



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2022 – 03:13 pm GMT

PDB ID : 7NRJ  
Title : Crystal Structure of a Class D carbapenemase complexed with iodide  
Authors : Zhou, Q.; He, Y.; Jin, Y.  
Deposited on : 2021-03-04  
Resolution : 1.67 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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.27  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

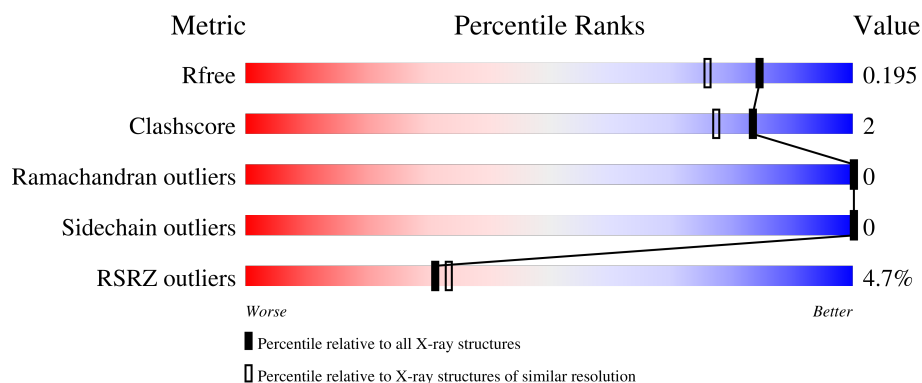
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.67 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	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (1.70-1.66)

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	<div> <div>2%</div> <div>88%</div> <div>5%</div> <div>7%</div> </div>
1	BBB	260	<div> <div>2%</div> <div>92%</div> <div>•</div> <div>7%</div> </div>
1	CCC	260	<div> <div>7%</div> <div>89%</div> <div>•</div> <div>7%</div> </div>
1	DDD	260	<div> <div>7%</div> <div>92%</div> <div>•</div> <div>7%</div> </div>

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
2	1BO	AAA	301	-	-	X	-
2	1BO	CCC	301	-	-	X	-
4	GOL	CCC	303	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16960 atoms, of which 7947 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
1	AAA	242	Total	C	H	N	O	S	48	3	0
			3967	1275	1961	352	371	8			
1	BBB	242	Total	C	H	N	O	S	48	3	0
			3969	1275	1964	352	369	9			
1	CCC	241	Total	C	H	N	O	S	50	3	0
			3955	1271	1957	353	366	8			
1	DDD	242	Total	C	H	N	O	S	48	2	0
			3952	1270	1955	351	368	8			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	6	MET	-	initiating methionine	UNP A0A482LRD5
AAA	7	HIS	-	expression tag	UNP A0A482LRD5
AAA	8	HIS	-	expression tag	UNP A0A482LRD5
AAA	9	HIS	-	expression tag	UNP A0A482LRD5
AAA	10	HIS	-	expression tag	UNP A0A482LRD5
AAA	11	HIS	-	expression tag	UNP A0A482LRD5
AAA	12	HIS	-	expression tag	UNP A0A482LRD5
AAA	13	SER	-	expression tag	UNP A0A482LRD5
AAA	14	ALA	-	expression tag	UNP A0A482LRD5
AAA	15	GLY	-	expression tag	UNP A0A482LRD5
AAA	16	GLU	-	expression tag	UNP A0A482LRD5
AAA	17	ASN	-	expression tag	UNP A0A482LRD5
AAA	18	LEU	-	expression tag	UNP A0A482LRD5
AAA	19	TYR	-	expression tag	UNP A0A482LRD5
AAA	20	PHE	-	expression tag	UNP A0A482LRD5
AAA	21	GLN	-	expression tag	UNP A0A482LRD5
AAA	22	GLY	-	expression tag	UNP A0A482LRD5
BBB	6	MET	-	initiating methionine	UNP A0A482LRD5
BBB	7	HIS	-	expression tag	UNP A0A482LRD5
BBB	8	HIS	-	expression tag	UNP A0A482LRD5
BBB	9	HIS	-	expression tag	UNP A0A482LRD5

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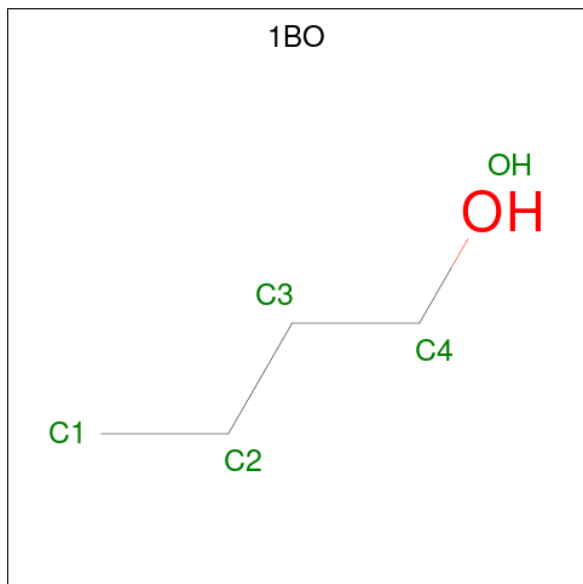
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	10	HIS	-	expression tag	UNP A0A482LRD5
BBB	11	HIS	-	expression tag	UNP A0A482LRD5
BBB	12	HIS	-	expression tag	UNP A0A482LRD5
BBB	13	SER	-	expression tag	UNP A0A482LRD5
BBB	14	ALA	-	expression tag	UNP A0A482LRD5
BBB	15	GLY	-	expression tag	UNP A0A482LRD5
BBB	16	GLU	-	expression tag	UNP A0A482LRD5
BBB	17	ASN	-	expression tag	UNP A0A482LRD5
BBB	18	LEU	-	expression tag	UNP A0A482LRD5
BBB	19	TYR	-	expression tag	UNP A0A482LRD5
BBB	20	PHE	-	expression tag	UNP A0A482LRD5
BBB	21	GLN	-	expression tag	UNP A0A482LRD5
BBB	22	GLY	-	expression tag	UNP A0A482LRD5
CCC	6	MET	-	initiating methionine	UNP A0A482LRD5
CCC	7	HIS	-	expression tag	UNP A0A482LRD5
CCC	8	HIS	-	expression tag	UNP A0A482LRD5
CCC	9	HIS	-	expression tag	UNP A0A482LRD5
CCC	10	HIS	-	expression tag	UNP A0A482LRD5
CCC	11	HIS	-	expression tag	UNP A0A482LRD5
CCC	12	HIS	-	expression tag	UNP A0A482LRD5
CCC	13	SER	-	expression tag	UNP A0A482LRD5
CCC	14	ALA	-	expression tag	UNP A0A482LRD5
CCC	15	GLY	-	expression tag	UNP A0A482LRD5
CCC	16	GLU	-	expression tag	UNP A0A482LRD5
CCC	17	ASN	-	expression tag	UNP A0A482LRD5
CCC	18	LEU	-	expression tag	UNP A0A482LRD5
CCC	19	TYR	-	expression tag	UNP A0A482LRD5
CCC	20	PHE	-	expression tag	UNP A0A482LRD5
CCC	21	GLN	-	expression tag	UNP A0A482LRD5
CCC	22	GLY	-	expression tag	UNP A0A482LRD5
DDD	6	MET	-	initiating methionine	UNP A0A482LRD5
DDD	7	HIS	-	expression tag	UNP A0A482LRD5
DDD	8	HIS	-	expression tag	UNP A0A482LRD5
DDD	9	HIS	-	expression tag	UNP A0A482LRD5
DDD	10	HIS	-	expression tag	UNP A0A482LRD5
DDD	11	HIS	-	expression tag	UNP A0A482LRD5
DDD	12	HIS	-	expression tag	UNP A0A482LRD5
DDD	13	SER	-	expression tag	UNP A0A482LRD5
DDD	14	ALA	-	expression tag	UNP A0A482LRD5
DDD	15	GLY	-	expression tag	UNP A0A482LRD5
DDD	16	GLU	-	expression tag	UNP A0A482LRD5
DDD	17	ASN	-	expression tag	UNP A0A482LRD5

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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	18	LEU	-	expression tag	UNP A0A482LRD5
DDD	19	TYR	-	expression tag	UNP A0A482LRD5
DDD	20	PHE	-	expression tag	UNP A0A482LRD5
DDD	21	GLN	-	expression tag	UNP A0A482LRD5
DDD	22	GLY	-	expression tag	UNP A0A482LRD5

- Molecule 2 is 1-BUTANOL (three-letter code: 1BO) (formula: C<sub>4</sub>H<sub>10</sub>O).

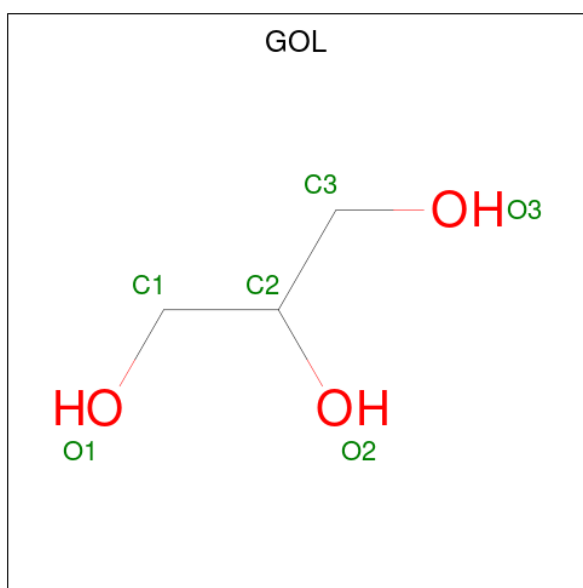


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	H	O	0	0
			15	4	10	1		
2	BBB	1	Total	C	H	O	0	0
			15	4	10	1		
2	BBB	1	Total	C	H	O	0	0
			15	4	10	1		
2	CCC	1	Total	C	H	O	0	0
			15	4	10	1		
2	CCC	1	Total	C	H	O	0	0
			15	4	10	1		
2	DDD	1	Total	C	H	O	0	0
			15	4	10	1		
2	DDD	1	Total	C	H	O	0	0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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	5	Total I 7 7	0	2
3	BBB	5	Total I 6 6	0	1
3	CCC	3	Total I 3 3	0	0
3	DDD	3	Total I 3 3	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	BBB	1	Total C H O 28 6 16 6	4	1
4	BBB	1	Total C H O 14 3 8 3	2	0
4	CCC	1	Total C H O 14 3 8 3	2	0
4	DDD	1	Total C H O 14 3 8 3	2	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	239	Total O 240 240	0	1
5	BBB	266	Total O 266 266	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	CCC	222	Total 223	O 223	0	1
5	DDD	194	Total 194	O 194	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.

