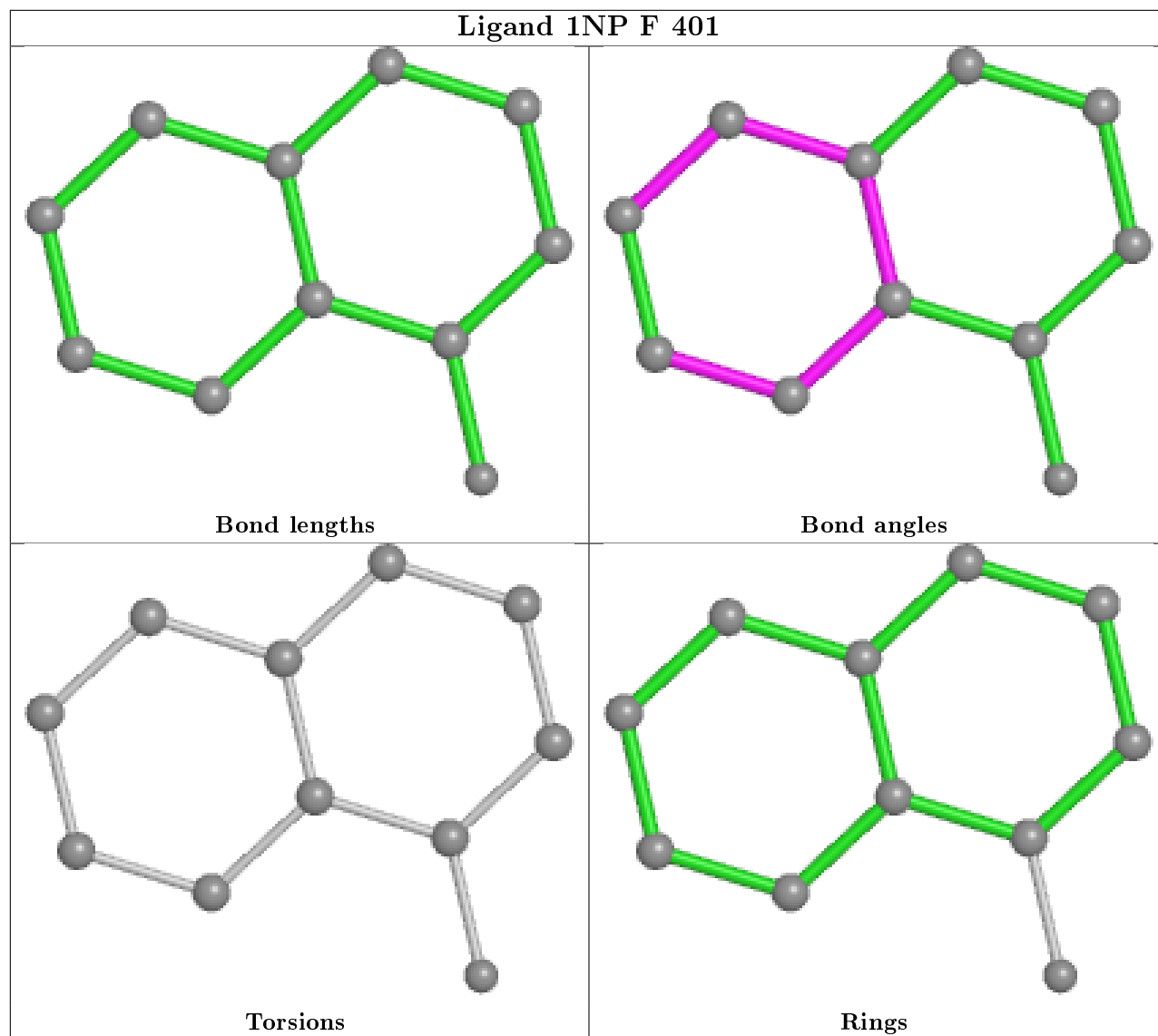
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	603	1NP	1	0
2	A	602	PO4	1	0
3	E	505	1NP	1	0
3	F	402	1NP	1	0
3	B	602	1NP	1	0
2	C	602	PO4	1	0
3	D	604	1NP	2	0
3	A	603	1NP	2	0
3	C	604	1NP	2	0

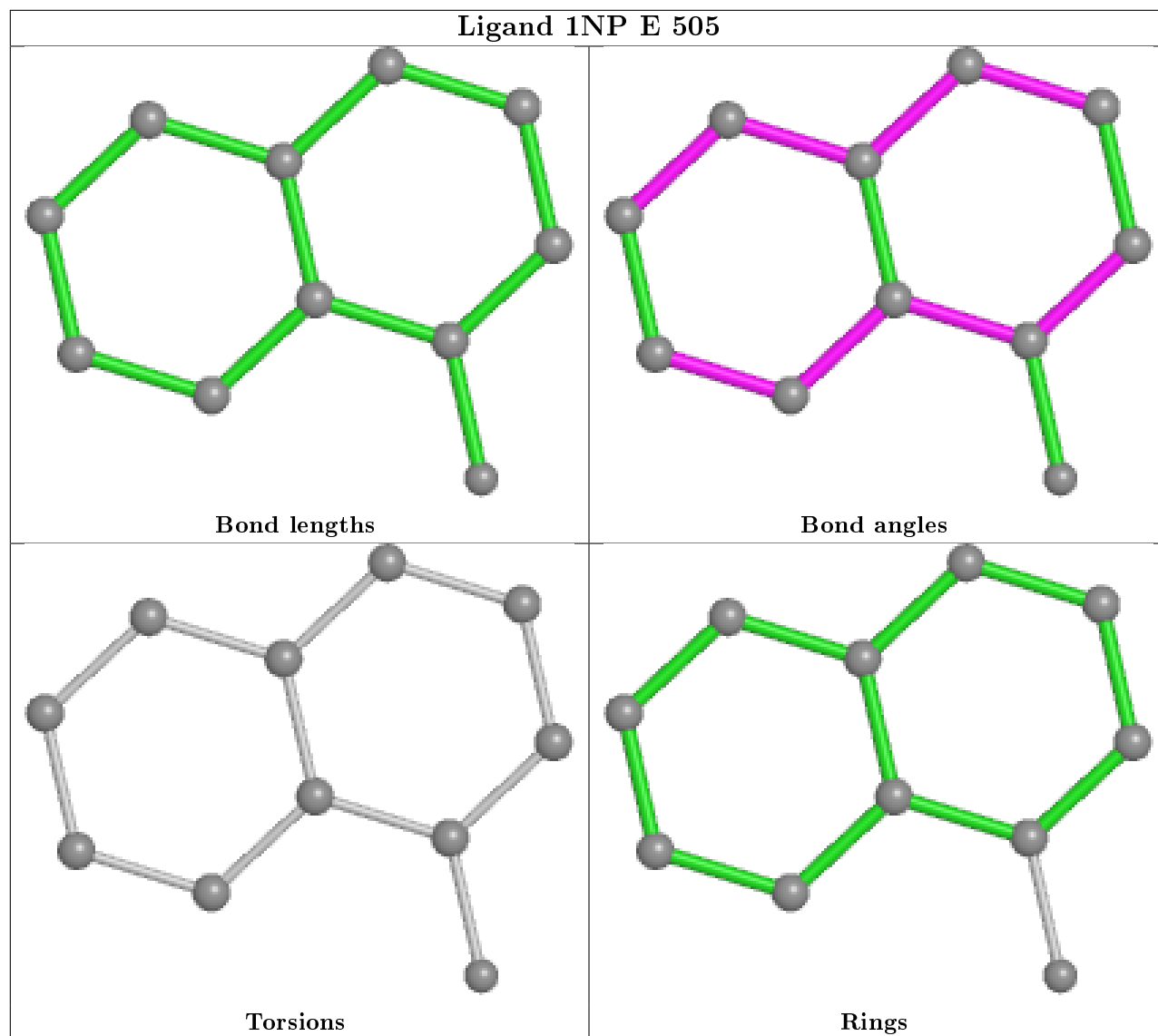
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

