



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 21, 2024 – 12:24 pm GMT

PDB ID : 7O5Q  
Title : Crystal Structure of a Class D Carbapenemase Complexed with Hydrolyzed Oxacillin  
Authors : Zhou, Q.; He, Y.; Jin, Y.  
Deposited on : 2021-04-09  
Resolution : 1.85 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 : 1.8.4, 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

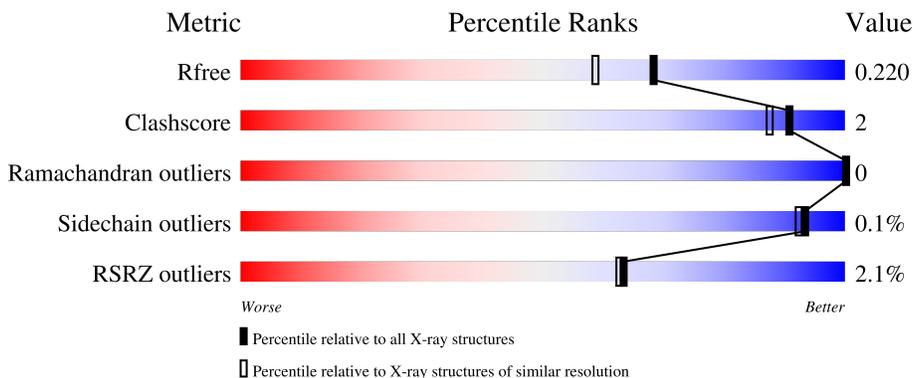
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

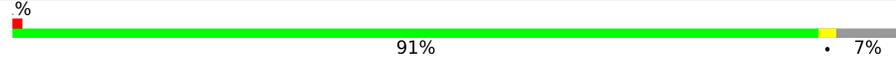
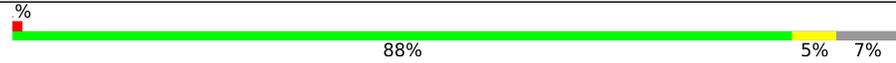
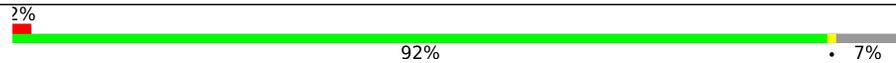
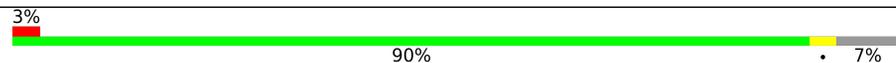
The reported resolution of this entry is 1.85 Å.

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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	AAA	260	 91% 7%
1	BBB	260	 88% 5% 7%
1	CCC	260	 92% 7%
1	DDD	260	 90% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IOD	AAA	305	-	-	X	-
3	IOD	BBB	303[B]	-	-	X	-

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 16875 atoms, of which 7987 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 Beta-lactamase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	AAA	242	3974	1276	1968	353	369	8	48	3	0
1	BBB	242	3982	1278	1971	356	369	8	47	3	0
1	CCC	242	3952	1270	1955	351	368	8	48	2	0
1	DDD	242	3952	1270	1955	351	368	8	48	2	0

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	6	MET	-	initiating methionine	UNP Q6XEC0
AAA	7	HIS	-	expression tag	UNP Q6XEC0
AAA	8	HIS	-	expression tag	UNP Q6XEC0
AAA	9	HIS	-	expression tag	UNP Q6XEC0
AAA	10	HIS	-	expression tag	UNP Q6XEC0
AAA	11	HIS	-	expression tag	UNP Q6XEC0
AAA	12	HIS	-	expression tag	UNP Q6XEC0
AAA	13	SER	-	expression tag	UNP Q6XEC0
AAA	14	ALA	-	expression tag	UNP Q6XEC0
AAA	15	GLY	-	expression tag	UNP Q6XEC0
AAA	16	GLU	-	expression tag	UNP Q6XEC0
AAA	17	ASN	-	expression tag	UNP Q6XEC0
AAA	18	LEU	-	expression tag	UNP Q6XEC0
AAA	19	TYR	-	expression tag	UNP Q6XEC0
AAA	20	PHE	-	expression tag	UNP Q6XEC0
AAA	21	GLN	-	expression tag	UNP Q6XEC0
AAA	22	GLY	-	expression tag	UNP Q6XEC0
BBB	6	MET	-	initiating methionine	UNP Q6XEC0
BBB	7	HIS	-	expression tag	UNP Q6XEC0
BBB	8	HIS	-	expression tag	UNP Q6XEC0
BBB	9	HIS	-	expression tag	UNP Q6XEC0

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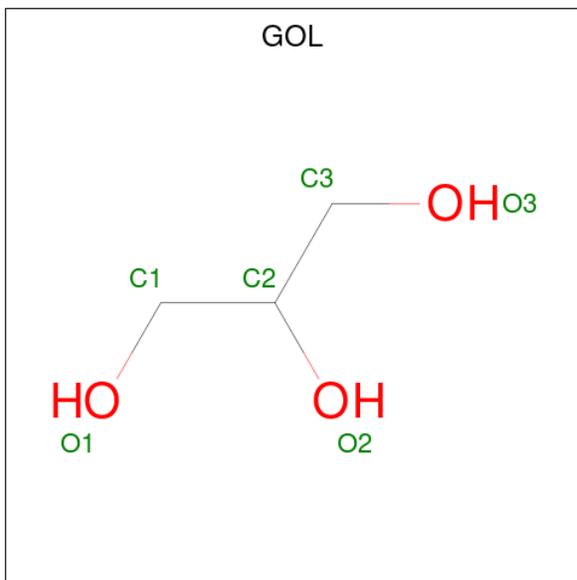
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	10	HIS	-	expression tag	UNP Q6XEC0
BBB	11	HIS	-	expression tag	UNP Q6XEC0
BBB	12	HIS	-	expression tag	UNP Q6XEC0
BBB	13	SER	-	expression tag	UNP Q6XEC0
BBB	14	ALA	-	expression tag	UNP Q6XEC0
BBB	15	GLY	-	expression tag	UNP Q6XEC0
BBB	16	GLU	-	expression tag	UNP Q6XEC0
BBB	17	ASN	-	expression tag	UNP Q6XEC0
BBB	18	LEU	-	expression tag	UNP Q6XEC0
BBB	19	TYR	-	expression tag	UNP Q6XEC0
BBB	20	PHE	-	expression tag	UNP Q6XEC0
BBB	21	GLN	-	expression tag	UNP Q6XEC0
BBB	22	GLY	-	expression tag	UNP Q6XEC0
CCC	6	MET	-	initiating methionine	UNP Q6XEC0
CCC	7	HIS	-	expression tag	UNP Q6XEC0
CCC	8	HIS	-	expression tag	UNP Q6XEC0
CCC	9	HIS	-	expression tag	UNP Q6XEC0
CCC	10	HIS	-	expression tag	UNP Q6XEC0
CCC	11	HIS	-	expression tag	UNP Q6XEC0
CCC	12	HIS	-	expression tag	UNP Q6XEC0
CCC	13	SER	-	expression tag	UNP Q6XEC0
CCC	14	ALA	-	expression tag	UNP Q6XEC0
CCC	15	GLY	-	expression tag	UNP Q6XEC0
CCC	16	GLU	-	expression tag	UNP Q6XEC0
CCC	17	ASN	-	expression tag	UNP Q6XEC0
CCC	18	LEU	-	expression tag	UNP Q6XEC0
CCC	19	TYR	-	expression tag	UNP Q6XEC0
CCC	20	PHE	-	expression tag	UNP Q6XEC0
CCC	21	GLN	-	expression tag	UNP Q6XEC0
CCC	22	GLY	-	expression tag	UNP Q6XEC0
DDD	6	MET	-	initiating methionine	UNP Q6XEC0
DDD	7	HIS	-	expression tag	UNP Q6XEC0
DDD	8	HIS	-	expression tag	UNP Q6XEC0
DDD	9	HIS	-	expression tag	UNP Q6XEC0
DDD	10	HIS	-	expression tag	UNP Q6XEC0
DDD	11	HIS	-	expression tag	UNP Q6XEC0
DDD	12	HIS	-	expression tag	UNP Q6XEC0
DDD	13	SER	-	expression tag	UNP Q6XEC0
DDD	14	ALA	-	expression tag	UNP Q6XEC0
DDD	15	GLY	-	expression tag	UNP Q6XEC0
DDD	16	GLU	-	expression tag	UNP Q6XEC0
DDD	17	ASN	-	expression tag	UNP Q6XEC0

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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	18	LEU	-	expression tag	UNP Q6XEC0
DDD	19	TYR	-	expression tag	UNP Q6XEC0
DDD	20	PHE	-	expression tag	UNP Q6XEC0
DDD	21	GLN	-	expression tag	UNP Q6XEC0
DDD	22	GLY	-	expression tag	UNP Q6XEC0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	H			O
2	AAA	1	14	3	8	3	2	0
2	BBB	1	14	3	8	3	2	0
2	CCC	1	14	3	8	3	2	0

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I) (labeled as "Ligand of Interest" by depositor).

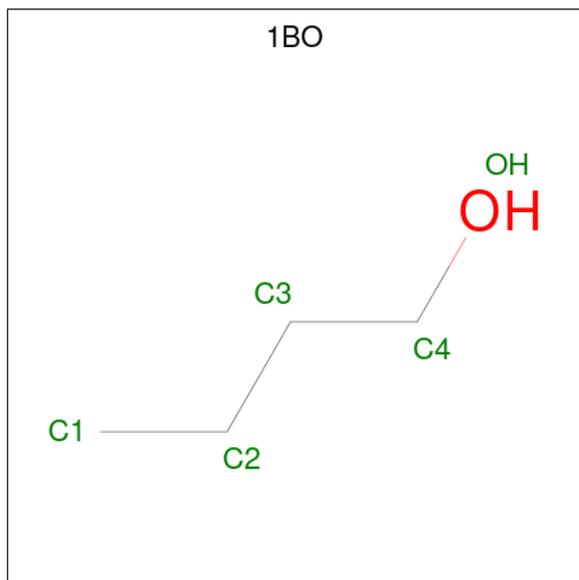
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	I		
3	AAA	4	5	5	0	1
3	BBB	5	6	6	0	1
3	CCC	4	4	4	0	0

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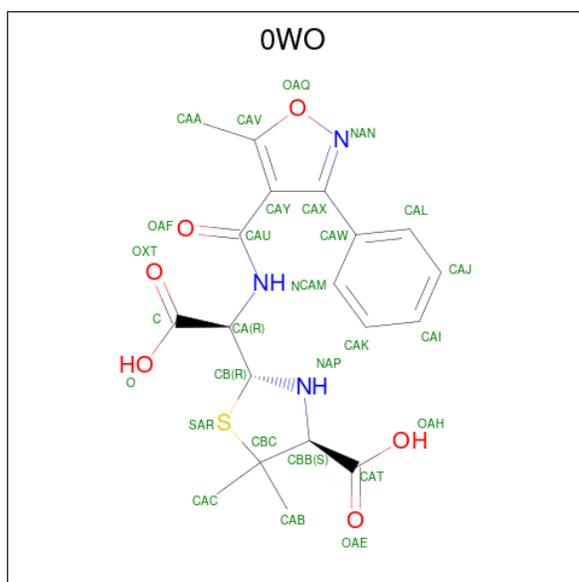
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	DDD	2	Total I 2 2	0	0

- Molecule 4 is 1-BUTANOL (three-letter code: 1BO) (formula: C<sub>4</sub>H<sub>10</sub>O).