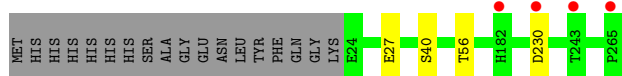
- Molecule 1: Beta-lactamase

Chain AAA: 



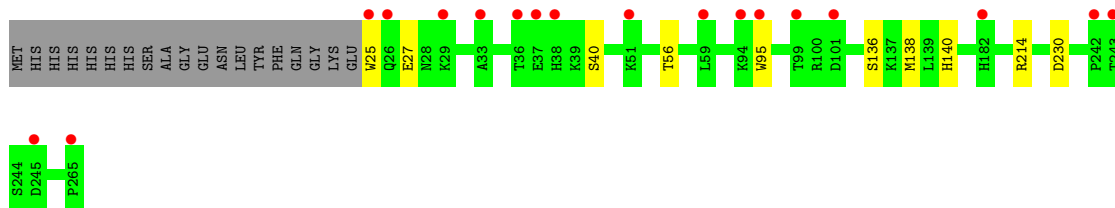
- Molecule 1: Beta-lactamase

Chain BBB: 



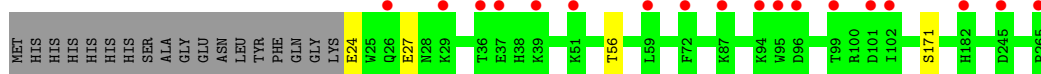
- Molecule 1: Beta-lactamase

Chain CCC: 



- Molecule 1: Beta-lactamase

Chain DDD: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.76Å 126.86Å 111.10Å 90.00° 98.35° 90.00°	Depositor
Resolution (Å)	19.74 – 1.67 19.78 – 1.67	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.74-1.67) 99.9 (19.78-1.67)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 1.67Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.166 , 0.197 0.165 , 0.195	Depositor DCC
$R_{free}$ test set	7450 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.6	Xtriage
Anisotropy	0.837	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16960	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.43% 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: IOD, KCX, 1BO, 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	0.81	1/2760 (0.0%)
1	BBB	0.89	0/2041	0.81	0/2758
1	CCC	0.85	0/2035	0.81	0/2751
1	DDD	0.83	0/2033	0.80	0/2748
All	All	0.86	0/8151	0.81	1/11017 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	128	ARG	NE-CZ-NH1	-6.19	117.20	120.30

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	1961	1948	11	0
1	BBB	2005	1964	1952	3	0
1	CCC	1998	1957	1944	9	0
1	DDD	1997	1955	1944	3	0
2	AAA	5	10	10	6	0
2	BBB	10	20	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	CCC	10	20	19	9	0
2	DDD	10	20	19	4	0
3	AAA	7	0	0	1	0
3	BBB	6	0	0	0	0
3	CCC	3	0	0	1	0
3	DDD	3	0	0	0	0
4	BBB	18	24	24	0	0
4	CCC	6	8	8	5	0
4	DDD	6	8	8	0	0
5	AAA	240	0	0	4	0
5	BBB	266	0	0	2	0
5	CCC	223	0	0	6	0
5	DDD	194	0	0	4	0
All	All	9013	7947	7896	38	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 (38) 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	5:BBB:584:HOH:O	1.76	0.83
1:BBB:230:ASP:OD1	5:BBB:501:HOH:O	1.98	0.81
1:AAA:137:LYS:HD3	3:AAA:306[A]:IOD:I	2.52	0.80
1:AAA:96:ASP:H	2:AAA:301:1BO:H13	1.50	0.75
1:CCC:25:TRP:N	5:CCC:402:HOH:O	2.23	0.71
1:CCC:138:MET:SD	5:CCC:598:HOH:O	2.47	0.71
2:AAA:301:1BO:H11	5:AAA:520:HOH:O	1.91	0.71
2:DDD:303:1BO:H12	5:DDD:468:HOH:O	1.94	0.66
1:CCC:230:ASP:OD1	5:CCC:401:HOH:O	2.13	0.66
2:DDD:301:1BO:C1	5:DDD:502:HOH:O	2.47	0.63
1:AAA:67:LEU:HD11	1:AAA:215:ILE:HD12	1.83	0.60
2:CCC:301:1BO:C1	5:CCC:503:HOH:O	2.51	0.58
2:DDD:301:1BO:H12	5:DDD:502:HOH:O	2.03	0.57
1:AAA:40:SER:HB2	5:AAA:484:HOH:O	2.05	0.56
2:CCC:301:1BO:H12	4:CCC:303:GOL:H11	1.88	0.55
1:CCC:136:SER:O	1:CCC:140[B]:HIS:HD2	1.94	0.49
1:AAA:230:ASP:OD1	5:AAA:401:HOH:O	2.20	0.49
2:CCC:301:1BO:H21	5:CCC:493:HOH:O	2.12	0.49
2:CCC:301:1BO:H32	4:CCC:303:GOL:C1	2.44	0.47
2:CCC:301:1BO:H12	4:CCC:303:GOL:C1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:95:TRP:HA	2:CCC:302:1BO:H11	1.97	0.46
1:AAA:96:ASP:N	2:AAA:301:1BO:H13	2.25	0.46
2:AAA:301:1BO:H41	5:AAA:605:HOH:O	2.17	0.45
1:CCC:27:GLU:HA	1:CCC:56:THR:O	2.17	0.45
1:CCC:214:ARG:HE	2:CCC:301:1BO:H22	1.82	0.44
1:CCC:40:SER:HB2	5:CCC:492:HOH:O	2.18	0.44
1:AAA:95:TRP:HA	2:AAA:301:1BO:H13	1.99	0.44
1:CCC:214:ARG:HH21	2:CCC:301:1BO:H31	1.82	0.44
1:DDD:171[A]:SER:OG	2:DDD:303:1BO:H31	2.18	0.43
1:AAA:65:ALA:HB1	1:AAA:163:ARG:HB3	2.00	0.43
2:CCC:301:1BO:H32	4:CCC:303:GOL:H11	2.00	0.43
1:AAA:27:GLU:HA	1:AAA:56:THR:O	2.18	0.43
1:AAA:24[A]:GLU:HG2	1:AAA:25:TRP:CD1	2.54	0.42
4:CCC:303:GOL:O3	3:CCC:304:IOD:I	3.06	0.42
1:DDD:24:GLU:N	5:DDD:408:HOH:O	2.52	0.42
1:AAA:96:ASP:H	2:AAA:301:1BO:C1	2.26	0.41
1:BBB:27:GLU:HA	1:BBB:56:THR:O	2.20	0.41
1:DDD:27:GLU:HA	1:DDD:56:THR:O	2.19	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	241/260 (93%)	235 (98%)	6 (2%)	0	100	100
1	BBB	242/260 (93%)	237 (98%)	5 (2%)	0	100	100
1	CCC	241/260 (93%)	236 (98%)	5 (2%)	0	100	100
1	DDD	241/260 (93%)	236 (98%)	5 (2%)	0	100	100
All	All	965/1040 (93%)	944 (98%)	21 (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%)	213 (100%)	0	100	100
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%)	850 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	BBB	73	1	7,11,12	0.55	0	4,12,14	0.26	0
1	KCX	DDD	73	1	7,11,12	0.57	0	4,12,14	0.95	0
1	KCX	AAA	73	1	7,11,12	0.53	0	4,12,14	0.46	0
1	KCX	CCC	73	1	7,11,12	0.67	0	4,12,14	0.59	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	BBB	73	1	-	0/7/10/12	-
1	KCX	DDD	73	1	-	0/7/10/12	-
1	KCX	AAA	73	1	-	0/7/10/12	-
1	KCX	CCC	73	1	-	0/7/10/12	-

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 31 ligands modelled in this entry, 19 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	GOL	BBB	402[A]	-	5,5,5	0.10	0	5,5,5	0.23	0
4	GOL	BBB	403	-	5,5,5	0.09	0	5,5,5	0.29	0
4	GOL	DDD	302	-	5,5,5	0.08	0	5,5,5	0.32	0
2	1BO	CCC	302	-	4,4,4	0.14	0	3,3,3	0.22	0
4	GOL	CCC	303	-	5,5,5	0.10	0	5,5,5	0.29	0
2	1BO	BBB	401	-	4,4,4	0.17	0	3,3,3	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	1BO	AAA	301	-	4,4,4	0.22	0	3,3,3	0.34	0
2	1BO	CCC	301	-	4,4,4	1.14	0	3,3,3	0.37	0
2	1BO	BBB	404	-	4,4,4	0.29	0	3,3,3	0.43	0
2	1BO	DDD	303	-	4,4,4	0.14	0	3,3,3	0.12	0
4	GOL	BBB	402[B]	-	5,5,5	0.13	0	5,5,5	0.48	0
2	1BO	DDD	301	-	4,4,4	0.82	0	3,3,3	0.55	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	GOL	BBB	402[A]	-	-	2/4/4/4	-
4	GOL	BBB	403	-	-	1/4/4/4	-
4	GOL	DDD	302	-	-	0/4/4/4	-
2	1BO	CCC	302	-	-	0/2/2/2	-
4	GOL	CCC	303	-	-	4/4/4/4	-
2	1BO	BBB	401	-	-	1/2/2/2	-
2	1BO	AAA	301	-	-	0/2/2/2	-
2	1BO	CCC	301	-	-	1/2/2/2	-
2	1BO	BBB	404	-	-	1/2/2/2	-
2	1BO	DDD	303	-	-	1/2/2/2	-
4	GOL	BBB	402[B]	-	-	1/4/4/4	-
2	1BO	DDD	301	-	-	1/2/2/2	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	BBB	402[A]	GOL	C1-C2-C3-O3
4	BBB	402[A]	GOL	O2-C2-C3-O3
4	CCC	303	GOL	C1-C2-C3-O3
4	BBB	403	GOL	C1-C2-C3-O3
4	CCC	303	GOL	O1-C1-C2-C3
2	BBB	404	1BO	C2-C3-C4-OH
4	CCC	303	GOL	O1-C1-C2-O2
4	CCC	303	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	DDD	303	1BO	C2-C3-C4-OH
2	CCC	301	1BO	C2-C3-C4-OH
2	DDD	301	1BO	C2-C3-C4-OH
2	BBB	401	1BO	C2-C3-C4-OH
4	BBB	402[B]	GOL	C1-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	CCC	302	1BO	1	0
4	CCC	303	GOL	5	0
2	AAA	301	1BO	6	0
2	CCC	301	1BO	8	0
2	DDD	303	1BO	2	0
2	DDD	301	1BO	2	0