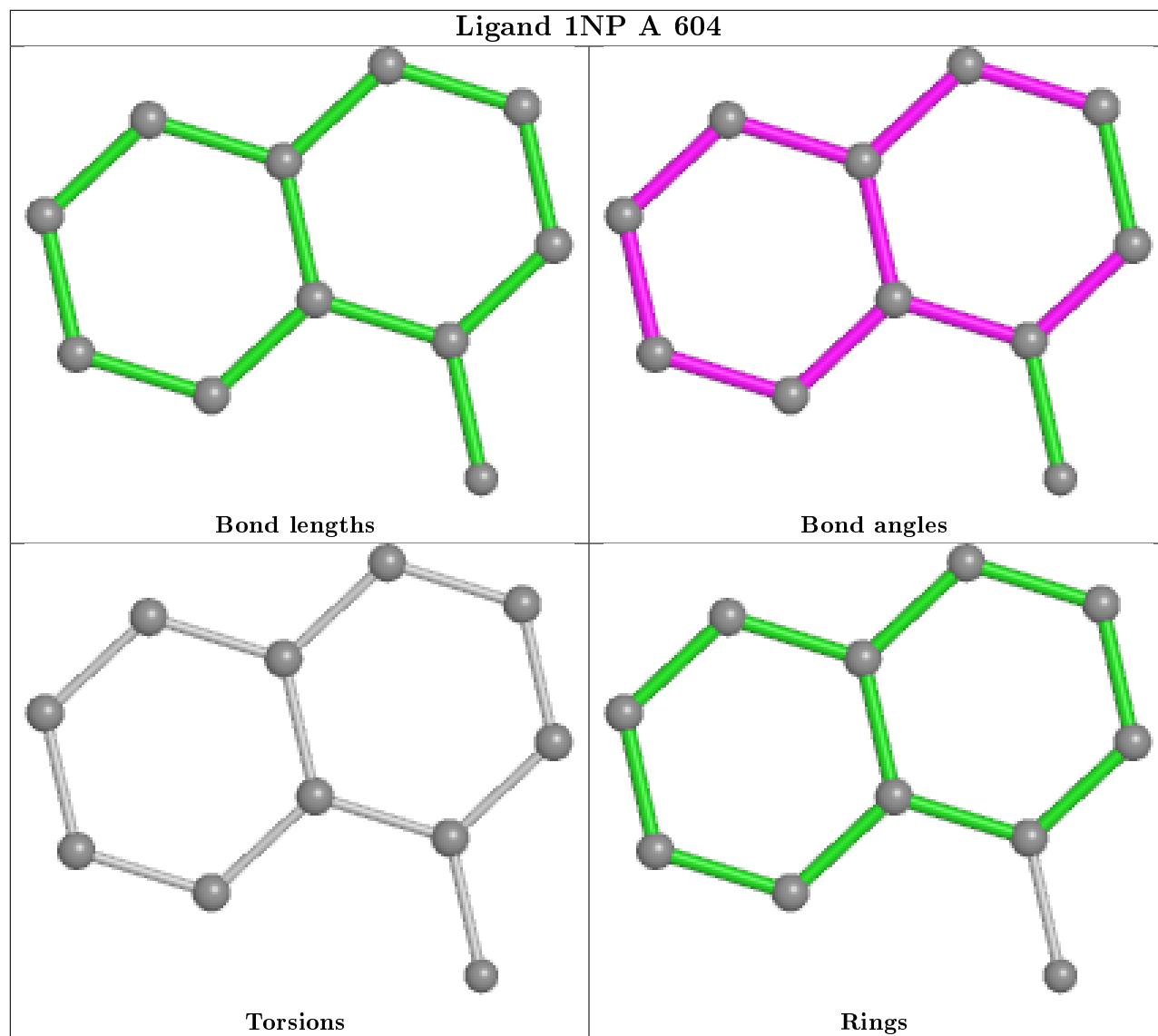
equivalents in the CSD to analyse the geometry.