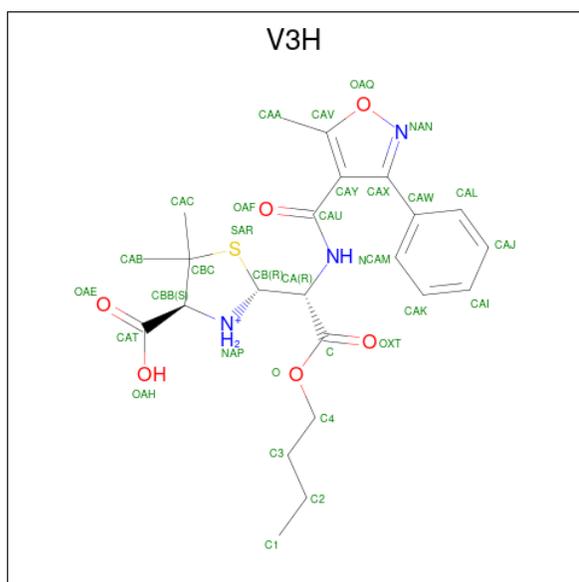
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	BBB	1	15	4	10	1	0	0
4	DDD	1	15	4	10	1	0	0

- Molecule 5 is (2R,4S)-2-[(R)-carboxy{[(5-methyl-3-phenyl-1,2-oxazol-4-yl)carbonyl]amino}methyl]-5,5-dimethyl-1,3-thiazolidine-4-carboxylic acid (three-letter code: 0WO) (formula: C<sub>19</sub>H<sub>21</sub>N<sub>3</sub>O<sub>6</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	CCC	1	Total	C	H	N	O	S	0	0
			48	19	19	3	6	1		
5	DDD	1	Total	C	H	N	O	S	0	0
			48	19	19	3	6	1		

- Molecule 6 is (2R,4S)-2-[(1R)-2-butoxy-1-[(5-methyl-3-phenyl-1,2-oxazol-4-yl)carbonylamino]-2-oxidanylidene-ethyl]-5,5-dimethyl-1,3-thiazolidin-3-ium-4-carboxylic acid (three-letter code: V3H) (formula: C<sub>23</sub>H<sub>30</sub>N<sub>3</sub>O<sub>6</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
6	CCC	1	Total	C	H	N	O	S	0	0
			61	23	28	3	6	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O	S		
6	DDD	1	61	23	28	3	6	1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	AAA	204	205	205	0	1
7	BBB	190	192	192	0	2
7	CCC	168	169	169	0	1
7	DDD	141	142	142	0	1

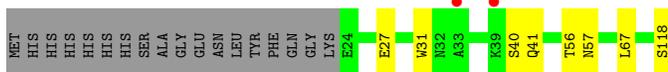
### 3 Residue-property plots [i](#)

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: Beta-lactamase



- Molecule 1: Beta-lactamase



- Molecule 1: Beta-lactamase



- Molecule 1: Beta-lactamase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.05Å 126.90Å 111.20Å 90.00° 98.29° 90.00°	Depositor
Resolution (Å)	19.81 – 1.85 19.80 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.81-1.85) 100.0 (19.80-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 1.85Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.173 , 0.211 0.185 , 0.220	Depositor DCC
$R_{free}$ test set	5465 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.6	Xtrriage
Anisotropy	0.889	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 56.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	16875	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.75% 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: V3H, KCX, IOD, 1BO, 0WO, GOL

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	AAA	0.86	0/2042	0.86	0/2759
1	BBB	0.87	0/2047	0.84	0/2766
1	CCC	0.86	0/2033	0.81	0/2748
1	DDD	0.85	0/2033	0.80	0/2748
All	All	0.86	0/8155	0.83	0/11021

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	AAA	2006	1968	1956	7	0
1	BBB	2011	1971	1959	8	0
1	CCC	1997	1955	1944	2	0
1	DDD	1997	1955	1944	6	0
2	AAA	6	8	8	0	0
2	BBB	6	8	8	1	0
2	CCC	6	8	8	0	0
3	AAA	5	0	0	3	0
3	BBB	6	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	CCC	4	0	0	1	0
3	DDD	2	0	0	1	0
4	BBB	5	10	10	1	0
4	DDD	5	10	10	0	0
5	CCC	29	19	19	0	0
5	DDD	29	19	19	0	0
6	CCC	33	28	0	2	0
6	DDD	33	28	0	1	0
7	AAA	205	0	0	3	0
7	BBB	192	0	0	4	0
7	CCC	169	0	0	2	0
7	DDD	142	0	0	0	0
All	All	8888	7987	7885	28	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 (28) 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:BBB:40:SER:HB2	7:BBB:457:HOH:O	1.77	0.83
3:BBB:304:IOD:I	7:BBB:578:HOH:O	2.71	0.78
4:BBB:302:1BO:H12	7:BBB:479:HOH:O	1.90	0.70
1:AAA:40:SER:HB2	7:AAA:471:HOH:O	1.95	0.67
6:CCC:403:V3H:CAB	3:CCC:406:IOD:I	3.17	0.62
1:AAA:137:LYS:HD3	3:AAA:305:IOD:I	2.73	0.58
1:BBB:67:LEU:HD11	1:BBB:215:ILE:HG13	1.89	0.54
6:DDD:503:V3H:CAB	3:DDD:504:IOD:I	3.30	0.50
6:CCC:403:V3H:C1	7:CCC:583:HOH:O	2.60	0.50
1:BBB:121:PRO:HB2	2:BBB:301:GOL:H31	1.94	0.49
1:BBB:27:GLU:HA	1:BBB:56:THR:O	2.12	0.49
1:CCC:41:GLN:NE2	7:CCC:503:HOH:O	2.46	0.49
3:BBB:303[B]:IOD:I	1:DDD:206:ARG:NH2	3.12	0.47
1:AAA:129:GLN:NE2	7:AAA:403:HOH:O	2.49	0.46
3:BBB:303[B]:IOD:I	1:DDD:206:ARG:NH1	3.15	0.45
1:AAA:137:LYS:CE	3:AAA:305:IOD:I	3.35	0.44
1:BBB:220:GLY:O	1:BBB:238:ASN:HA	2.17	0.43
1:DDD:220:GLY:O	1:DDD:238:ASN:HA	2.18	0.43
1:DDD:31:TRP:HB2	1:DDD:57:ASN:HB3	2.01	0.43
1:AAA:65:ALA:HB1	1:AAA:163:ARG:HB3	2.01	0.42
1:BBB:41[A]:GLN:NE2	7:BBB:407:HOH:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:120:VAL:HB	1:DDD:121:PRO:HD3	2.00	0.42
1:DDD:124:GLN:HG2	1:DDD:154:ASP:O	2.19	0.42
1:AAA:94[A]:LYS:CD	7:AAA:404:HOH:O	2.67	0.42
1:CCC:27:GLU:HA	1:CCC:56:THR:O	2.20	0.42
1:AAA:137:LYS:NZ	3:AAA:305:IOD:I	3.18	0.41
1:BBB:247:LEU:HD22	1:BBB:250:ARG:CZ	2.50	0.41
1:BBB:31:TRP:HB2	1:BBB:57:ASN:HB3	2.02	0.41

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	AAA	242/260 (93%)	237 (98%)	5 (2%)	0	100	100
1	BBB	242/260 (93%)	236 (98%)	6 (2%)	0	100	100
1	CCC	241/260 (93%)	234 (97%)	7 (3%)	0	100	100
1	DDD	241/260 (93%)	235 (98%)	6 (2%)	0	100	100
All	All	966/1040 (93%)	942 (98%)	24 (2%)	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	AAA	213/225 (95%)	213 (100%)	0	100	100
1	BBB	213/225 (95%)	212 (100%)	1 (0%)	88	86
1	CCC	212/225 (94%)	212 (100%)	0	100	100
1	DDD	212/225 (94%)	212 (100%)	0	100	100
All	All	850/900 (94%)	849 (100%)	1 (0%)	93	92

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	118	SER

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](#)

4 non-standard protein/DNA/RNA residues 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
1	KCX	CCC	73	1	9,11,12	0.62	0	5,12,14	0.54	0
1	KCX	BBB	73	1	9,11,12	0.37	0	5,12,14	0.40	0
1	KCX	DDD	73	1	9,11,12	0.56	0	5,12,14	0.70	0
1	KCX	AAA	73	1	9,11,12	0.59	0	5,12,14	0.62	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
1	KCX	CCC	73	1	-	0/9/10/12	-
1	KCX	BBB	73	1	-	0/9/10/12	-
1	KCX	DDD	73	1	-	0/9/10/12	-
1	KCX	AAA	73	1	-	0/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 17 are monoatomic - leaving 9 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
5	OWO	CCC	401	-	24,31,31	1.18	2 (8%)	28,46,46	0.69	0
2	GOL	AAA	301	-	5,5,5	0.18	0	5,5,5	0.29	0
6	V3H	CCC	403	-	28,35,35	0.99	2 (7%)	32,50,50	0.82	2 (6%)
4	1BO	BBB	302	-	4,4,4	0.15	0	3,3,3	0.37	0
5	OWO	DDD	501	-	24,31,31	1.00	2 (8%)	28,46,46	0.81	0
6	V3H	DDD	503	-	28,35,35	0.90	1 (3%)	32,50,50	0.71	0
2	GOL	BBB	301	-	5,5,5	0.20	0	5,5,5	0.43	0
4	1BO	DDD	502	-	4,4,4	0.22	0	3,3,3	0.15	0
2	GOL	CCC	402	-	5,5,5	0.05	0	5,5,5	0.35	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
5	0WO	CCC	401	-	-	4/16/39/39	0/3/3/3
2	GOL	AAA	301	-	-	2/4/4/4	-
6	V3H	CCC	403	-	-	4/21/44/44	0/3/3/3
4	1BO	BBB	302	-	-	1/2/2/2	-
5	0WO	DDD	501	-	-	4/16/39/39	0/3/3/3
6	V3H	DDD	503	-	-	2/21/44/44	0/3/3/3
2	GOL	BBB	301	-	-	1/4/4/4	-
4	1BO	DDD	502	-	-	0/2/2/2	-
2	GOL	CCC	402	-	-	4/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	CCC	401	0WO	CAY-CAU	-4.02	1.45	1.51
6	CCC	403	V3H	CAY-CAU	-3.59	1.45	1.51
6	DDD	503	V3H	CAY-CAU	-3.39	1.46	1.51
5	DDD	501	0WO	CAY-CAU	-2.92	1.46	1.51
5	DDD	501	0WO	OAH-CAT	-2.85	1.21	1.30
5	CCC	401	0WO	OAH-CAT	-2.69	1.21	1.30
6	CCC	403	V3H	OAH-CAT	-2.12	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	CCC	403	V3H	CBC-SAR-CB	-2.62	88.38	93.99
6	CCC	403	V3H	C4-O-C	2.09	121.00	116.58

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	301	GOL	O1-C1-C2-C3
2	CCC	402	GOL	O1-C1-C2-O2
2	CCC	402	GOL	O1-C1-C2-C3
2	CCC	402	GOL	C1-C2-C3-O3
2	CCC	402	GOL	O2-C2-C3-O3

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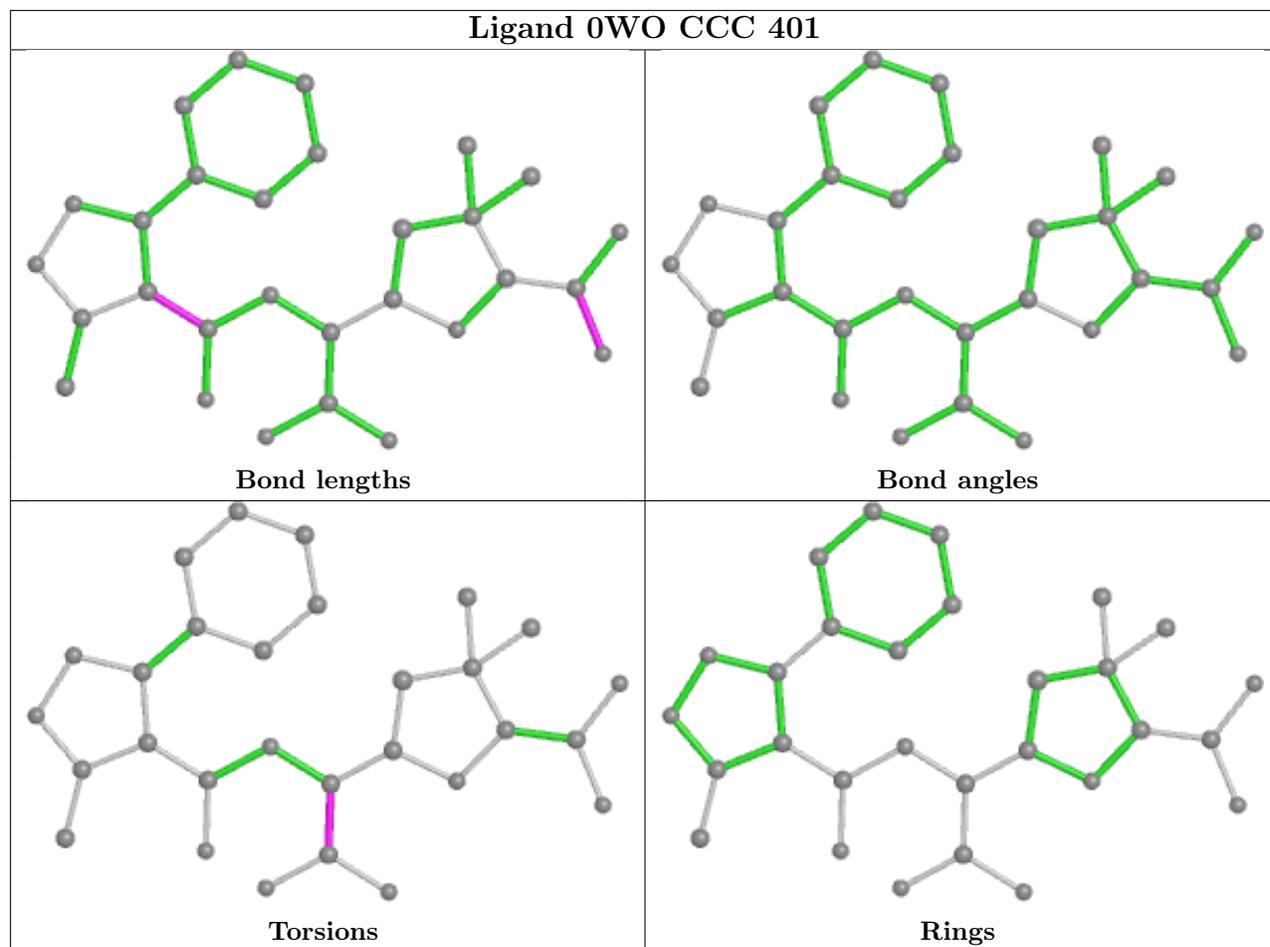
Mol	Chain	Res	Type	Atoms
5	CCC	401	0WO	OXT-C-CA-N
6	CCC	403	V3H	CA-C-O-C4
6	CCC	403	V3H	OXT-C-O-C4
6	DDD	503	V3H	CA-C-O-C4
6	DDD	503	V3H	OXT-C-O-C4
2	AAA	301	GOL	O1-C1-C2-O2
4	BBB	302	1BO	C1-C2-C3-C4
5	DDD	501	0WO	O-C-CA-N
5	DDD	501	0WO	OXT-C-CA-N
6	CCC	403	V3H	CAM-CAW-CAX-NAN
5	CCC	401	0WO	O-C-CA-N
5	CCC	401	0WO	O-C-CA-CB
5	CCC	401	0WO	OXT-C-CA-CB
5	DDD	501	0WO	O-C-CA-CB
5	DDD	501	0WO	OXT-C-CA-CB
6	CCC	403	V3H	CAL-CAW-CAX-NAN
2	BBB	301	GOL	O1-C1-C2-C3