## 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%)	0.39	5 (2%)	63	67	14, 21, 36, 56	2 (0%)
1	BBB	241/260 (92%)	0.45	4 (1%)	70	74	15, 22, 37, 51	2 (0%)
1	CCC	240/260 (92%)	0.50	18 (7%)	14	15	14, 22, 45, 59	1 (0%)
1	DDD	241/260 (92%)	0.65	18 (7%)	14	15	16, 25, 45, 57	2 (0%)
All	All	963/1040 (92%)	0.50	45 (4%)	31	33	14, 23, 43, 59	7 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	39	LYS	4.6
1	AAA	265	PRO	4.2
1	CCC	265	PRO	4.1
1	CCC	36	THR	3.8
1	BBB	182	HIS	3.6
1	DDD	36	THR	3.5
1	BBB	265	PRO	3.5
1	DDD	101	ASP	3.5
1	CCC	59	LEU	3.3
1	DDD	102	ILE	3.3
1	CCC	26	GLN	3.1
1	DDD	265	PRO	3.1
1	DDD	95	TRP	2.9
1	DDD	245	ASP	2.9
1	AAA	262	LYS	2.9
1	CCC	101	ASP	2.8
1	DDD	99	THR	2.8
1	CCC	94	LYS	2.8
1	DDD	26	GLN	2.7
1	CCC	245	ASP	2.6
1	CCC	25	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	AAA	243	THR	2.6
1	BBB	243	THR	2.6
1	CCC	29	LYS	2.5
1	DDD	39	LYS	2.5
1	AAA	72	PHE	2.5
1	DDD	94	LYS	2.4
1	CCC	51	LYS	2.4
1	CCC	33	ALA	2.3
1	CCC	182	HIS	2.3
1	DDD	72	PHE	2.3
1	DDD	29	LYS	2.3
1	BBB	230	ASP	2.2
1	CCC	242	PRO	2.2
1	CCC	99	THR	2.2
1	CCC	243	THR	2.2
1	DDD	96	ASP	2.2
1	DDD	59	LEU	2.1
1	DDD	182	HIS	2.1
1	DDD	51	LYS	2.1
1	CCC	38	HIS	2.1
1	CCC	37	GLU	2.0
1	DDD	87	LYS	2.0
1	DDD	37	GLU	2.0
1	CCC	95	TRP	2.0

## 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	0.93	0.11	13,17,20,20	1
1	KCX	DDD	73	12/13	0.93	0.12	17,21,24,25	1
1	KCX	CCC	73	12/13	0.94	0.11	14,18,20,22	1
1	KCX	BBB	73	12/13	0.94	0.12	14,16,19,20	1

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

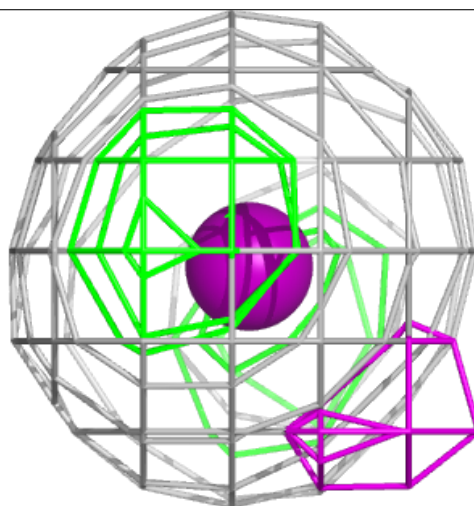
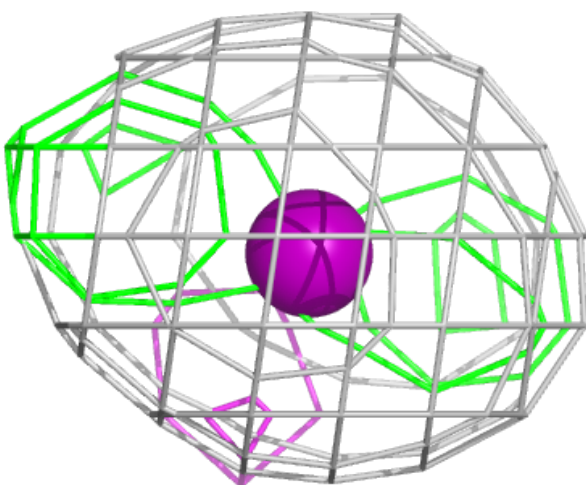
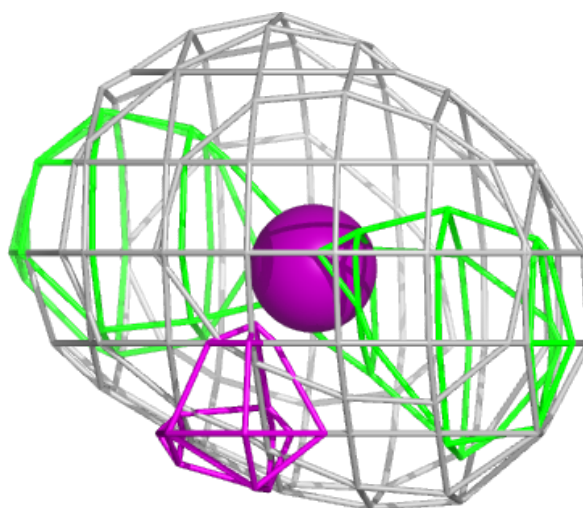
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	1BO	BBB	404	5/5	0.45	0.33	43,46,49,51	0
2	1BO	DDD	303	5/5	0.50	0.28	50,55,56,57	0
4	GOL	CCC	303	6/6	0.65	0.20	48,58,64,64	2
2	1BO	BBB	401	5/5	0.75	0.15	42,45,46,47	0
4	GOL	BBB	403	6/6	0.81	0.14	44,50,53,53	2
4	GOL	DDD	302	6/6	0.87	0.13	39,44,49,52	2
2	1BO	CCC	302	5/5	0.88	0.11	32,37,43,44	0
4	GOL	BBB	402[B]	6/6	0.89	0.15	22,23,24,24	14
4	GOL	BBB	402[A]	6/6	0.89	0.15	24,28,33,35	14
2	1BO	DDD	301	5/5	0.90	0.20	27,34,39,41	0
2	1BO	AAA	301	5/5	0.91	0.15	21,29,36,37	0
2	1BO	CCC	301	5/5	0.93	0.17	20,27,34,34	0
3	IOD	CCC	305	1/1	0.95	0.06	37,37,37,37	1
3	IOD	CCC	304	1/1	0.96	0.07	28,28,28,28	1
3	IOD	BBB	409	1/1	0.97	0.06	34,34,34,34	1
3	IOD	AAA	305	1/1	0.97	0.06	36,36,36,36	1
3	IOD	BBB	407	1/1	0.97	0.07	29,29,29,29	0
3	IOD	DDD	304	1/1	0.97	0.07	32,32,32,32	1
3	IOD	DDD	306	1/1	0.97	0.09	64,64,64,64	1
3	IOD	AAA	304	1/1	0.98	0.06	26,26,26,26	0
3	IOD	AAA	302	1/1	0.98	0.07	23,23,23,23	1
3	IOD	AAA	306[A]	1/1	0.98	0.07	46,46,46,46	1
3	IOD	DDD	305	1/1	0.98	0.06	39,39,39,39	1
3	IOD	AAA	306[B]	1/1	0.98	0.07	80,80,80,80	1
3	IOD	BBB	405	1/1	0.98	0.06	27,27,27,27	1
3	IOD	BBB	406[A]	1/1	0.98	0.11	17,17,17,17	1
3	IOD	BBB	406[B]	1/1	0.98	0.11	20,20,20,20	1
3	IOD	AAA	303[A]	1/1	0.98	0.09	15,15,15,15	1
3	IOD	AAA	303[B]	1/1	0.98	0.09	26,26,26,26	1
3	IOD	BBB	408	1/1	0.99	0.04	37,37,37,37	1
3	IOD	CCC	306	1/1	0.99	0.06	31,31,31,31	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.

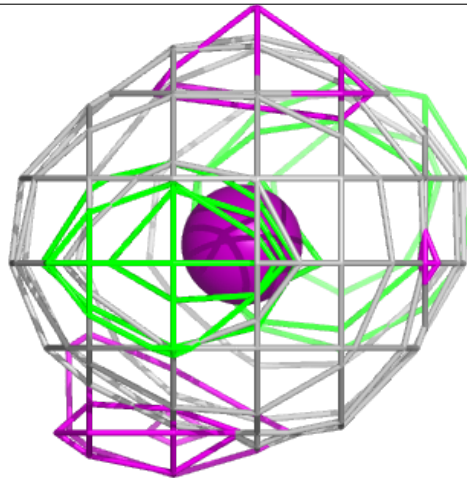
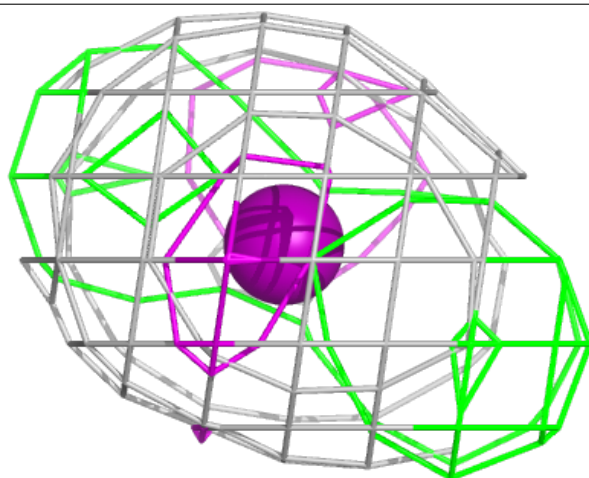
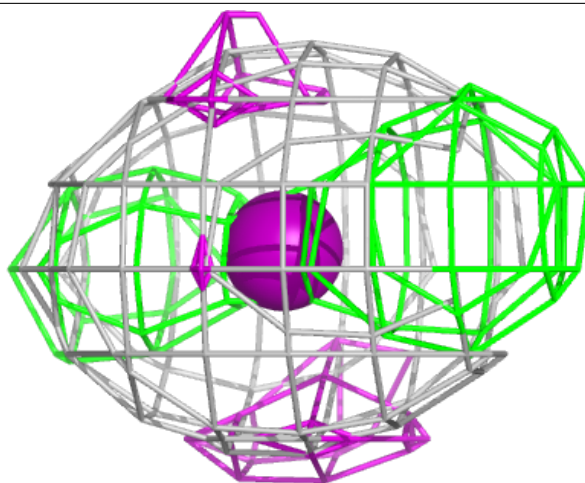
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and green (positive)



