



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2023 – 01:37 AM JST

PDB ID : 6KF1  
Title : Microbial Hormone-sensitive lipase- E53 mutant S162A  
Authors : Xiaochen, Y.; Zhengyang, L.; Xuewei, X.; Jixi, L.  
Deposited on : 2019-07-05  
Resolution : 2.00 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
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) : 2.36

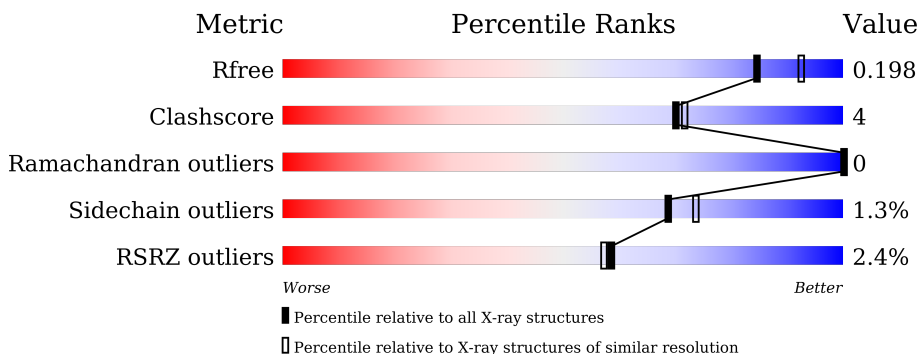
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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% 94% 6%
1	B	309	 5% 92% 7%
1	C	309	 2% 94% 6%
2	D	310	 2% 94% 6%

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10736 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 Lipase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	309	2275	1443	391	429	12	0	0	0
1	B	309	2280	1446	391	431	12	0	0	0
1	C	309	2272	1442	391	427	12	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	162	ALA	SER	engineered mutation	UNP A0A074MDU6
B	162	ALA	SER	engineered mutation	UNP A0A074MDU6
C	162	ALA	SER	engineered mutation	UNP A0A074MDU6

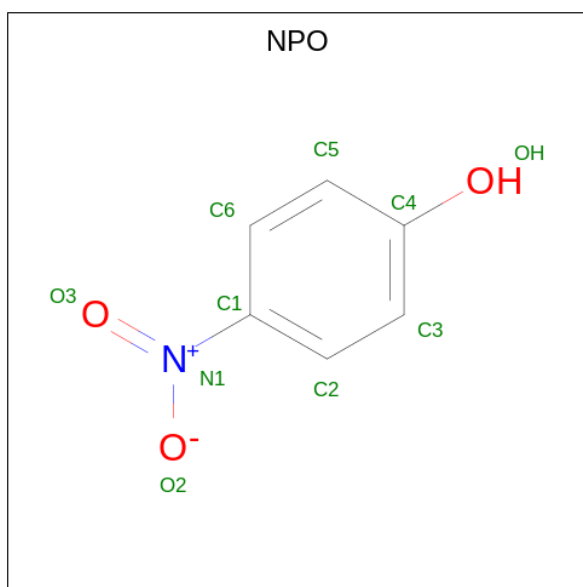
- Molecule 2 is a protein called Lipase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	310	2294	1453	392	437	12	0	0	0

There is a discrepancy between the modelled and reference sequences:

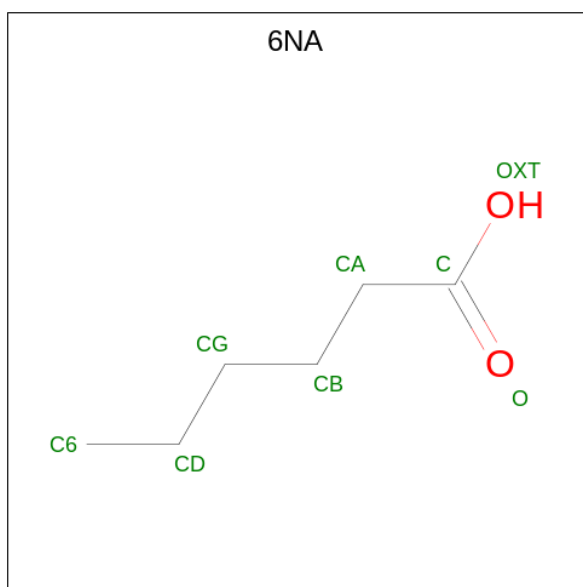
Chain	Residue	Modelled	Actual	Comment	Reference
D	162	ALA	SER	engineered mutation	UNP A0A074MDU6

- Molecule 3 is P-NITROPHENOL (three-letter code: NPO) (formula: C<sub>6</sub>H<sub>5</sub>NO<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



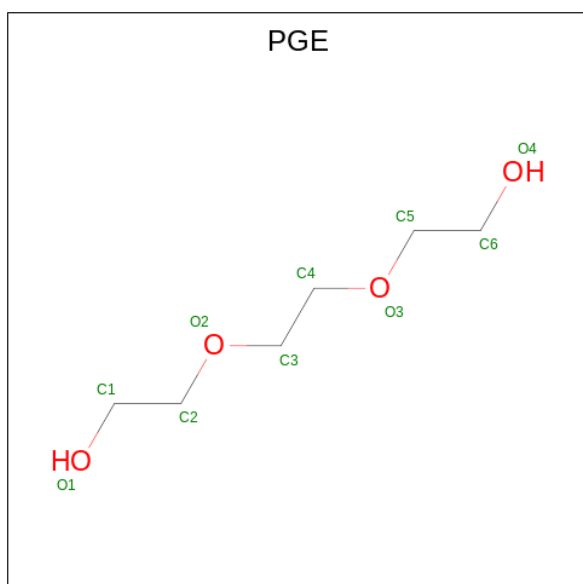
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	10	6	1	3	0	0
3	A	1	10	6	1	3	0	0
3	A	1	10	6	1	3	0	0
3	B	1	10	6	1	3	0	0
3	B	1	10	6	1	3	0	0
3	B	1	10	6	1	3	0	0
3	C	1	10	6	1	3	0	0
3	C	1	10	6	1	3	0	0
3	C	1	10	6	1	3	0	0
3	D	1	10	6	1	3	0	0
3	D	1	10	6	1	3	0	0

- Molecule 4 is HEXANOIC ACID (three-letter code: 6NA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>).



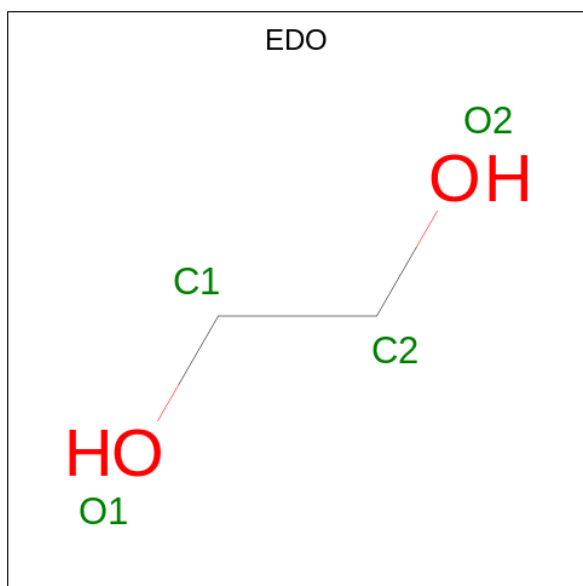
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0
4	C	1	Total C O 8 6 2	0	0
4	D	1	Total C O 8 6 2	0	0
4	D	1	Total C O 8 6 2	0	0

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



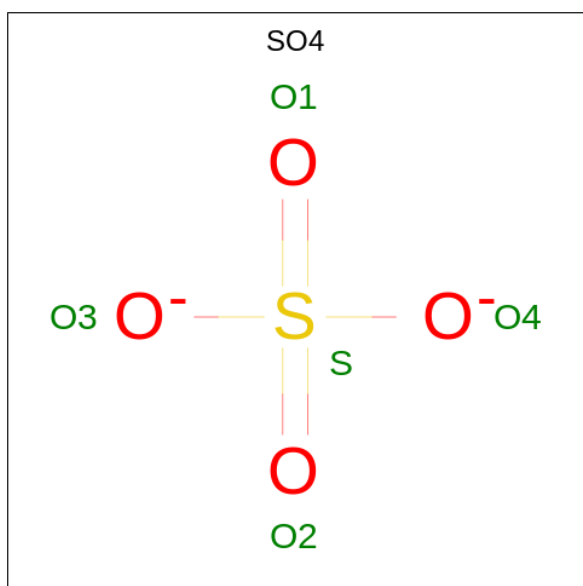
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



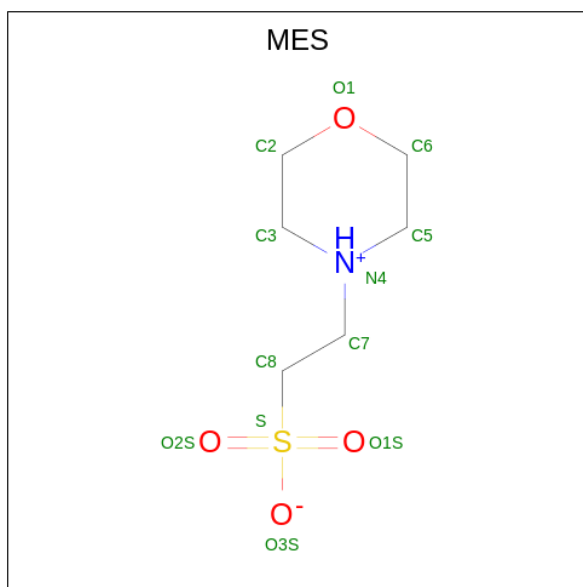
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

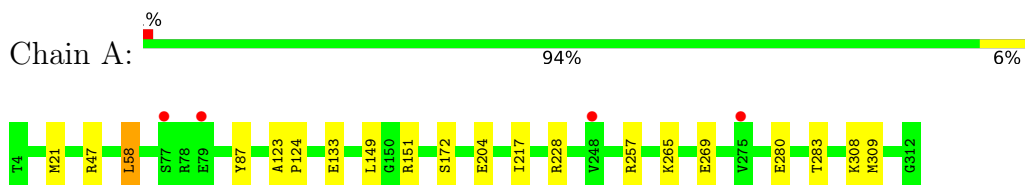
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	373	Total	O	0	0
			373	373		
9	B	315	Total	O	0	0
			315	315		
9	C	400	Total	O	0	0
			400	400		
9	D	341	Total	O	0	0
			341	341		

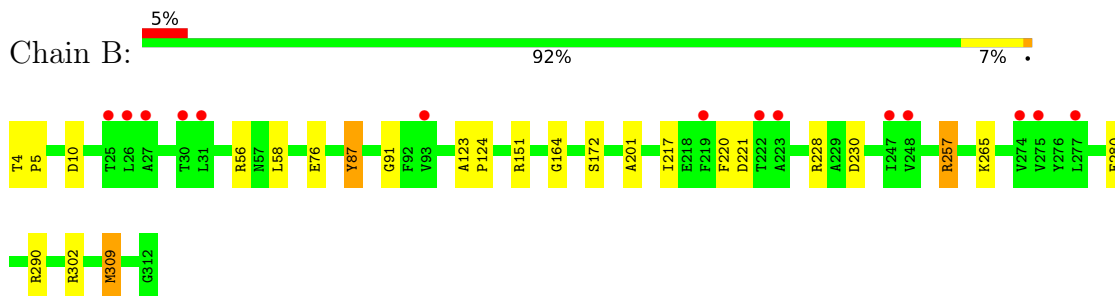
### 3 Residue-property plots [i](#)

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.

