



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 07:43 AM UTC

PDB ID : 8QNZ / pdb_00008qnz
Title : OXA-48 with carbamylated Lys73 in complex with hydrolysed Imipenem and bromide ion competing for binding with Arg250 at neutral pH
Authors : Zhou, Q.; He, Y.; Jin, Y.
Deposited on : 2023-09-27
Resolution : 1.53 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

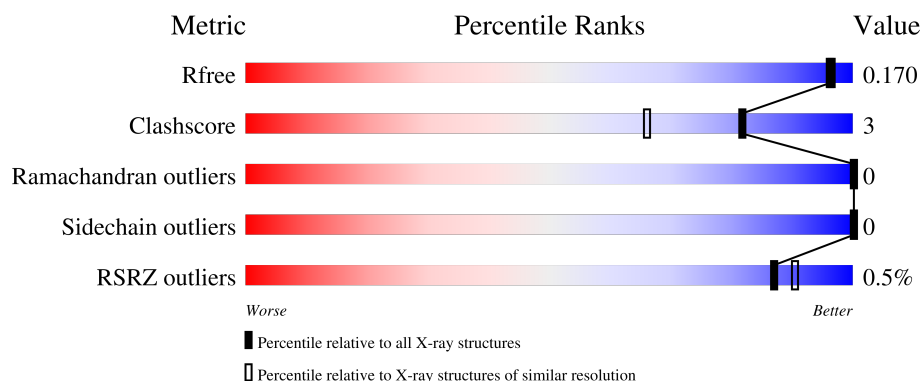
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.53 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}	180053	1003 (1.54-1.54)
Clashscore	190562	1025 (1.54-1.54)
Ramachandran outliers	187476	1007 (1.54-1.54)
Sidechain outliers	187428	1007 (1.54-1.54)
RSRZ outliers	180081	1002 (1.54-1.54)

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 ≥ 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	90% 7%
1	BBB	260	89% 5% 7%
1	CCC	260	90% 7%
1	DDD	260	% 87% 8% 5%

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	BR	AAA	302[B]	-	-	X	-
3	BR	BBB	303[B]	-	-	X	-
3	BR	CCC	301[B]	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17322 atoms, of which 8058 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	243	Total	C	H	N	O	S	50	5	0
			4011	1287	1984	356	376	8			
1	BBB	243	Total	C	H	N	O	S	51	6	0
			4022	1290	1989	357	378	8			
1	CCC	243	Total	C	H	N	O	S	48	5	0
			4038	1293	2003	362	373	7			
1	DDD	248	Total	C	H	N	O	S	52	4	0
			4087	1316	2021	363	379	8			

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

Continued on next page...

Continued from previous page...

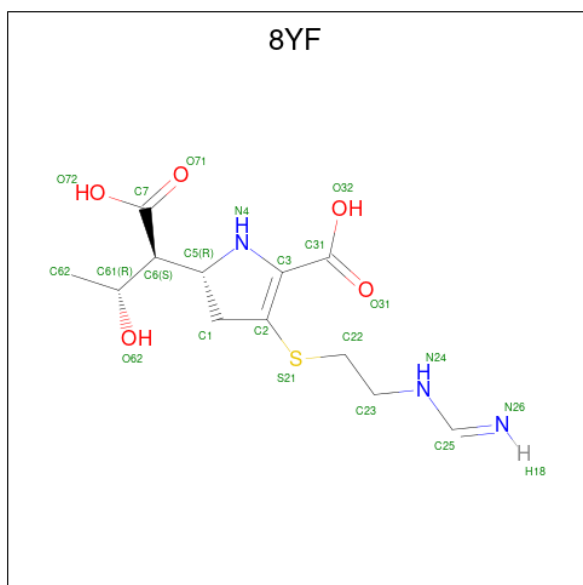
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	10	HIS	-	expression tag	UNP Q6XEC0
BBB	11	HIS	-	expression tag	UNP Q6XEC0
BBB	12	HIS	-	expression tag	UNP Q6XEC0
BBB	13	SER	-	expression tag	UNP Q6XEC0
BBB	14	ALA	-	expression tag	UNP Q6XEC0
BBB	15	GLY	-	expression tag	UNP Q6XEC0
BBB	16	GLU	-	expression 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

Continued on next page...

Continued from previous page...

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 (2R)-2-[(2S,3R)-1,3-bis(oxidanyl)-1-oxidanylidene-butan-2-yl]-4-(2-methanimidamidoethylsulfanyl)-2,3-dihydro-1H-pyrrole -5-carboxylic acid (CCD ID: 8YF) (formula: C₁₂H₁₉N₃O₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	AAA	1	Total 38	C 12	H 17	N 3	O 5	S 1	2	0
2	BBB	1	Total 38	C 12	H 17	N 3	O 5	S 1	2	0
2	DDD	1	Total 38	C 12	H 17	N 3	O 5	S 1	2	0

- Molecule 3 is BROMIDE ION (CCD ID: BR) (formula: Br) (labeled as "Ligand of Interest" by depositor).

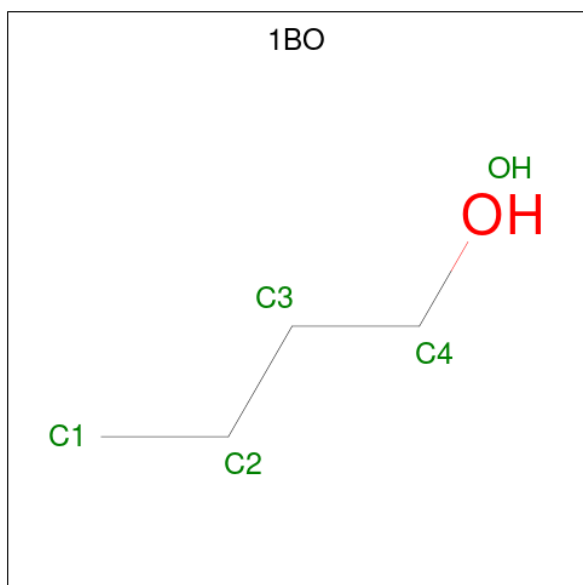
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	5	Total	Br	0	2
			7	7		
3	BBB	3	Total	Br	0	1
			4	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	CCC	2	Total	Br	0	1
			3	3		
3	DDD	1	Total	Br	0	0
			1	1		

- Molecule 4 is 1-BUTANOL (CCD ID: 1BO) (formula: $C_4H_{10}O$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	285	Total	O	0	0
			285	285		
5	BBB	280	Total	O	0	0
			280	280		
5	CCC	218	Total	O	0	0
			218	218		
5	DDD	236	Total	O	0	1
			237	237		

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:  90% 7%



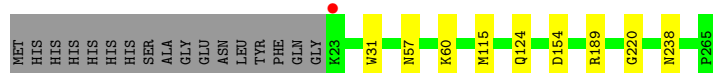
- Molecule 1: Beta-lactamase

Chain BBB:  89% 5% 7%



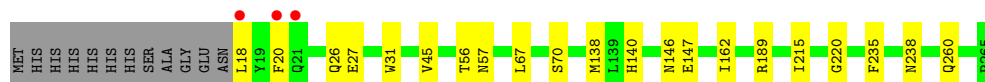
- Molecule 1: Beta-lactamase

Chain CCC:  90% 7%



- Molecule 1: Beta-lactamase

Chain DDD:  87% 8% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.31Å 105.97Å 124.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.42 – 1.53 62.42 – 1.53	Depositor EDS
% Data completeness (in resolution range)	98.1 (62.42-1.53) 98.1 (62.42-1.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 1.53Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.146 , 0.199 (Not available) , 0.170	Depositor DCC
R_{free} test set	7991 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	16.5	Xtriage
Anisotropy	0.627	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	17322	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.83 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0428e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: KCX, 1BO, 8YF, BR

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	1.01	2/2063 (0.1%)	1.15	2/2787 (0.1%)
1	BBB	0.99	0/2069	1.14	0/2795
1	CCC	1.03	0/2074	1.15	0/2800
1	DDD	0.99	0/2105	1.17	0/2844
All	All	1.01	2/8311 (0.0%)	1.15	2/11226 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	186	ARG	C-O	5.50	1.30	1.24
1	AAA	189	ARG	C-O	5.11	1.30	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	100	ARG	CA-C-N	7.45	130.27	120.28
1	AAA	100	ARG	C-N-CA	7.45	130.27	120.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2027	1984	1970	5	0
1	BBB	2033	1989	1974	8	0
1	CCC	2035	2003	1991	6	0
1	DDD	2066	2021	2007	15	0
2	AAA	21	17	0	1	0
2	BBB	21	17	0	1	0
2	DDD	21	17	0	2	0
3	AAA	7	0	0	5	0
3	BBB	4	0	0	2	0
3	CCC	3	0	0	3	0
3	DDD	1	0	0	0	0
4	BBB	5	10	10	1	0
5	AAA	285	0	0	4	0
5	BBB	280	0	0	2	0
5	CCC	218	0	0	3	0
5	DDD	237	0	0	3	0
All	All	9264	8058	7952	41	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 41 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)
3:AAA:302[B]:BR:BR	5:AAA:629:HOH:O	2.50	0.83
3:BBB:303[B]:BR:BR	5:BBB:620:HOH:O	2.54	0.80
1:DDD:20:PHE:H	1:DDD:26:GLN:HE22	1.30	0.79
3:AAA:302[B]:BR:BR	5:DDD:1080:HOH:O	2.59	0.76
2:AAA:301:8YF:C5	5:AAA:413:HOH:O	2.36	0.73

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	245/260 (94%)	239 (98%)	6 (2%)	0	100	100
1	BBB	246/260 (95%)	240 (98%)	6 (2%)	0	100	100
1	CCC	245/260 (94%)	240 (98%)	5 (2%)	0	100	100
1	DDD	249/260 (96%)	242 (97%)	7 (3%)	0	100	100
All	All	985/1040 (95%)	961 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	216/225 (96%)	216 (100%)	0	100	100
1	BBB	217/225 (96%)	217 (100%)	0	100	100
1	CCC	216/225 (96%)	216 (100%)	0	100	100
1	DDD	219/225 (97%)	219 (100%)	0	100	100
All	All	868/900 (96%)	868 (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 ⓘ

There are no RNA molecules in this entry.