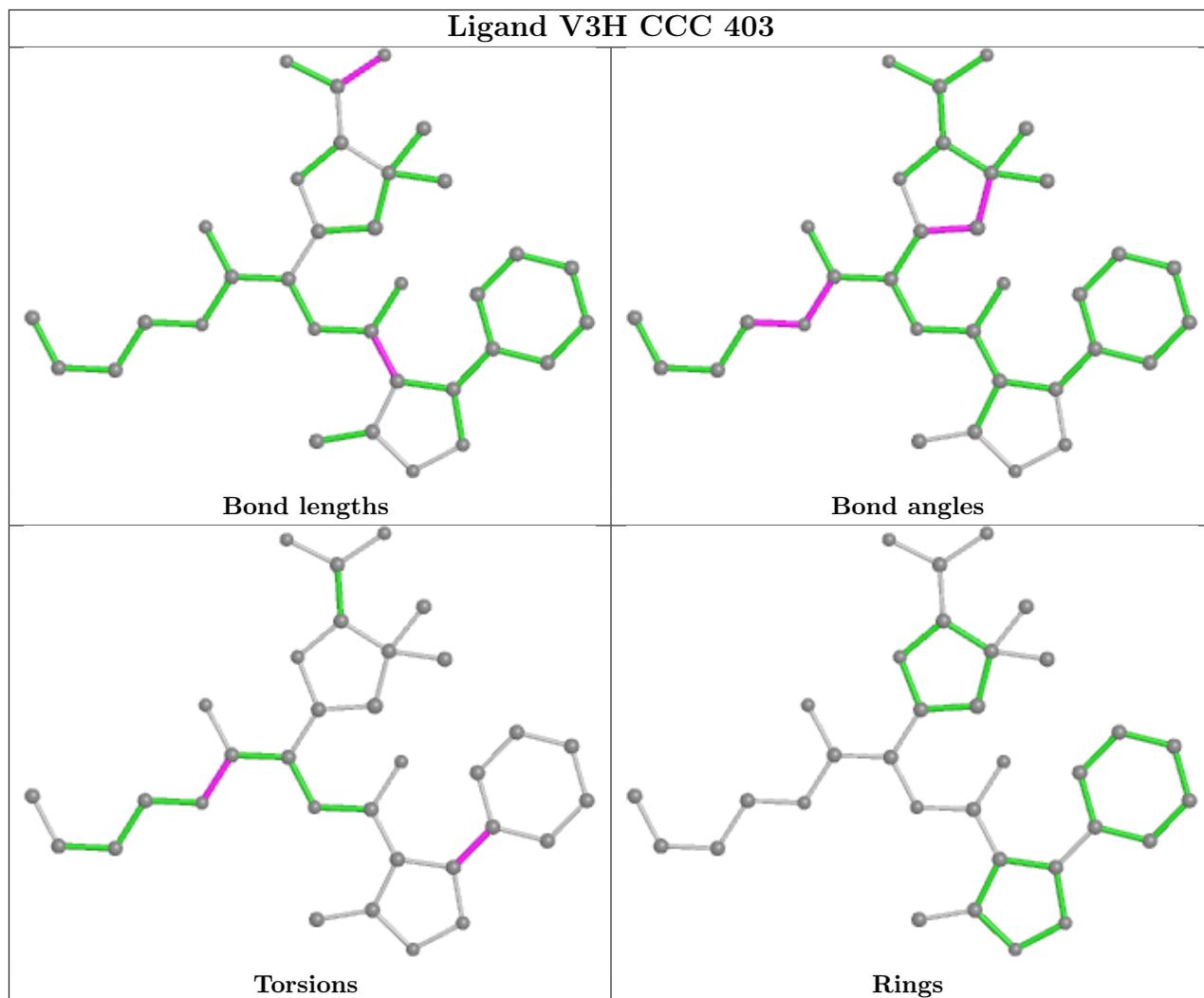
There are no ring outliers.

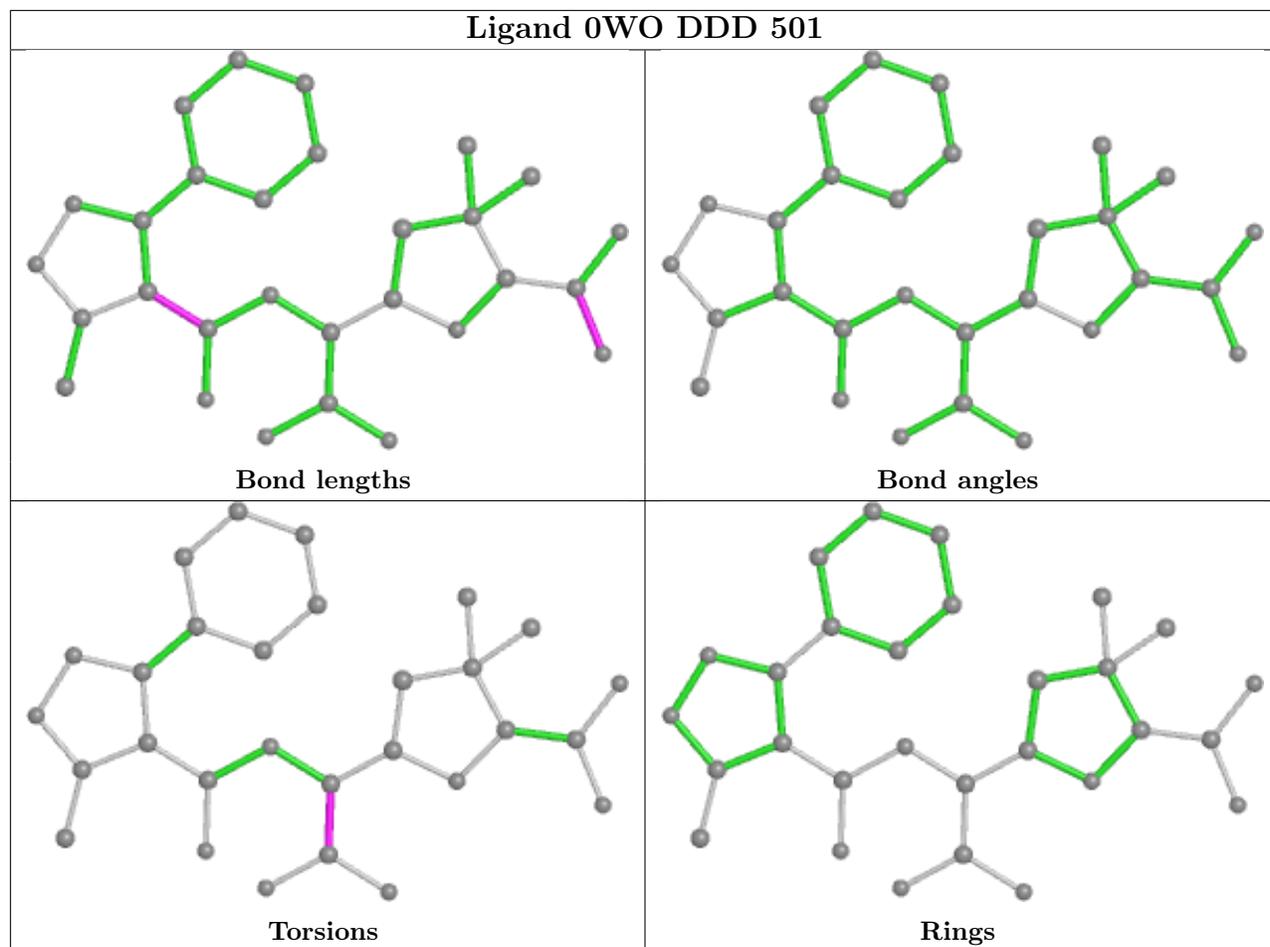
4 monomers are involved in 5 short contacts:

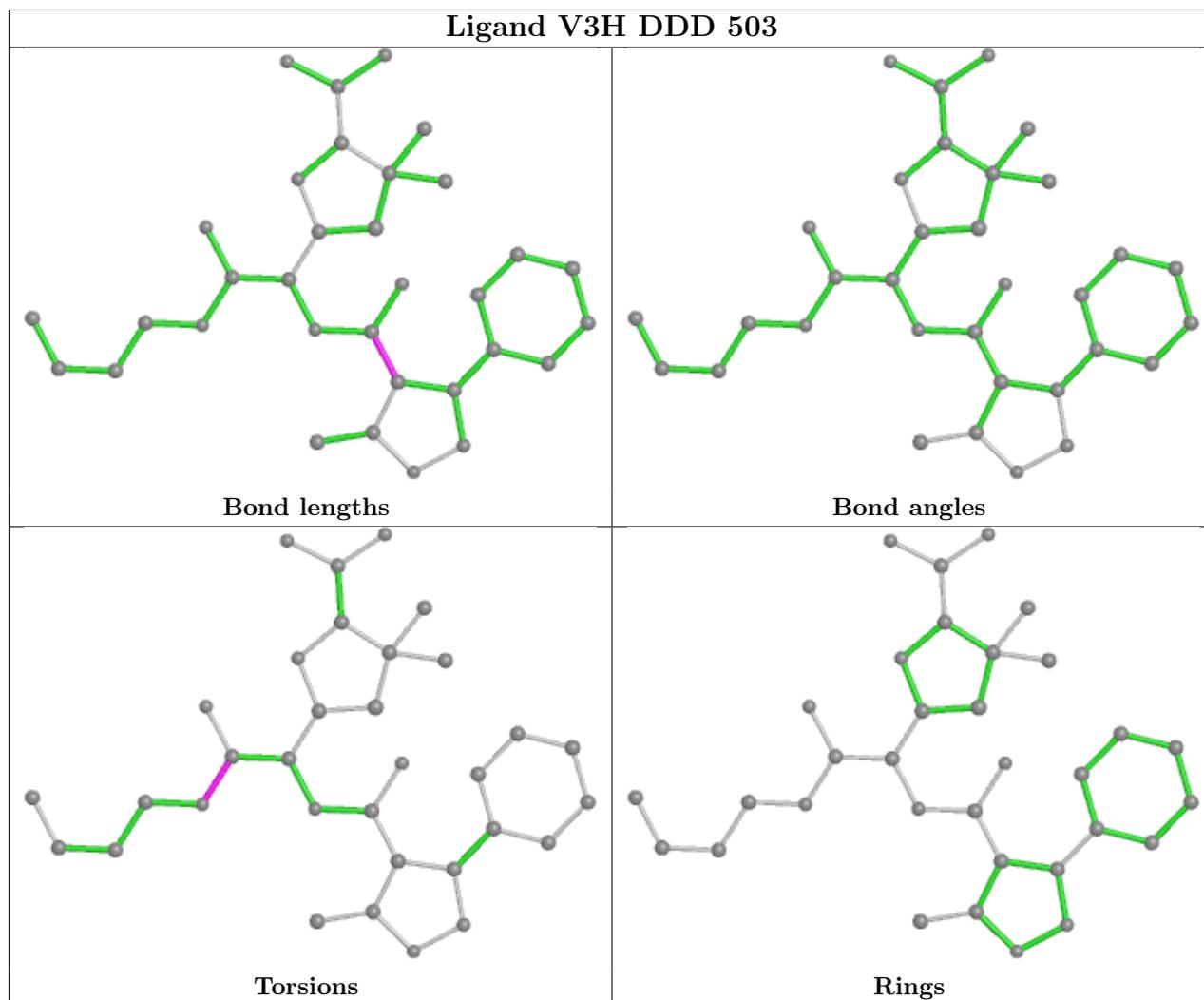
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	CCC	403	V3H	2	0
4	BBB	302	1BO	1	0
6	DDD	503	V3H	1	0
2	BBB	301	GOL	1	0

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

### 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	AAA	241/260 (92%)	-0.08	3 (1%) 79 79	16, 24, 41, 53	5 (2%)
1	BBB	241/260 (92%)	-0.05	3 (1%) 79 79	18, 27, 42, 54	3 (1%)
1	CCC	241/260 (92%)	0.06	6 (2%) 57 56	16, 26, 49, 63	3 (1%)
1	DDD	241/260 (92%)	0.08	8 (3%) 46 44	18, 29, 50, 63	0
All	All	964/1040 (92%)	0.00	20 (2%) 63 63	16, 27, 47, 63	11 (1%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	265	PRO	3.5
1	CCC	245	ASP	3.1
1	DDD	39	LYS	3.1
1	CCC	265	PRO	3.0
1	AAA	265	PRO	3.0
1	CCC	37	GLU	2.9
1	DDD	101	ASP	2.8
1	CCC	243	THR	2.8
1	AAA	39	LYS	2.6
1	BBB	265	PRO	2.5
1	DDD	36	THR	2.5
1	CCC	36	THR	2.4
1	BBB	33	ALA	2.3
1	DDD	29	LYS	2.3
1	DDD	245	ASP	2.2
1	DDD	97	GLY	2.2
1	CCC	39	LYS	2.2
1	BBB	39	LYS	2.1
1	AAA	262	LYS	2.1
1	DDD	94	LYS	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	KCX	AAA	73	12/13	0.96	0.09	15,18,21,24	1
1	KCX	DDD	73	12/13	0.96	0.13	19,25,30,33	1
1	KCX	CCC	73	12/13	0.97	0.11	16,21,27,27	1
1	KCX	BBB	73	12/13	0.97	0.09	17,19,22,23	1