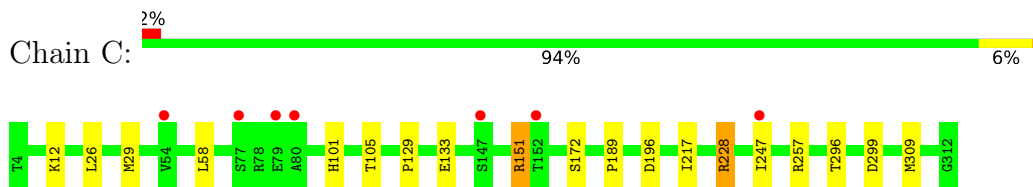
- Molecule 1: Lipase



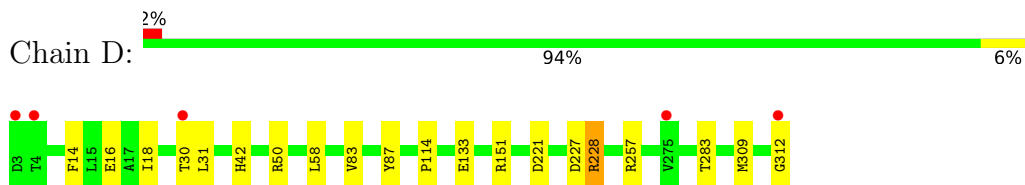
- Molecule 1: Lipase



- Molecule 1: Lipase



- Molecule 2: Lipase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.39Å 129.79Å 220.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.70 – 2.00 48.65 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.70-2.00) 99.8 (48.65-2.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.23 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.8.0253	Depositor
R, $R_{free}$	0.159 , 0.189 0.170 , 0.198	Depositor DCC
$R_{free}$ test set	6777 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.7	Xtrriage
Anisotropy	0.012	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 51.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10736	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.21% 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: EDO, SO4, MES, PGE, NPO, 6NA

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	0.84	1/2325 (0.0%)	0.91	0/3174
1	B	0.84	2/2331 (0.1%)	0.94	7/3182 (0.2%)
1	C	0.85	1/2323 (0.0%)	0.96	6/3172 (0.2%)
2	D	0.84	0/2345	0.93	3/3201 (0.1%)
All	All	0.84	4/9324 (0.0%)	0.94	16/12729 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	D	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	133	GLU	CD-OE2	-10.23	1.14	1.25
1	A	133	GLU	CD-OE2	-8.17	1.16	1.25
1	B	76	GLU	CD-OE2	6.70	1.33	1.25
1	B	280	GLU	CD-OE2	6.41	1.32	1.25

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	228	ARG	NE-CZ-NH1	-10.41	115.10	120.30
1	C	228	ARG	NE-CZ-NH2	8.70	124.65	120.30
2	D	228	ARG	NE-CZ-NH1	6.81	123.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	151	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	C	151	ARG	CG-CD-NE	6.24	124.90	111.80
1	C	151	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	B	257	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	B	302	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	B	290	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	B	10	ASP	CB-CA-C	5.50	121.40	110.40
2	D	228	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	B	56	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	290	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	C	228	ARG	CG-CD-NE	-5.12	101.05	111.80
2	D	312	GLY	CA-C-O	-5.09	111.44	120.60
1	B	309	MET	CG-SD-CE	5.05	108.28	100.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	283	THR	Peptide
2	D	283	THR	Peptide

## 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	2275	0	2251	22	0
1	B	2280	0	2261	19	0
1	C	2272	0	2253	17	0
2	D	2294	0	2274	19	0
3	A	30	0	14	1	0
3	B	30	0	15	1	0
3	C	30	0	14	1	0
3	D	20	0	9	0	0
4	A	8	0	11	1	0
4	B	8	0	11	4	0
4	C	8	0	11	3	0
4	D	16	0	22	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	10	0	14	1	0
6	B	4	0	6	0	0
7	C	5	0	0	0	0
7	D	5	0	0	0	0
8	D	12	0	13	0	0
9	A	373	0	0	9	0
9	B	315	0	0	3	4
9	C	400	0	0	4	0
9	D	341	0	0	5	2
All	All	10736	0	9179	67	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (67) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ARG:NH2	9:A:501:HOH:O	1.80	1.15
1:A:228:ARG:CZ	9:A:501:HOH:O	2.14	0.91
1:C:257:ARG:HH12	4:C:405:6NA:HBC1	1.39	0.87
1:C:309:MET:CE	2:D:309:MET:HE3	2.15	0.77
1:B:257:ARG:HH12	4:B:405:6NA:HBC1	1.51	0.74
1:B:230:ASP:OD1	9:B:501:HOH:O	2.06	0.73
1:A:280:GLU:OE1	9:A:502:HOH:O	2.06	0.72
1:C:309:MET:HE3	2:D:309:MET:HE3	1.72	0.72
1:A:257:ARG:HH12	4:A:404:6NA:HBC1	1.55	0.71
1:C:309:MET:HE3	2:D:309:MET:CE	2.23	0.69
1:C:12:LYS:HE2	9:C:762:HOH:O	1.93	0.68
1:A:309:MET:CE	1:B:309:MET:HE3	2.26	0.65
1:A:309:MET:HE2	1:B:309:MET:HE3	1.80	0.64
1:C:309:MET:CE	2:D:309:MET:CE	2.78	0.61
2:D:30:THR:HB	4:D:405:6NA:HAC2	1.83	0.61
1:C:257:ARG:NH1	4:C:405:6NA:HBC1	2.13	0.60
1:A:269:GLU:OE1	1:B:265:LYS:NZ	2.34	0.60
1:C:309:MET:HE2	2:D:309:MET:HE3	1.83	0.59
1:A:21:MET:HE1	9:C:872:HOH:O	2.03	0.57
1:A:309:MET:CE	1:B:309:MET:CE	2.82	0.57
1:A:309:MET:HE3	1:B:309:MET:CE	2.35	0.56
1:A:228:ARG:NE	9:A:501:HOH:O	2.28	0.55
2:D:257:ARG:HH22	4:D:406:6NA:HGC1	1.73	0.53
2:D:31:LEU:HB2	4:D:405:6NA:HAC1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:LEU:HD23	1:C:58:LEU:N	2.24	0.53
1:B:221:ASP:CG	1:B:228:ARG:HH22	2.12	0.52
1:A:149:LEU:HD23	9:A:583:HOH:O	2.08	0.52
1:C:196:ASP:OD2	1:C:228:ARG:HD2	2.11	0.51
2:D:14:PHE:CE2	2:D:18:ILE:HD11	2.47	0.49
4:C:405:6NA:HBC2	9:C:848:HOH:O	2.13	0.49
2:D:31:LEU:H	4:D:405:6NA:CA	2.26	0.49
1:C:172:SER:HB2	9:C:658:HOH:O	2.13	0.48
1:A:265:LYS:HE3	5:A:405:PGE:H6	1.94	0.48
1:B:172:SER:HB2	9:B:659:HOH:O	2.14	0.48
2:D:133:GLU:OE2	9:D:501:HOH:O	2.20	0.47
1:A:47:ARG:HD2	9:A:549:HOH:O	2.13	0.47
1:A:309:MET:HE3	1:B:309:MET:HE2	1.96	0.47
1:A:172:SER:HB2	9:A:642:HOH:O	2.15	0.46
1:B:123:ALA:HB1	1:B:124:PRO:HA	1.97	0.46
1:C:26:LEU:HA	1:C:29:MET:HE3	1.98	0.46
1:B:257:ARG:NH1	4:B:405:6NA:HBC1	2.25	0.46
1:C:309:MET:HE3	2:D:309:MET:HE2	1.98	0.46
1:B:201:ALA:HB1	4:B:405:6NA:H6C1	1.98	0.45
1:A:58:LEU:CD1	1:A:58:LEU:N	2.79	0.45
1:B:257:ARG:HH22	4:B:405:6NA:HDC1	1.82	0.45
1:A:308:LYS:NZ	9:A:507:HOH:O	2.47	0.45
2:D:16:GLU:HB2	9:D:520:HOH:O	2.16	0.44
1:C:217:ILE:HG23	3:C:402:NPO:C4	2.48	0.44
1:B:87:TYR:O	1:B:164:GLY:HA3	2.17	0.44
2:D:31:LEU:H	4:D:405:6NA:HAC1	1.81	0.44
2:D:257:ARG:HH12	4:D:406:6NA:HGC1	1.82	0.44
1:B:4:THR:N	9:B:523:HOH:O	2.52	0.43
2:D:221:ASP:CG	2:D:228:ARG:HH22	2.22	0.43
1:A:204:GLU:CB	9:A:865:HOH:O	2.66	0.43
2:D:50:ARG:NH1	9:D:511:HOH:O	2.46	0.42
4:D:405:6NA:H6C3	9:D:662:HOH:O	2.19	0.42
1:A:123:ALA:HB1	1:A:124:PRO:HA	2.02	0.42
2:D:227:ASP:HB3	9:D:713:HOH:O	2.19	0.42
1:A:217:ILE:HG23	3:A:401:NPO:C4	2.50	0.41
2:D:83:VAL:HG22	2:D:114:PRO:HG2	2.02	0.41
1:C:296:THR:HA	1:C:299:ASP:OD2	2.20	0.41
1:A:149:LEU:HD12	1:A:149:LEU:HA	1.92	0.41
1:B:217:ILE:HG23	3:B:402:NPO:C4	2.50	0.41
1:C:189:PRO:HD2	1:C:247:ILE:O	2.21	0.41
1:B:4:THR:HA	1:B:5:PRO:HD2	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:HIS:O	1:C:105:THR:HG23	2.22	0.40
1:B:91:GLY:HA3	1:B:220:PHE:CG	2.56	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:606:HOH:O	9:B:606:HOH:O[2_755]	1.10	1.10
9:D:520:HOH:O	9:D:520:HOH:O[2_556]	1.34	0.86
9:B:767:HOH:O	9:B:767:HOH:O[2_755]	1.60	0.60
9:B:794:HOH:O	9:B:794:HOH:O[2_755]	1.79	0.41
9:B:581:HOH:O	9:D:794:HOH:O[3_565]	2.06	0.14