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

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	AAA	73	1	10,11,12	0.40	0	6,12,14	0.85	0
1	KCX	CCC	73	1	10,11,12	0.47	0	6,12,14	0.36	0
1	KCX	BBB	73	1	10,11,12	0.56	0	6,12,14	0.53	0
1	KCX	DDD	73	1	10,11,12	0.55	0	6,12,14	0.34	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	AAA	73	1	-	0/9/10/12	-
1	KCX	CCC	73	1	-	1/9/10/12	-
1	KCX	BBB	73	1	-	0/9/10/12	-
1	KCX	DDD	73	1	-	0/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	CCC	73	KCX	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 15 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	8YF	BBB	301	-	18,21,21	0.86	1 (5%)	13,28,28	1.93	2 (15%)
2	8YF	AAA	301	-	18,21,21	1.03	1 (5%)	13,28,28	1.48	2 (15%)
4	1BO	BBB	302	-	4,4,4	0.21	0	3,3,3	0.41	0
2	8YF	DDD	801	-	18,21,21	1.03	2 (11%)	13,28,28	1.57	2 (15%)

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	8YF	BBB	301	-	-	5/22/34/34	0/1/1/1
2	8YF	AAA	301	-	-	6/22/34/34	0/1/1/1
4	1BO	BBB	302	-	-	1/2/2/2	-
2	8YF	DDD	801	-	-	4/22/34/34	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	DDD	801	8YF	O32-C31	-2.57	1.23	1.30
2	AAA	301	8YF	O32-C31	-2.44	1.23	1.30
2	BBB	301	8YF	O32-C31	-2.26	1.24	1.30
2	DDD	801	8YF	O71-C7	2.05	1.28	1.22

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	301	8YF	C31-C3-N4	5.34	127.02	120.41
2	DDD	801	8YF	C31-C3-N4	3.68	124.97	120.41
2	AAA	301	8YF	C1-C5-C6	3.54	119.99	113.78
2	BBB	301	8YF	O71-C7-C6	-2.61	116.17	122.84
2	AAA	301	8YF	O31-C31-C3	-2.27	116.24	120.20

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	301	8YF	C23-C22-S21-C2
2	AAA	301	8YF	N26-C25-N24-C23
2	BBB	301	8YF	C7-C6-C61-C62
2	BBB	301	8YF	C7-C6-C61-O62
2	BBB	301	8YF	S21-C22-C23-N24

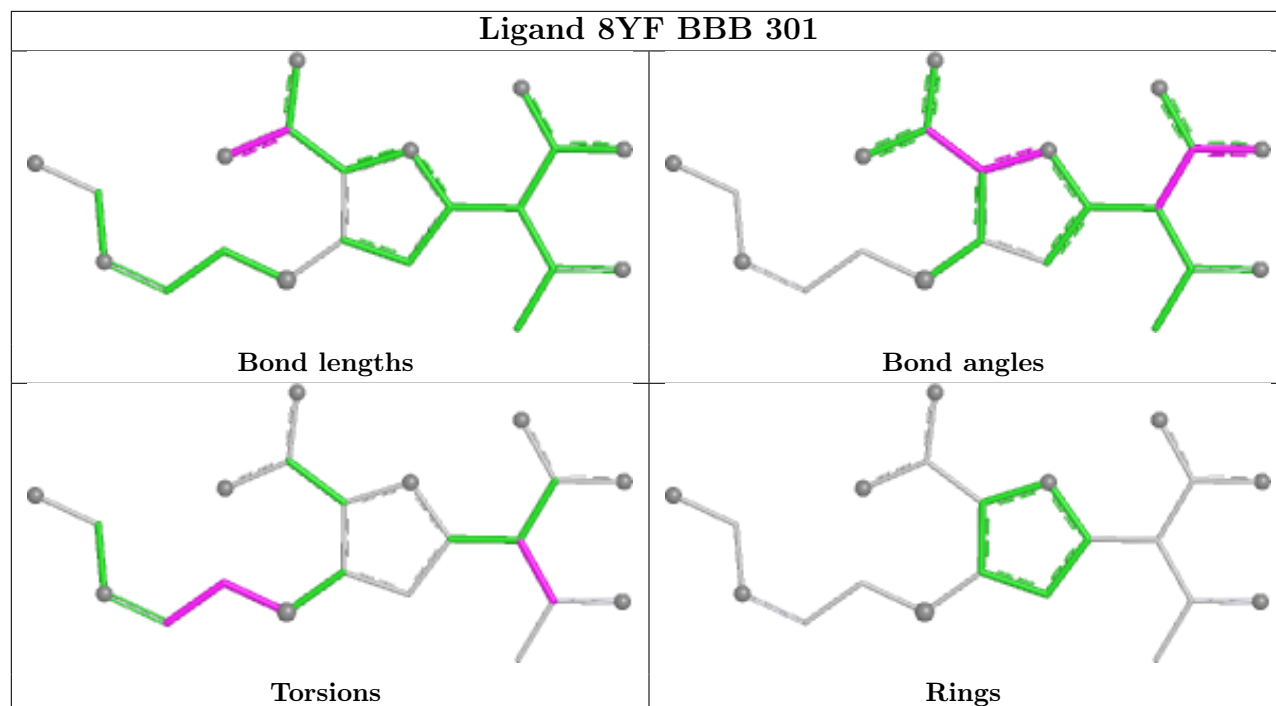
There are no ring outliers.

4 monomers are involved in 5 short contacts:

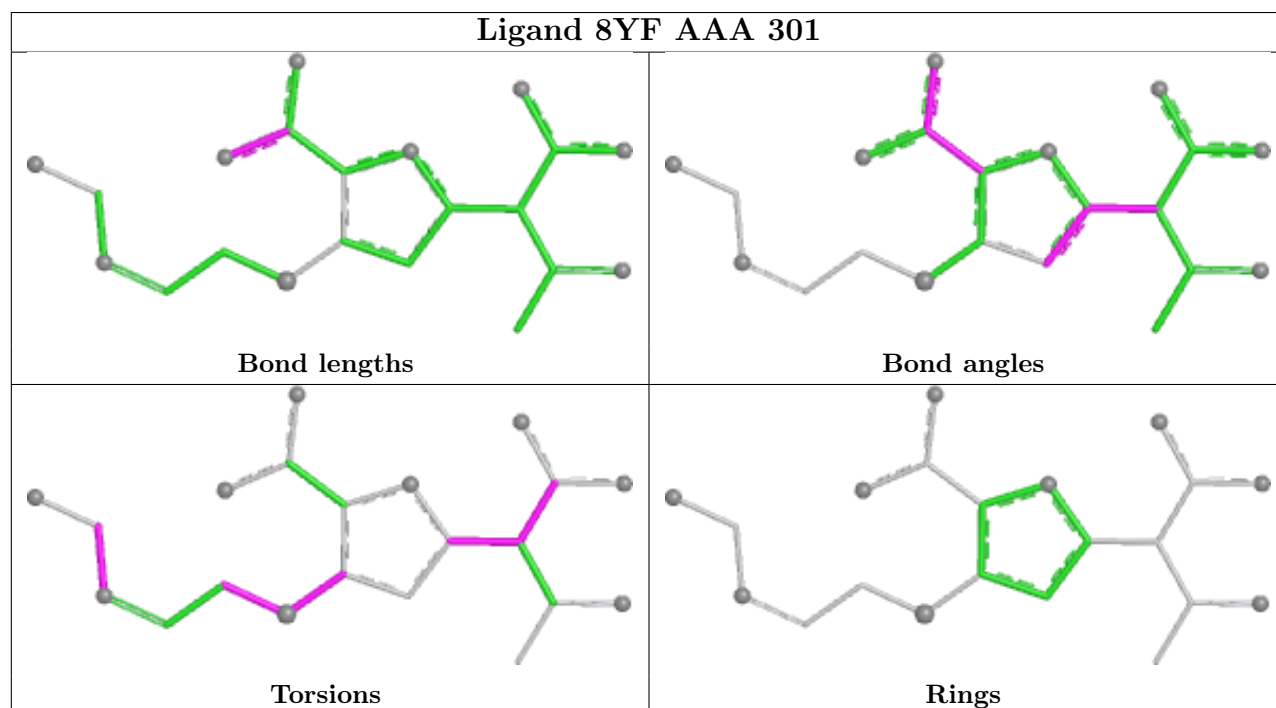
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	301	8YF	1	0
2	AAA	301	8YF	1	0
4	BBB	302	1BO	1	0
2	DDD	801	8YF	2	0

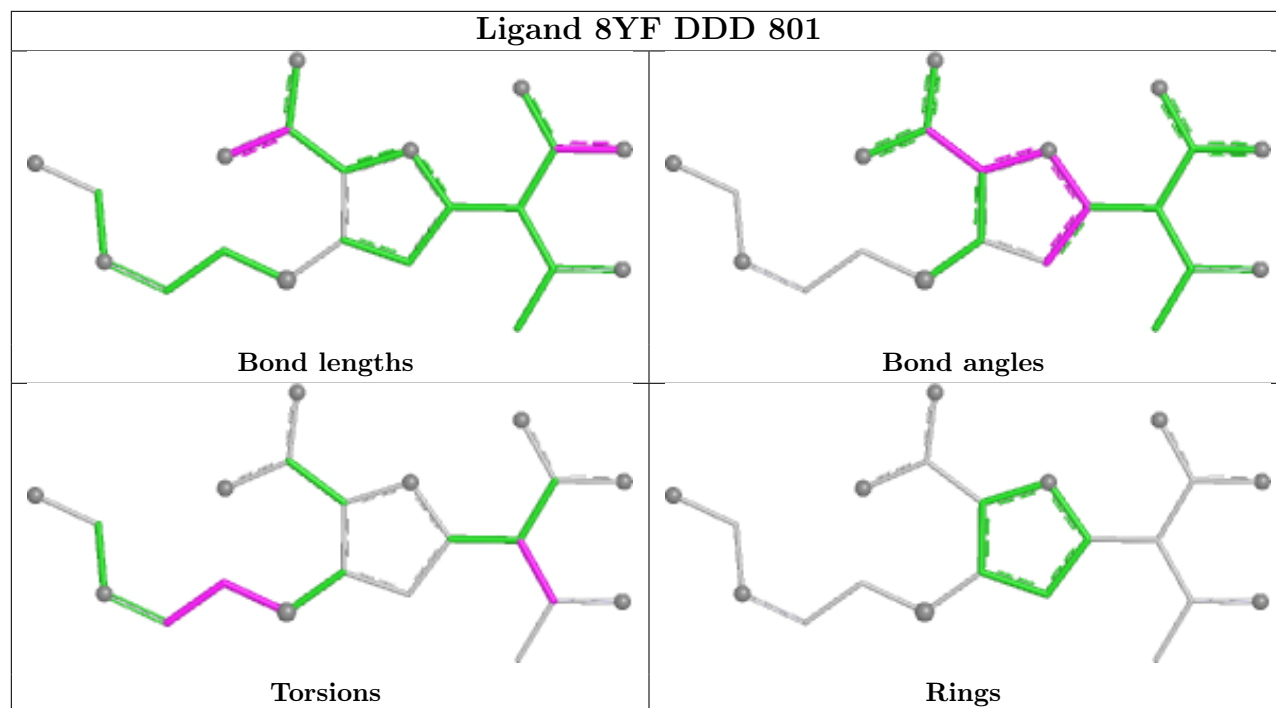
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 8YF BBB 301