## 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.

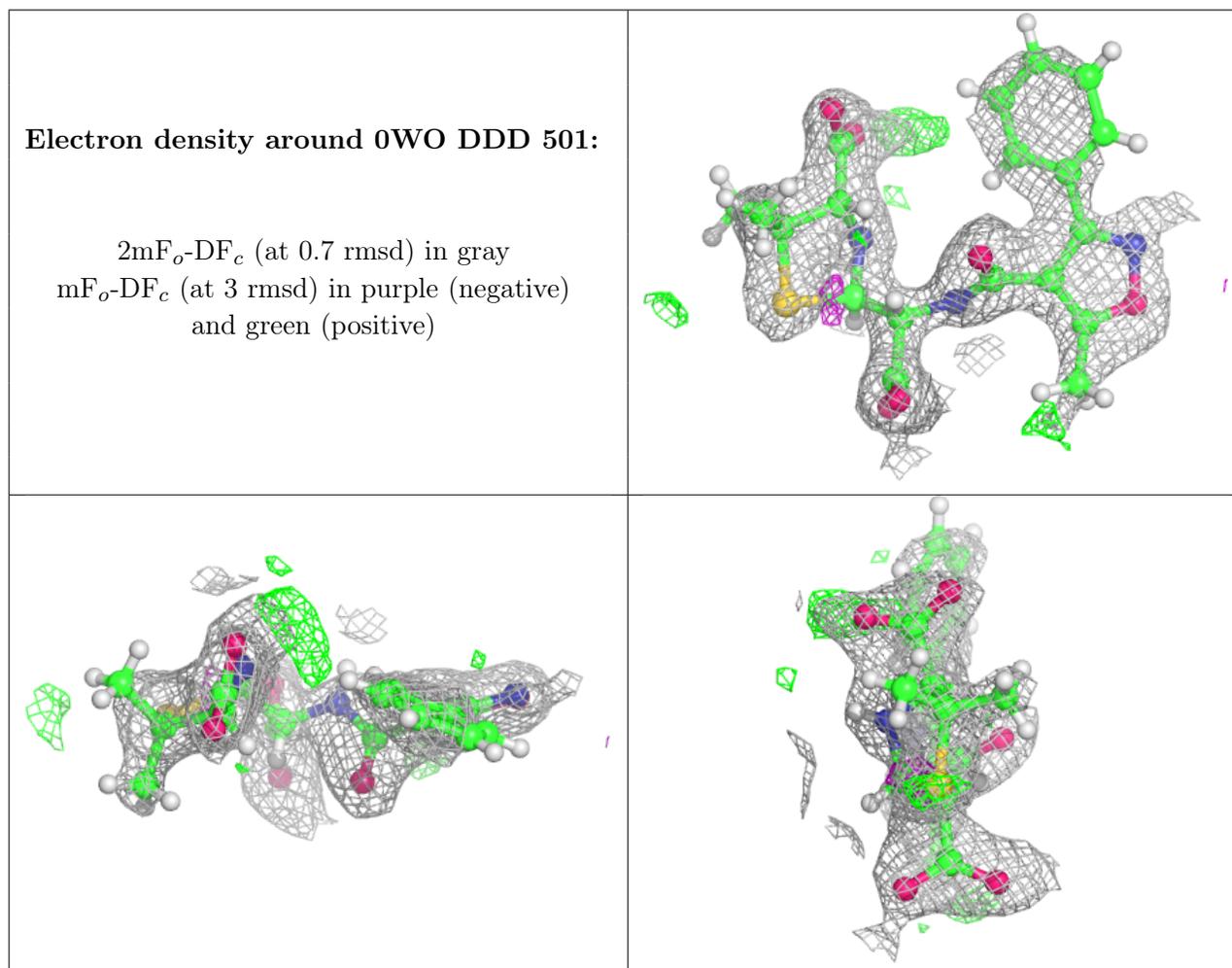
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	0WO	DDD	501	29/29	0.79	0.21	37,44,46,46	47
6	V3H	DDD	503	33/33	0.83	0.16	38,43,45,47	45
6	V3H	CCC	403	33/33	0.85	0.18	35,41,46,48	39
5	0WO	CCC	401	29/29	0.86	0.19	37,44,47,47	47
4	1BO	BBB	302	5/5	0.90	0.10	45,46,52,54	0
4	1BO	DDD	502	5/5	0.90	0.12	40,42,44,45	0
2	GOL	CCC	402	6/6	0.90	0.14	44,50,54,54	2
2	GOL	BBB	301	6/6	0.91	0.11	27,36,37,37	2
2	GOL	AAA	301	6/6	0.91	0.17	29,43,48,49	2
3	IOD	DDD	504	1/1	0.97	0.05	50,50,50,50	1
3	IOD	BBB	305	1/1	0.98	0.04	36,36,36,36	1
3	IOD	CCC	407	1/1	0.98	0.06	31,31,31,31	0
3	IOD	AAA	303	1/1	0.98	0.04	38,38,38,38	1
3	IOD	DDD	505	1/1	0.98	0.06	41,41,41,41	1
3	IOD	BBB	304	1/1	0.98	0.06	35,35,35,35	0
3	IOD	CCC	404	1/1	0.99	0.06	39,39,39,39	1
3	IOD	CCC	405	1/1	0.99	0.04	38,38,38,38	1
3	IOD	CCC	406	1/1	0.99	0.05	46,46,46,46	1

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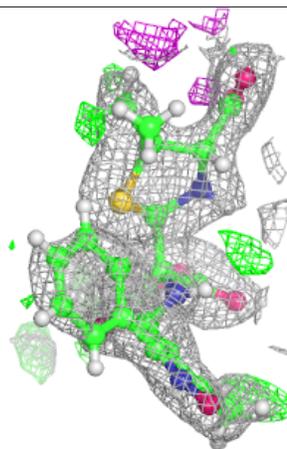
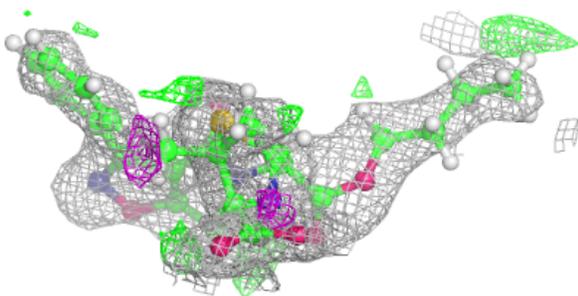
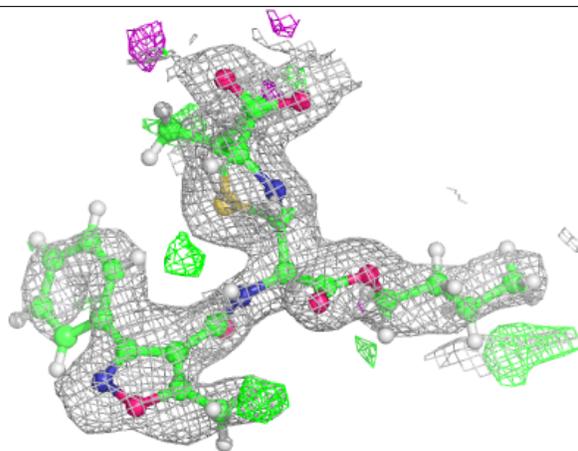
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	IOD	AAA	305	1/1	0.99	0.03	48,48,48,48	1
3	IOD	BBB	306	1/1	0.99	0.04	42,42,42,42	1
3	IOD	BBB	307	1/1	0.99	0.05	42,42,42,42	1
3	IOD	AAA	304[B]	1/1	1.00	0.08	23,23,23,23	1
3	IOD	AAA	302	1/1	1.00	0.03	34,34,34,34	1
3	IOD	BBB	303[A]	1/1	1.00	0.05	21,21,21,21	1
3	IOD	BBB	303[B]	1/1	1.00	0.05	22,22,22,22	1
3	IOD	AAA	304[A]	1/1	1.00	0.08	20,20,20,20	1

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.



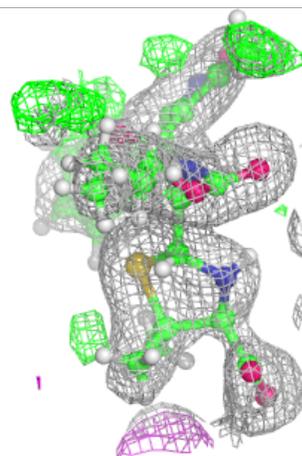
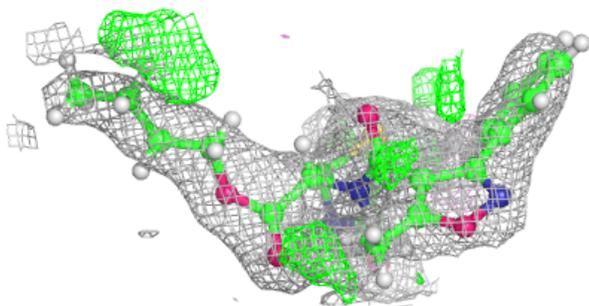
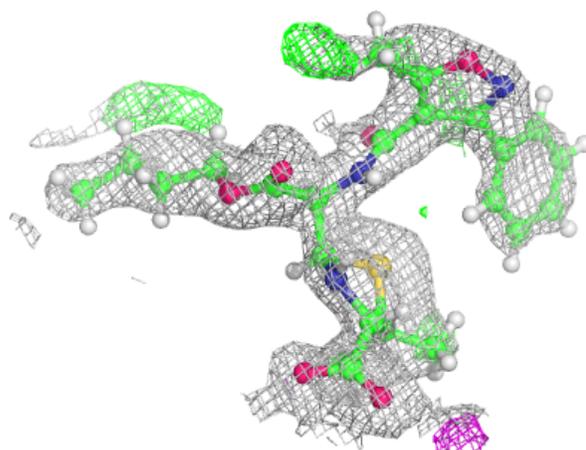
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and green (positive)



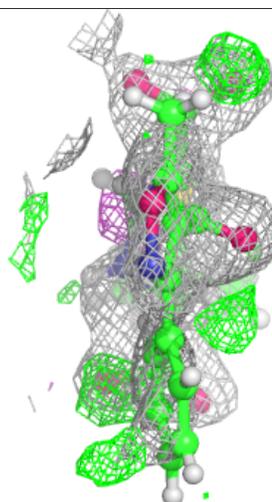
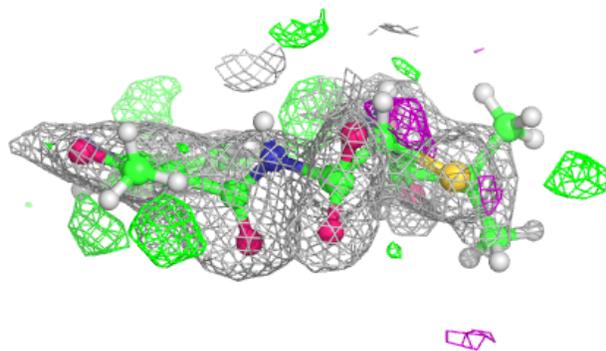
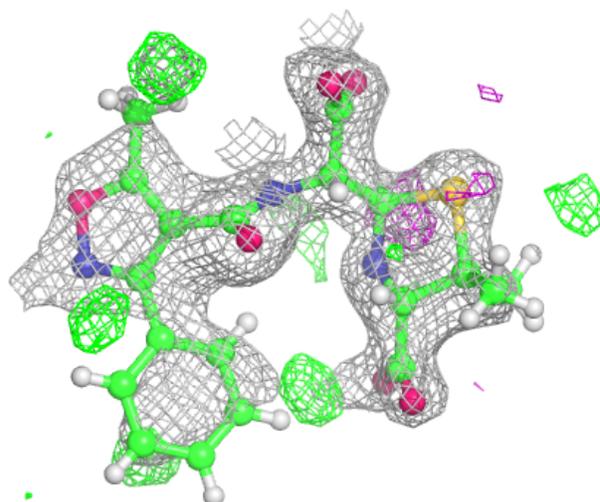
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and green (positive)