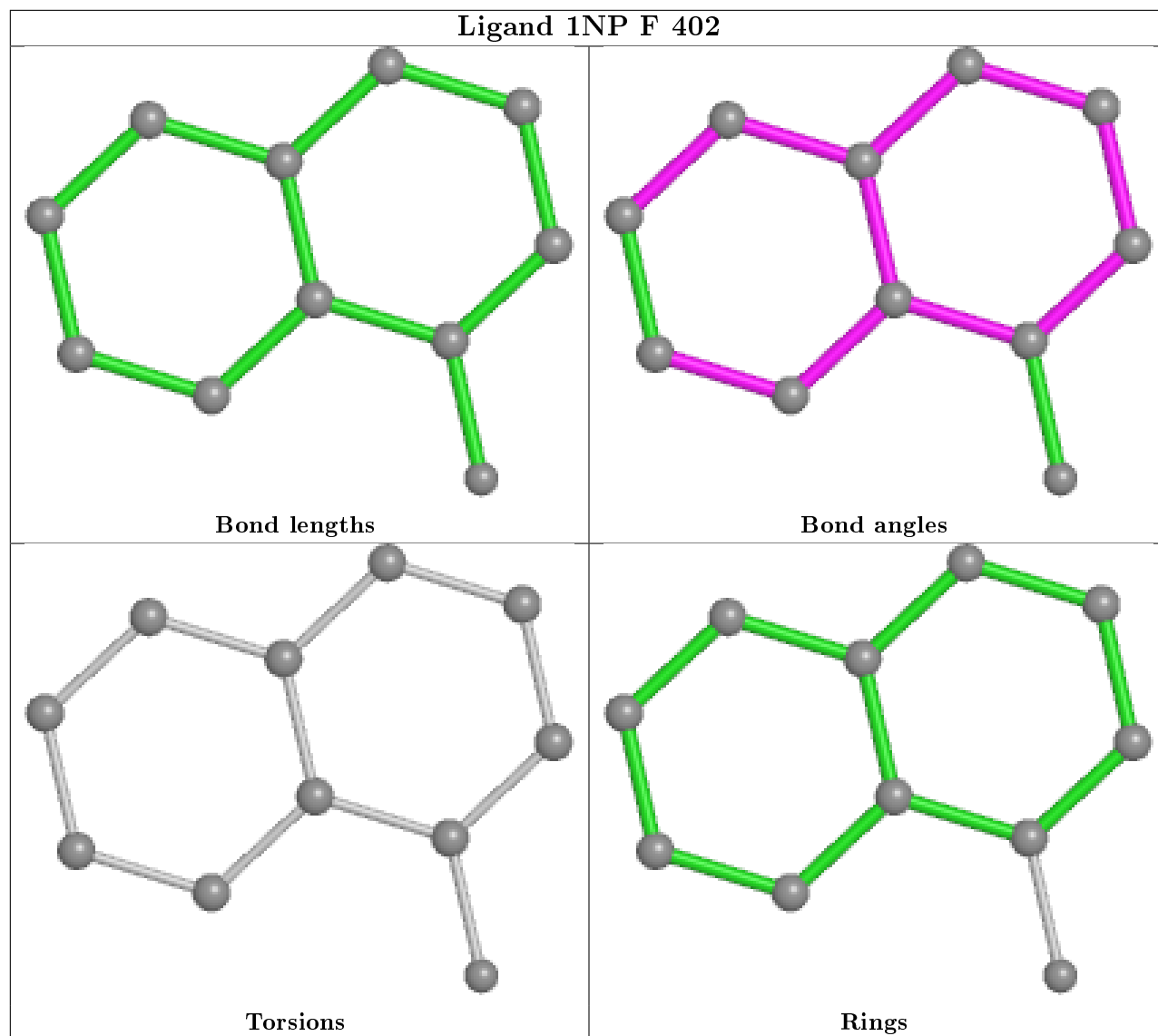


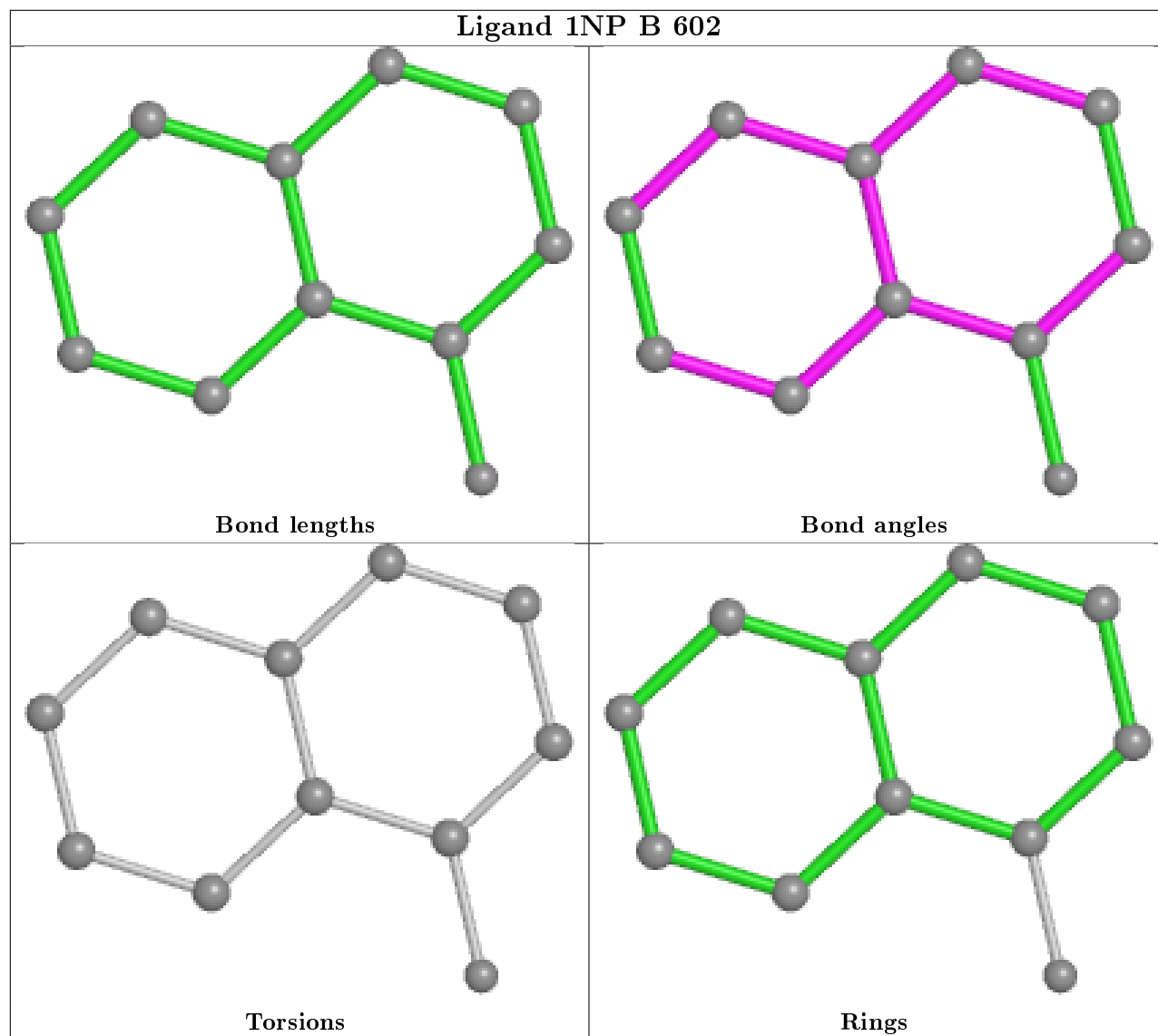


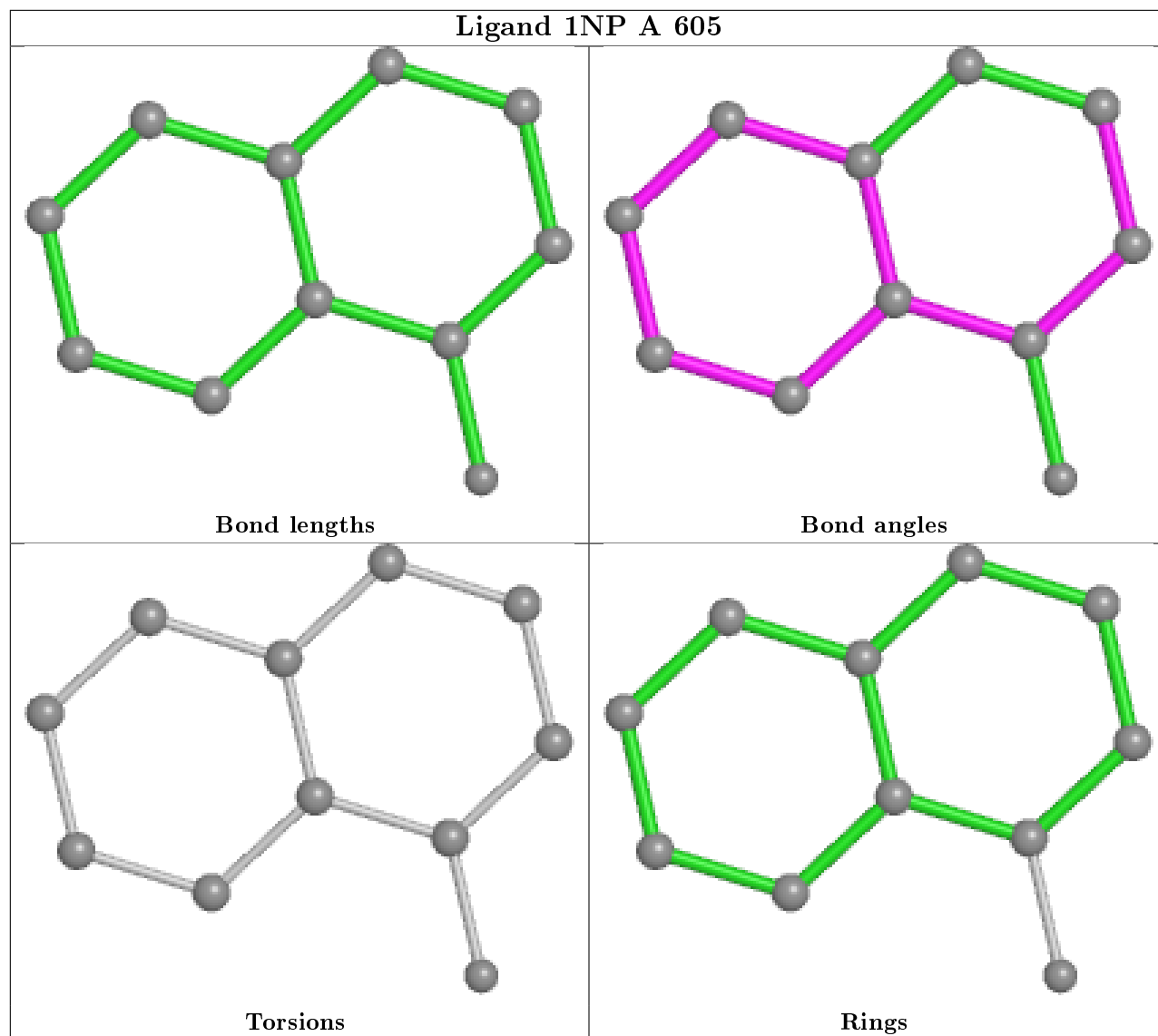


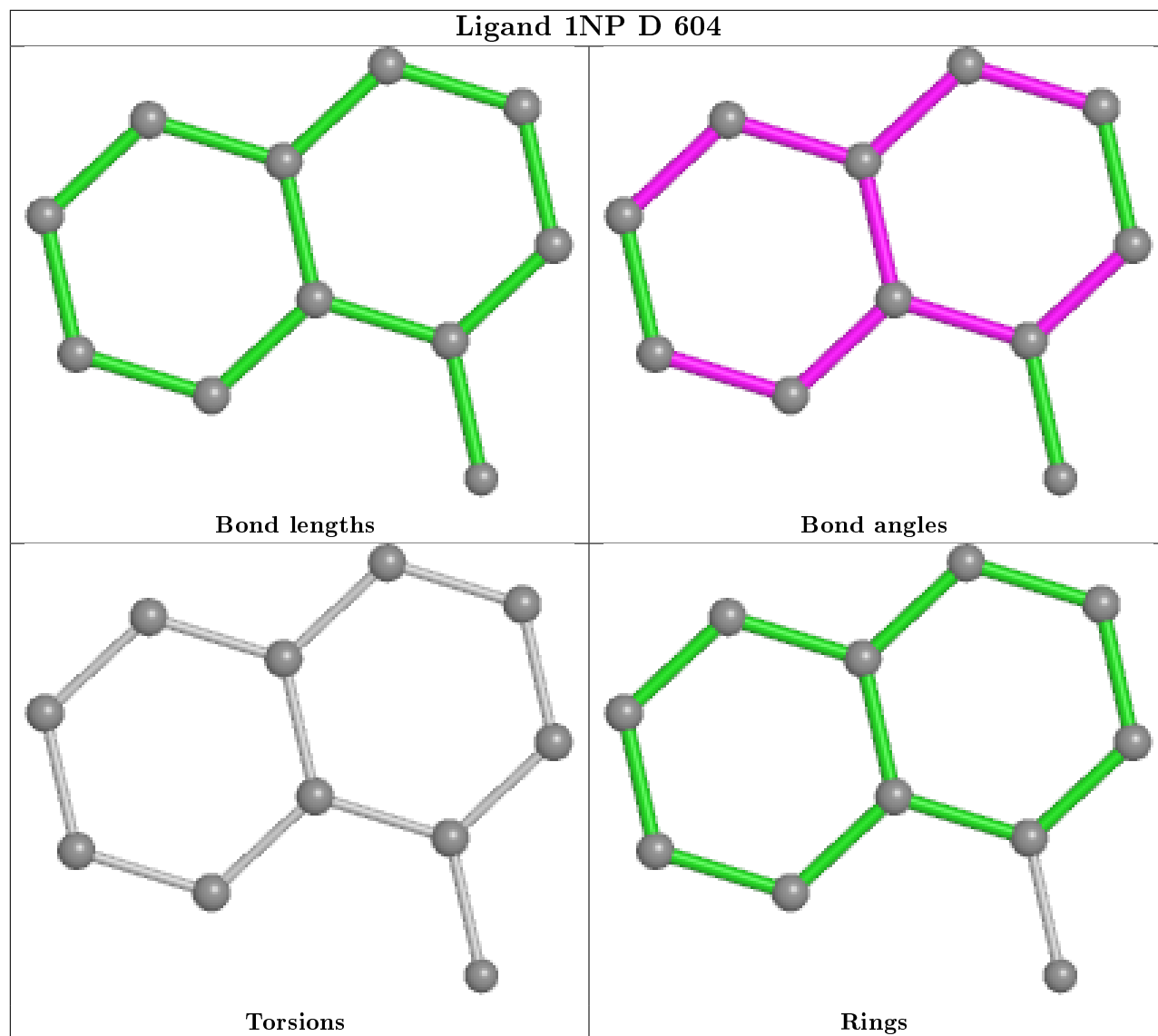


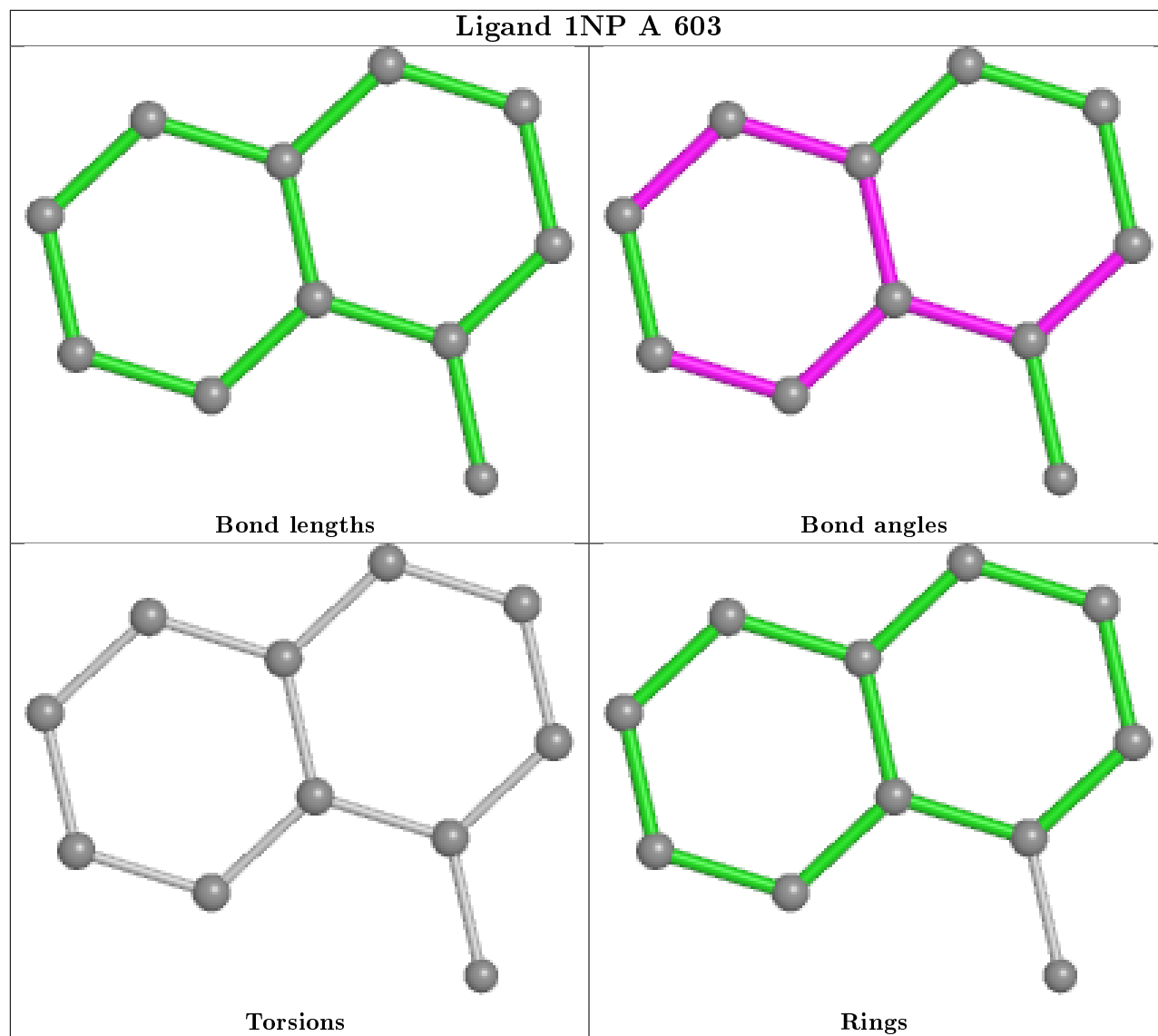


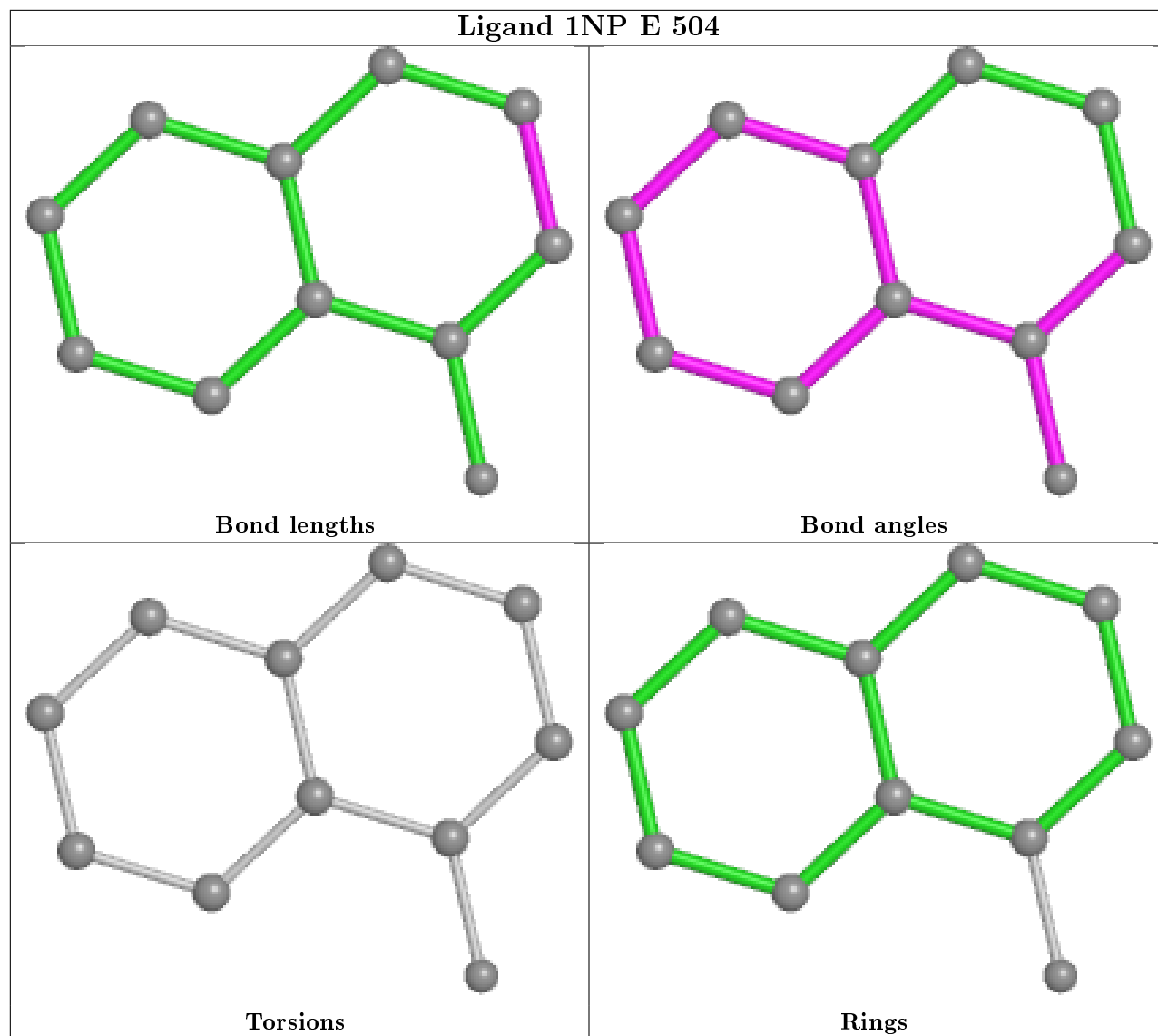


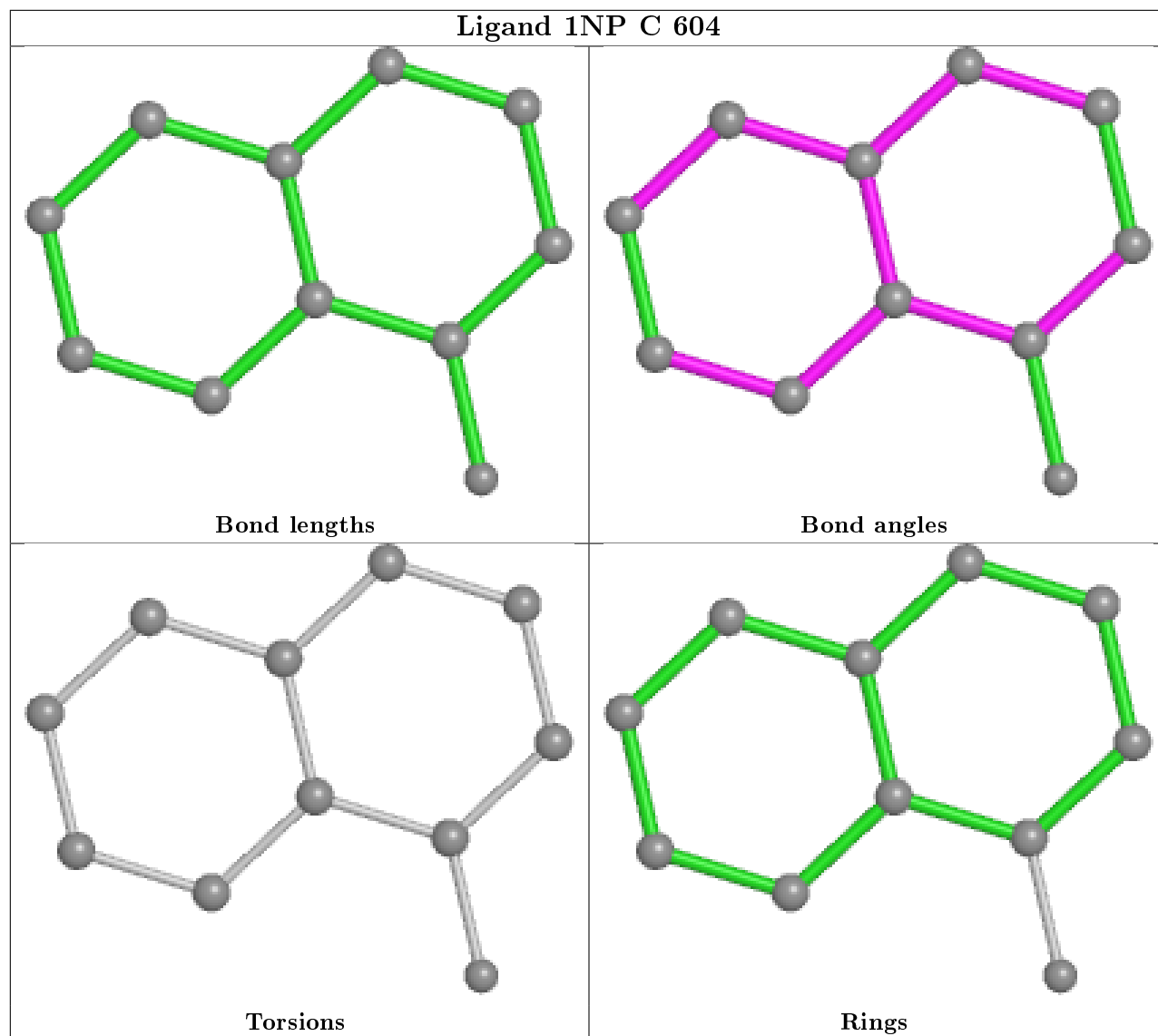












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	308/309 (99%)	-0.15	6 (1%) 66 68	18, 24, 39, 63	0
1	B	297/309 (96%)	-0.03	12 (4%) 38 39	19, 30, 49, 77	0
1	C	307/309 (99%)	-0.25	2 (0%) 87 88	18, 29, 43, 57	0
1	D	298/309 (96%)	-0.21	6 (2%) 65 66	20, 28, 42, 75	0
1	E	300/309 (97%)	-0.19	7 (2%) 60 62	19, 27, 43, 58	0
1	F	299/309 (96%)	-0.24	5 (1%) 70 71	19, 29, 43, 73	0
All	All	1809/1854 (97%)	-0.18	38 (2%) 63 65	18, 28, 43, 77	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	VAL	10.8
1	B	76	THR	7.4
1	B	74	GLY	5.9
1	A	0	SER	5.1
1	D	227	THR	4.8
1	A	80	ARG	3.9
1	F	227	THR	3.9
1	A	74	GLY	3.8