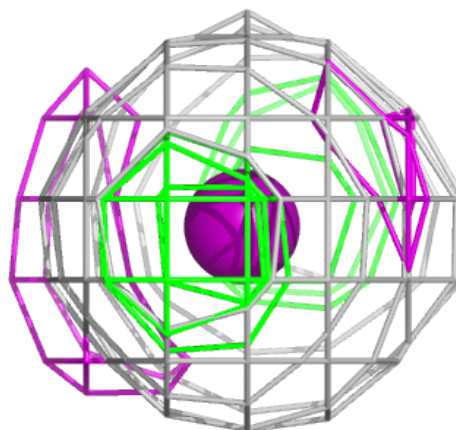
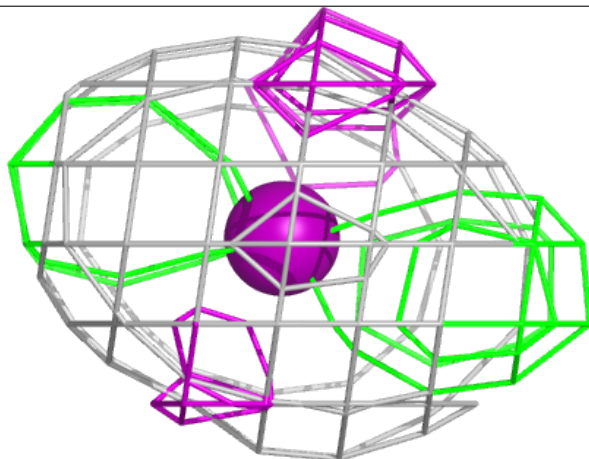
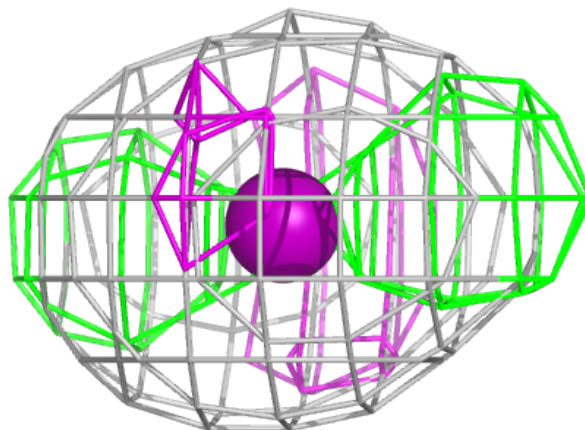
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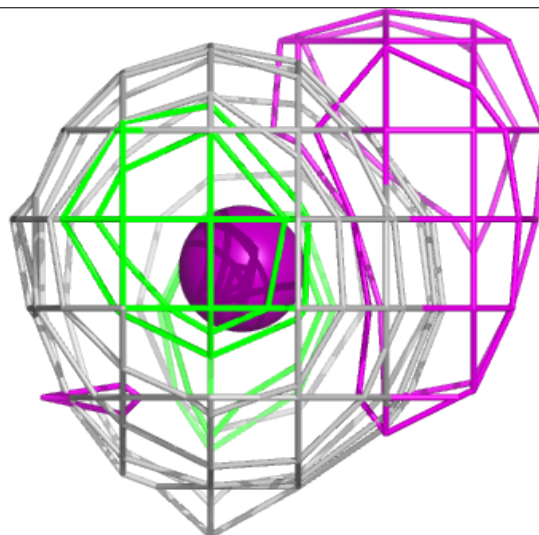
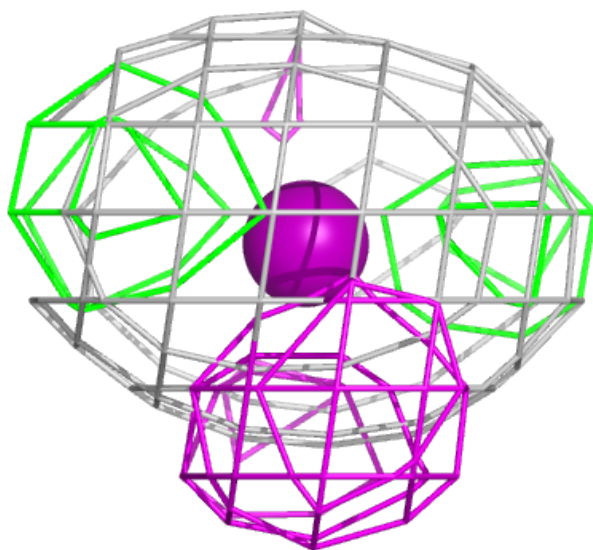
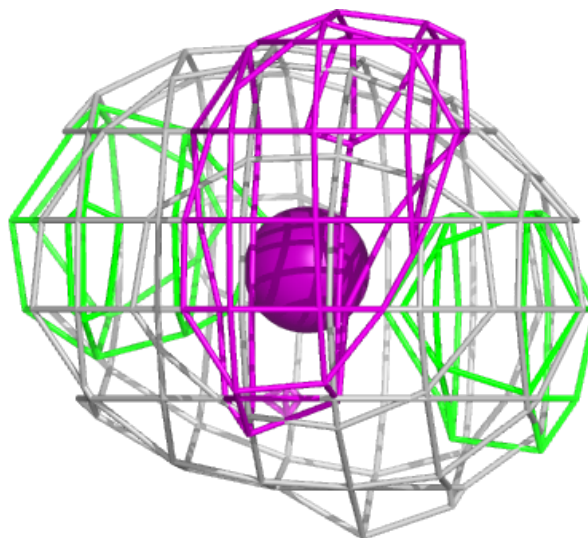
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and green (positive)





**Electron density around IOD AAA 305:**

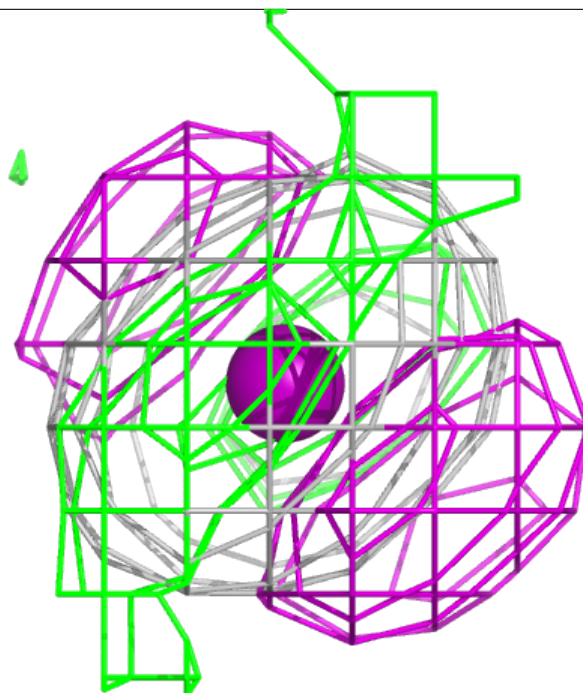
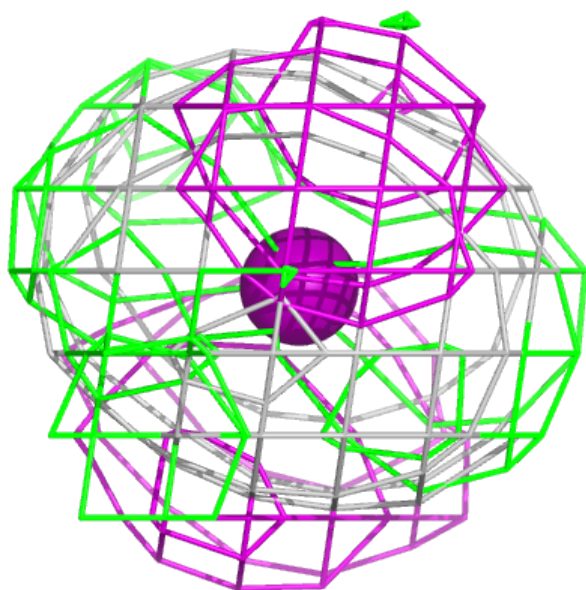
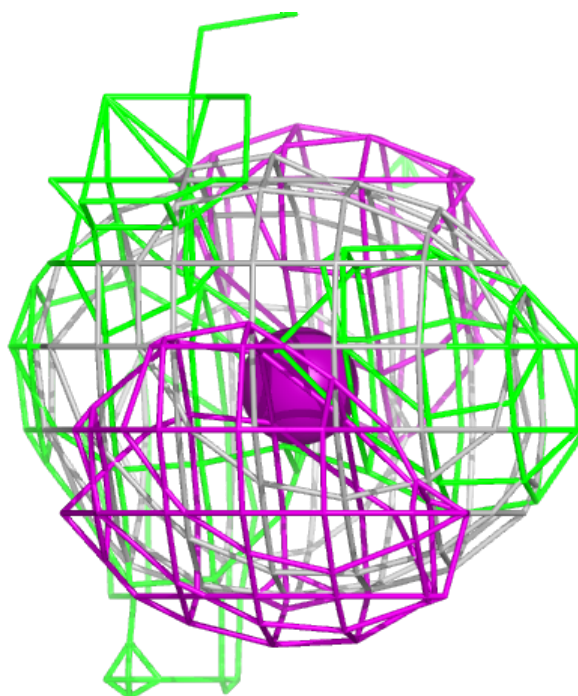
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and green (positive)