Ligand 8YF AAA 301





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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	242/260 (93%)	-0.78	0 100 100	7, 19, 32, 50	6 (2%)
1	BBB	242/260 (93%)	-0.79	1 (0%) 88 92	6, 18, 32, 51	7 (2%)
1	CCC	242/260 (93%)	-0.65	1 (0%) 88 92	8, 21, 38, 58	8 (3%)
1	DDD	247/260 (95%)	-0.61	3 (1%) 76 82	7, 20, 37, 58	8 (3%)
All	All	973/1040 (93%)	-0.71	5 (0%) 87 90	6, 19, 36, 58	29 (2%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	20	PHE	6.5
1	CCC	23	LYS	5.8
1	DDD	18	LEU	3.3
1	BBB	23	LYS	2.4
1	DDD	21	GLN	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	KCX	AAA	73	12/13	0.99	0.03	12,14,18,22	1
1	KCX	BBB	73	12/13	0.99	0.04	10,14,17,21	1
1	KCX	CCC	73	12/13	0.99	0.04	14,16,23,25	1
1	KCX	DDD	73	12/13	0.99	0.04	14,19,23,24	1

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

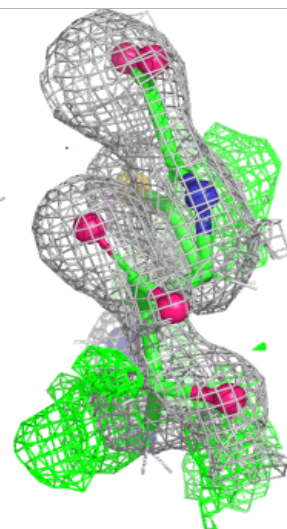
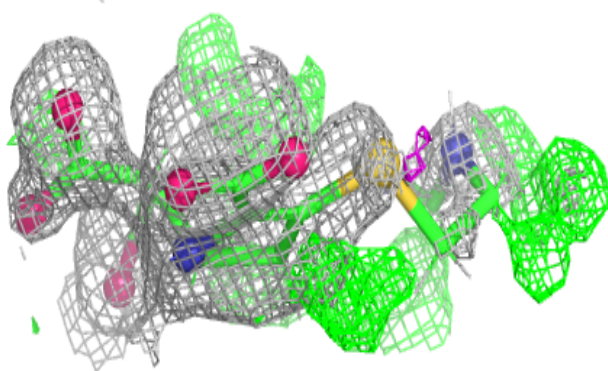
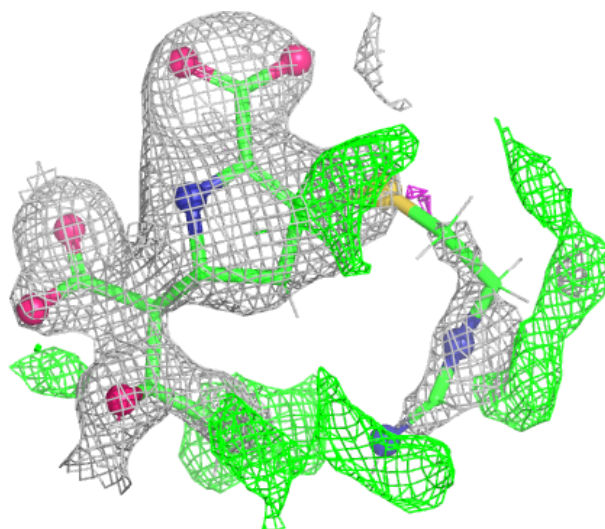
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	8YF	AAA	301	21/21	0.86	0.17	21,38,42,47	37
2	8YF	BBB	301	21/21	0.86	0.21	16,37,45,47	36
2	8YF	DDD	801	21/21	0.86	0.18	21,36,41,43	37
4	1BO	BBB	302	5/5	0.88	0.12	33,41,49,49	0
3	BR	AAA	305	1/1	0.98	0.06	40,40,40,40	1
3	BR	AAA	303[A]	1/1	0.99	0.04	28,28,28,28	1
3	BR	AAA	306	1/1	0.99	0.07	33,33,33,33	1
3	BR	BBB	304	1/1	0.99	0.04	33,33,33,33	1
3	BR	CCC	301[A]	1/1	0.99	0.07	24,24,24,24	1
3	BR	CCC	301[B]	1/1	0.99	0.07	32,32,32,32	1
3	BR	DDD	802	1/1	0.99	0.04	41,41,41,41	1
3	BR	AAA	303[B]	1/1	0.99	0.04	39,39,39,39	1
3	BR	AAA	304	1/1	1.00	0.02	31,31,31,31	1
3	BR	BBB	305	1/1	1.00	0.04	34,34,34,34	1
3	BR	AAA	302[A]	1/1	1.00	0.01	17,17,17,17	1
3	BR	AAA	302[B]	1/1	1.00	0.01	23,23,23,23	1
3	BR	CCC	302	1/1	1.00	0.04	38,38,38,38	0
3	BR	BBB	303[A]	1/1	1.00	0.02	15,15,15,15	1
3	BR	BBB	303[B]	1/1	1.00	0.02	12,12,12,12	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.

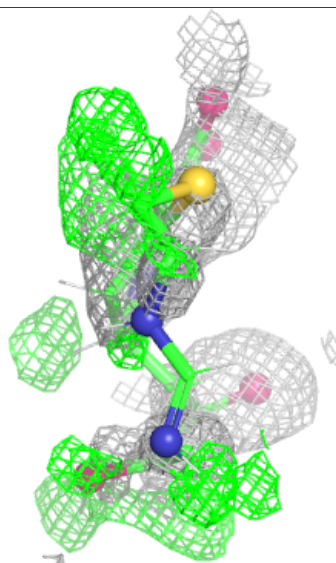
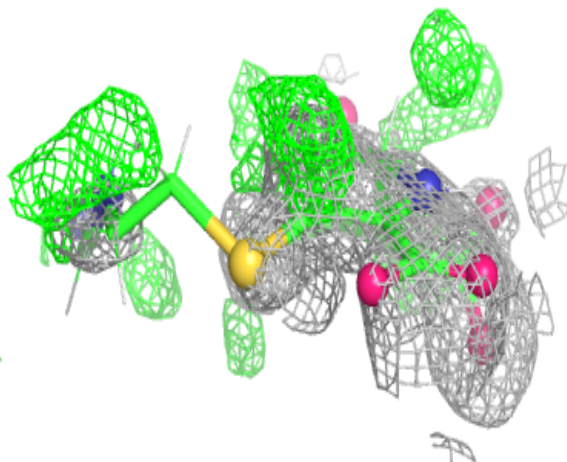
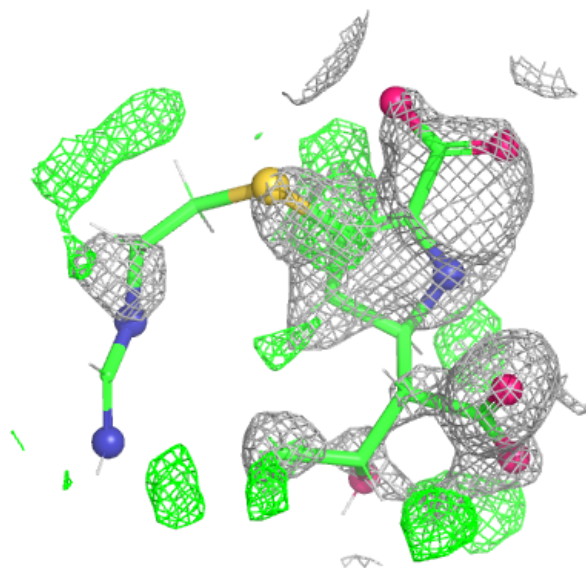
Electron density around 8YF AAA 301:

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



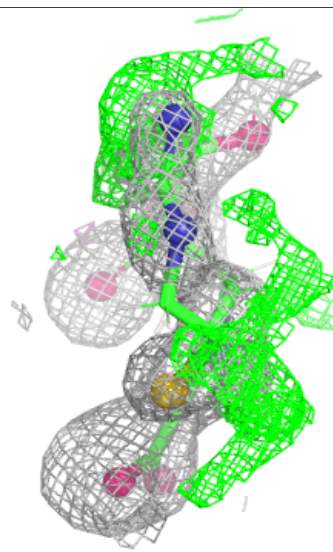
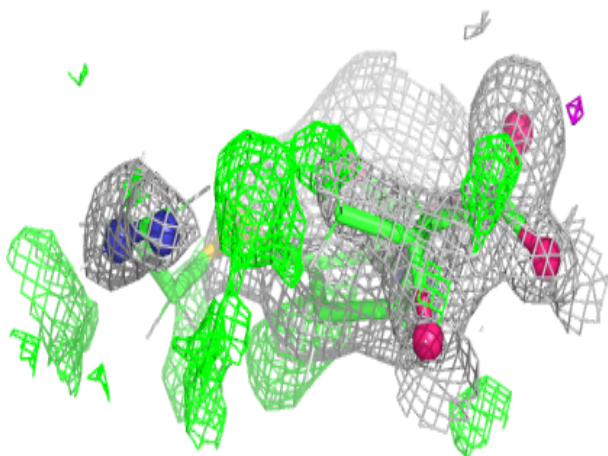
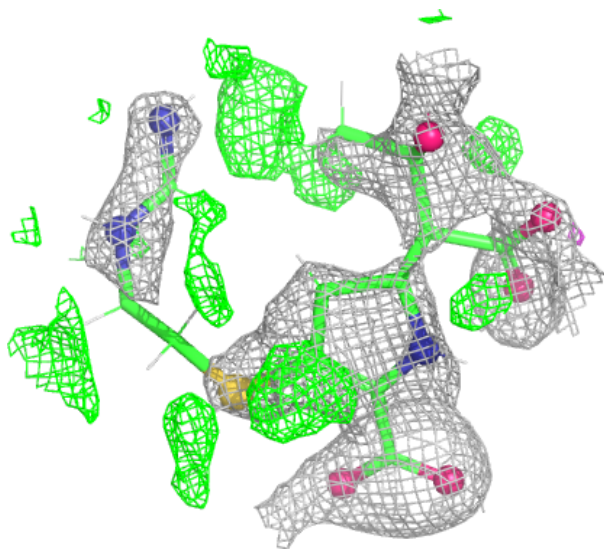
Electron density around 8YF BBB 301:

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



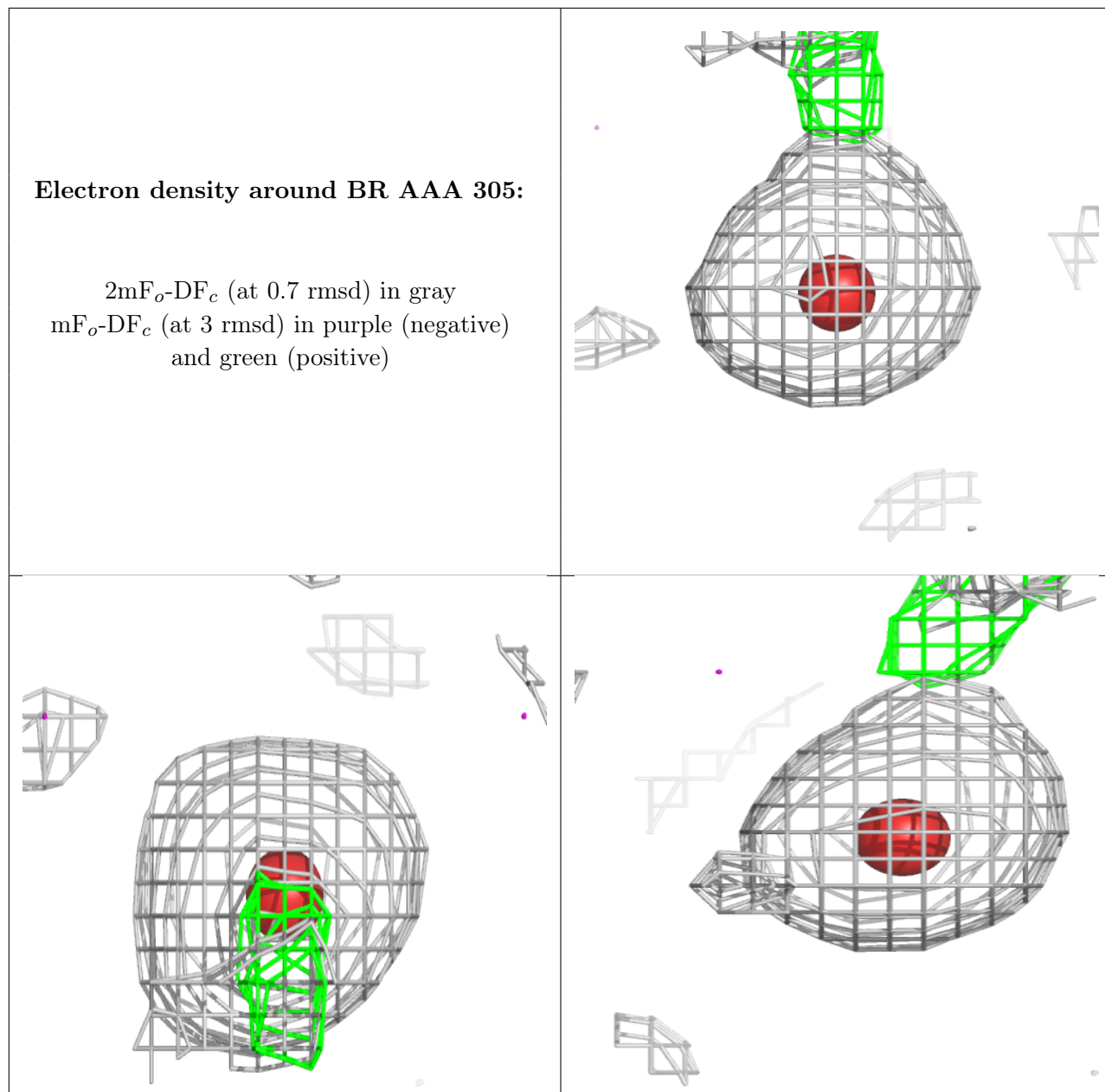
Electron density around 8YF DDD 801:

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



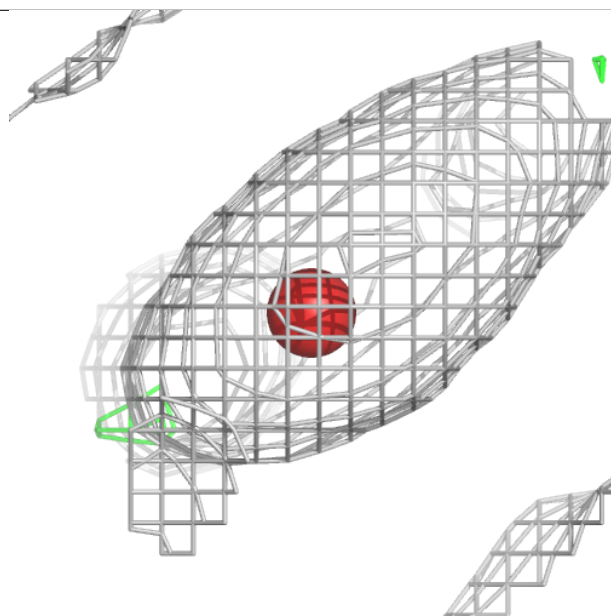
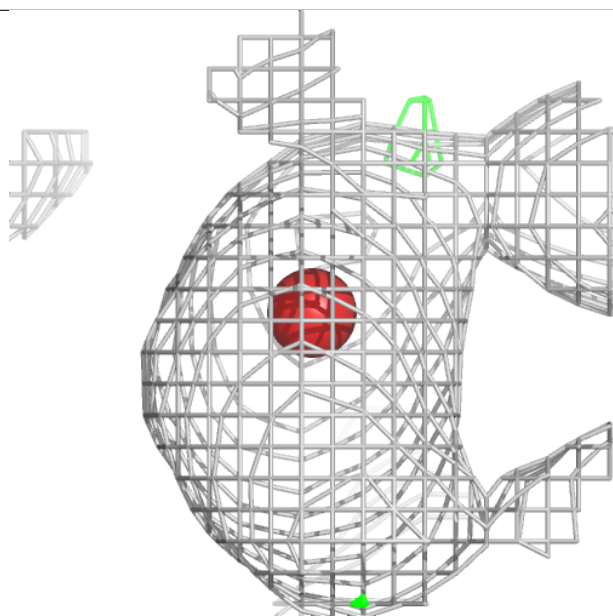
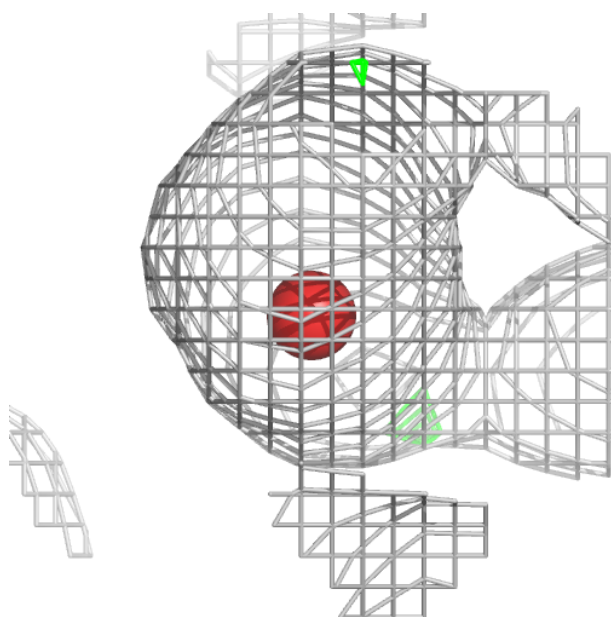
Electron density around BR AAA 305:

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



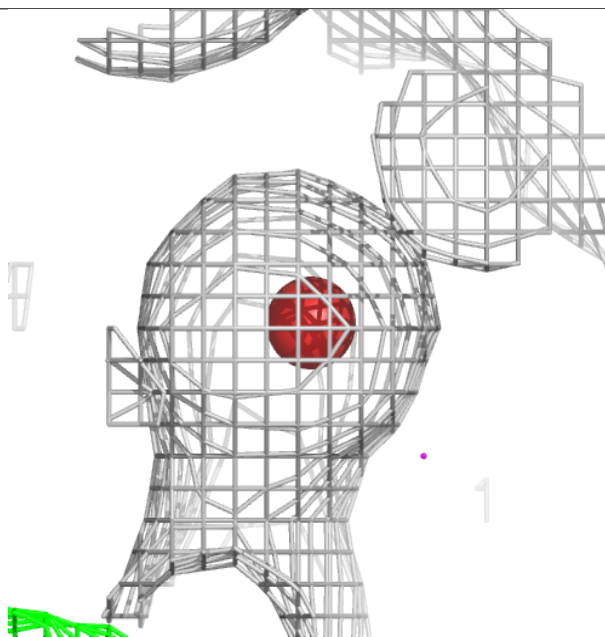
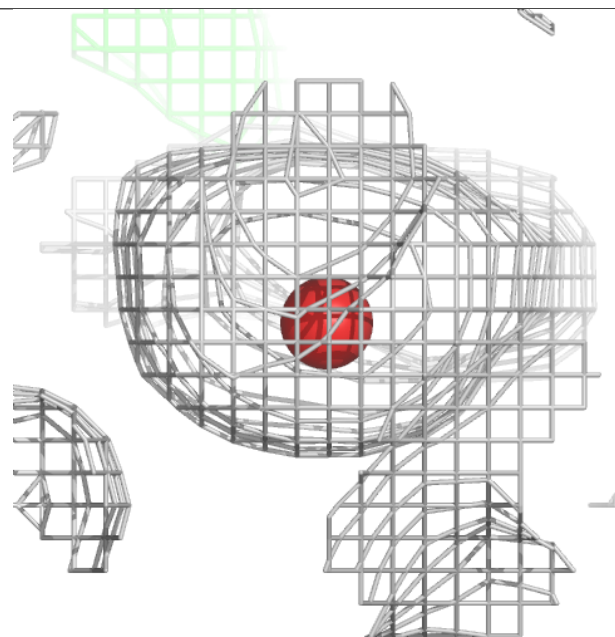
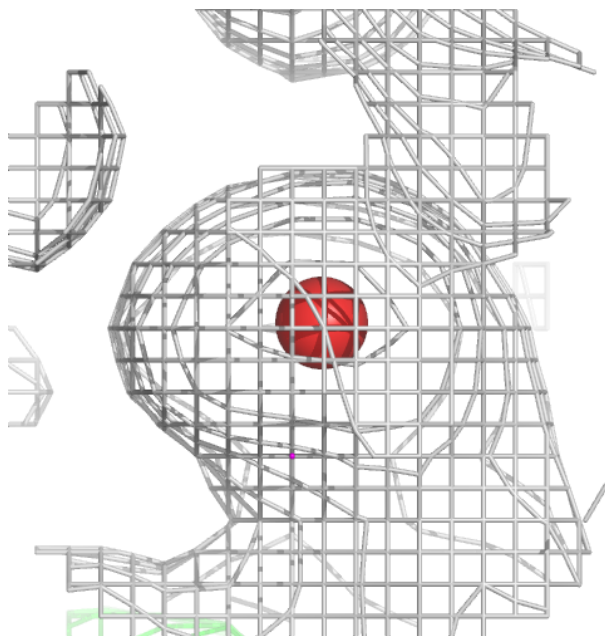
Electron density around BR AAA 303 (A):