## 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	307/309 (99%)	298 (97%)	9 (3%)	0	100	100
1	B	307/309 (99%)	296 (96%)	11 (4%)	0	100	100
1	C	307/309 (99%)	298 (97%)	9 (3%)	0	100	100
2	D	308/310 (99%)	295 (96%)	13 (4%)	0	100	100
All	All	1229/1237 (99%)	1187 (97%)	42 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	230/235 (98%)	227 (99%)	3 (1%)	69	74
1	B	232/235 (99%)	229 (99%)	3 (1%)	69	74
1	C	230/235 (98%)	228 (99%)	2 (1%)	78	83
2	D	235/236 (100%)	231 (98%)	4 (2%)	60	65
All	All	927/941 (98%)	915 (99%)	12 (1%)	69	74

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LEU
1	A	87	TYR
1	A	151	ARG
1	B	58	LEU
1	B	87	TYR
1	B	151	ARG
1	C	129	PRO
1	C	151	ARG
2	D	42	HIS
2	D	58	LEU
2	D	87	TYR
2	D	151	ARG

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

### 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

21 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
7	SO4	C	404	-	4,4,4	0.32	0	6,6,6	0.08	0
4	6NA	D	406	-	7,7,7	0.83	0	7,7,7	1.02	0
6	EDO	B	404	-	3,3,3	0.11	0	2,2,2	0.14	0
3	NPO	D	401	-	9,10,10	0.57	0	11,13,13	0.61	0
3	NPO	A	401	-	9,10,10	0.58	0	11,13,13	1.09	1 (9%)
3	NPO	C	401	-	9,10,10	0.40	0	11,13,13	1.49	2 (18%)
8	MES	D	403	-	12,12,12	0.83	0	14,16,16	1.12	1 (7%)
3	NPO	A	403	-	9,10,10	0.52	0	11,13,13	1.01	0
3	NPO	A	402	-	9,10,10	0.45	0	11,13,13	1.07	0
4	6NA	A	404	-	7,7,7	0.79	0	7,7,7	0.85	0
3	NPO	B	401	-	9,10,10	0.63	0	11,13,13	1.22	2 (18%)
4	6NA	D	405	-	7,7,7	0.83	0	7,7,7	1.47	1 (14%)
7	SO4	D	404	-	4,4,4	0.33	0	6,6,6	0.10	0
3	NPO	B	402	-	9,10,10	0.73	0	11,13,13	0.77	0
3	NPO	C	403	-	9,10,10	0.23	0	11,13,13	1.04	1 (9%)
3	NPO	D	402	-	9,10,10	0.69	0	11,13,13	0.79	0
4	6NA	C	405	-	7,7,7	1.13	1 (14%)	7,7,7	0.98	0
3	NPO	B	403	-	9,10,10	0.28	0	11,13,13	0.79	0
5	PGE	A	405	-	9,9,9	0.95	0	8,8,8	0.98	0
4	6NA	B	405	-	7,7,7	1.27	1 (14%)	7,7,7	0.66	0
3	NPO	C	402	-	9,10,10	1.13	1 (11%)	11,13,13	0.81	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
4	6NA	D	406	-	-	5/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	B	404	-	-	1/1/1/1	-
3	NPO	D	401	-	-	0/2/4/4	0/1/1/1
3	NPO	A	401	-	-	0/2/4/4	0/1/1/1
3	NPO	C	401	-	-	0/2/4/4	0/1/1/1
8	MES	D	403	-	-	0/6/14/14	0/1/1/1
3	NPO	A	403	-	-	0/2/4/4	0/1/1/1
3	NPO	A	402	-	-	0/2/4/4	0/1/1/1
4	6NA	A	404	-	-	5/5/5/5	-
3	NPO	B	401	-	-	0/2/4/4	0/1/1/1
4	6NA	D	405	-	-	1/5/5/5	-
3	NPO	B	402	-	-	0/2/4/4	0/1/1/1
3	NPO	C	403	-	-	0/2/4/4	0/1/1/1
3	NPO	D	402	-	-	0/2/4/4	0/1/1/1
4	6NA	C	405	-	-	5/5/5/5	-
3	NPO	B	403	-	-	0/2/4/4	0/1/1/1
5	PGE	A	405	-	-	3/7/7/7	-
4	6NA	B	405	-	-	4/5/5/5	-
3	NPO	C	402	-	-	0/2/4/4	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	NPO	C1-N1	2.81	1.51	1.45
4	B	405	6NA	O-C	2.62	1.30	1.22
4	C	405	6NA	O-C	2.22	1.29	1.22

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	405	6NA	CB-CA-C	3.34	122.89	114.47
3	C	401	NPO	C2-C1-N1	-3.04	117.09	119.38
8	D	403	MES	O1S-S-C8	-3.04	103.25	106.92
3	B	401	NPO	C2-C1-N1	-2.23	117.70	119.38
3	A	401	NPO	C6-C1-N1	2.21	121.04	119.38
3	C	403	NPO	C6-C1-N1	-2.11	117.79	119.38
3	B	401	NPO	C6-C1-N1	2.08	120.94	119.38
3	C	401	NPO	C5-C6-C1	-2.02	117.27	120.08

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	405	PGE	C1-C2-O2-C3
4	A	404	6NA	C-CA-CB-CG
4	C	405	6NA	C-CA-CB-CG
4	B	405	6NA	C-CA-CB-CG
4	A	404	6NA	CA-CB-CG-CD
4	D	406	6NA	CA-CB-CG-CD
4	D	406	6NA	C-CA-CB-CG
6	B	404	EDO	O1-C1-C2-O2
4	B	405	6NA	C6-CD-CG-CB
4	A	404	6NA	C6-CD-CG-CB
4	C	405	6NA	C6-CD-CG-CB
4	D	406	6NA	C6-CD-CG-CB
5	A	405	PGE	O2-C3-C4-O3
4	D	405	6NA	C6-CD-CG-CB
4	C	405	6NA	CA-CB-CG-CD
5	A	405	PGE	C3-C4-O3-C5
4	D	406	6NA	O-C-CA-CB
4	C	405	6NA	O-C-CA-CB
4	D	406	6NA	OXT-C-CA-CB
4	C	405	6NA	OXT-C-CA-CB
4	B	405	6NA	OXT-C-CA-CB
4	A	404	6NA	OXT-C-CA-CB
4	A	404	6NA	O-C-CA-CB
4	B	405	6NA	O-C-CA-CB

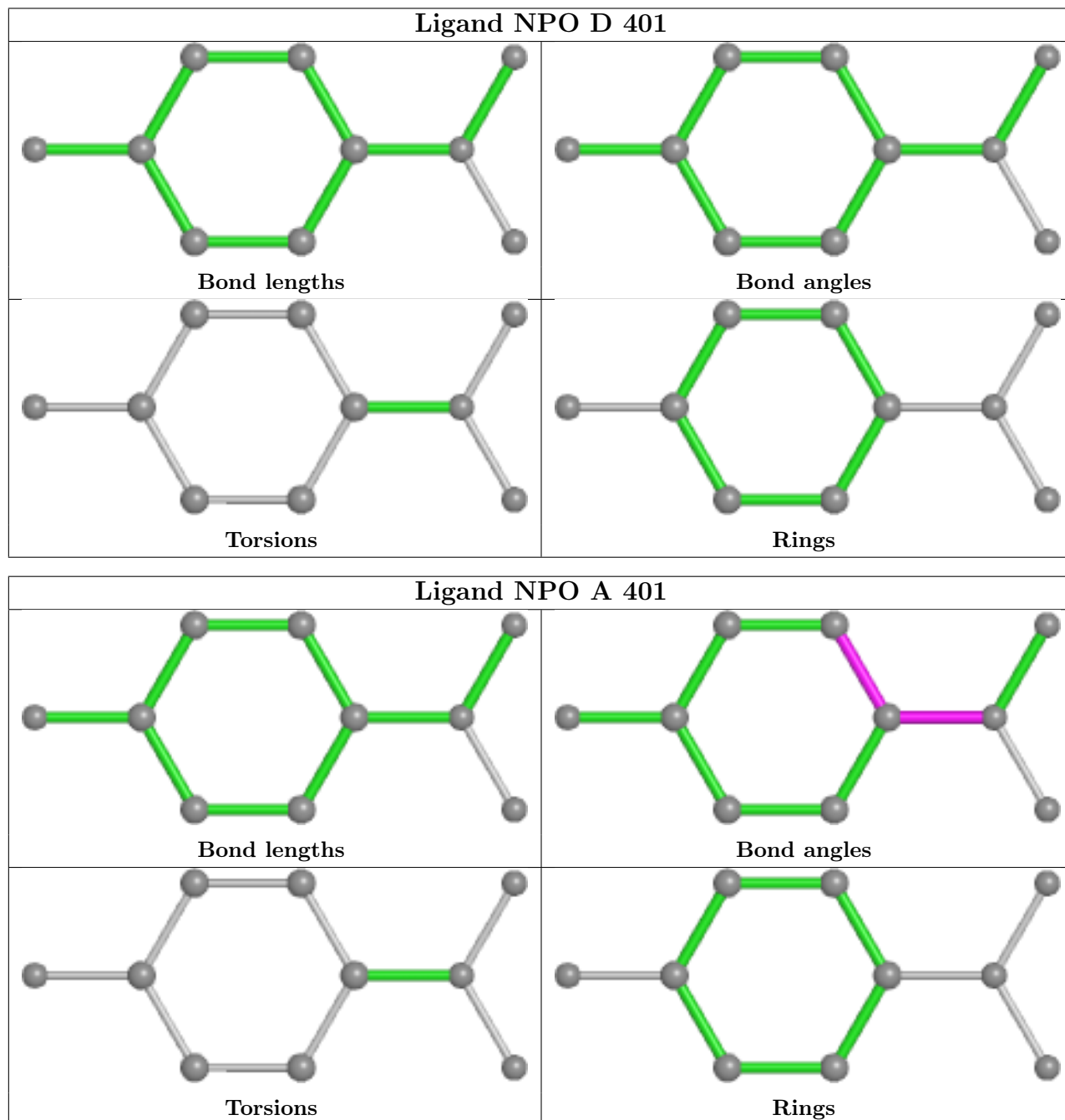
There are no ring outliers.