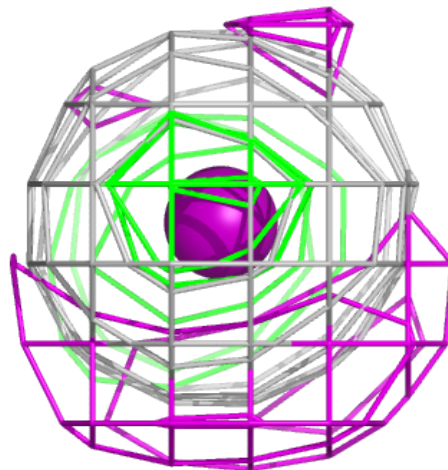
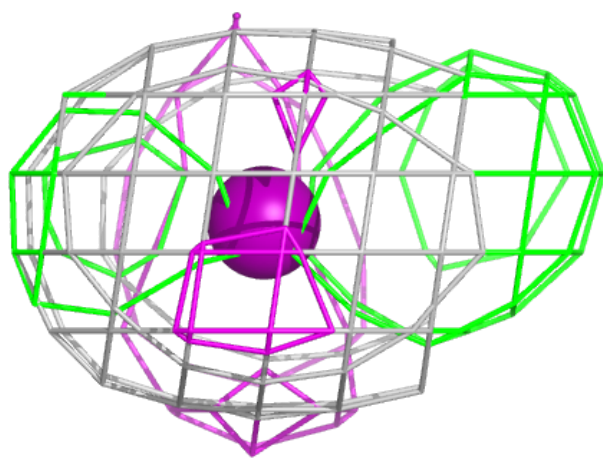
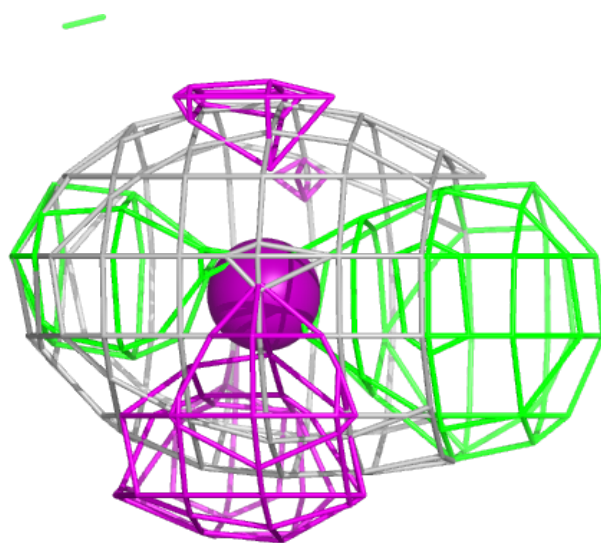
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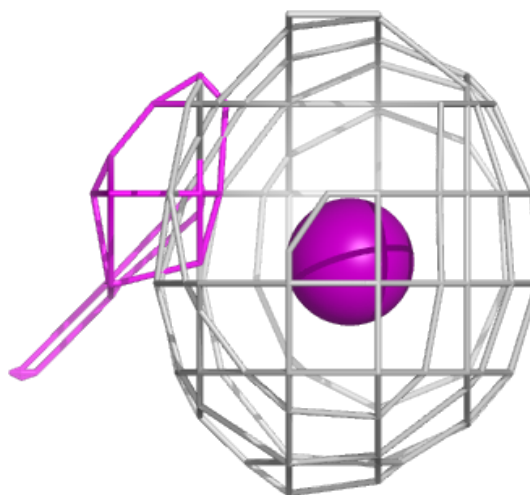
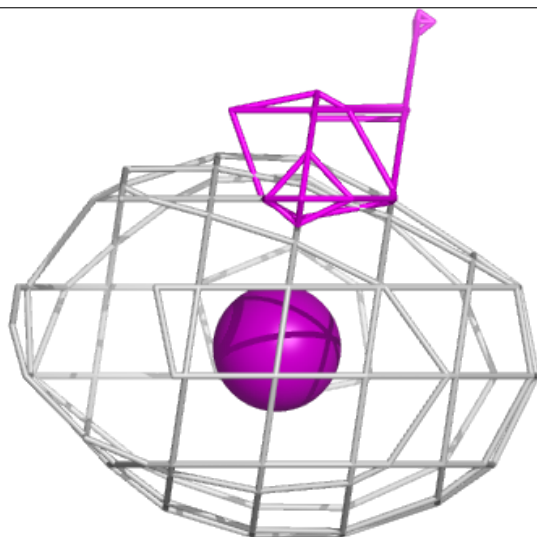
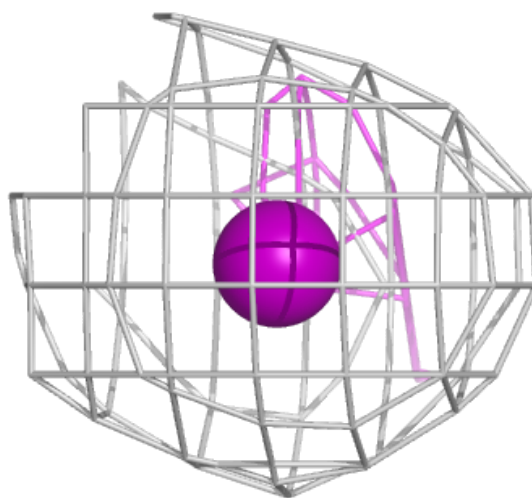
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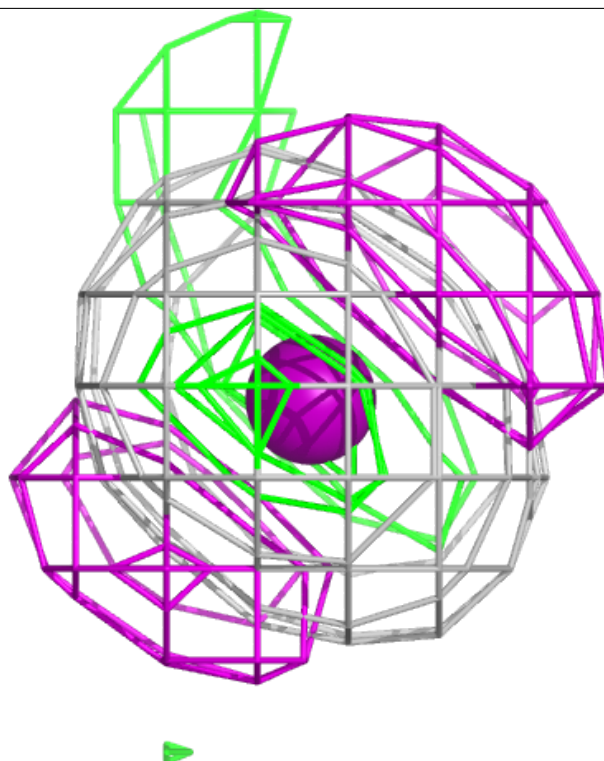
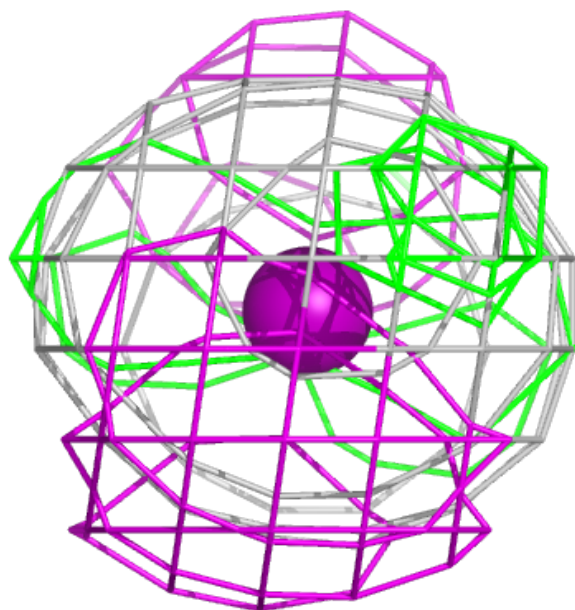
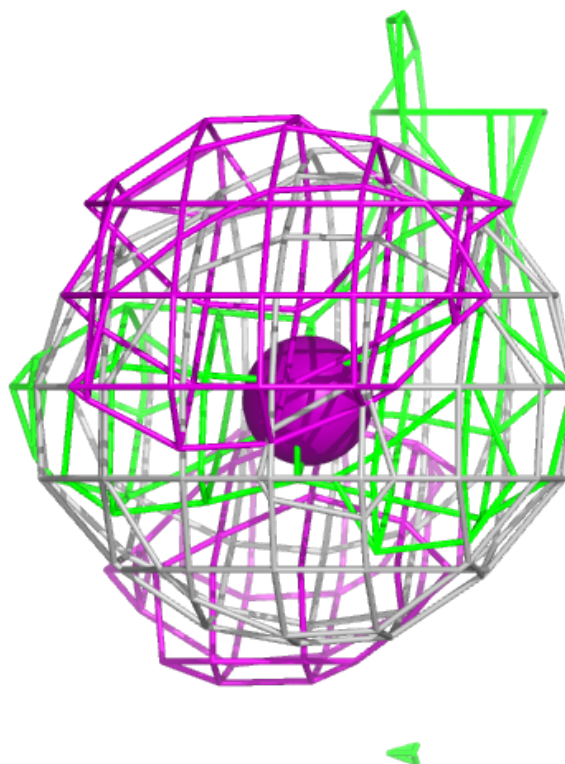
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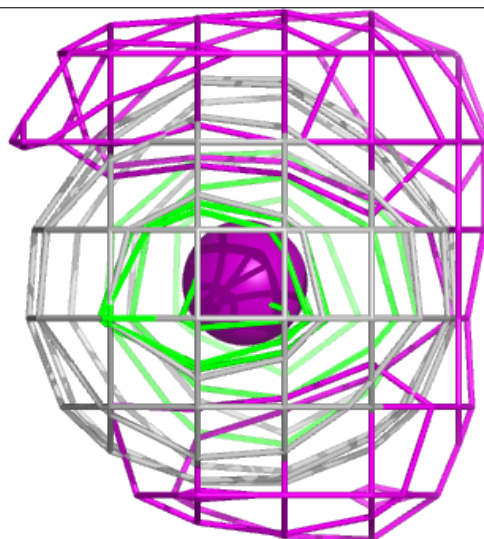
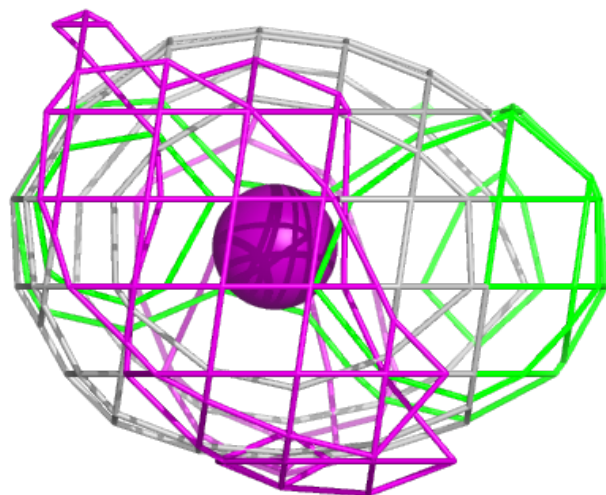
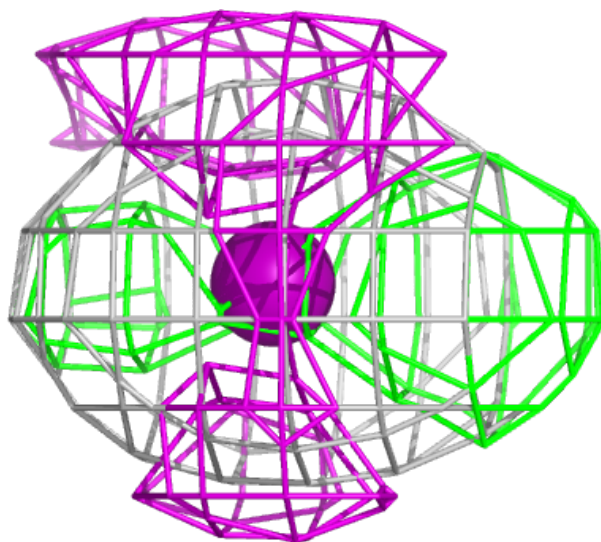
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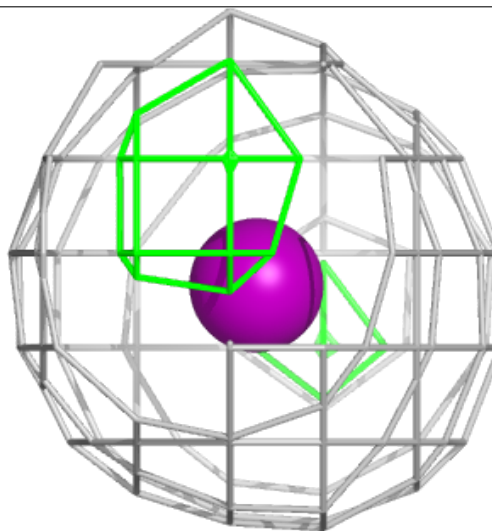
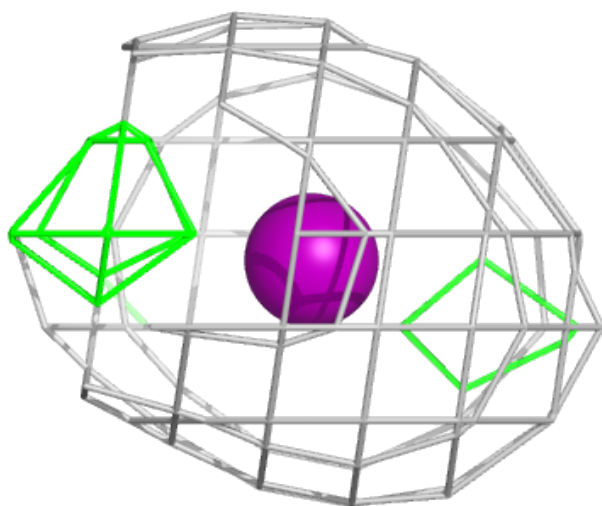
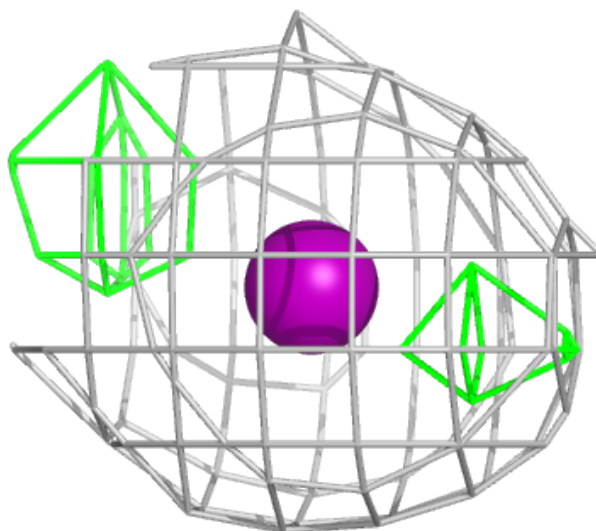
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and green (positive)