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



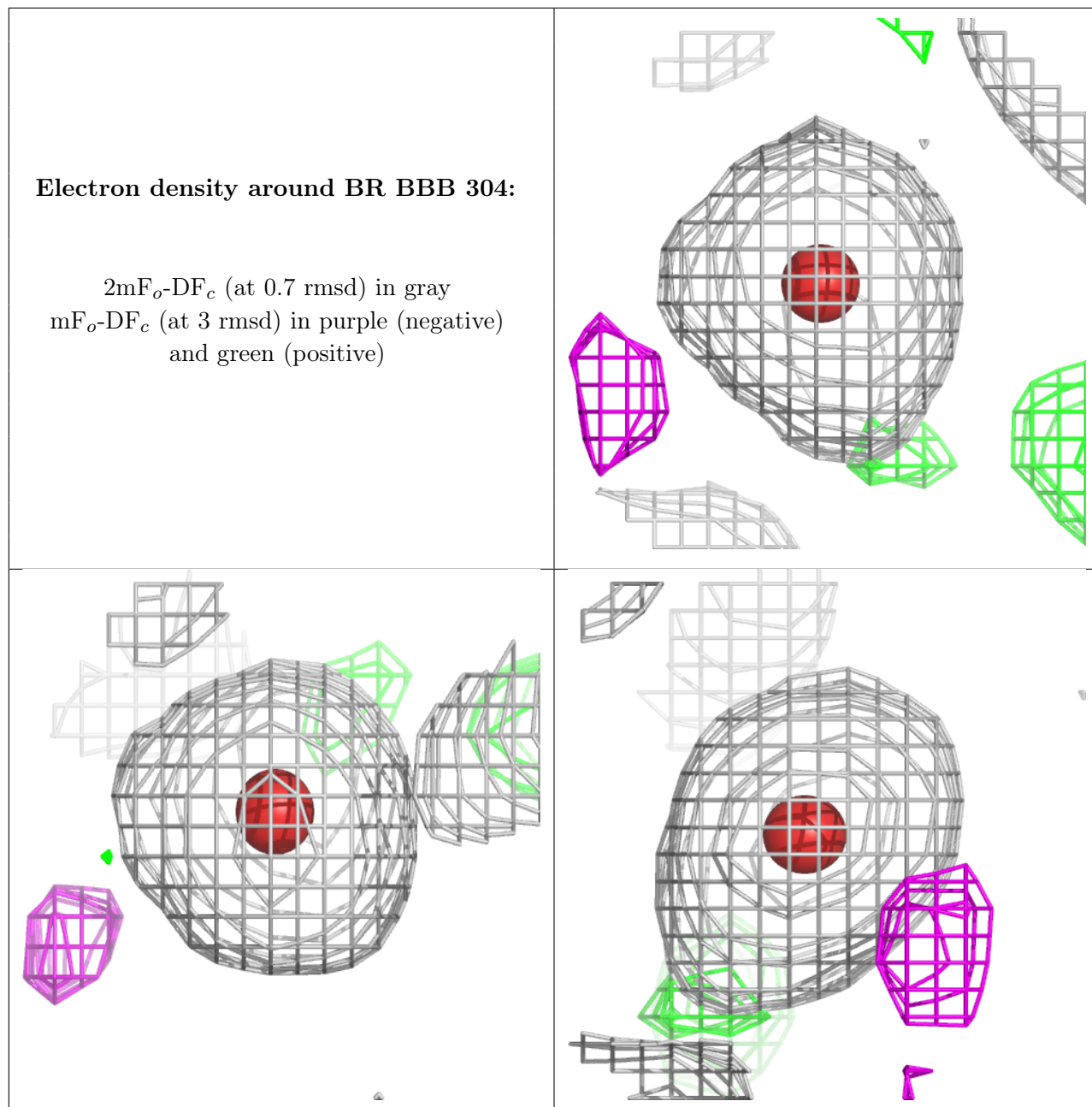
Electron density around BR AAA 306:

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



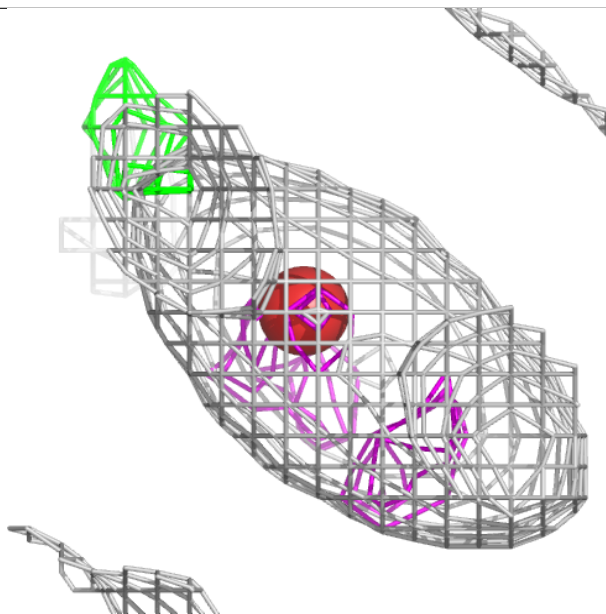
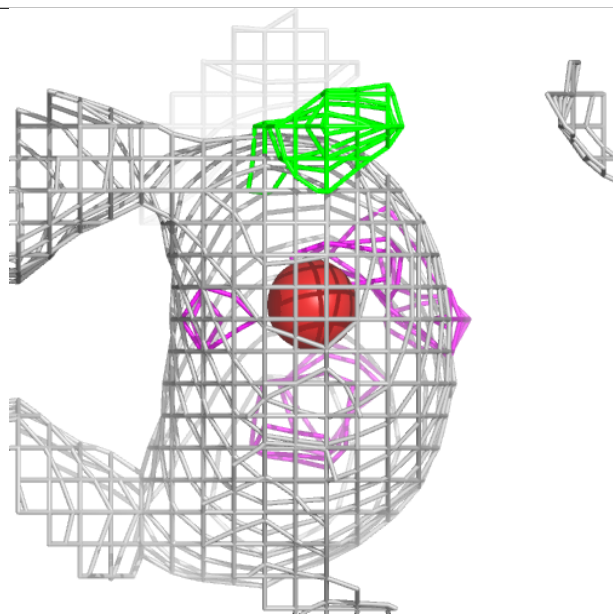
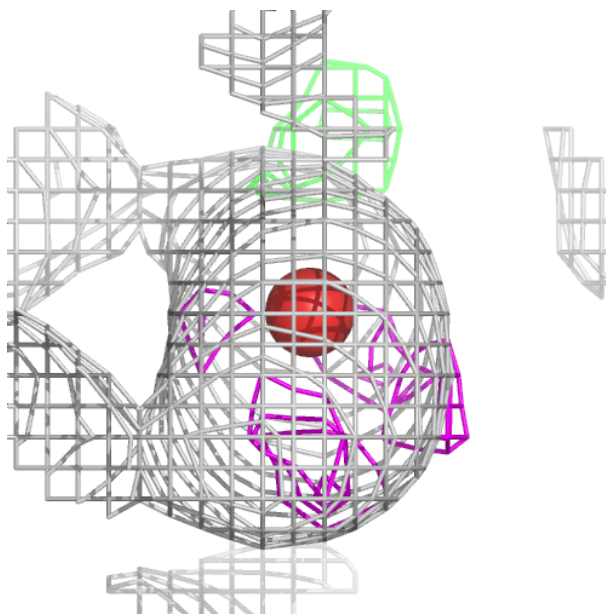
Electron density around BR BBB 304:

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



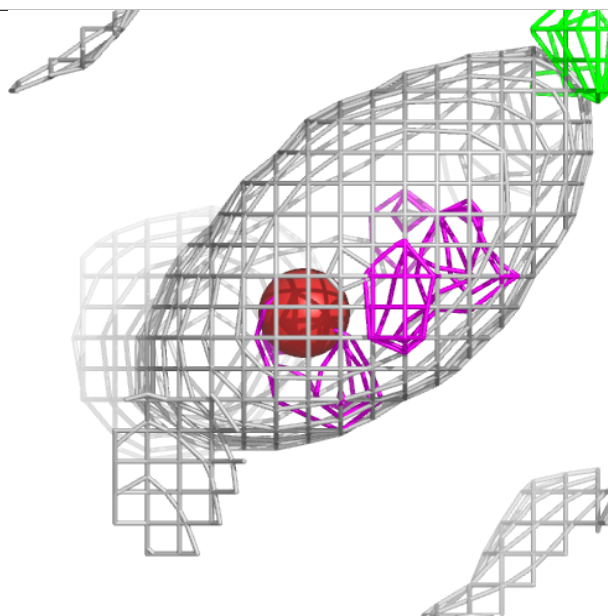
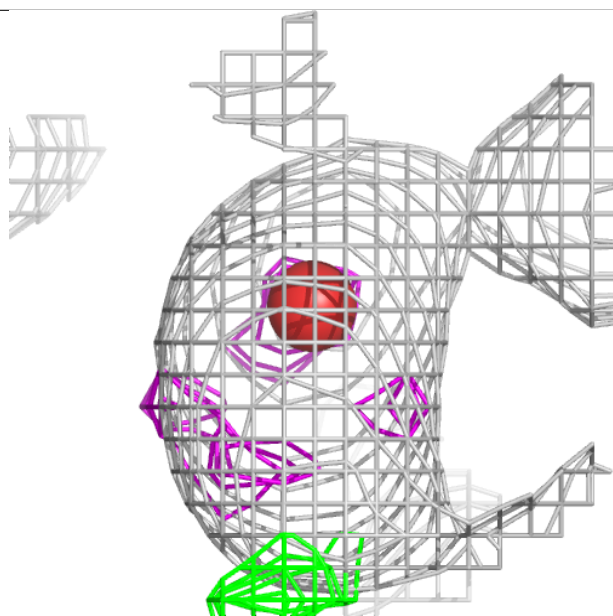
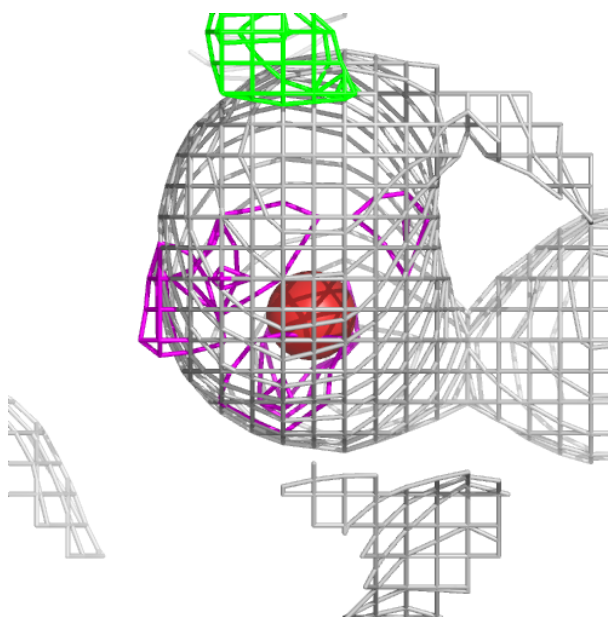
Electron density around BR CCC 301 (A):