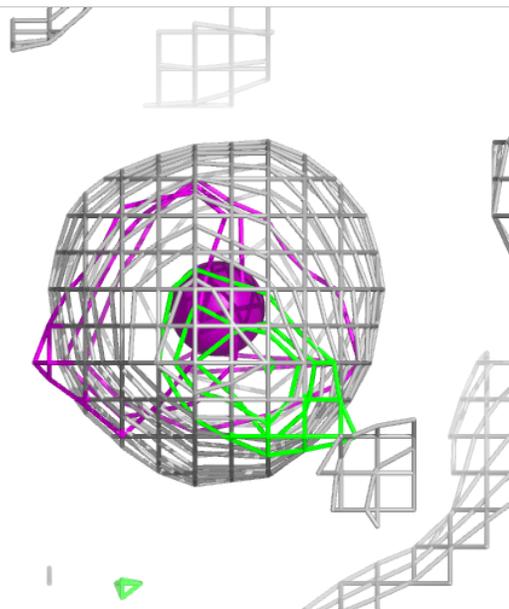
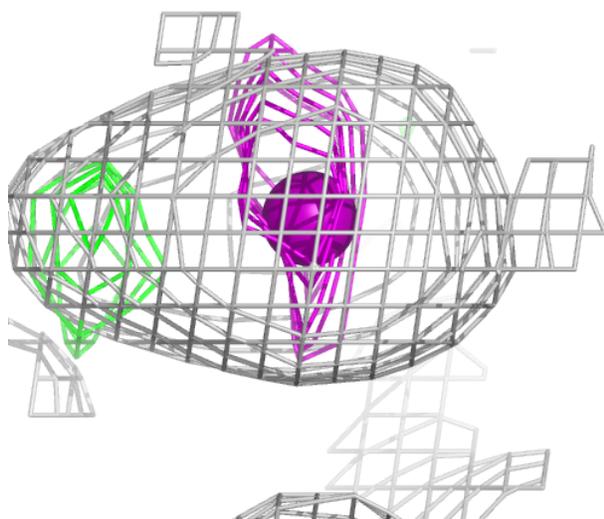
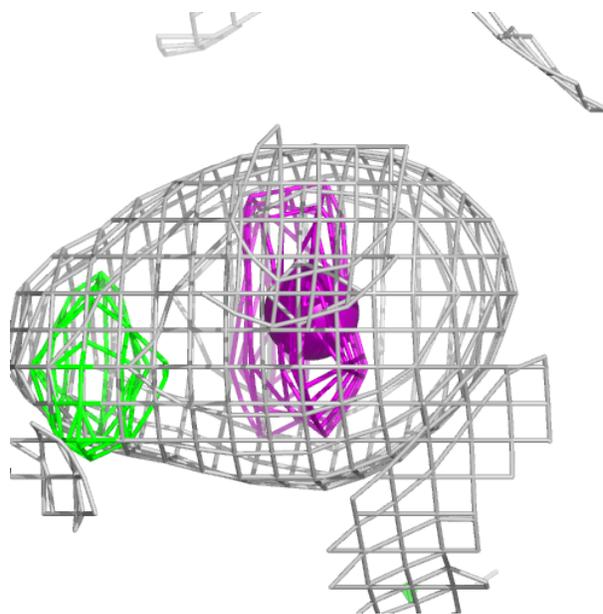
**Electron density around 0WO CCC 401:**

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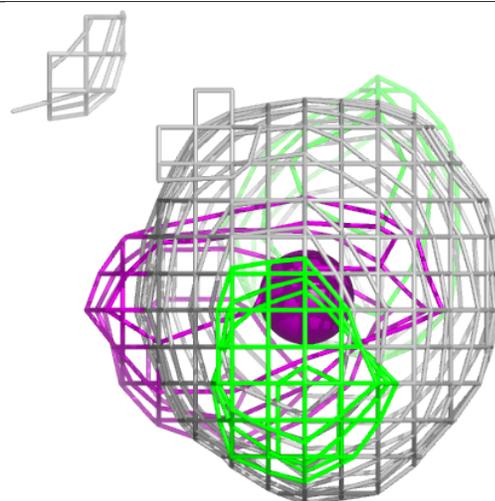
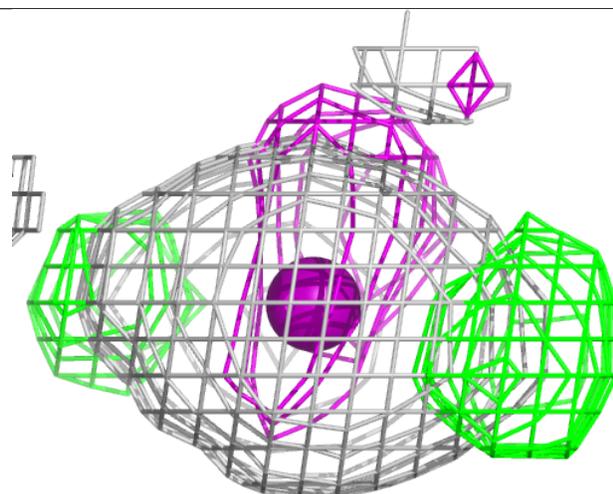
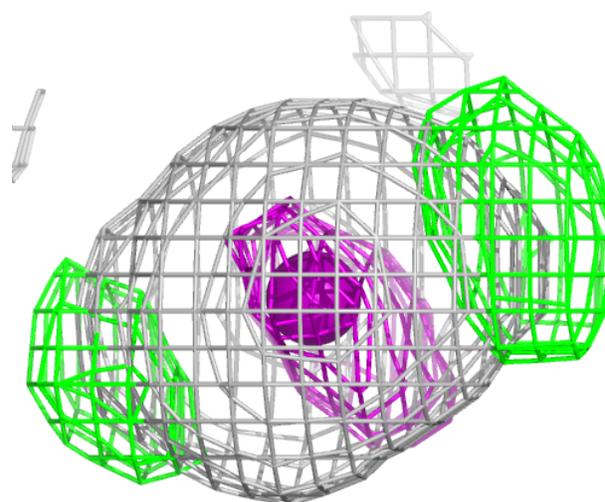
**Electron density around IOD DDD 504:**

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and green (positive)



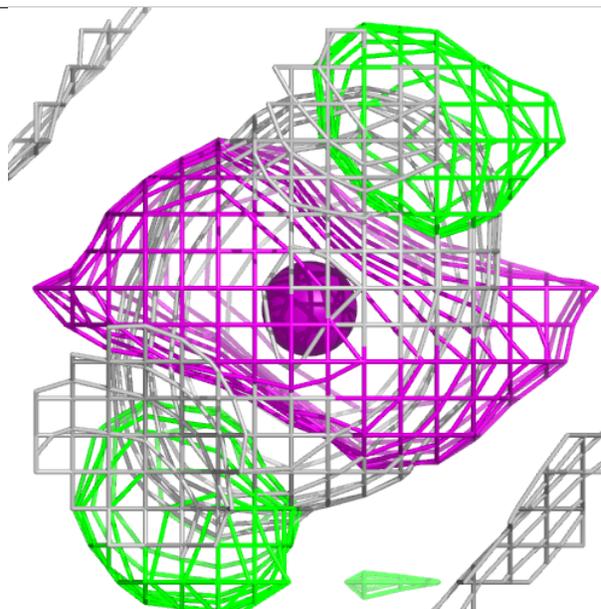
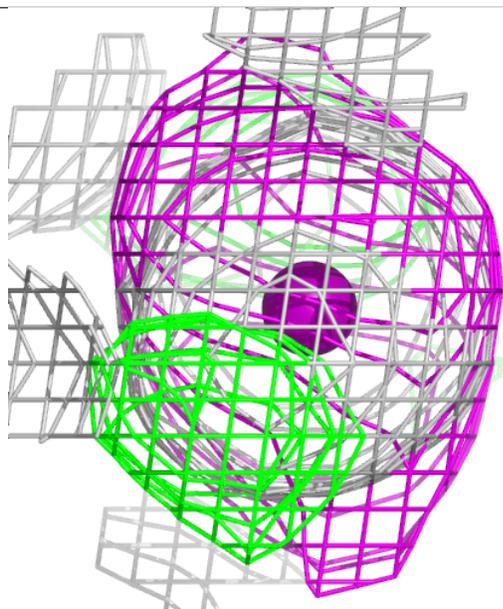
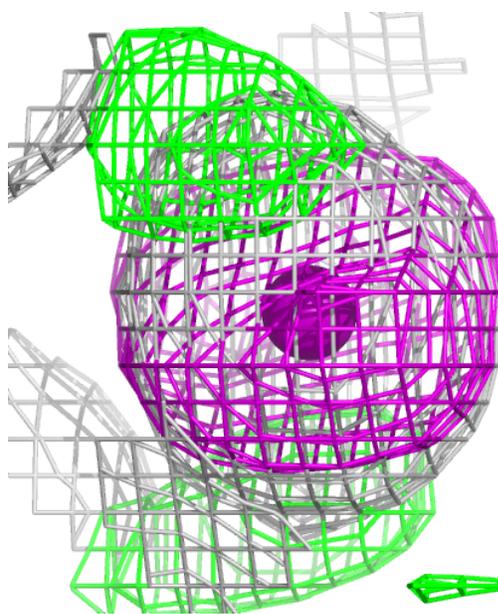
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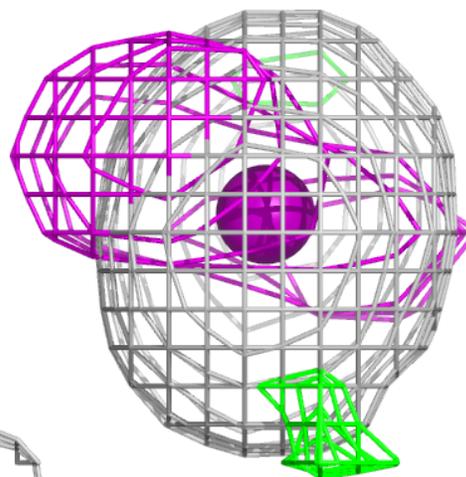
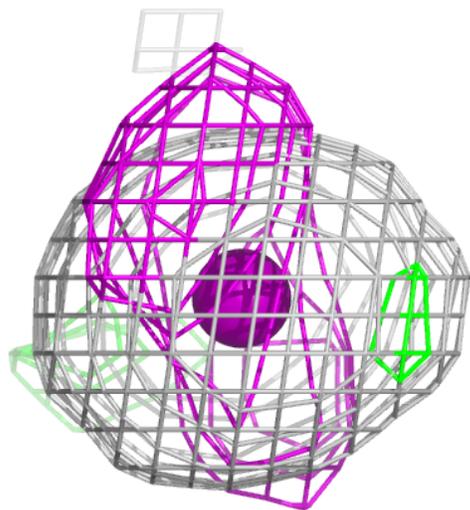
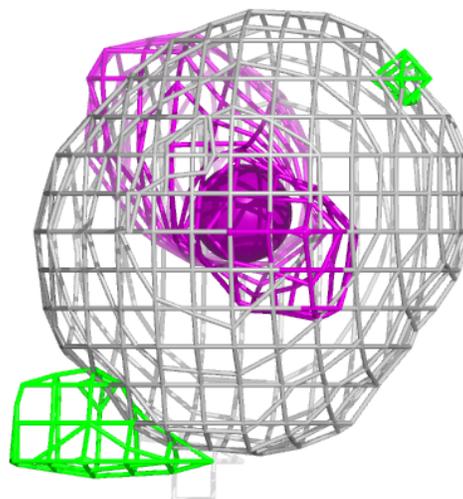
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and green (positive)



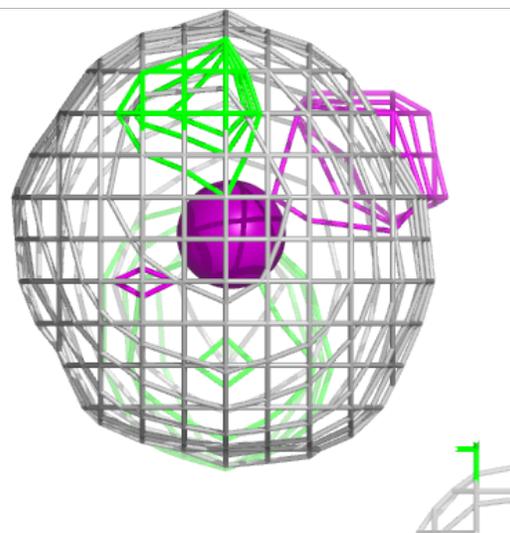
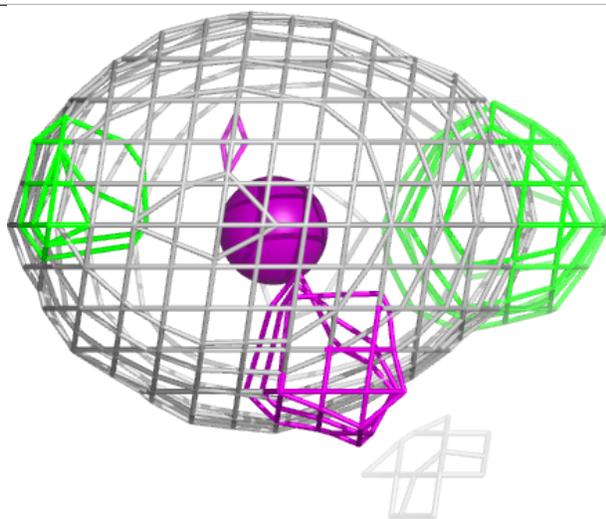
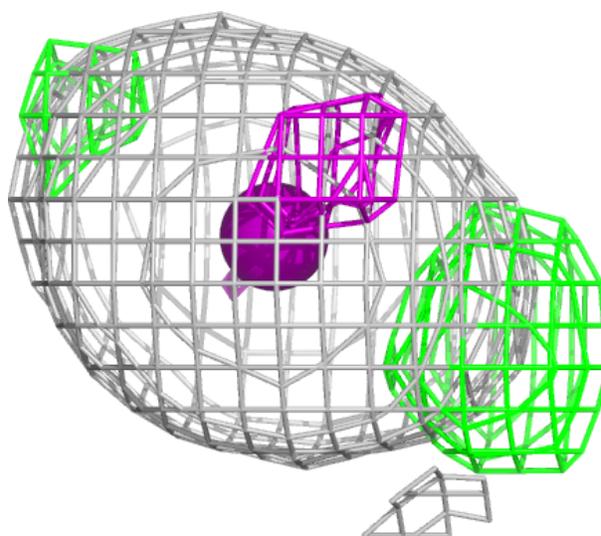
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and green (positive)