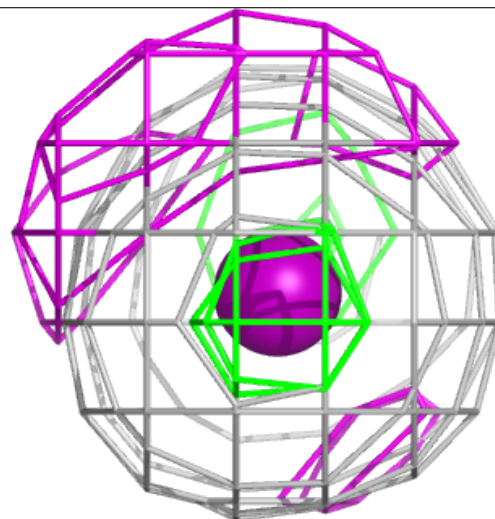
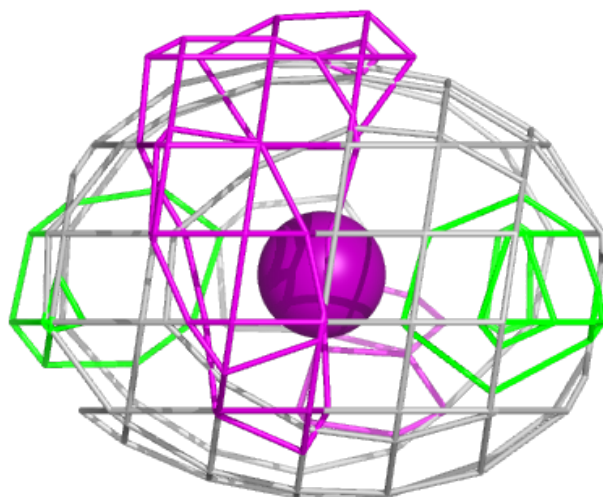
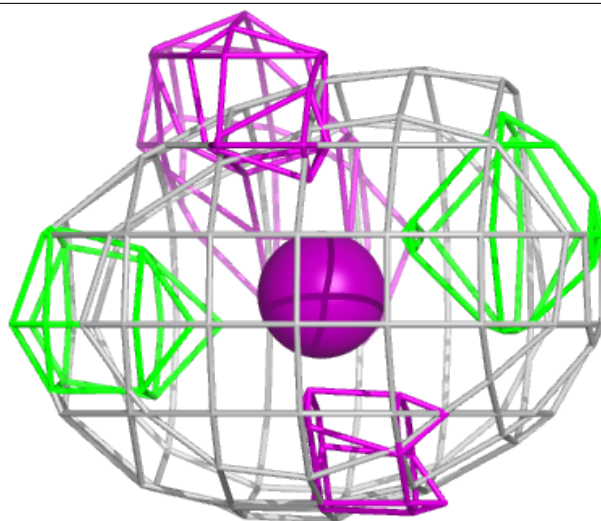
**Electron density around IOD AAA 306 (A):**

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



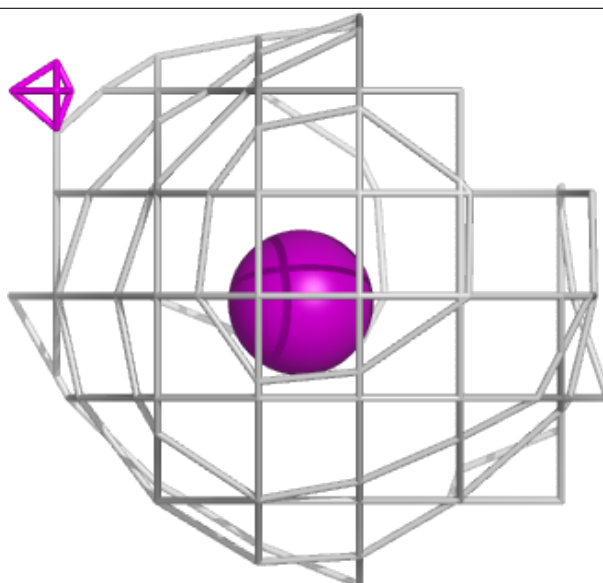
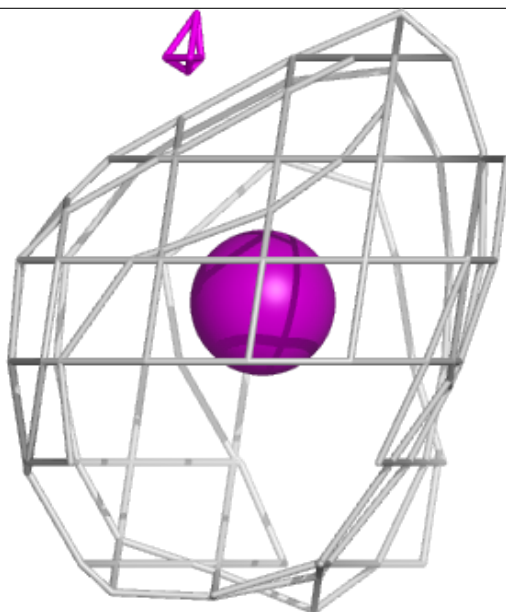
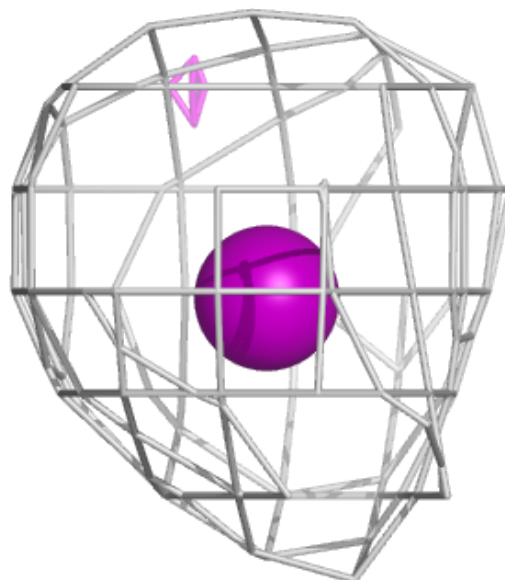
**Electron density around IOD DDD 305:**