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



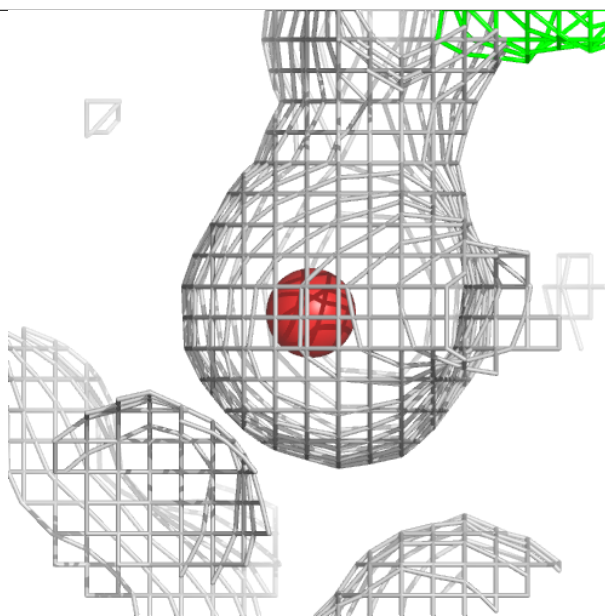
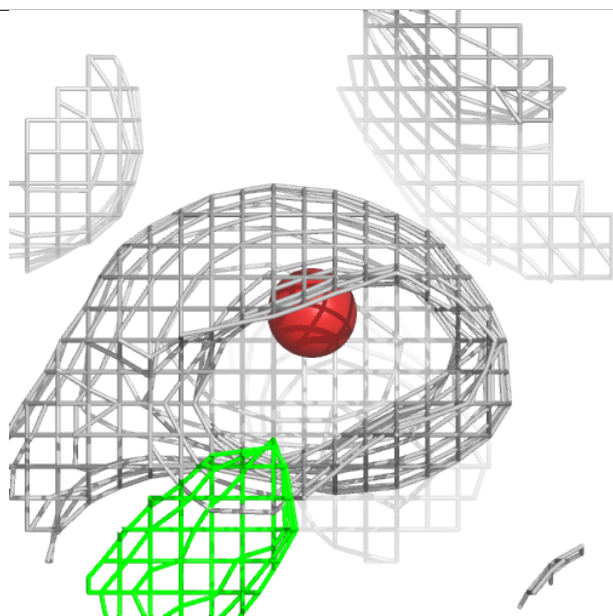
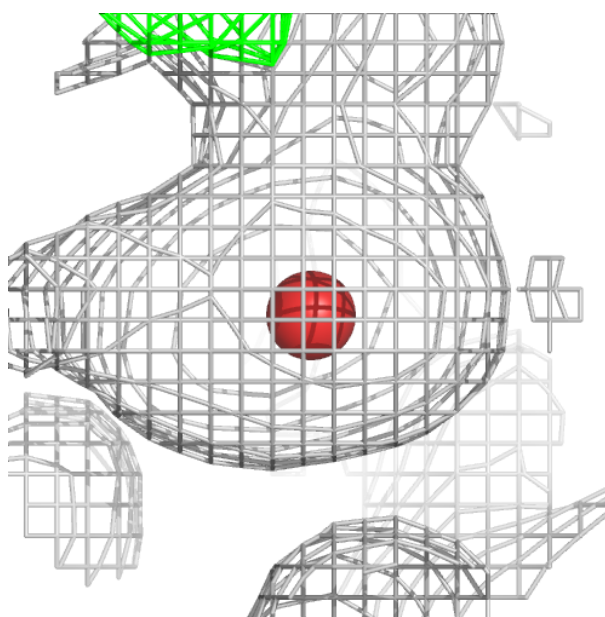
Electron density around BR CCC 301 (B):

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



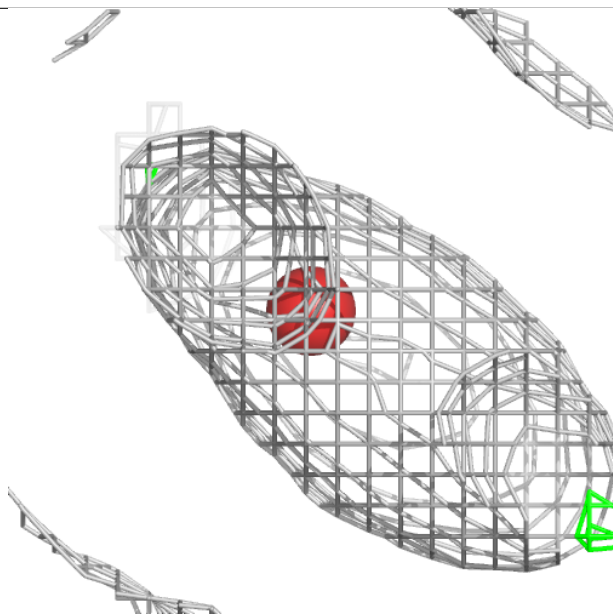
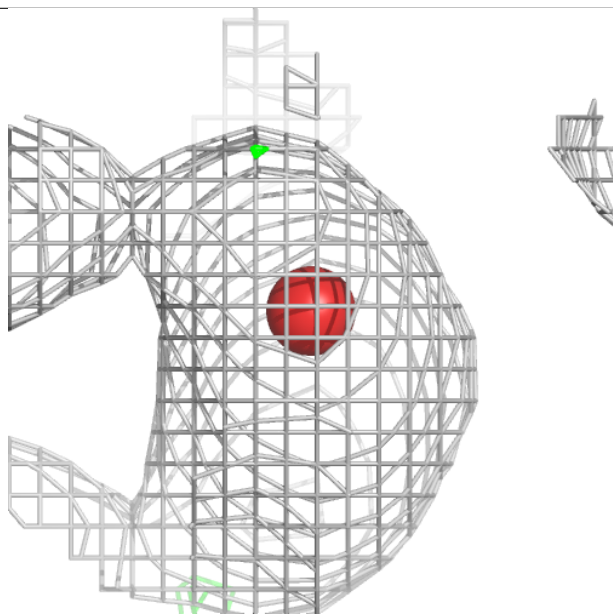
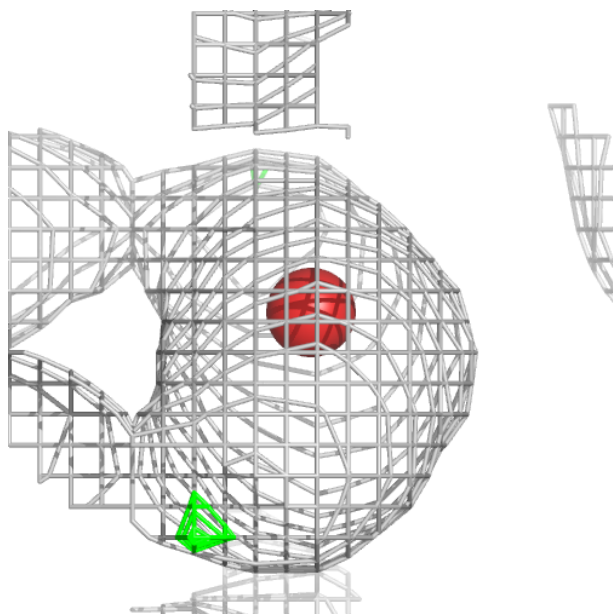
Electron density around BR DDD 802:

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



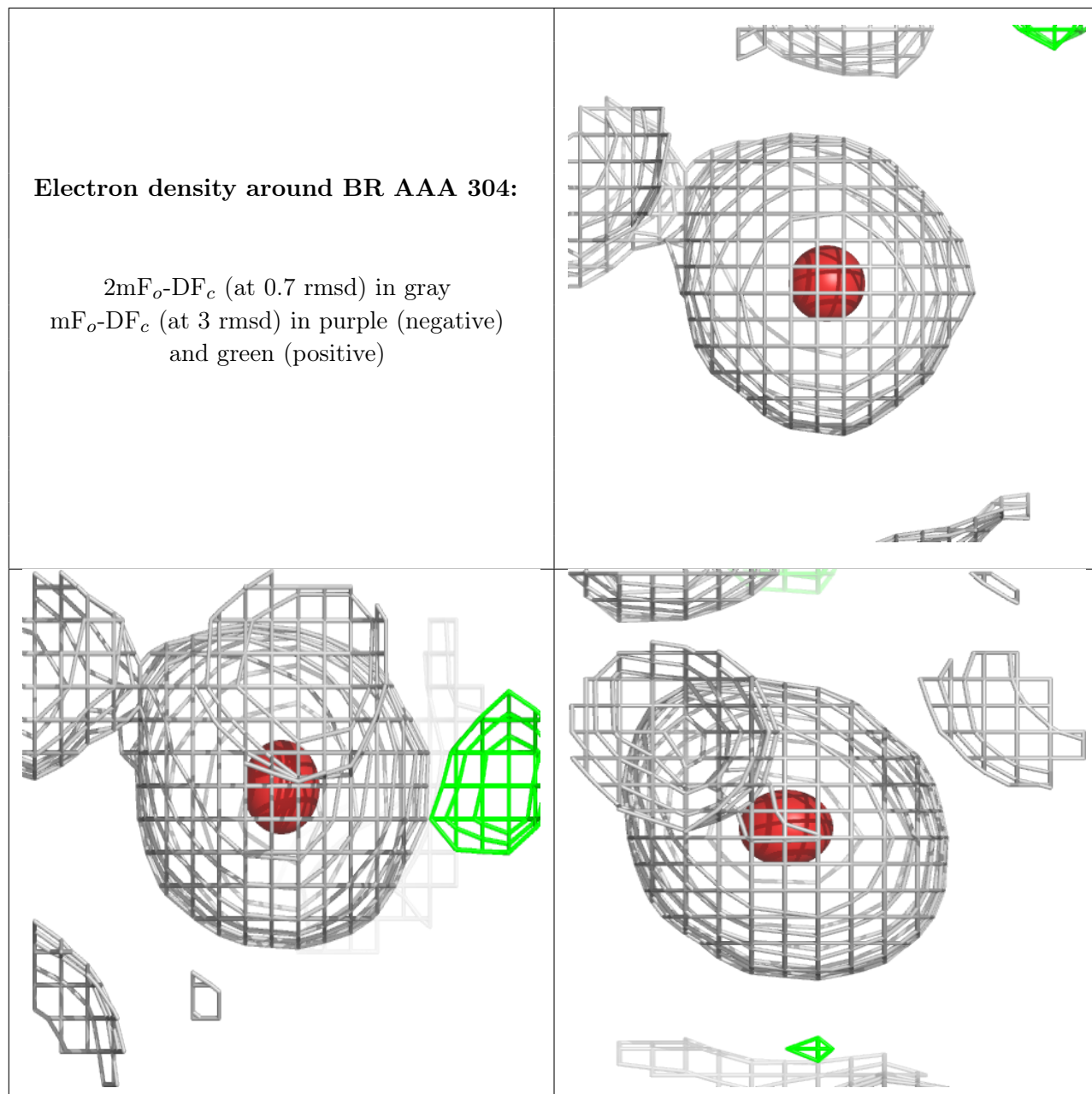
Electron density around BR AAA 303 (B):