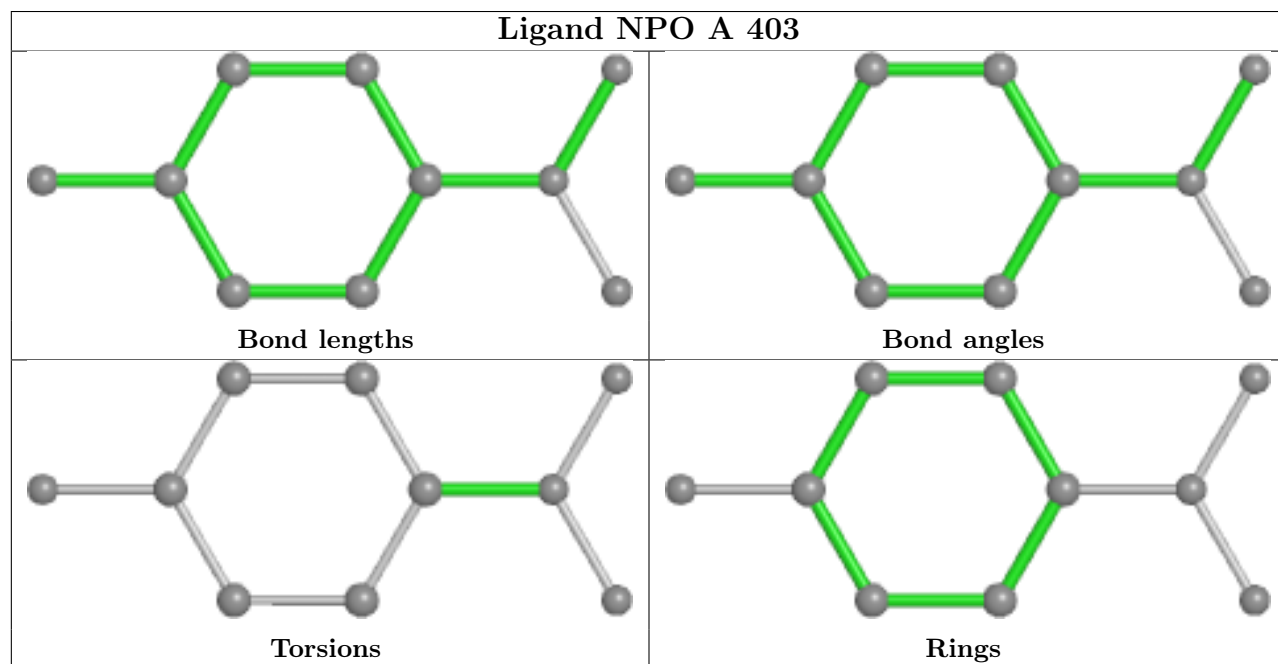
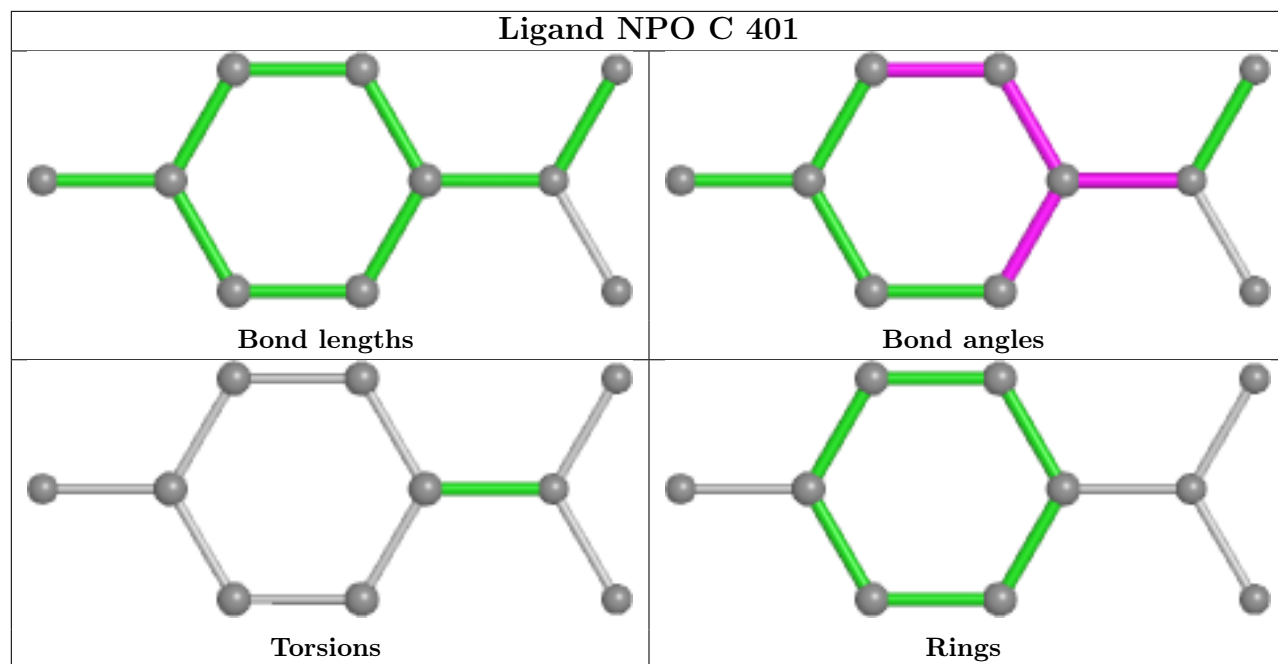
9 monomers are involved in 19 short contacts:

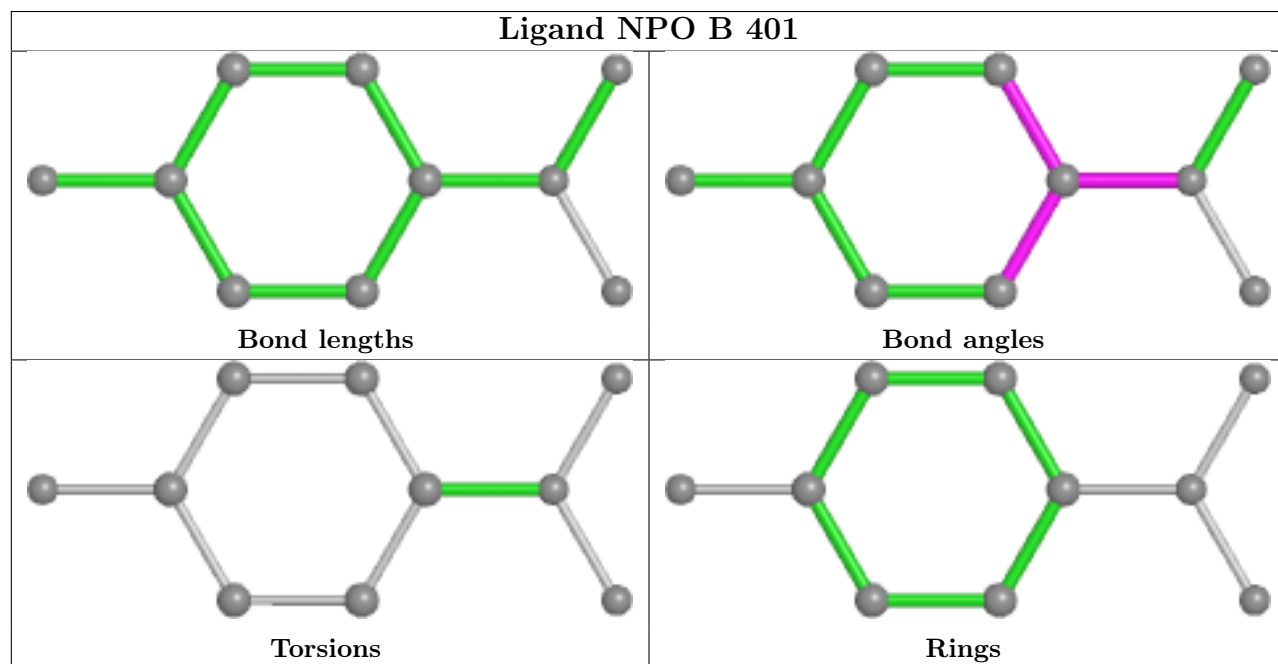
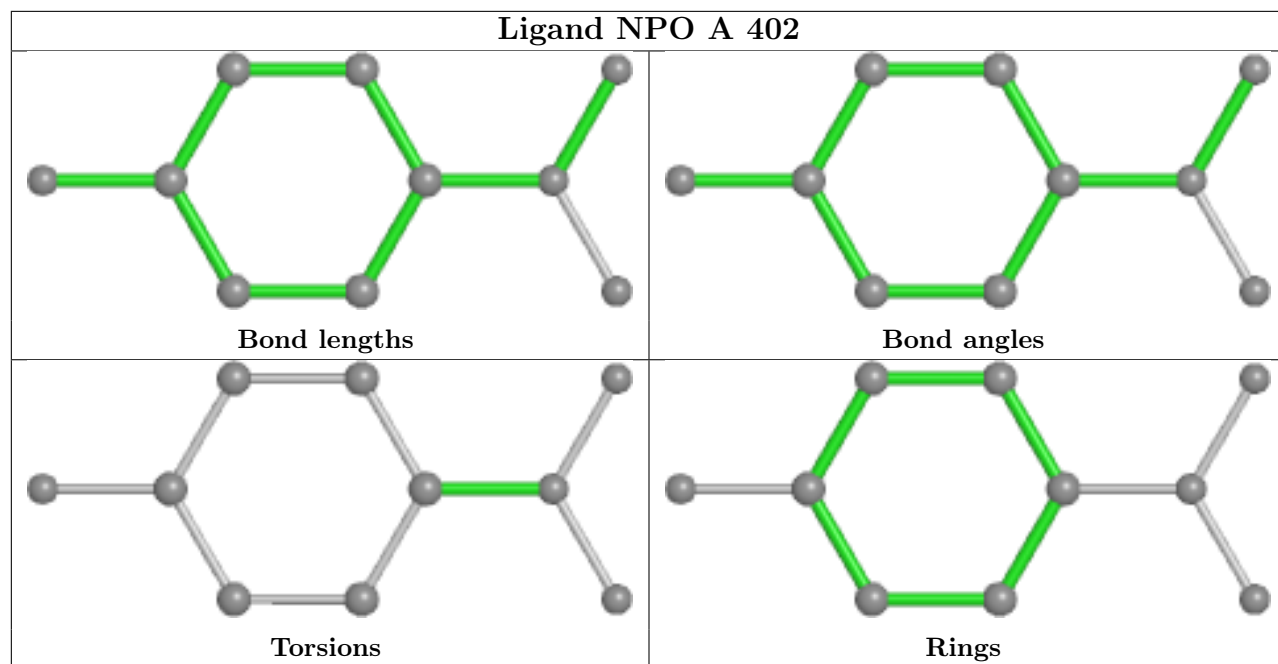
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	406	6NA	2	0
3	A	401	NPO	1	0
4	A	404	6NA	1	0
4	D	405	6NA	5	0
3	B	402	NPO	1	0
4	C	405	6NA	3	0
5	A	405	PGE	1	0
4	B	405	6NA	4	0
3	C	402	NPO	1	0