1	B	75	SER	3.6
1	D	0	SER	3.6
1	B	73	SER	3.5
1	D	239	VAL	3.4
1	E	81	ASP	3.3
1	B	227	THR	3.1
1	A	76	THR	3.1
1	B	238	ARG	3.0
1	A	229	MET	2.9
1	D	74	GLY	2.8
1	E	80	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	74	GLY	2.7
1	C	230	GLY	2.6
1	F	81	ASP	2.6
1	F	0	SER	2.5
1	B	240	LYS	2.5
1	D	238	ARG	2.5
1	D	78	LEU	2.5
1	E	1	VAL	2.5
1	C	81	ASP	2.4
1	A	81	ASP	2.4
1	B	307	SER	2.3
1	B	182	GLU	2.2
1	E	227	THR	2.2
1	B	250	ARG	2.2
1	B	80	ARG	2.2
1	E	257	SER	2.1
1	E	235	GLY	2.0
1	E	238	ARG	2.0
1	F	238	ARG	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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	1NP	D	604	11/11	0.73	0.34	42,47,55,56	0
3	1NP	D	603	11/11	0.82	0.17	33,36,38,40	0
3	1NP	C	603	11/11	0.82	0.13	32,35,39,40	0
3	1NP	E	504	11/11	0.83	0.13	33,39,41,44	0

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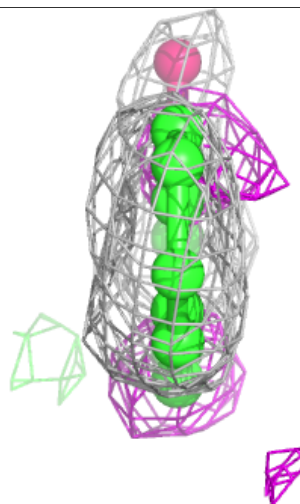
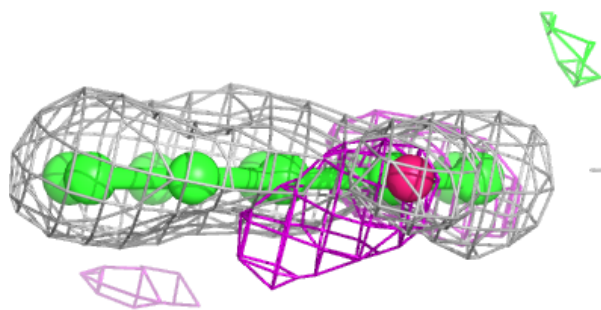