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



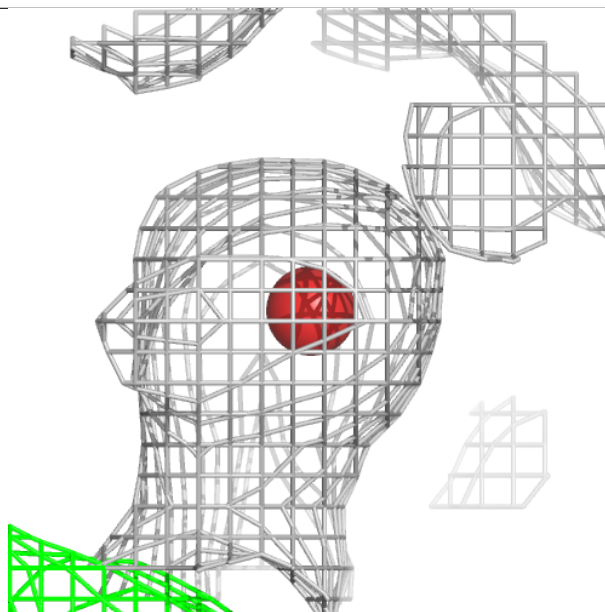
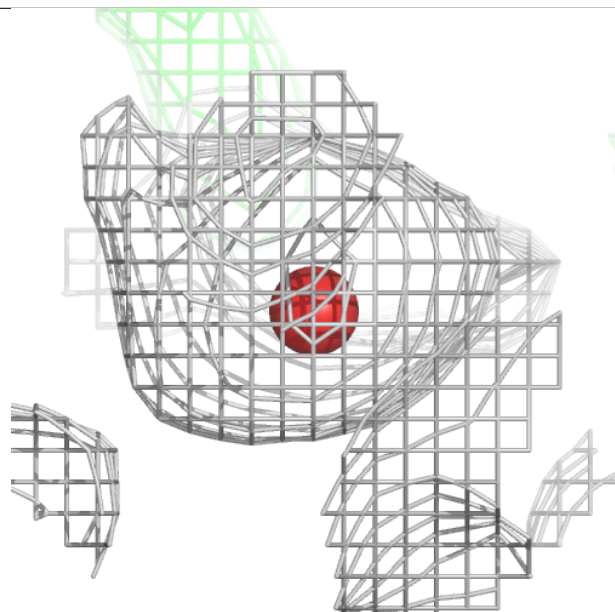
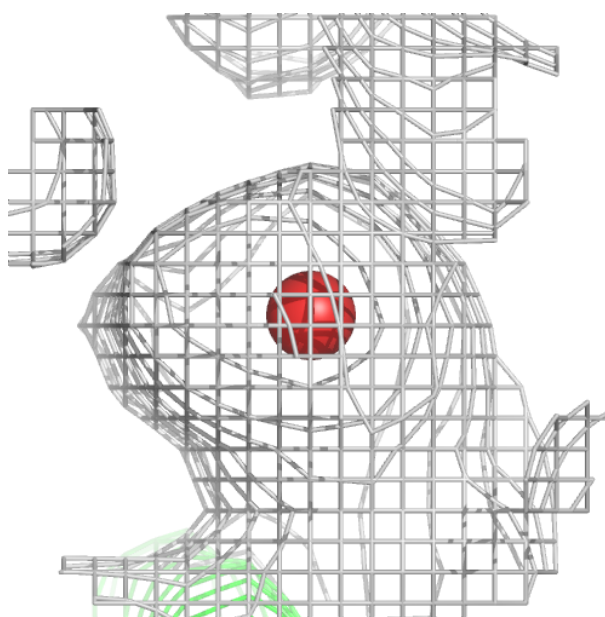
Electron density around BR AAA 304:

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



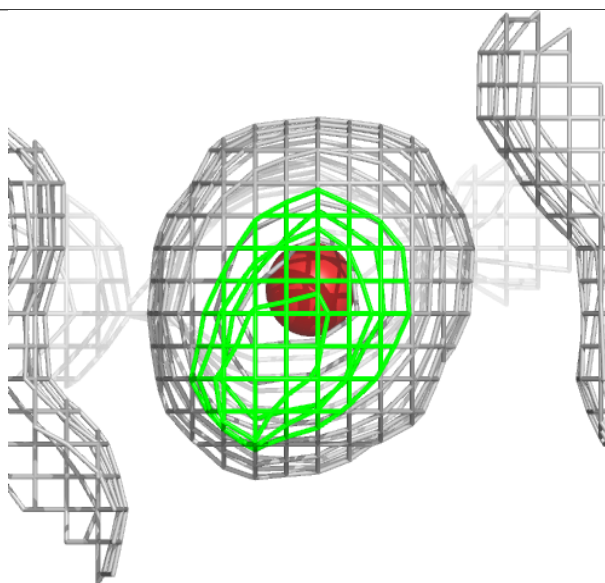
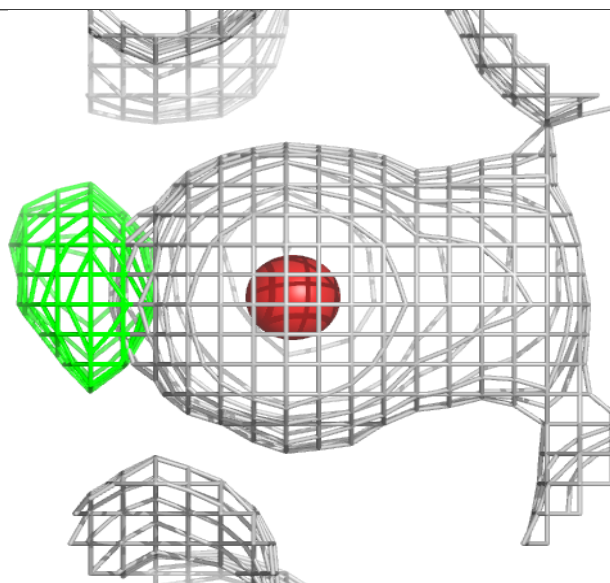
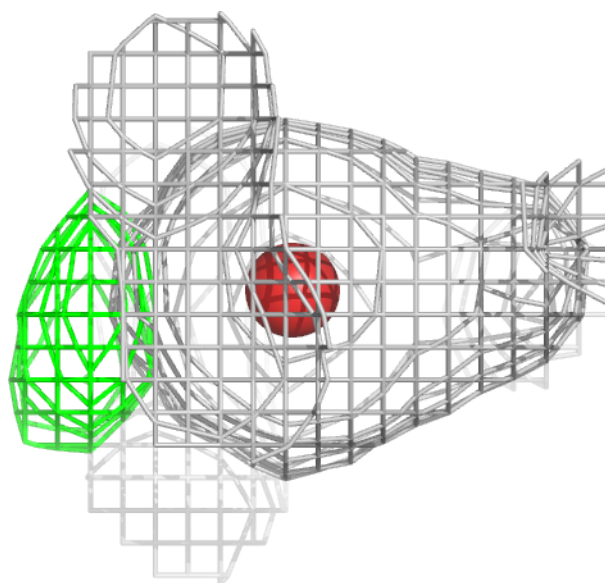
Electron density around BR BBB 305:

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



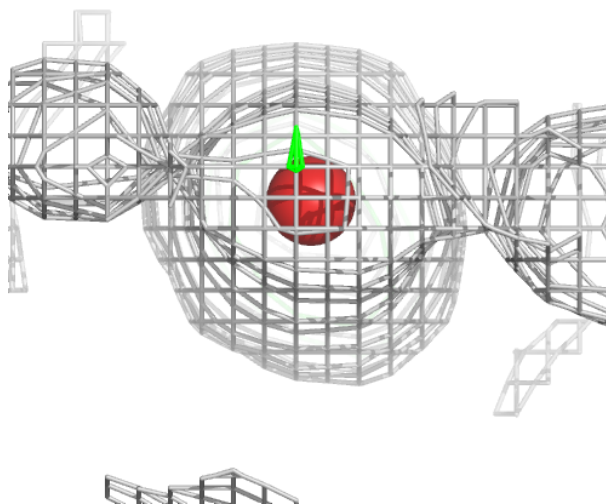
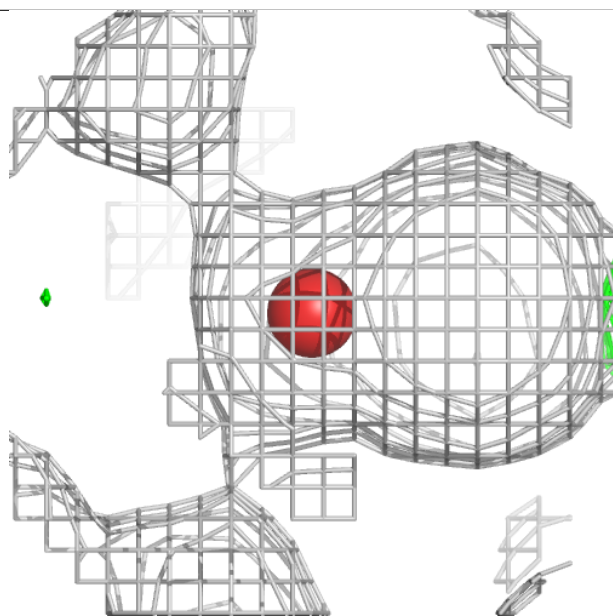
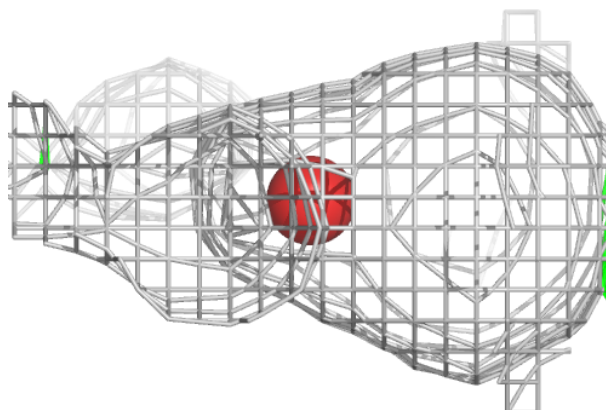
Electron density around BR AAA 302 (A):