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



**Electron density around IOD AAA 306 (B):**

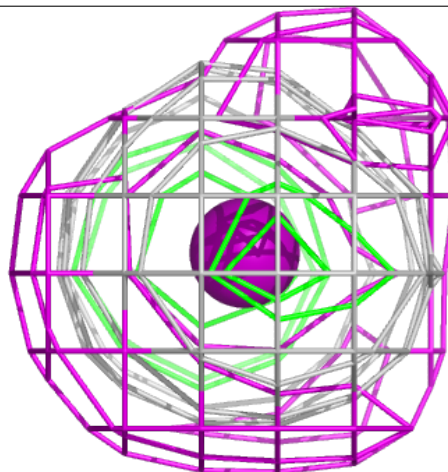
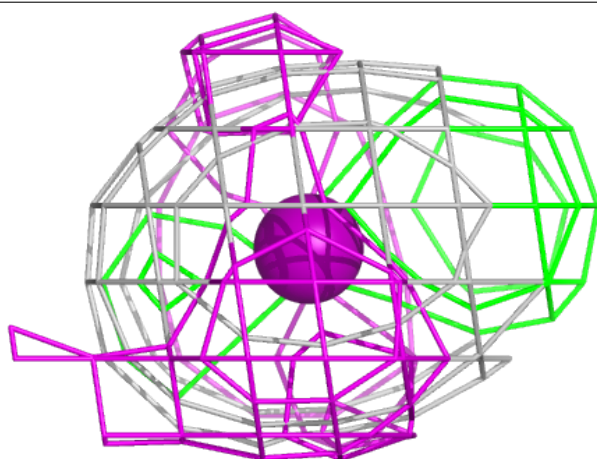
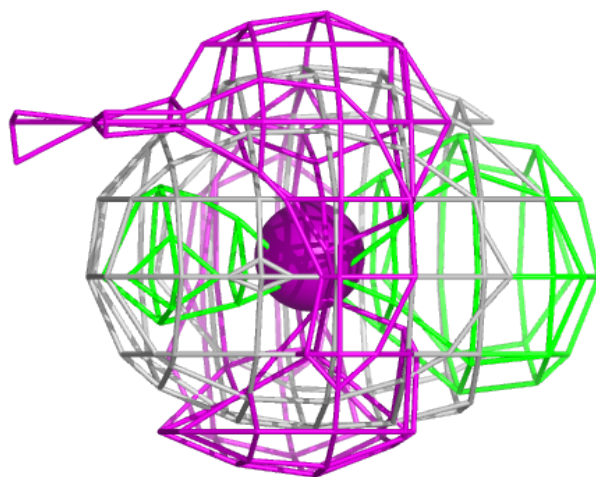
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





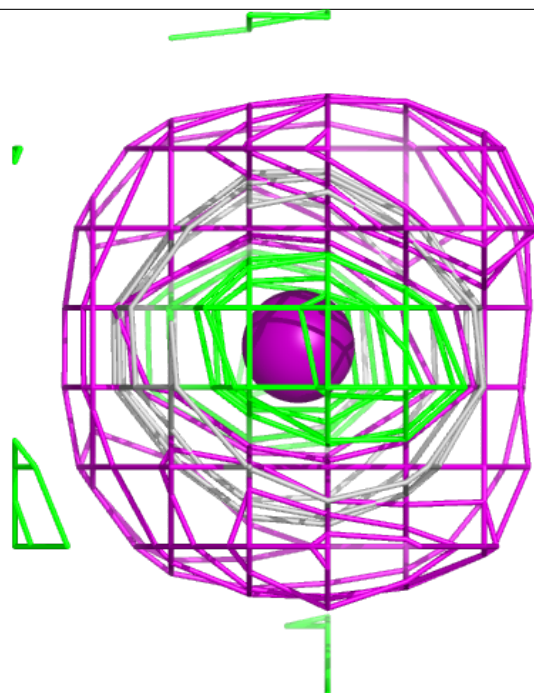
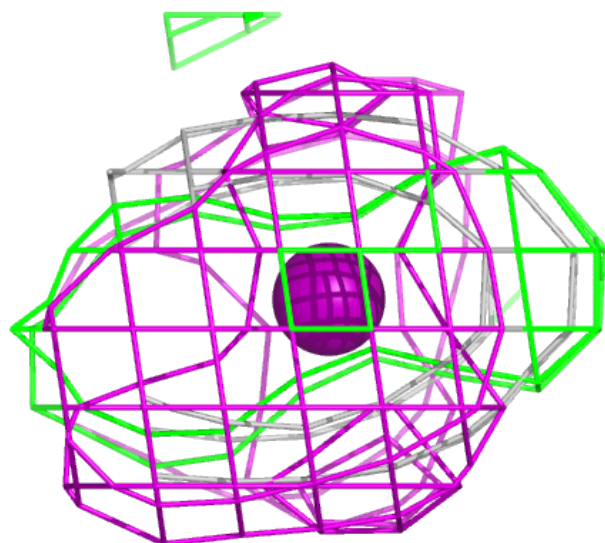
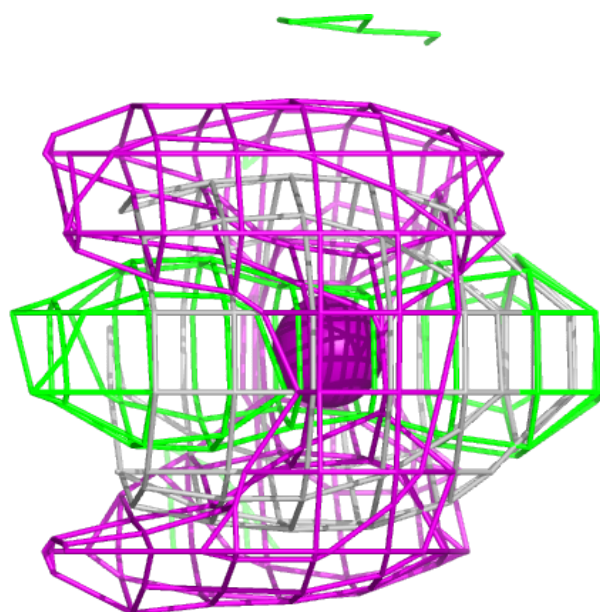
**Electron density around IOD BBB 405:**

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



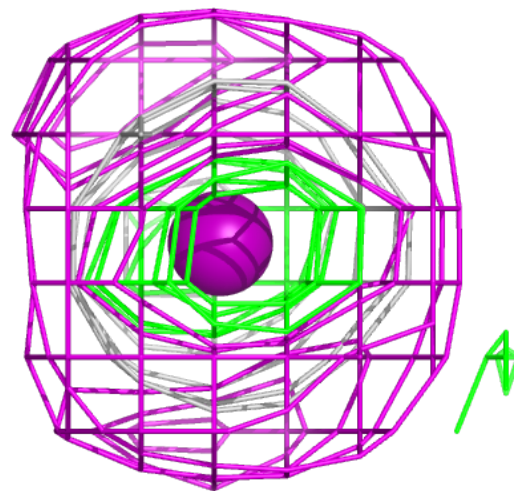
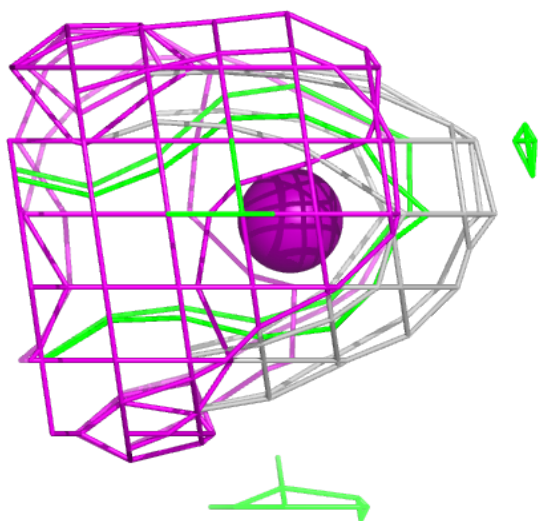
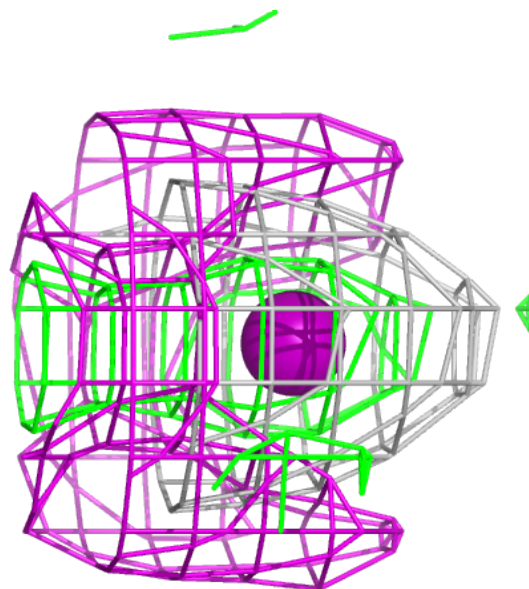
**Electron density around IOD BBB 406 (A):**

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



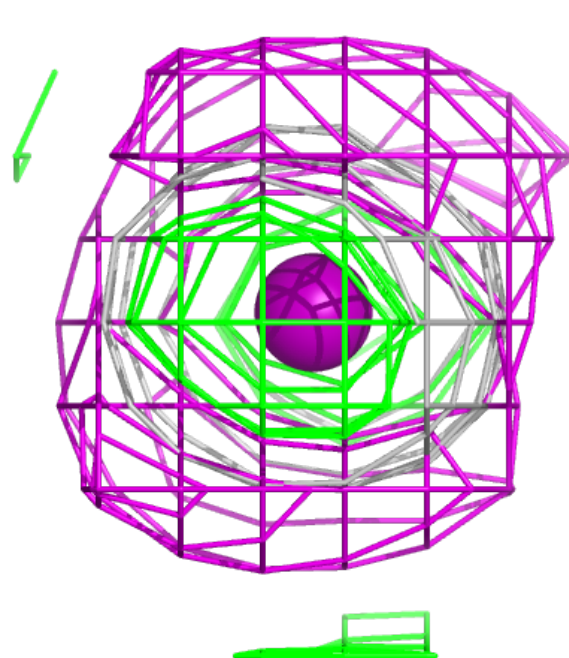
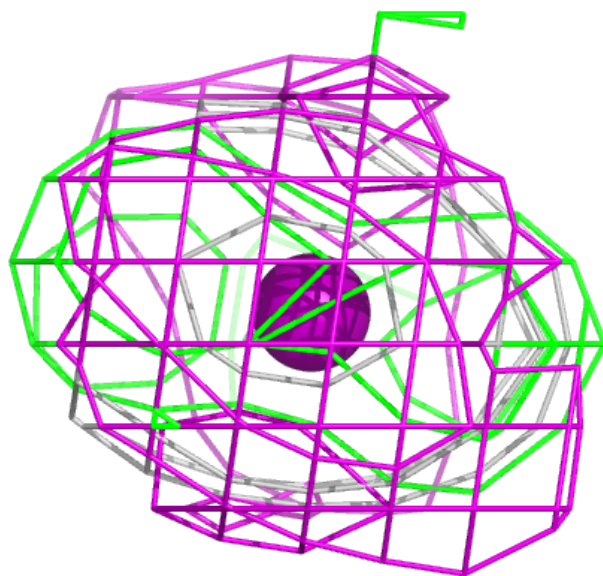
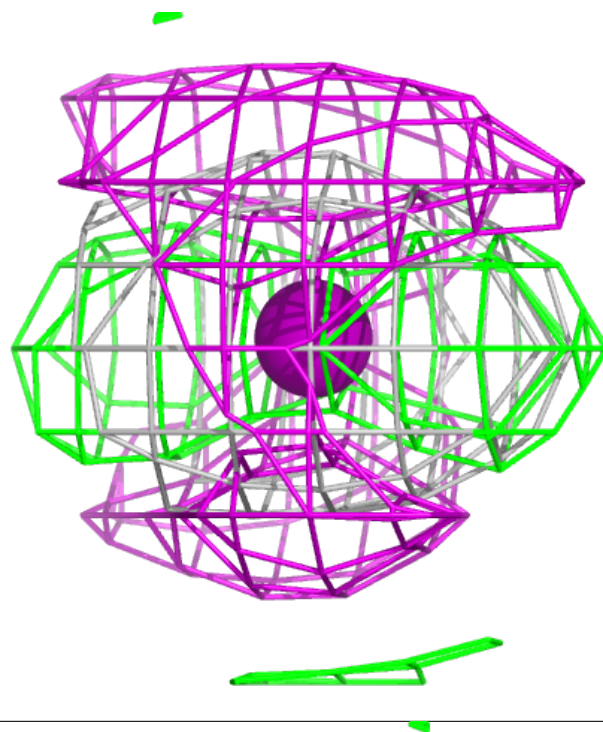
**Electron density around IOD BBB 406 (B):**