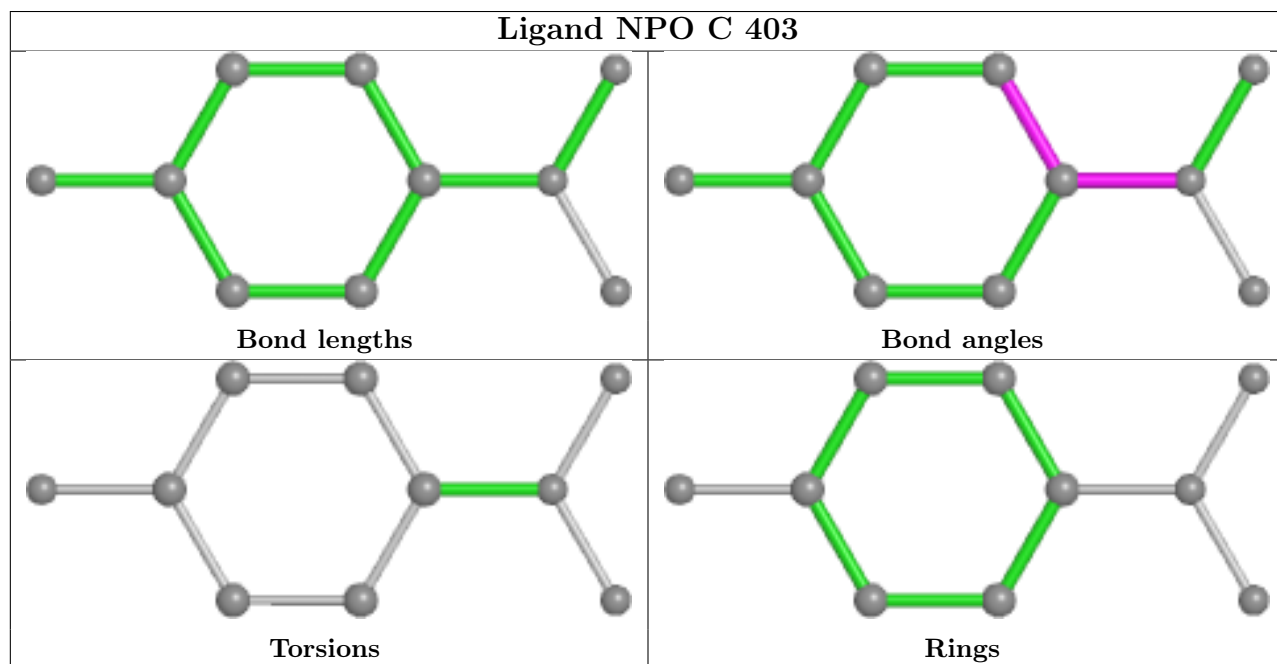
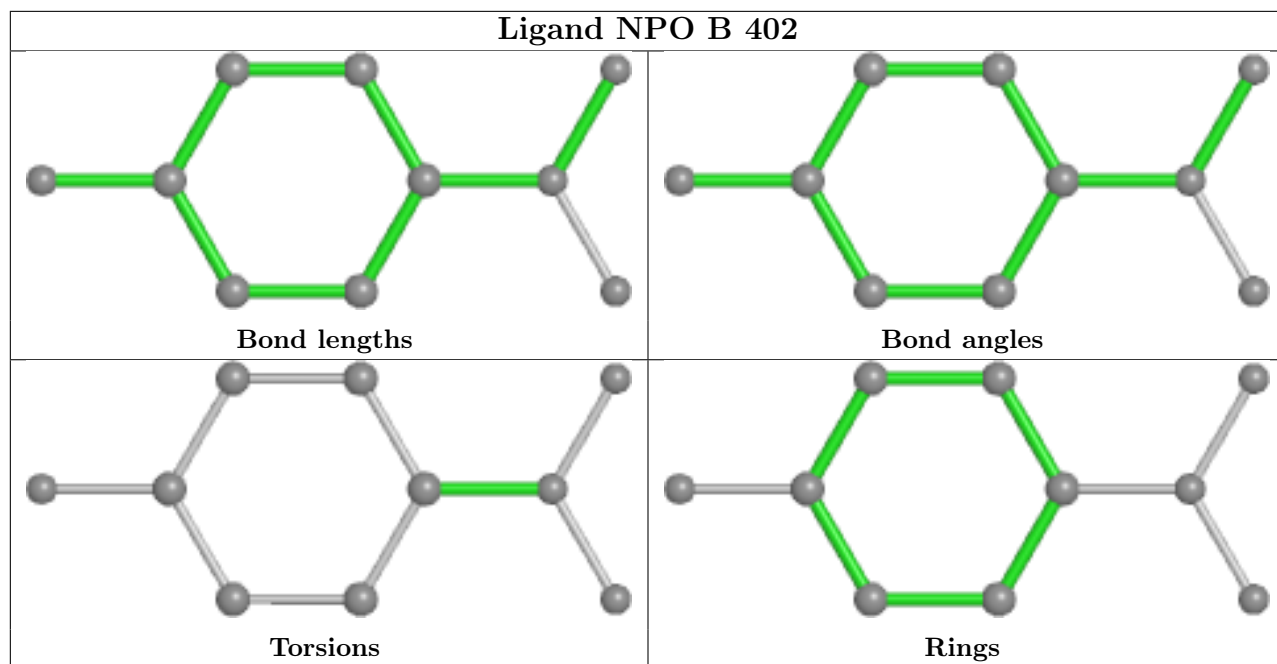
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

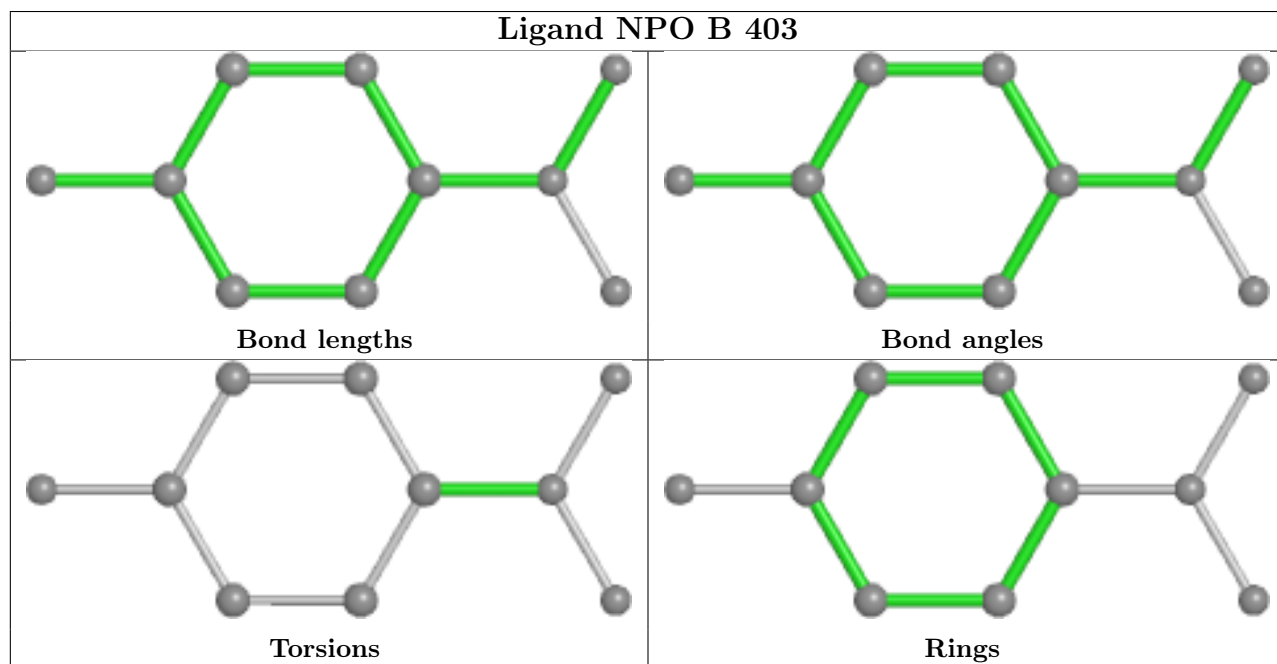
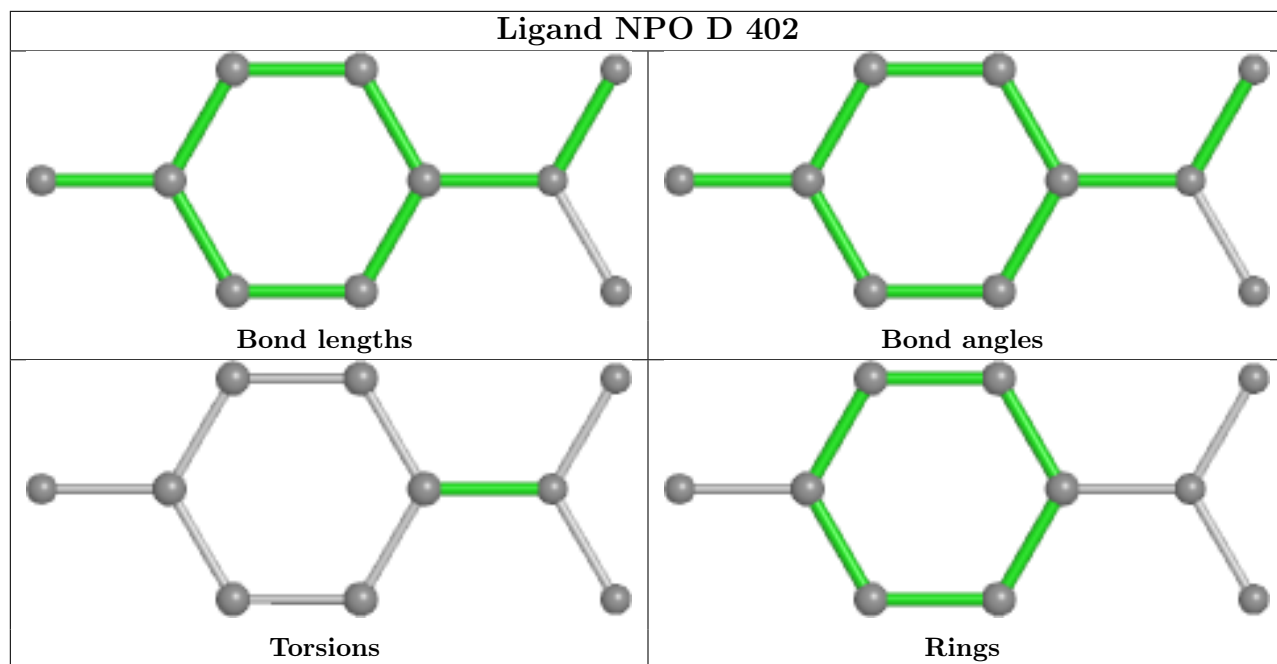
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