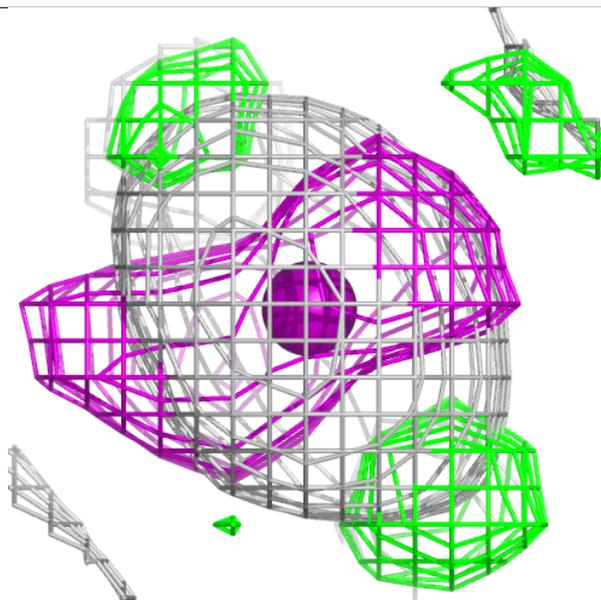
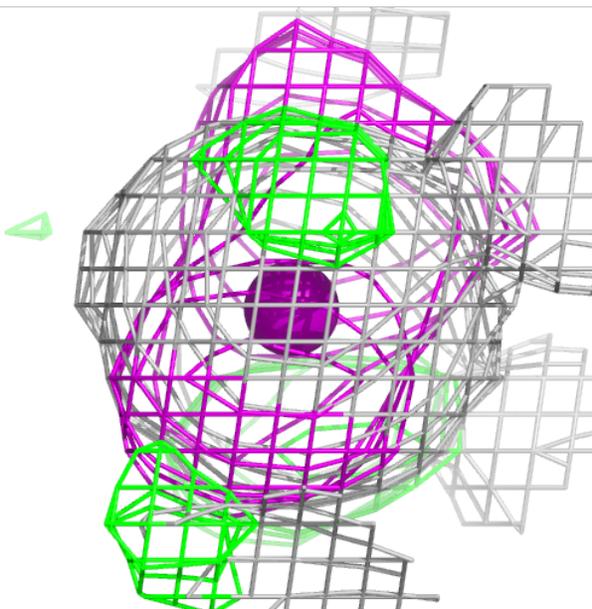
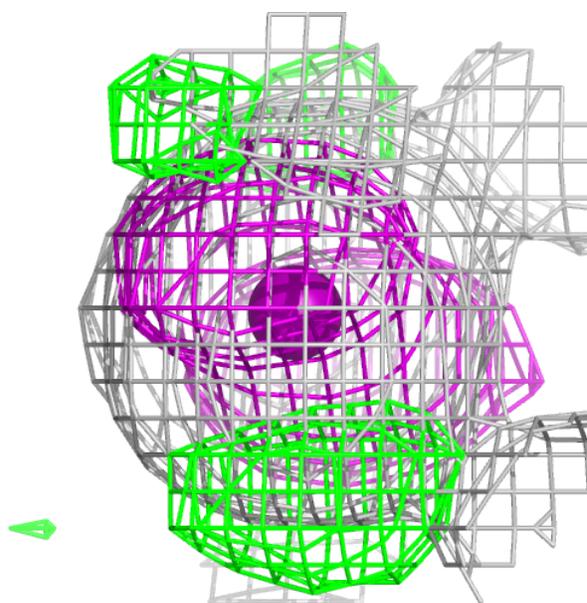
**Electron density around IOD DDD 505:**

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



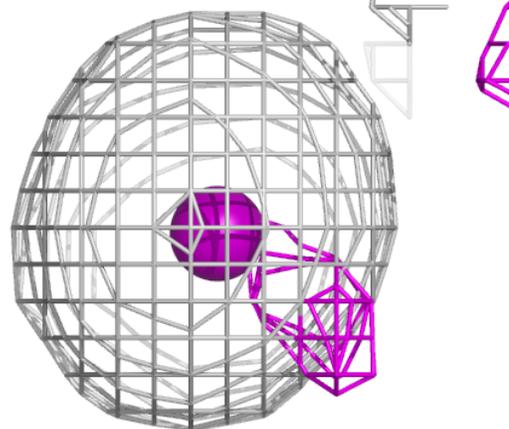
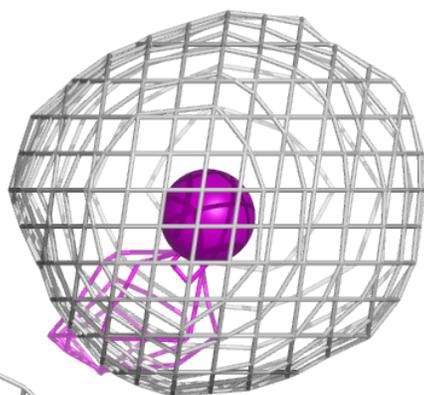
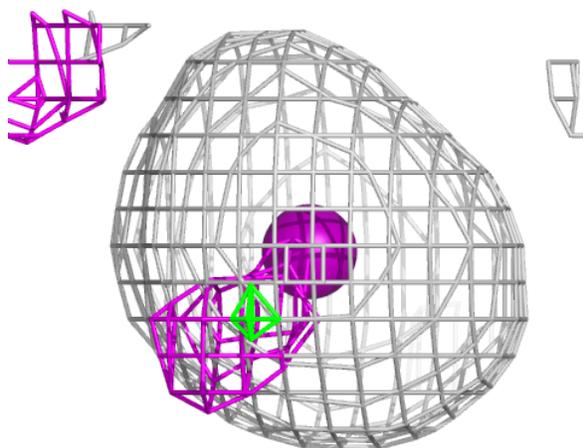
**Electron density around IOD BBB 304:**

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



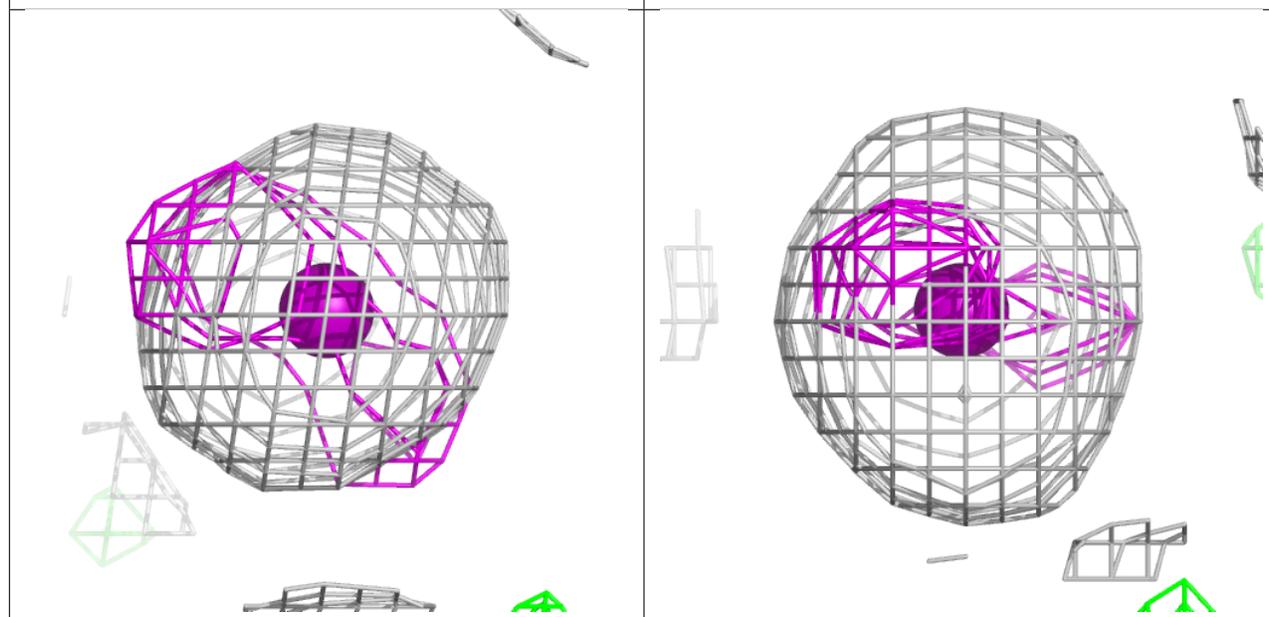
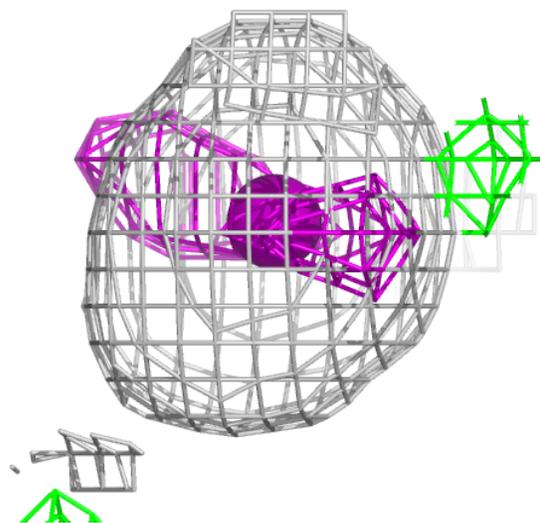
**Electron density around IOD CCC 404:**

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



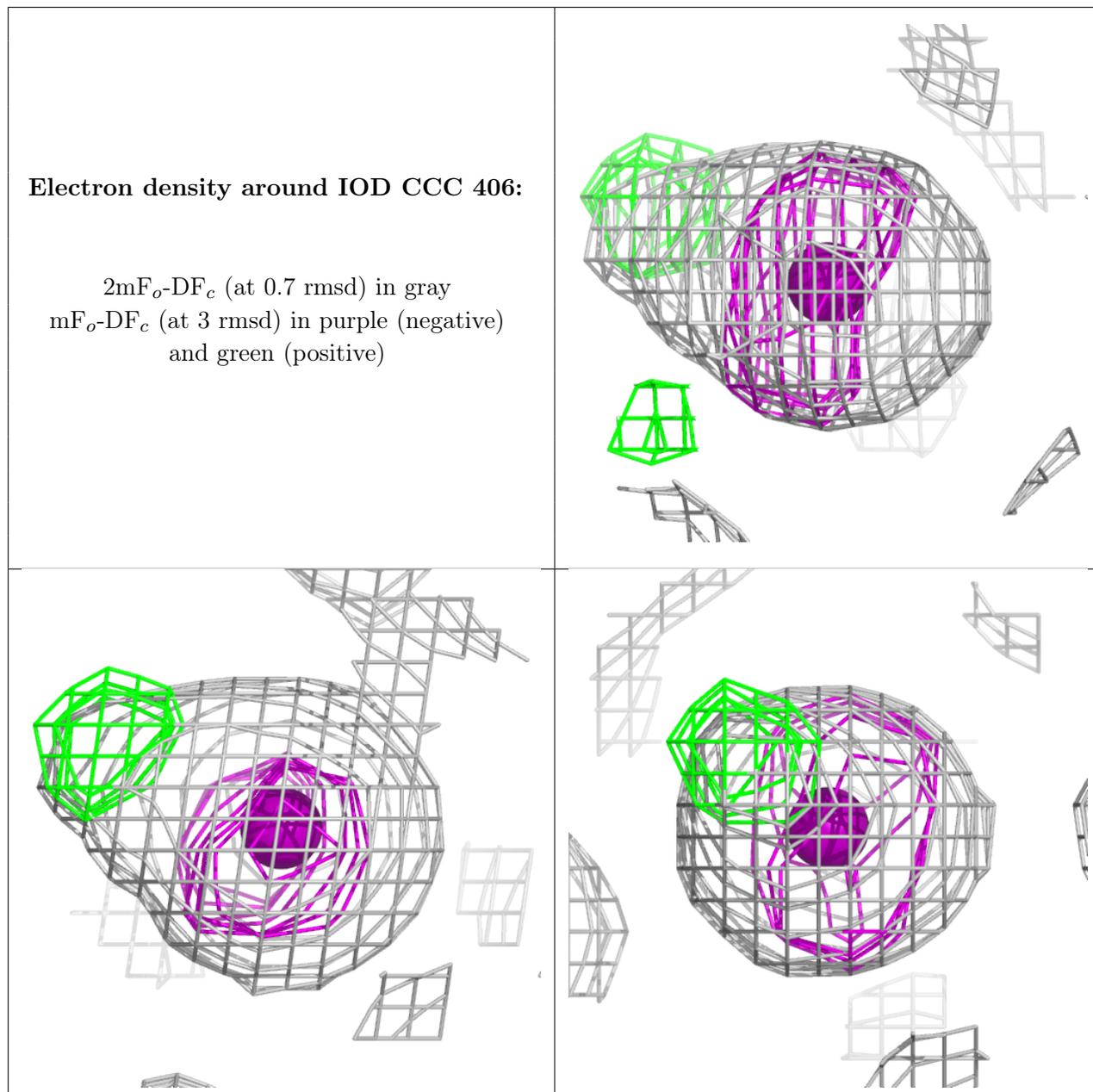
**Electron density around IOD CCC 405:**