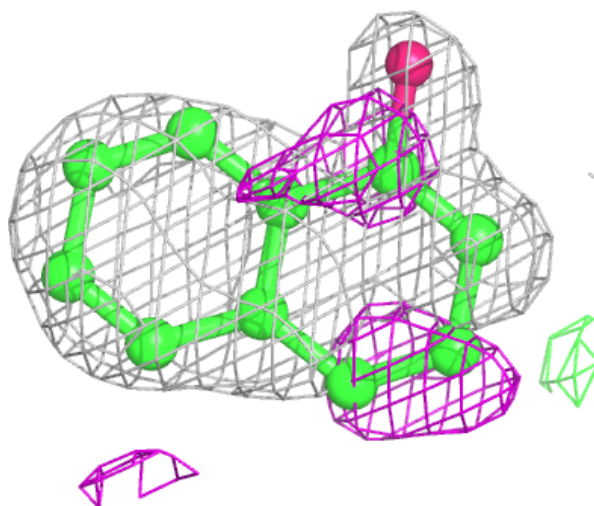
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	1NP	A	603	11/11	0.85	0.18	38,40,44,48	0
3	1NP	F	401	11/11	0.86	0.11	27,32,35,36	0
3	1NP	B	602	11/11	0.87	0.25	39,41,50,53	0
3	1NP	A	605	11/11	0.87	0.14	31,35,37,38	0
3	1NP	F	402	11/11	0.87	0.11	32,37,40,40	0
3	1NP	E	505	11/11	0.88	0.12	34,39,45,46	0
2	PO4	E	503	5/5	0.90	0.30	47,54,58,62	0
3	1NP	C	604	11/11	0.90	0.19	39,41,44,47	0
2	PO4	D	602	5/5	0.93	0.21	39,49,52,55	0
2	PO4	E	502	5/5	0.93	0.18	34,43,48,49	0
2	PO4	A	602	5/5	0.93	0.24	41,49,56,60	0
2	PO4	B	601	5/5	0.93	0.13	49,50,52,57	0
3	1NP	A	604	11/11	0.93	0.09	25,29,32,34	0
2	PO4	D	601	5/5	0.95	0.07	36,38,41,41	0
2	PO4	A	606	5/5	0.96	0.17	38,38,42,43	0
2	PO4	C	602	5/5	0.96	0.17	44,49,59,59	0
2	PO4	C	601	5/5	0.98	0.06	35,37,41,42	0
2	PO4	A	601	5/5	0.99	0.06	30,32,36,38	0
2	PO4	E	501	5/5	0.99	0.05	29,30,36,37	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.