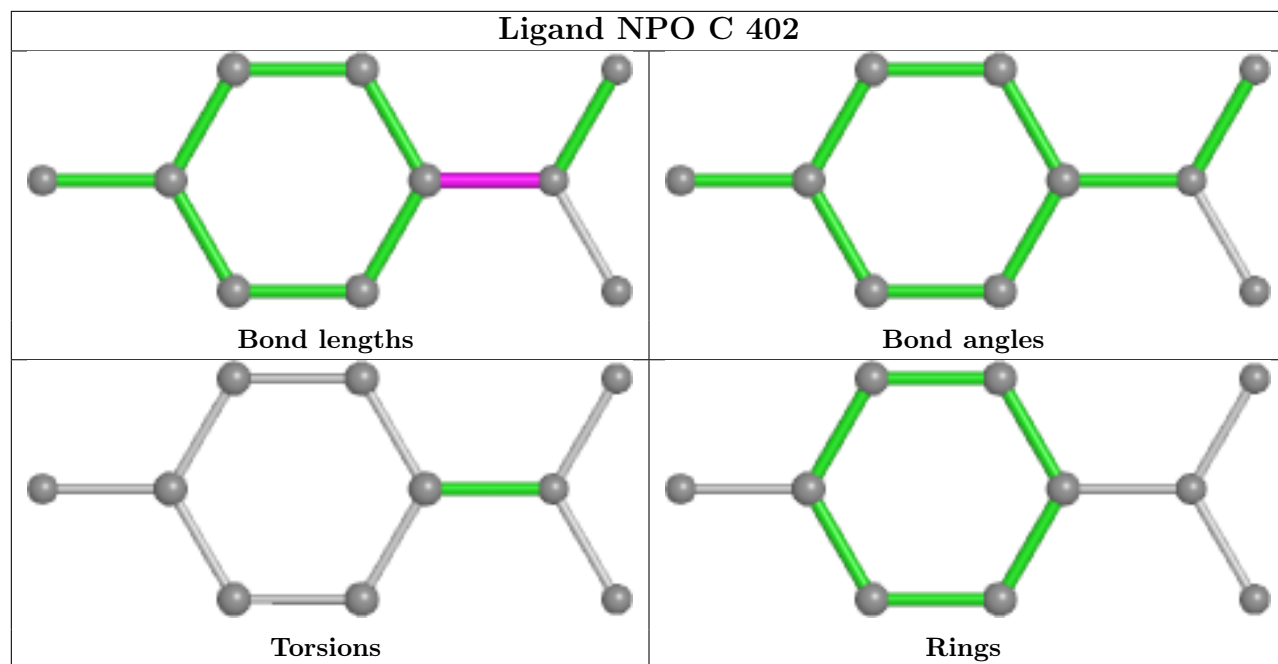












## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	309/309 (100%)	-0.08	4 (1%) 77 76	22, 29, 45, 58	0
1	B	309/309 (100%)	0.15	14 (4%) 33 32	26, 34, 55, 73	0
1	C	309/309 (100%)	-0.07	7 (2%) 60 59	23, 29, 44, 63	0
2	D	310/310 (100%)	-0.07	5 (1%) 72 70	25, 32, 50, 91	0
All	All	1237/1237 (100%)	-0.02	30 (2%) 59 57	22, 31, 49, 91	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	77	SER	3.7
1	B	219	PHE	3.5
1	C	77	SER	3.3
1	B	222	THR	3.3
1	B	27	ALA	3.2
1	B	275	VAL	3.2
1	B	247	ILE	3.1
1	C	147	SER	3.0
2	D	3	ASP	3.0
1	B	30	THR	2.9
1	C	54	VAL	2.9
2	D	312	GLY	2.8
1	C	80	ALA	2.8
1	C	79	GLU	2.8
1	C	247	ILE	2.6
1	B	248	VAL	2.4
1	A	275	VAL	2.4
1	B	223	ALA	2.4
1	B	277	LEU	2.3
2	D	30	THR	2.3
1	B	26	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	79	GLU	2.3
1	A	248	VAL	2.3
1	B	274	VAL	2.2
1	B	31	LEU	2.1
1	B	25	THR	2.1
2	D	4	THR	2.1
1	B	93	VAL	2.1
1	C	152	THR	2.0
2	D	275	VAL	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.

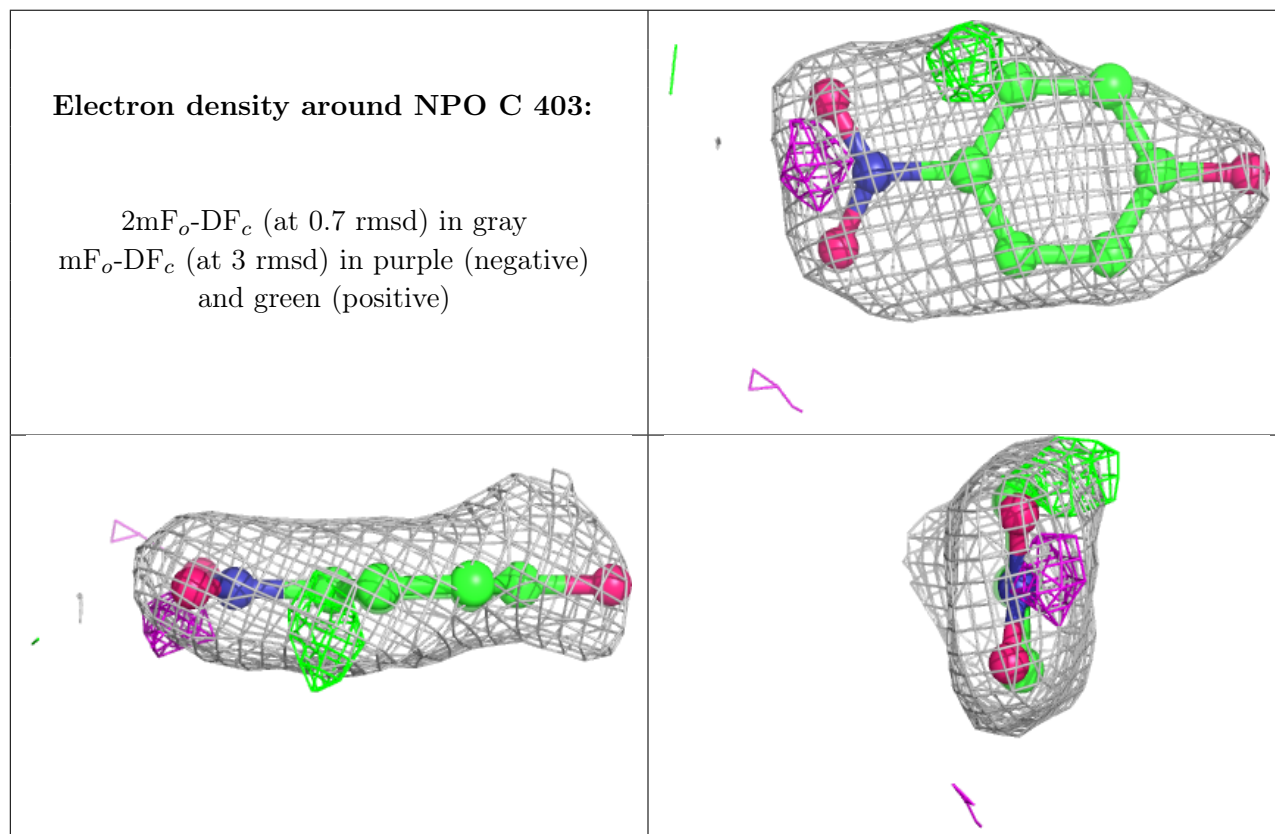
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	6NA	C	405	8/8	0.81	0.18	41,50,56,59	0
4	6NA	B	405	8/8	0.83	0.16	43,49,55,62	0
5	PGE	A	405	10/10	0.83	0.24	46,56,67,72	0
4	6NA	A	404	8/8	0.84	0.16	40,54,58,59	0
4	6NA	D	405	8/8	0.86	0.36	52,68,75,84	0
4	6NA	D	406	8/8	0.88	0.12	35,49,53,54	0
3	NPO	C	403	10/10	0.89	0.17	51,66,76,86	0
3	NPO	B	403	10/10	0.91	0.17	60,72,79,94	0
3	NPO	A	403	10/10	0.91	0.18	54,62,67,68	0
7	SO4	D	404	5/5	0.92	0.27	79,79,87,95	0
6	EDO	B	404	4/4	0.93	0.29	55,65,68,74	0
3	NPO	C	401	10/10	0.94	0.18	35,42,44,46	0
8	MES	D	403	12/12	0.94	0.17	35,44,65,70	0
3	NPO	A	402	10/10	0.95	0.14	38,41,46,48	0