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



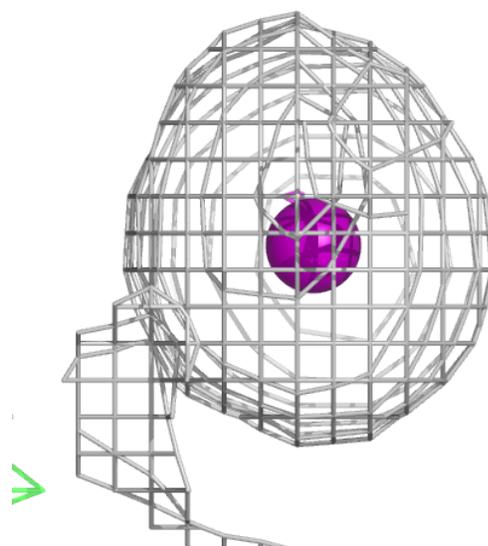
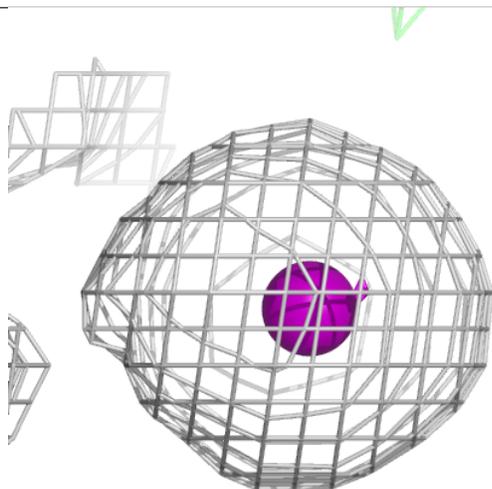
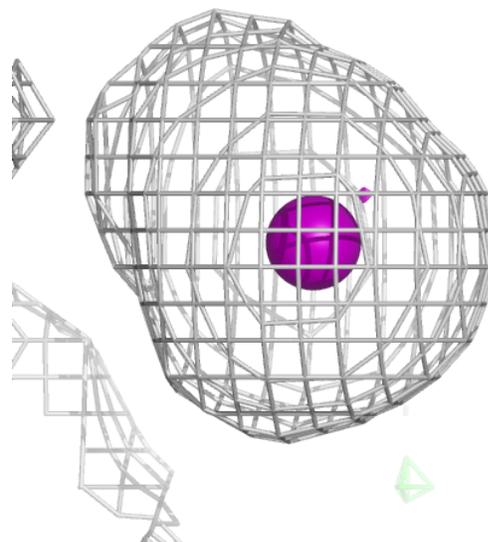
**Electron density around IOD CCC 406:**

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



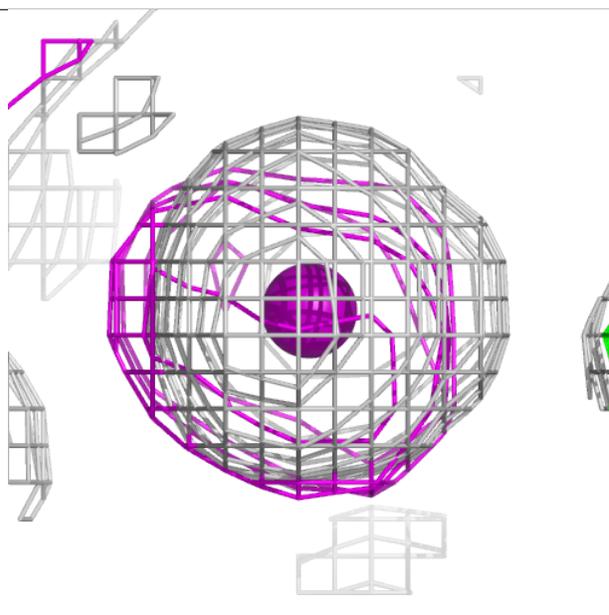
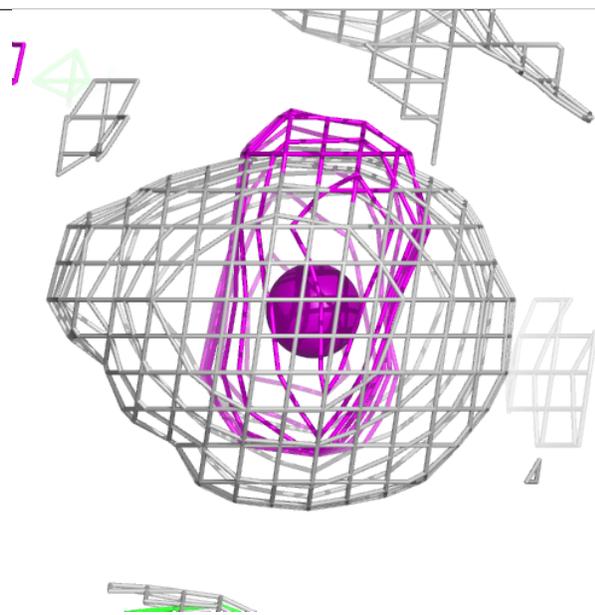
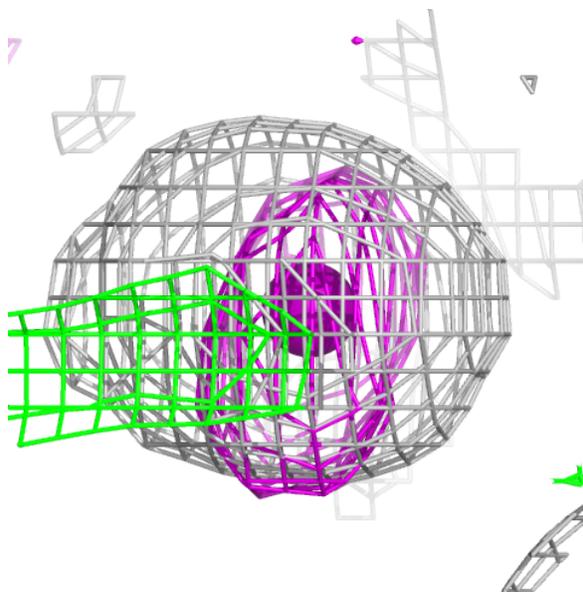
**Electron density around IOD AAA 305:**

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



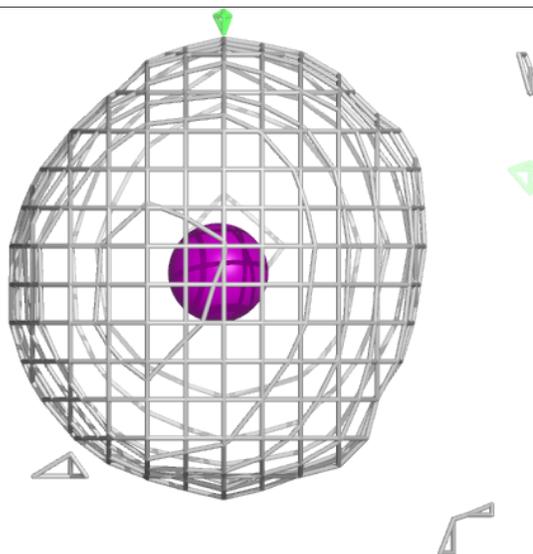
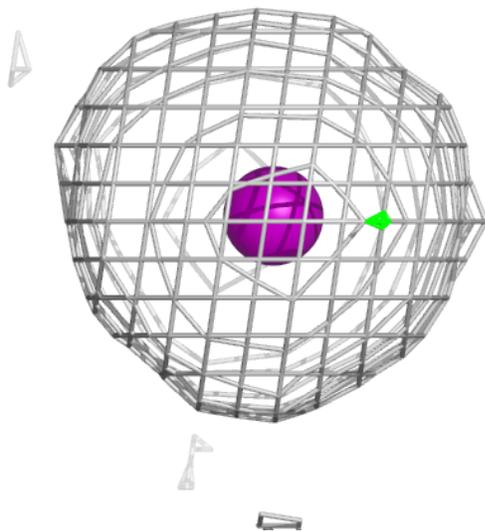
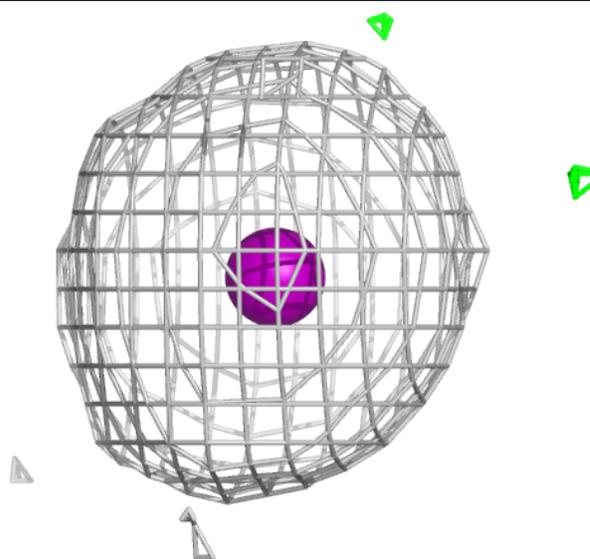
**Electron density around IOD BBB 306:**

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



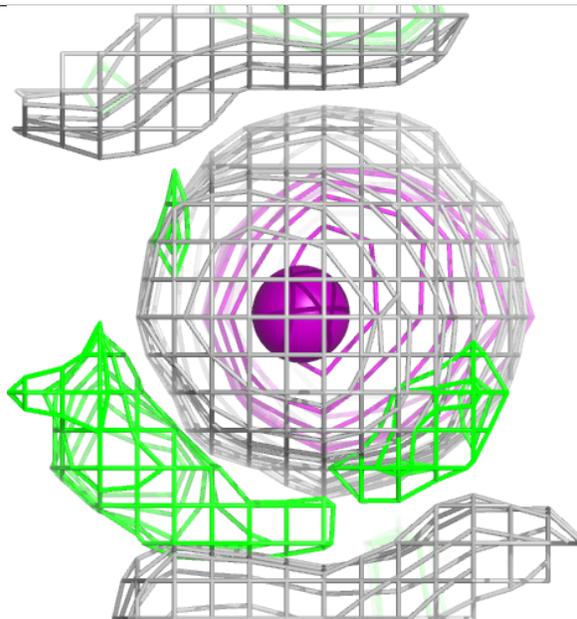
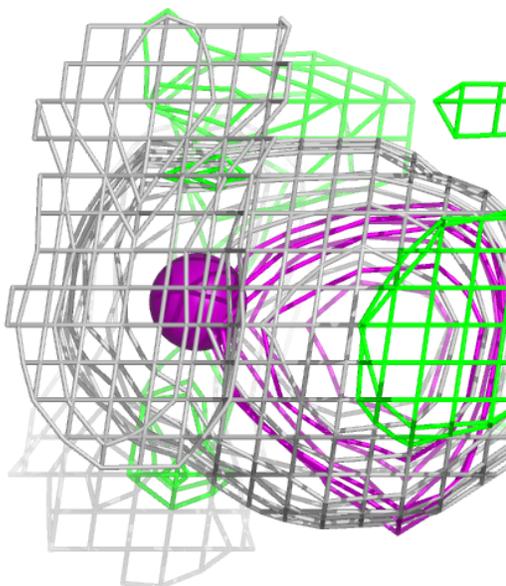
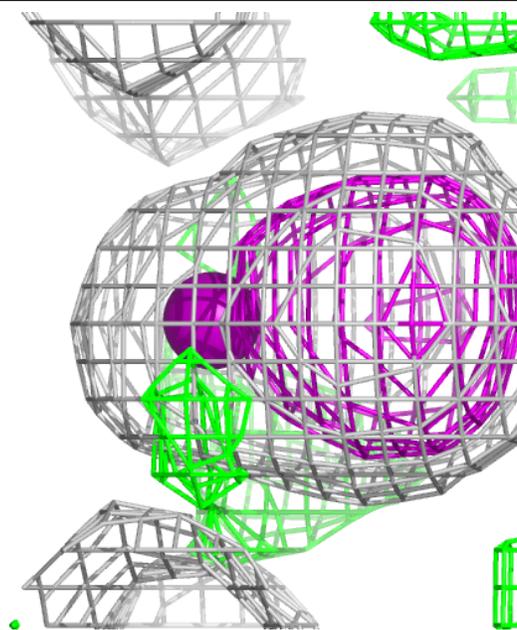
**Electron density around IOD BBB 307:**