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



**Electron density around IOD AAA 303 (A):**

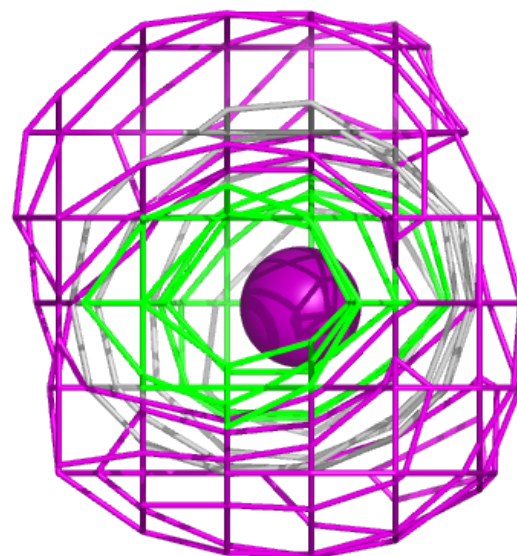
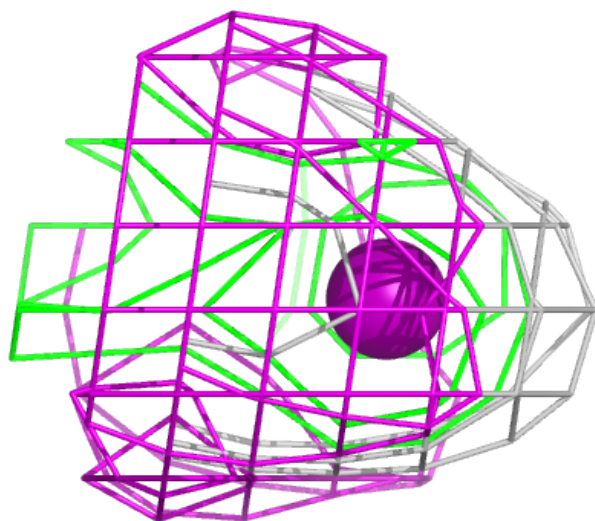
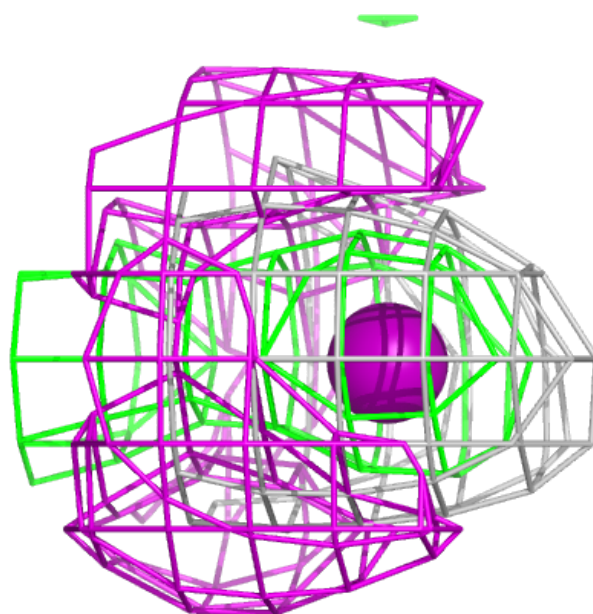
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





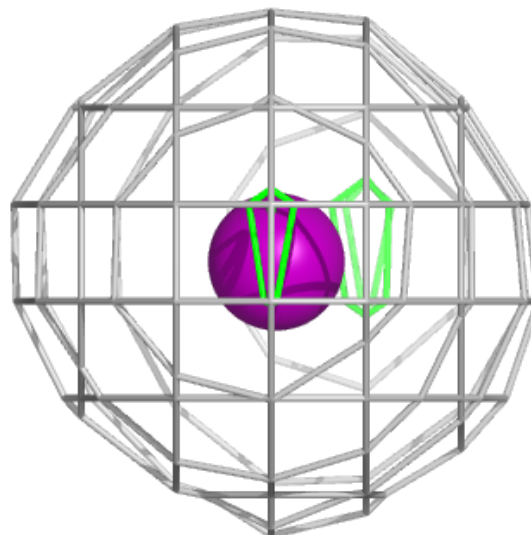
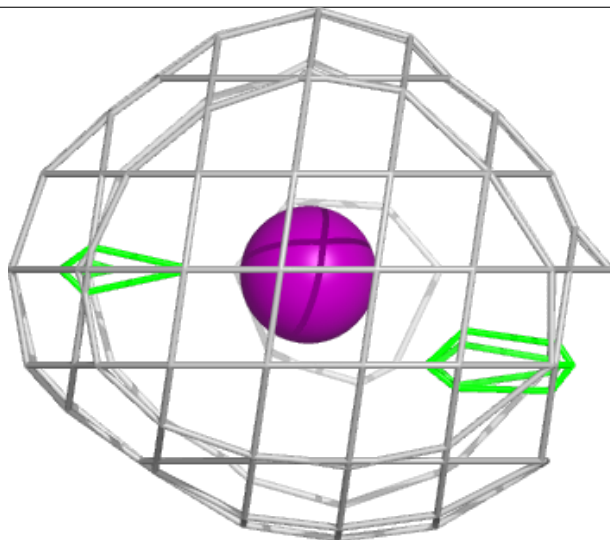
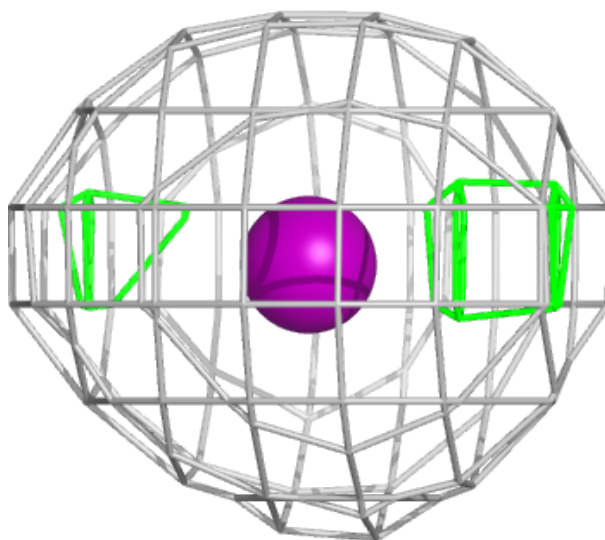
**Electron density around IOD AAA 303 (B):**

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



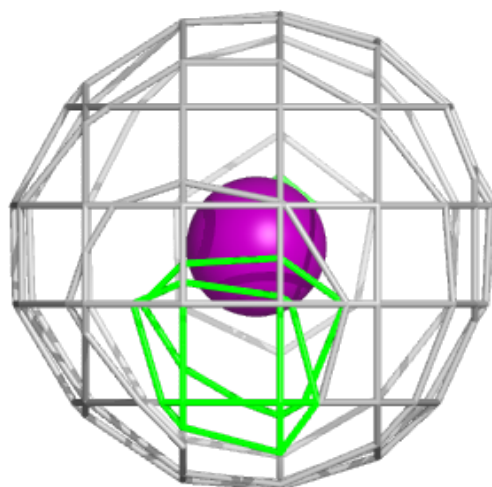
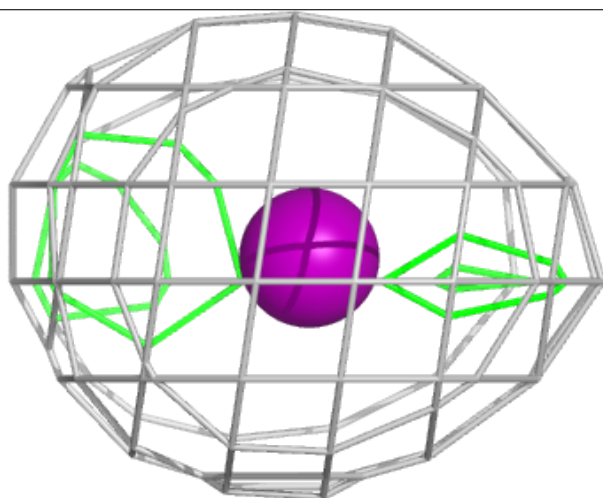
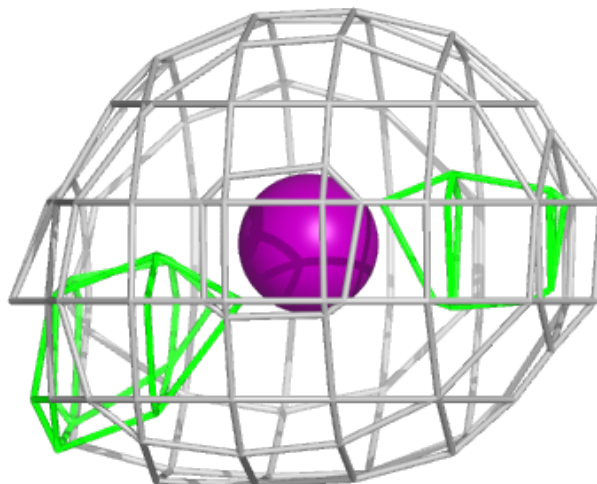
**Electron density around IOD BBB 408:**

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



**Electron density around IOD CCC 306:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.