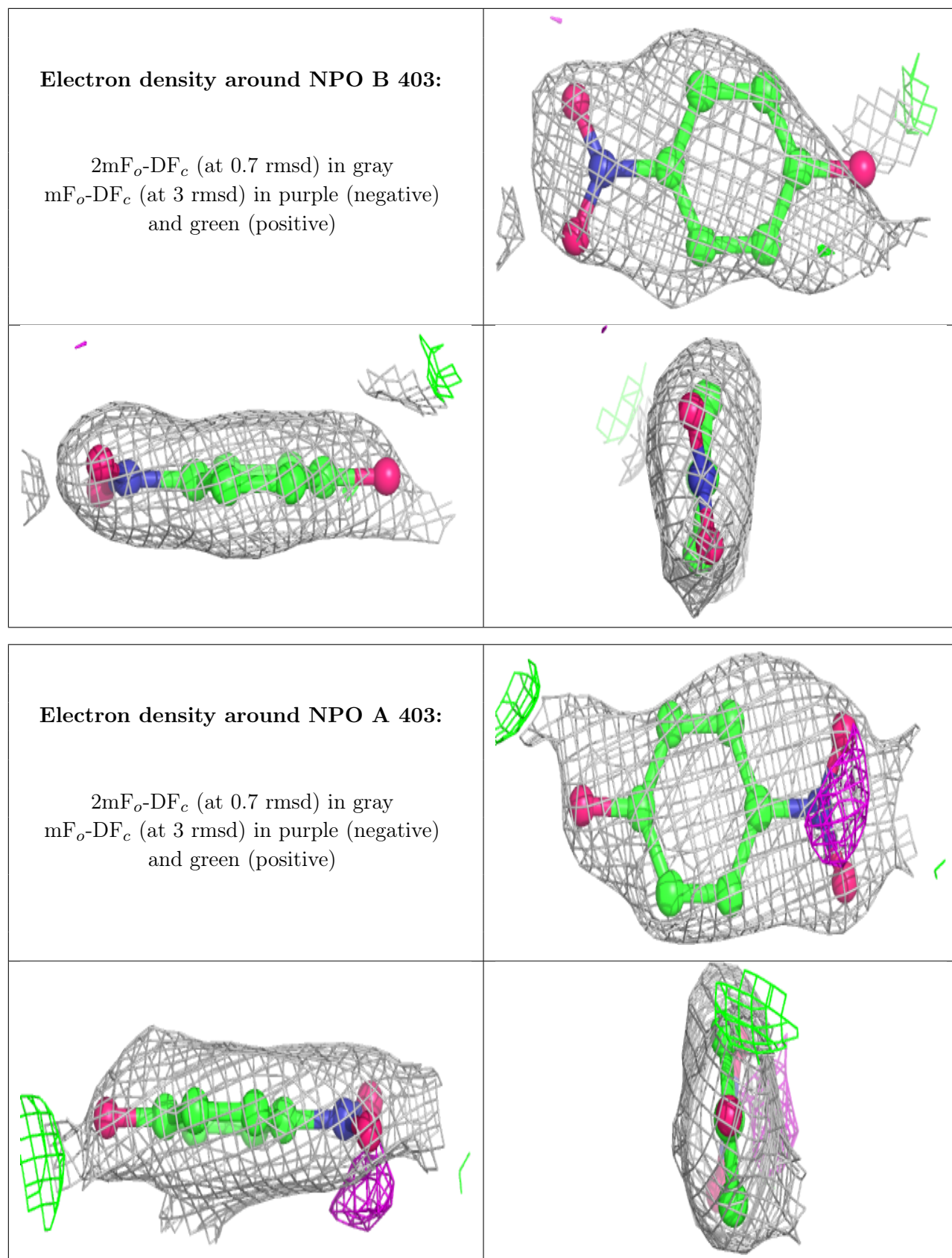
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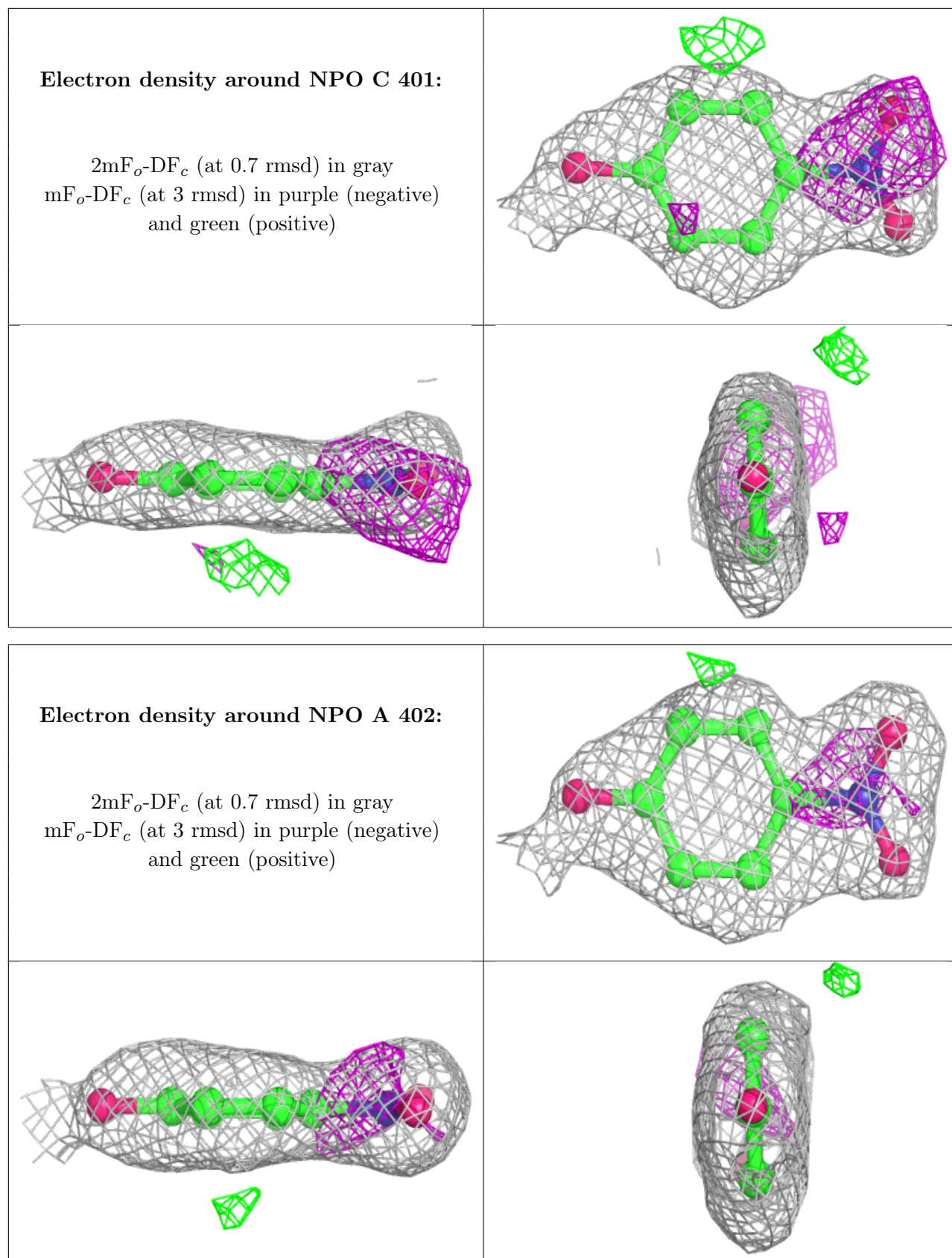
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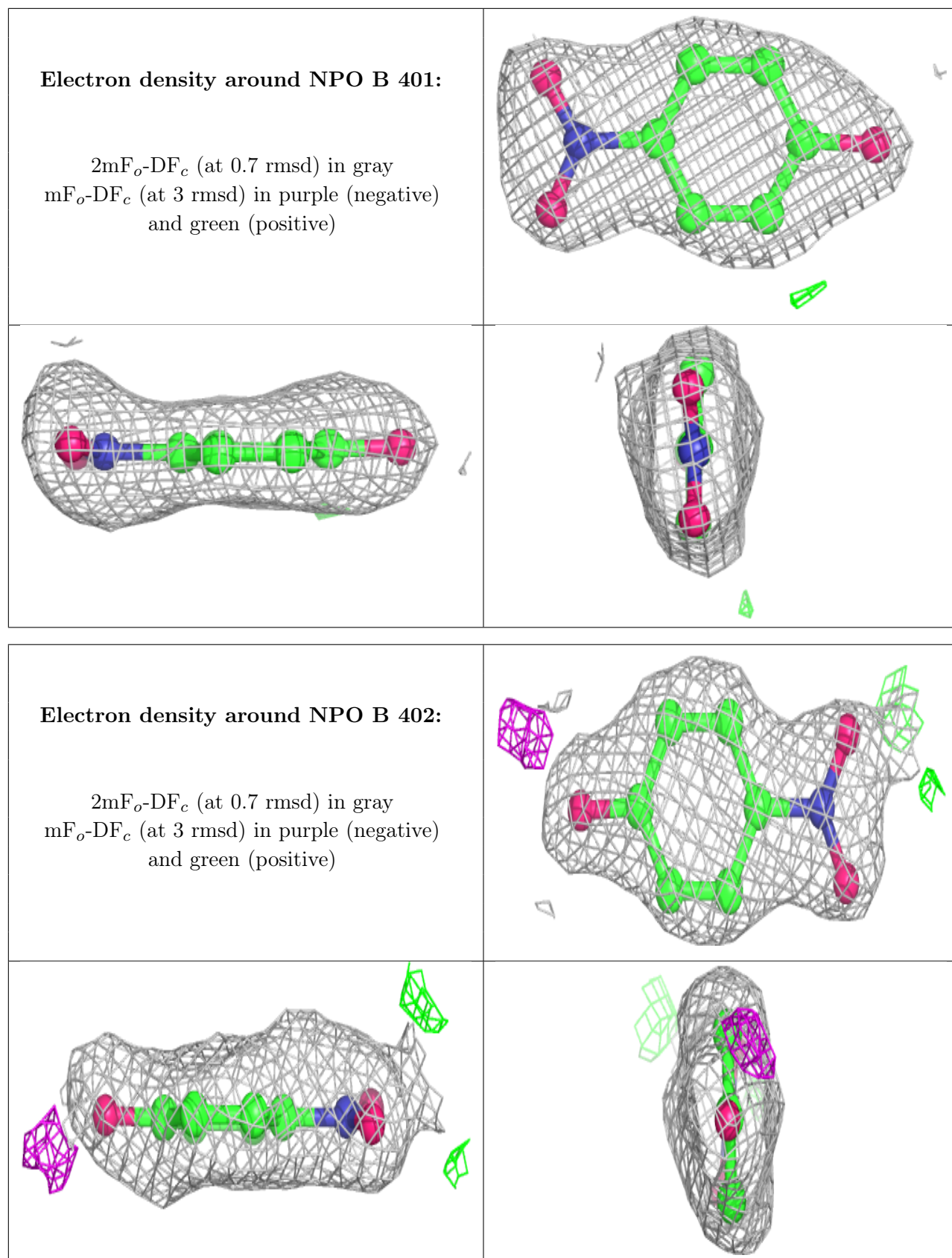
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	SO4	C	404	5/5	0.95	0.12	82,85,95,99	0
3	NPO	B	401	10/10	0.95	0.20	50,53,56,60	0
3	NPO	B	402	10/10	0.95	0.18	45,50,60,65	0
3	NPO	C	402	10/10	0.96	0.11	34,37,45,47	0
3	NPO	A	401	10/10	0.96	0.14	32,38,41,48	0
3	NPO	D	401	10/10	0.97	0.13	38,41,50,56	0
3	NPO	D	402	10/10	0.97	0.22	42,44,51,52	0