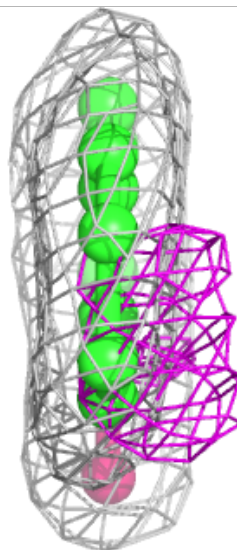
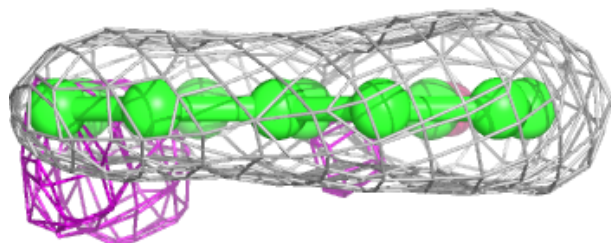
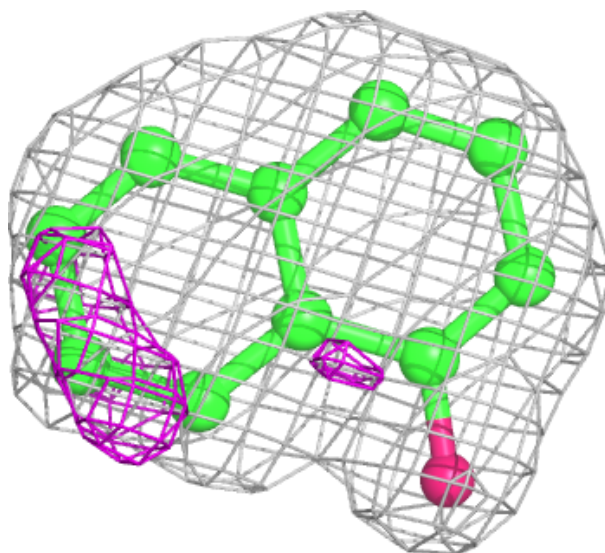
**Electron density around 1NP D 604:**

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



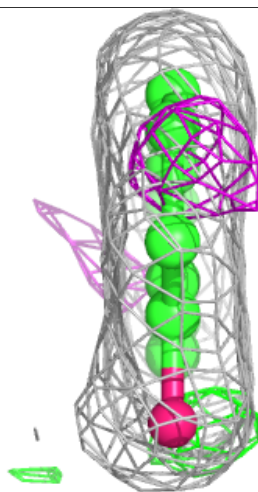
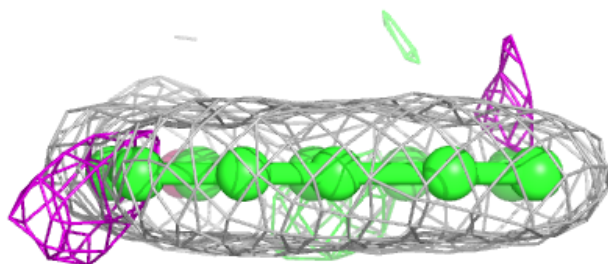
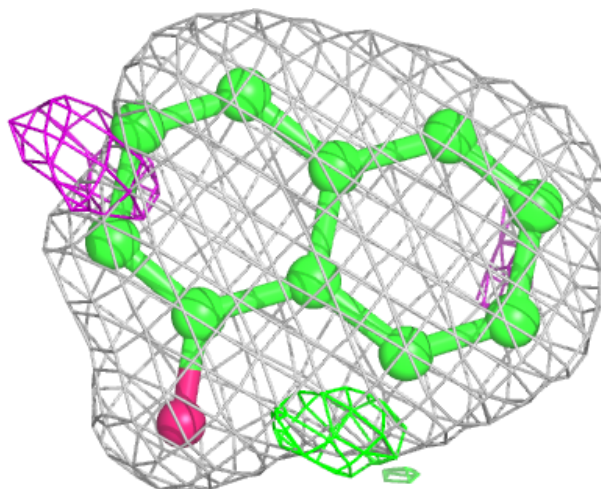
**Electron density around 1NP D 603:**

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



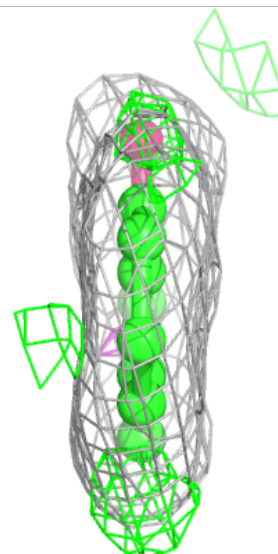
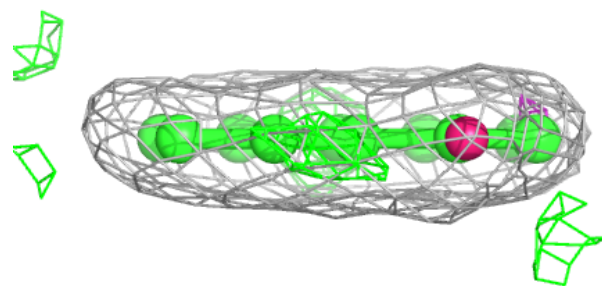
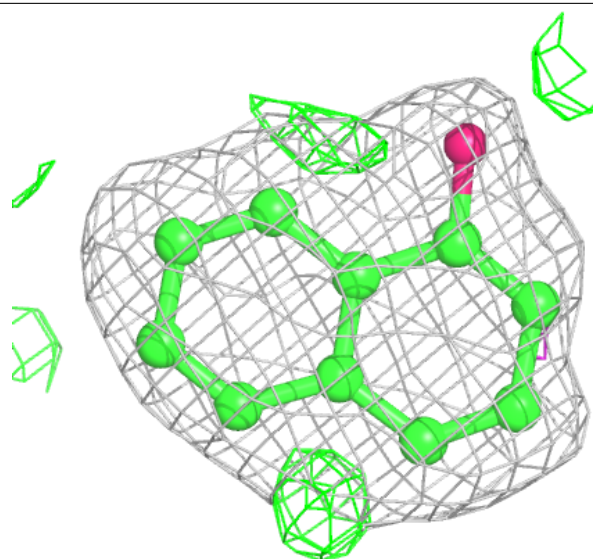
**Electron density around 1NP C 603:**

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



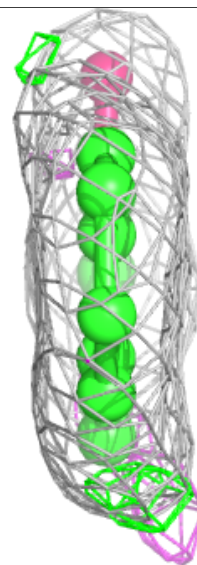
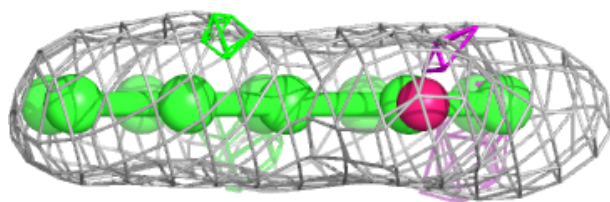
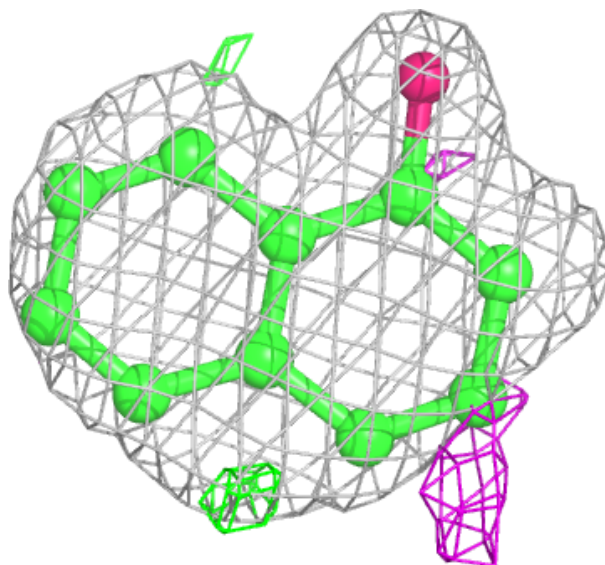
**Electron density around 1NP E 504:**