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



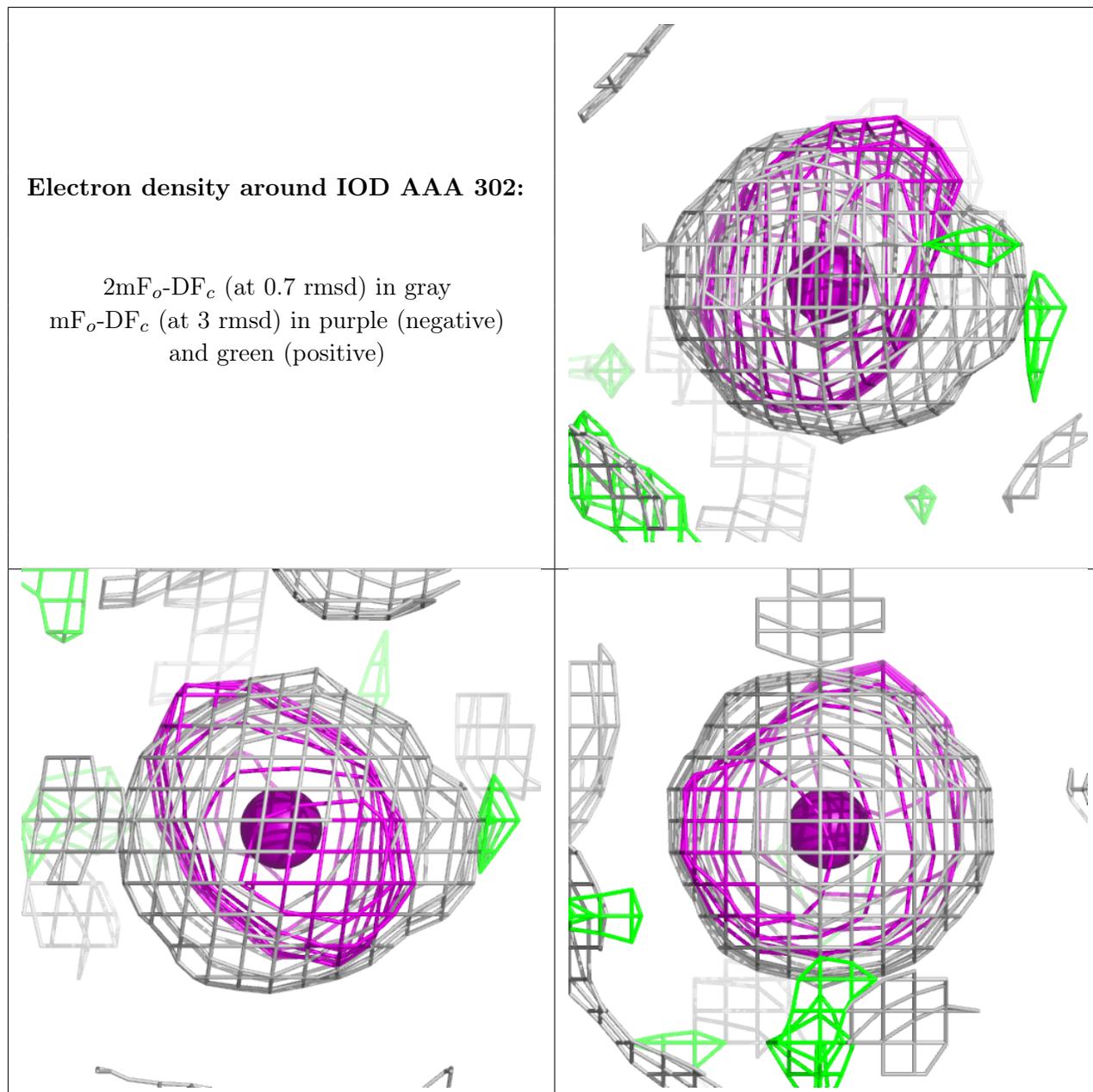
**Electron density around IOD AAA 304 (B):**

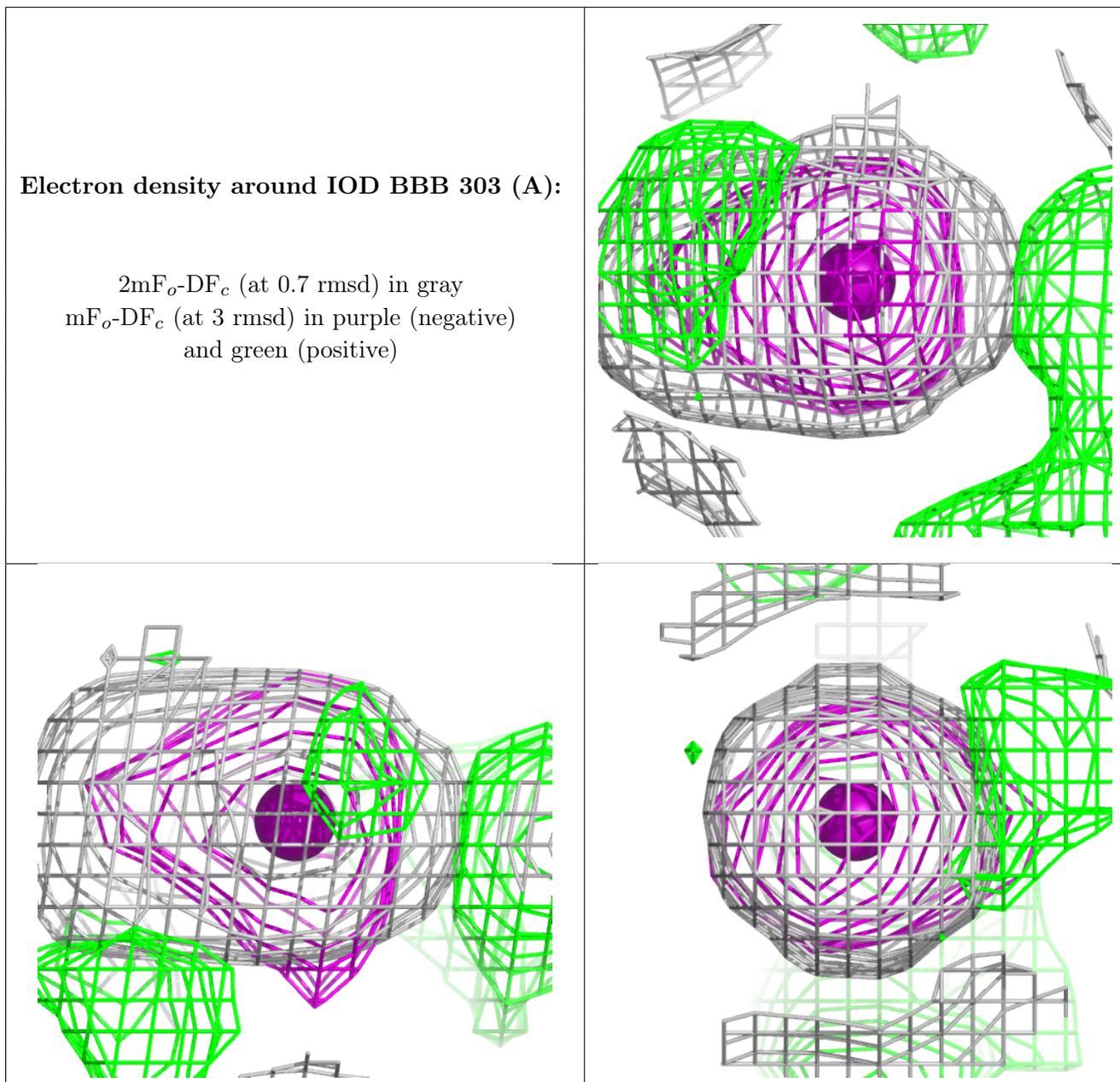
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around IOD AAA 302:**

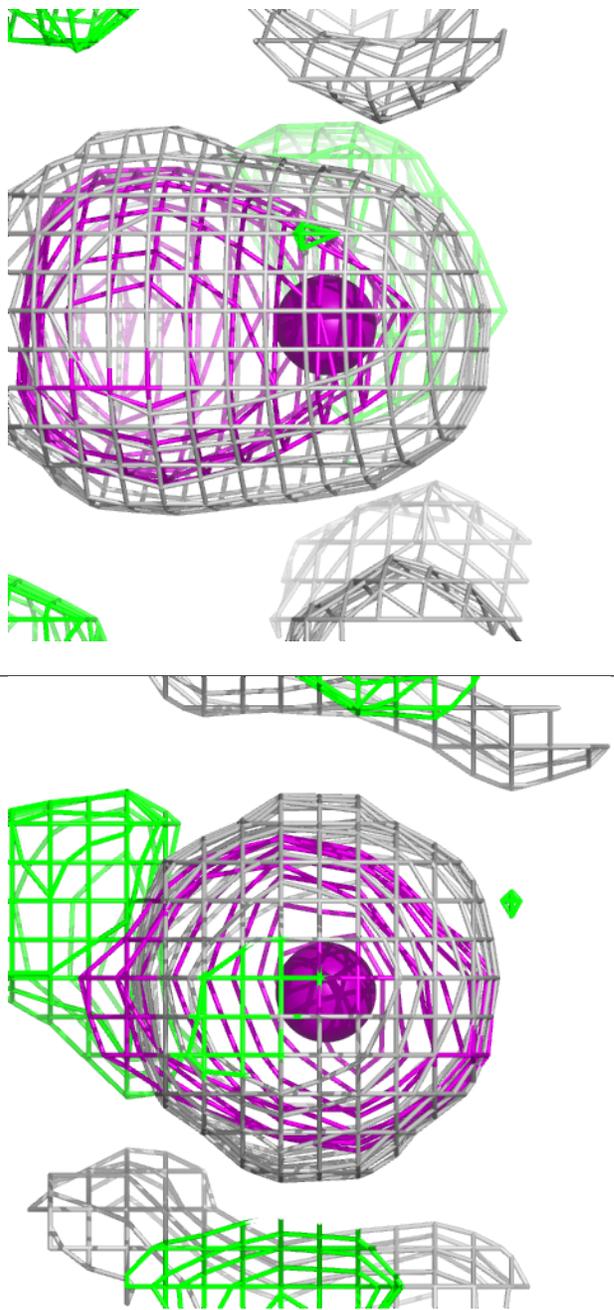
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

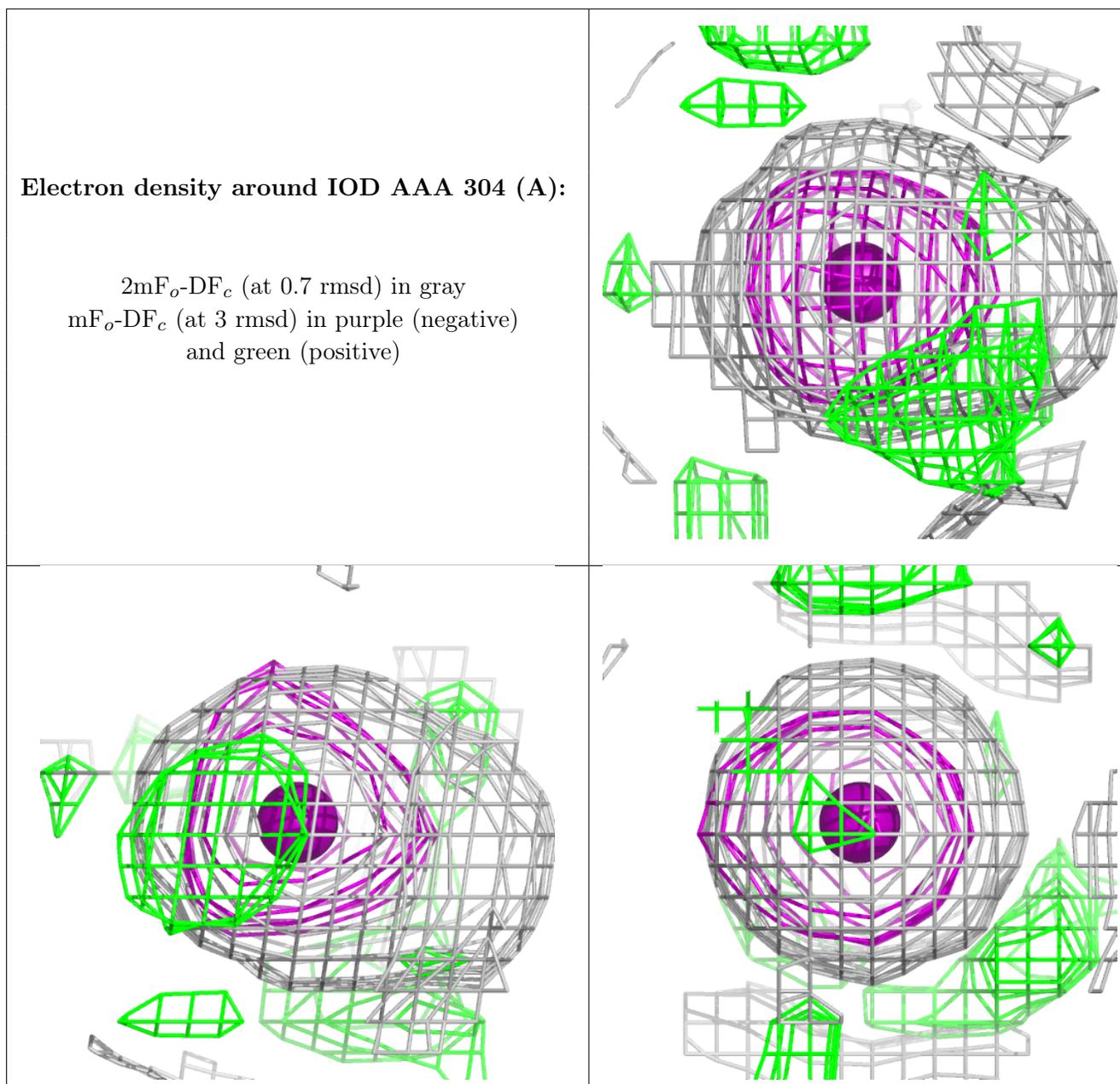




**Electron density around IOD BBB 303 (B):**

$2mF_o-DF_c$  (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.