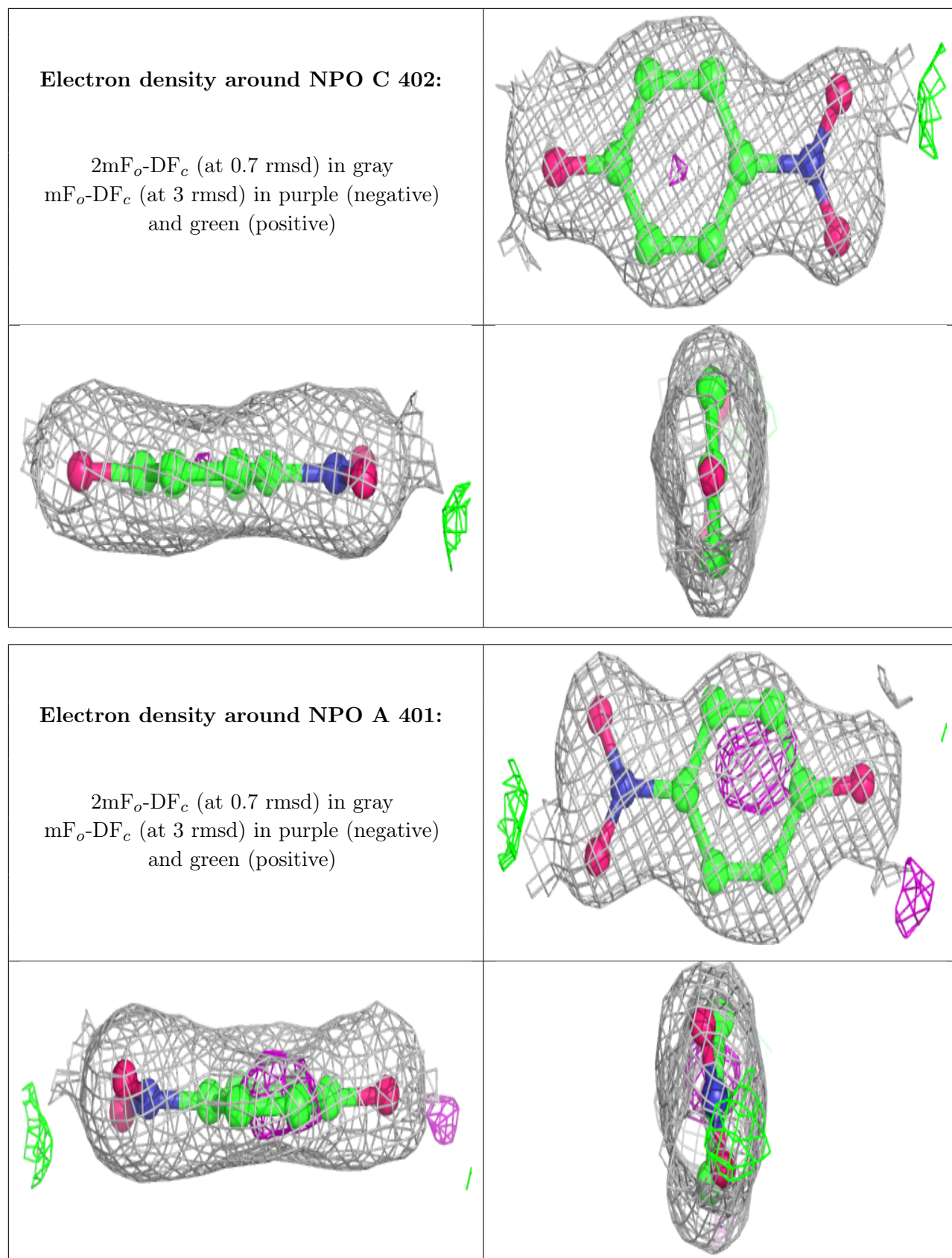
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

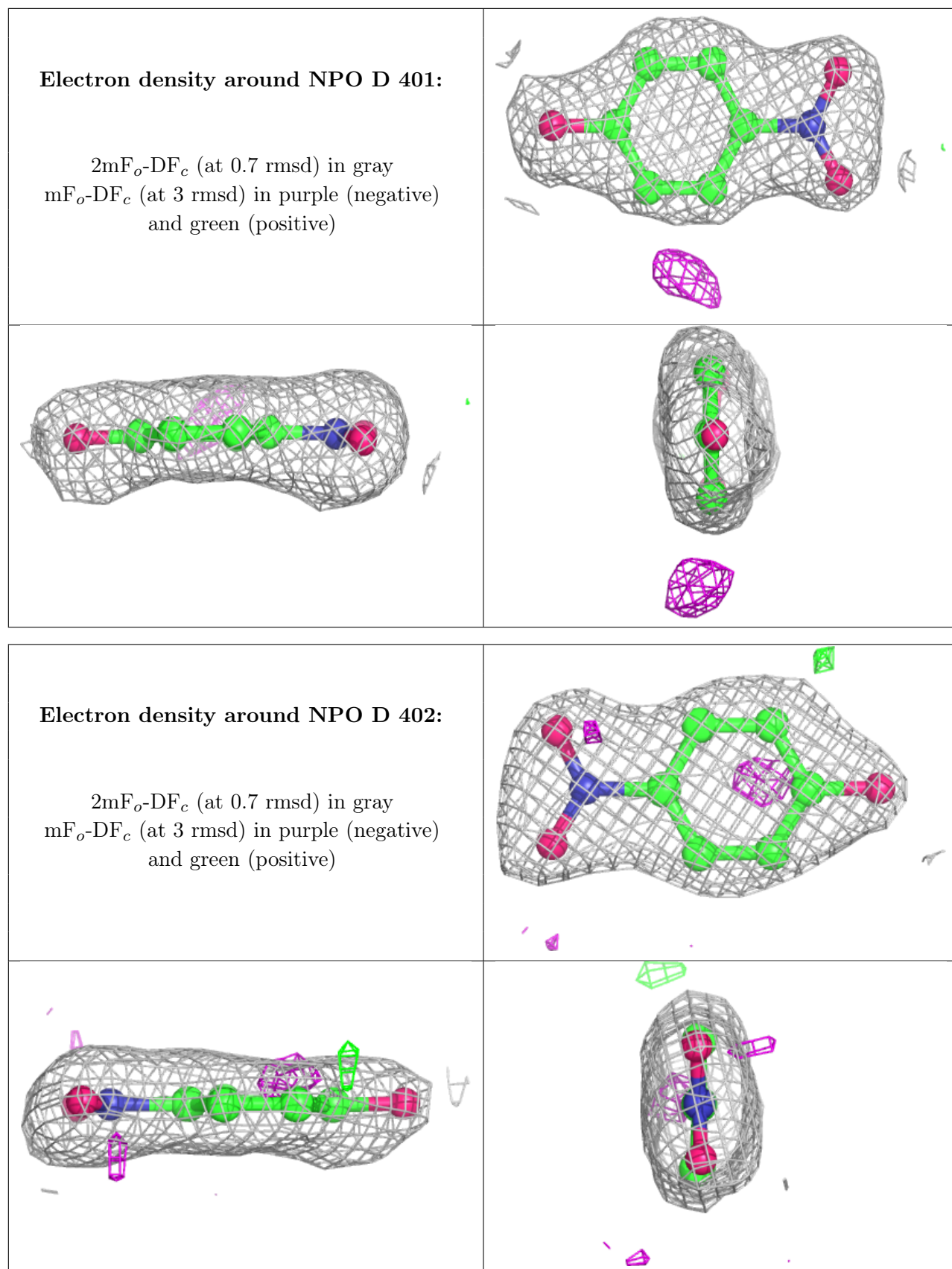














## 6.5 Other polymers [i](#)

There are no such residues in this entry.