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



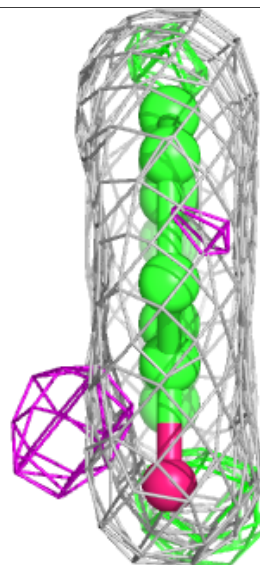
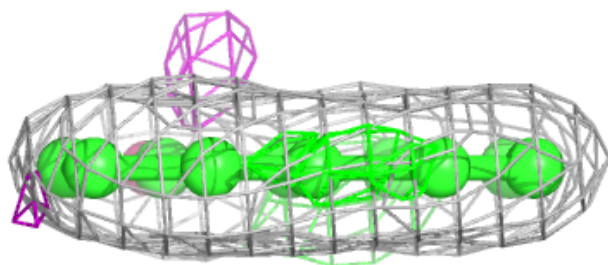
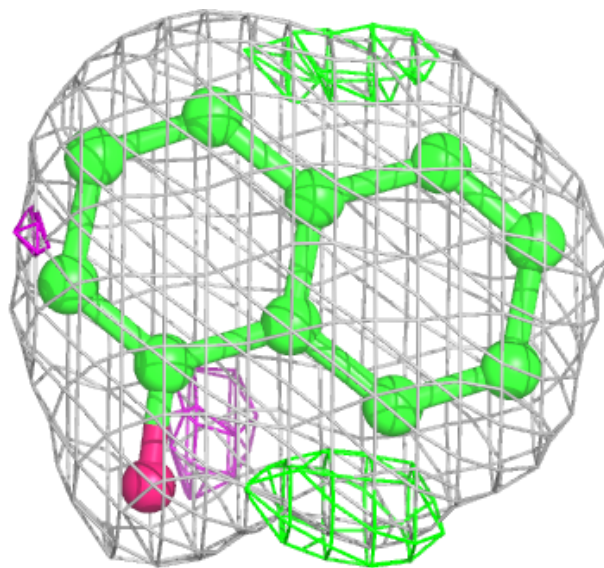
**Electron density around 1NP A 603:**

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



**Electron density around 1NP F 401:**

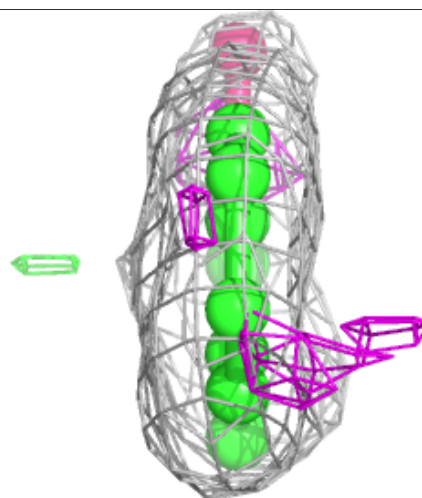
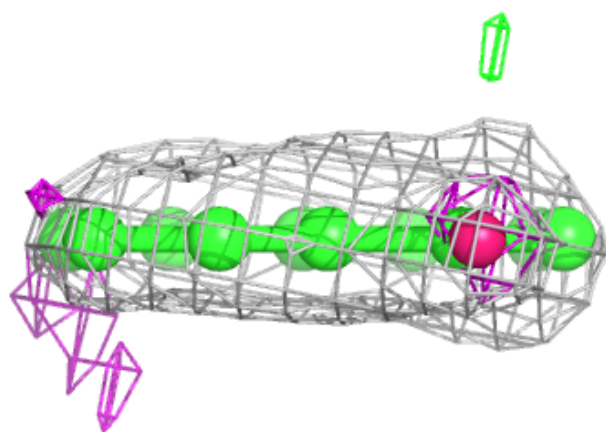
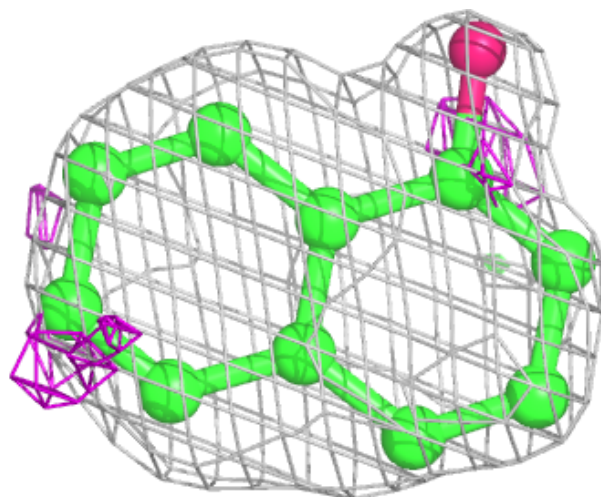
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





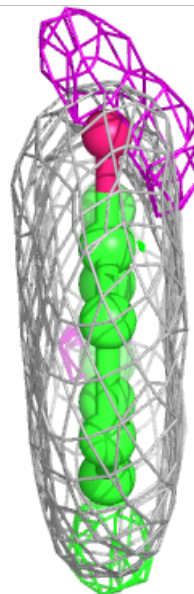
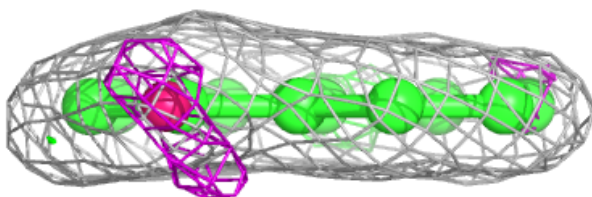
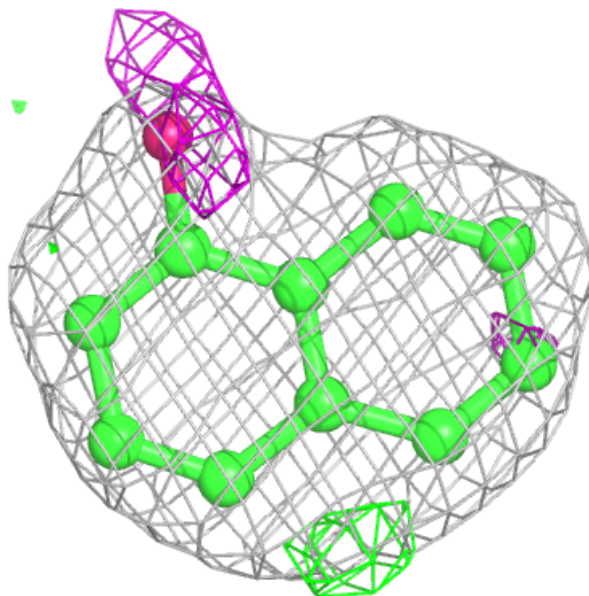
**Electron density around 1NP B 602:**