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



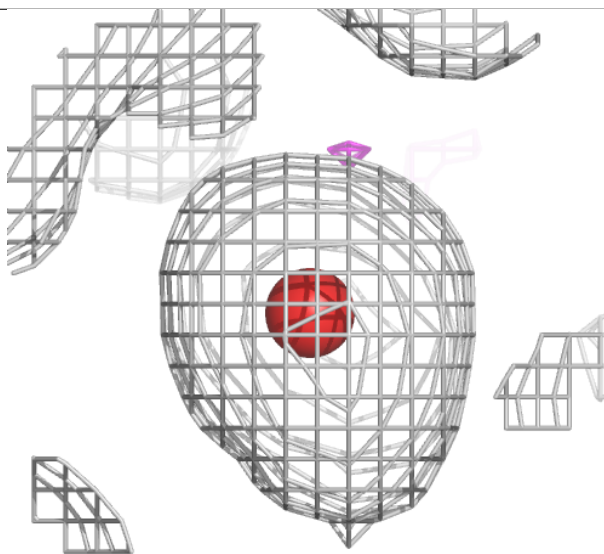
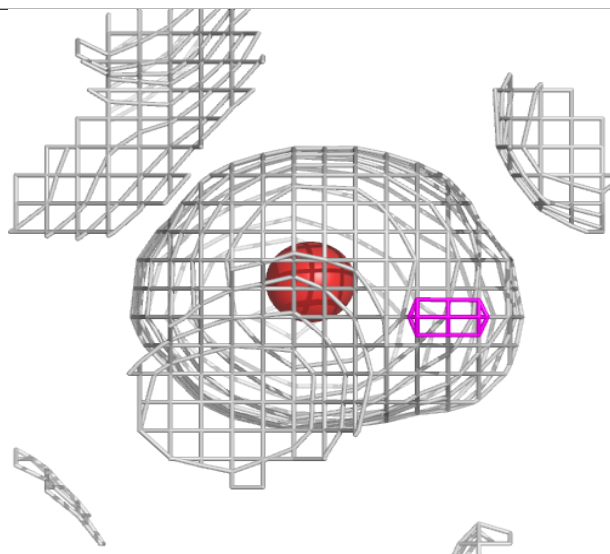
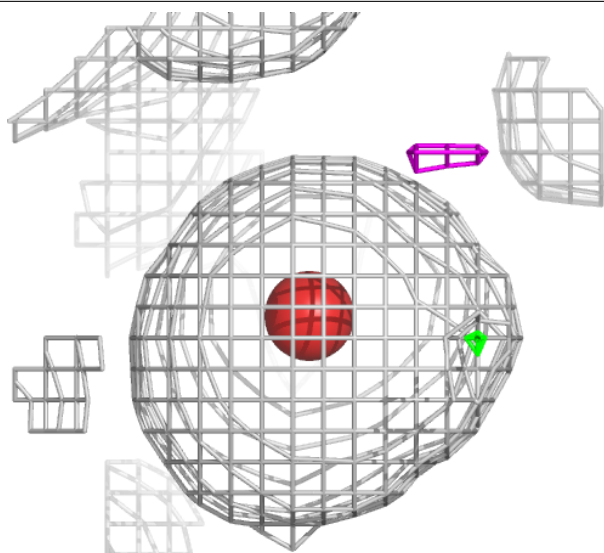
Electron density around BR AAA 302 (B):

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



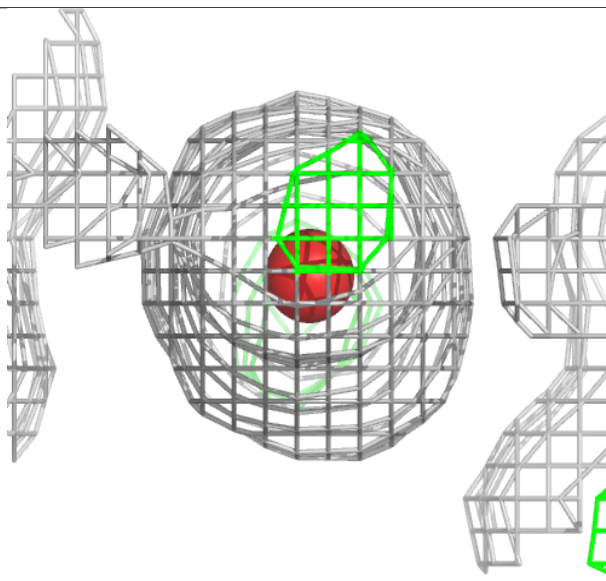
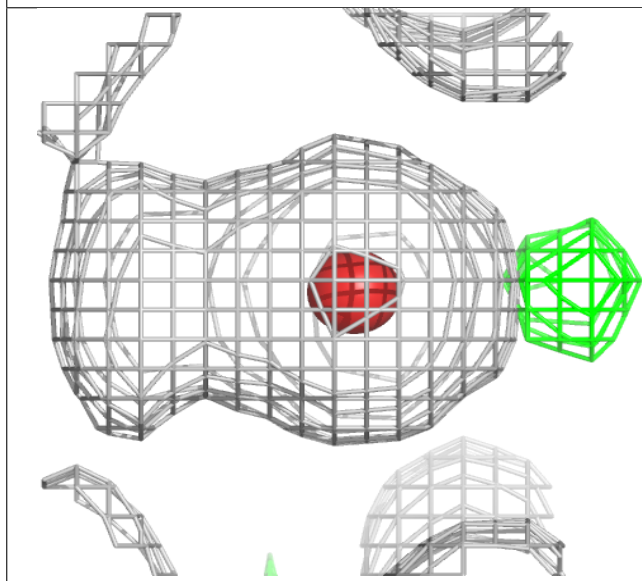
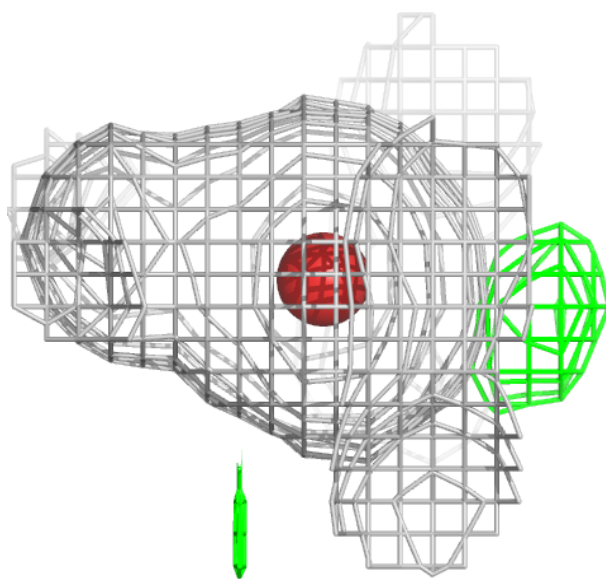
Electron density around BR CCC 302:

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



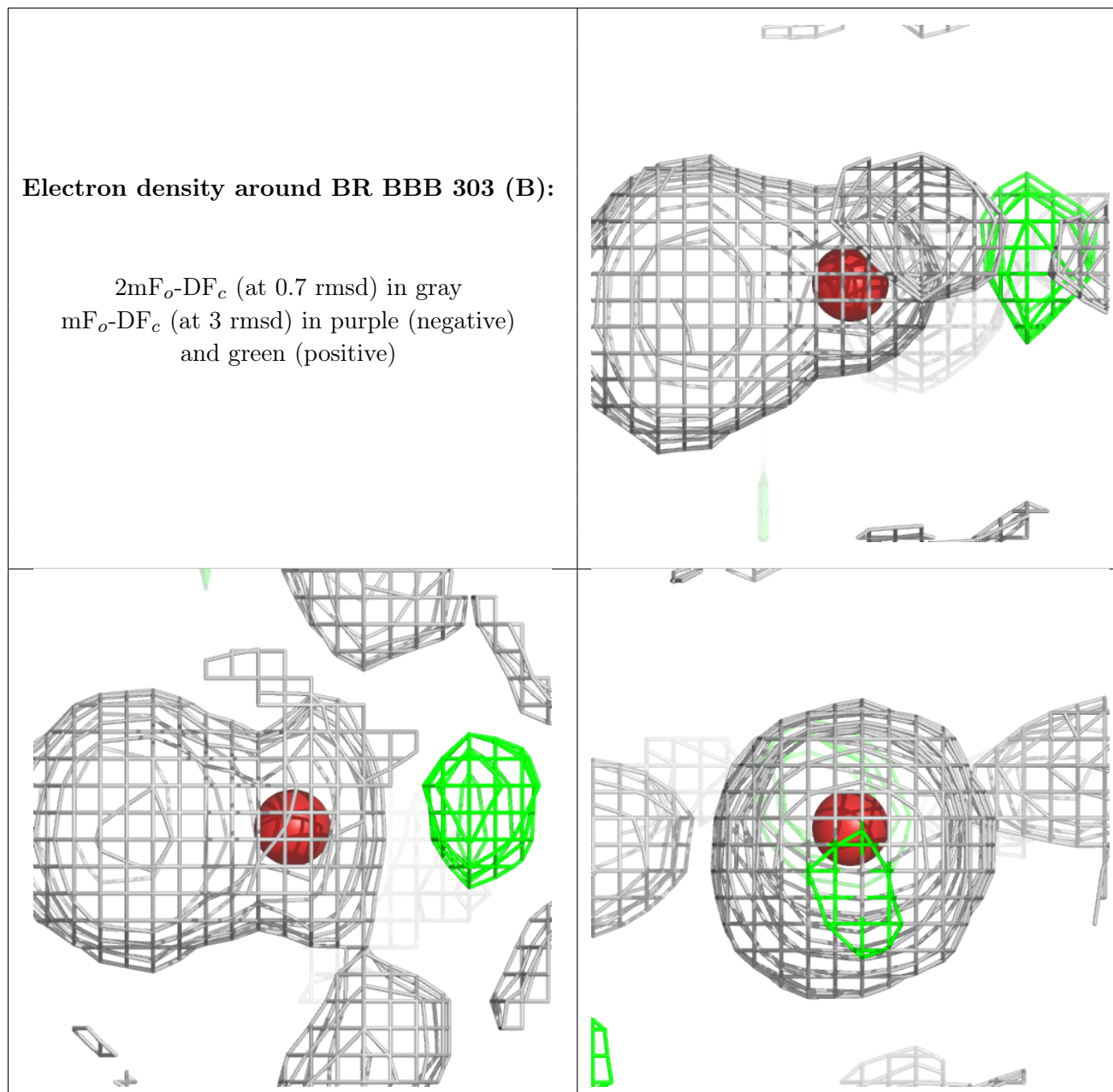
Electron density around BR BBB 303 (A):

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



Electron density around BR 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.