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



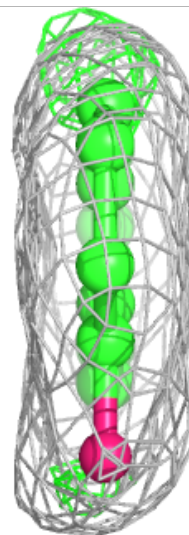
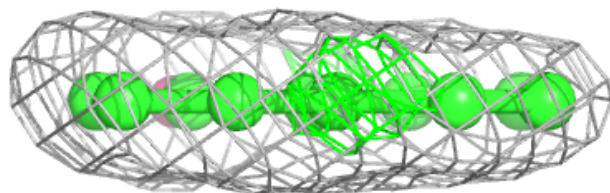
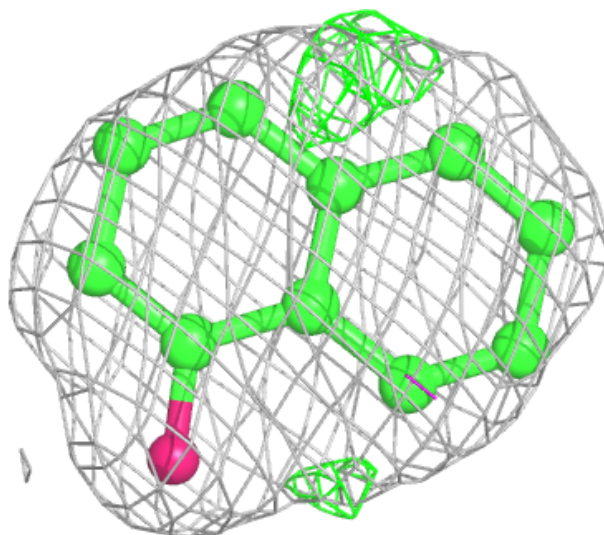
**Electron density around 1NP A 605:**

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



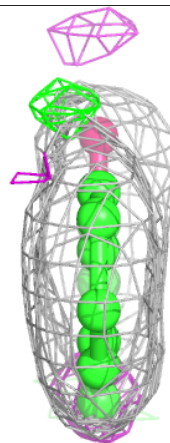
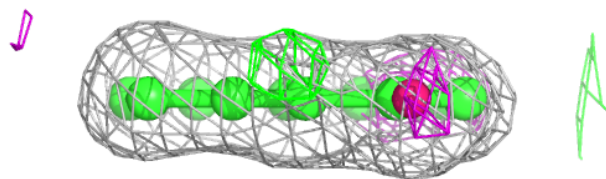
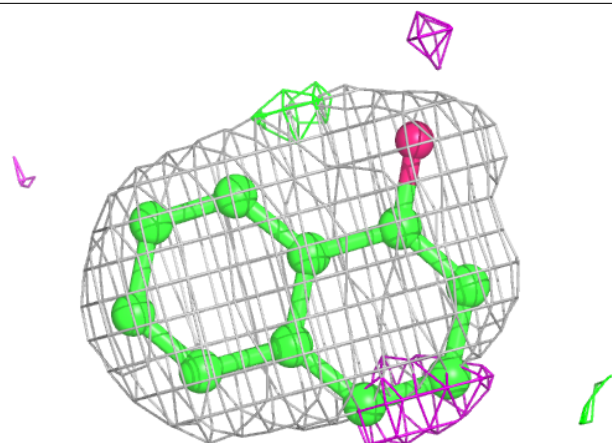
**Electron density around 1NP F 402:**

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



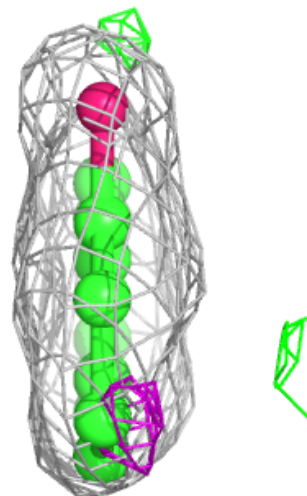
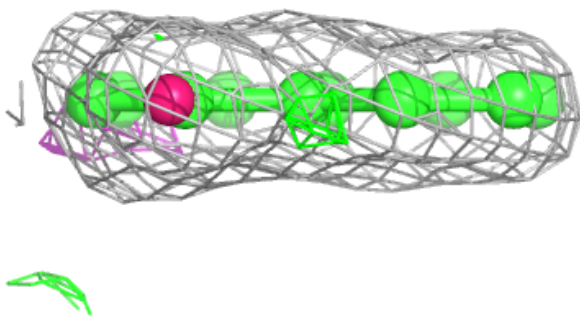
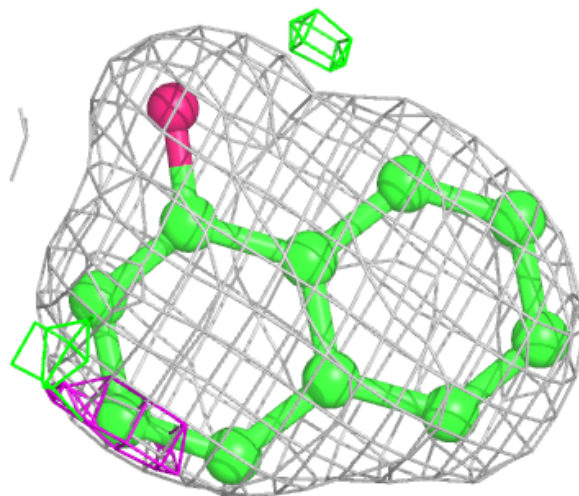
**Electron density around 1NP E 505:**

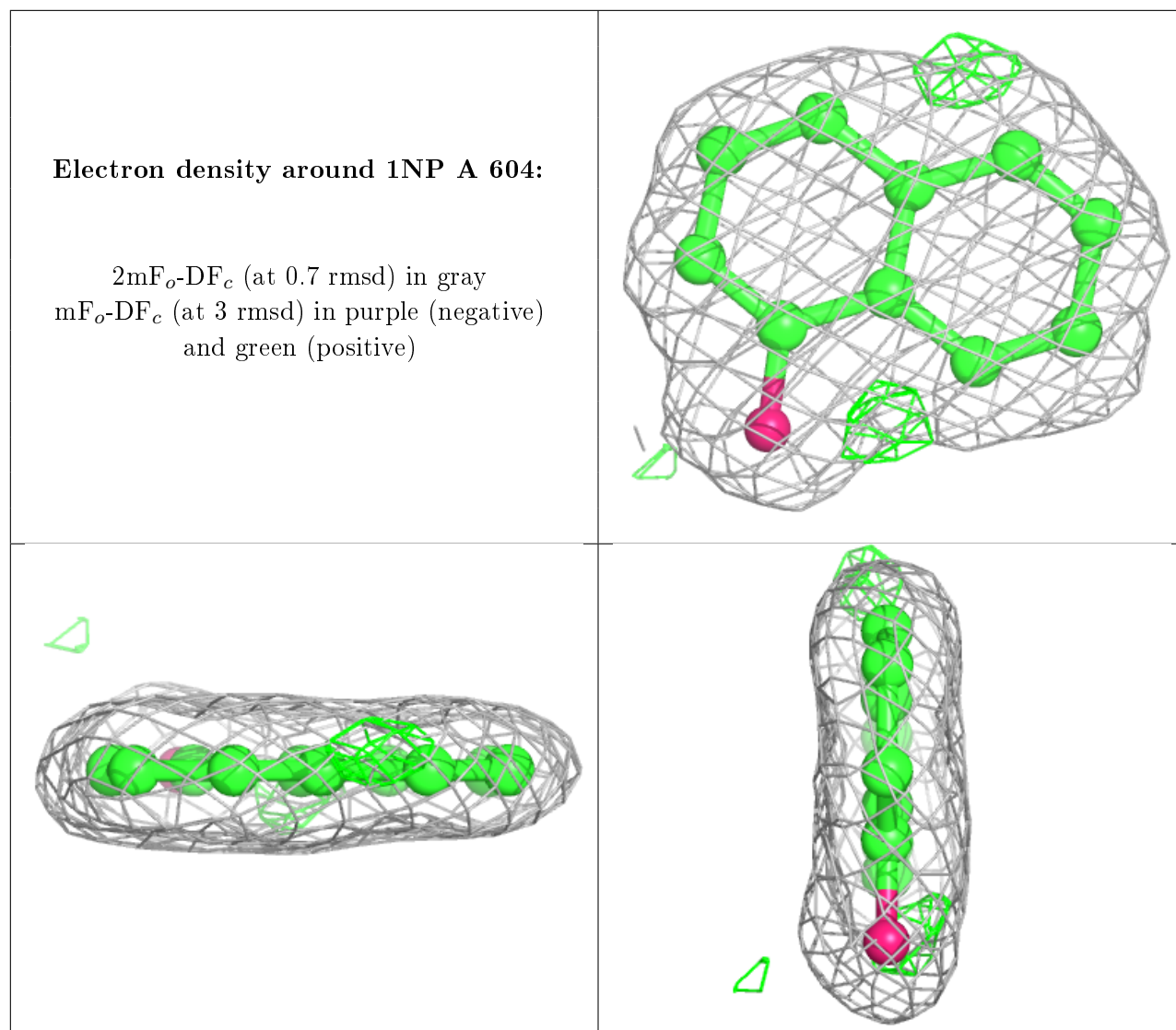
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 1NP C 604:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.