Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 08:09 am GMT

PDB ID	:	7Q14
Title	:	Crystal Structure of a Class D Carbapenemase_K73ALY Complexed with Imipenem
Authors	:	Zhou, Q.; He, Y.; Jin, Y.
Deposited on	:	2021-10-18
Resolution	:	2.15 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*
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:

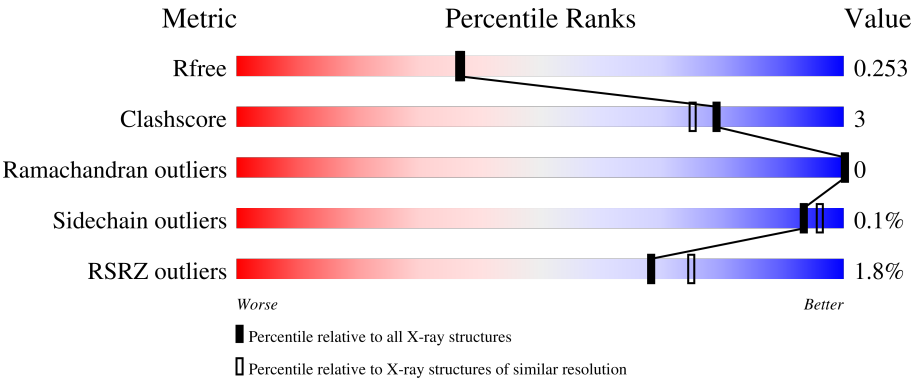
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 <=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	2% 83% 7% 9%
1	BBB	260	2% 82% 8% 10%
1	CCC	260	% 88% 5% 7%
1	DDD	260	3% 89% • 7%
1	EEE	260	89% • 7%

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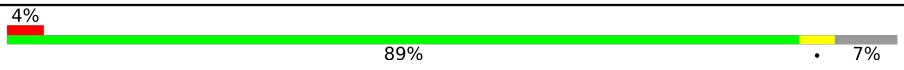
Mol	Chain	Length	Quality of chain
1	FFF	260	
1	GGG	260	
1	HHH	260	

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	1BO	AAA	302	-	-	X	-
4	BR	BBB	306[A]	-	-	X	-
4	BR	BBB	306[B]	-	-	X	-
4	BR	HHH	305[A]	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 32404 atoms, of which 15802 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	236	Total	C	H	N	O	S	44	0	0
			3852	1240	1911	343	351	7			
1	BBB	235	Total	C	H	N	O	S	44	0	0
			3840	1236	1907	342	348	7			
1	CCC	243	Total	C	H	N	O	S	47	1	0
			3964	1275	1963	354	365	7			
1	DDD	242	Total	C	H	N	O	S	45	0	0
			3924	1263	1942	349	363	7			
1	EEE	242	Total	C	H	N	O	S	47	1	0
			3942	1269	1950	352	364	7			
1	FFF	242	Total	C	H	N	O	S	45	0	0
			3924	1263	1942	349	363	7			
1	GGG	243	Total	C	H	N	O	S	45	0	0
			3946	1269	1955	351	364	7			
1	HHH	242	Total	C	H	N	O	S	45	0	0
			3924	1263	1942	349	363	7			

There are 136 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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

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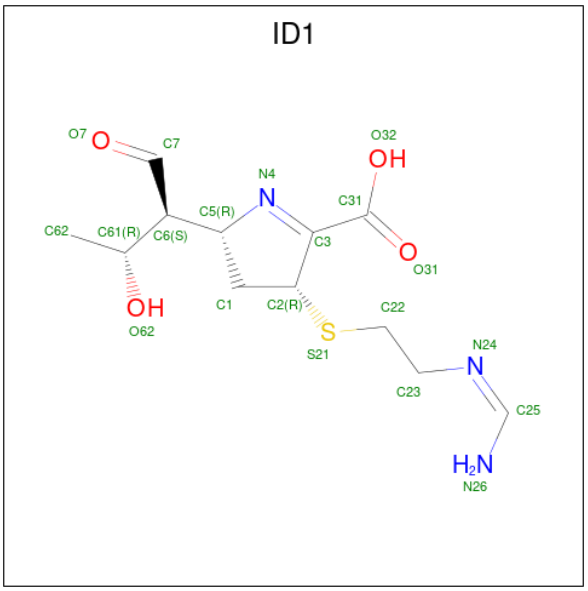
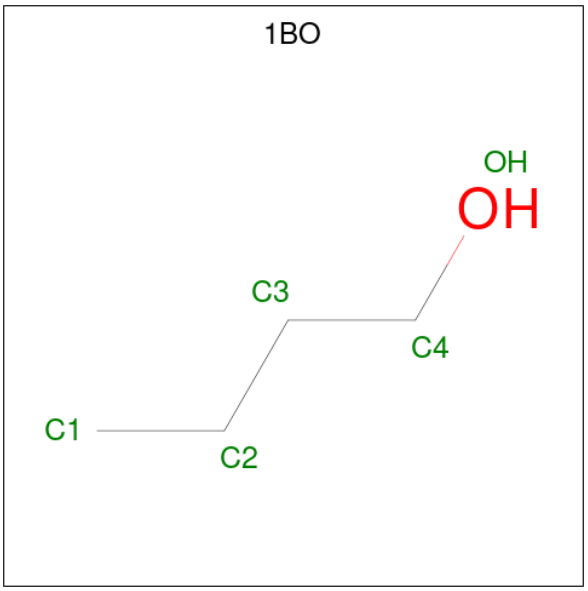
Chain	Residue	Modelled	Actual	Comment	Reference
FFF	18	LEU	-	expression tag	UNP A0A482LRD5
FFF	19	TYR	-	expression tag	UNP A0A482LRD5
FFF	20	PHE	-	expression tag	UNP A0A482LRD5
FFF	21	GLN	-	expression tag	UNP A0A482LRD5
FFF	22	GLY	-	expression tag	UNP A0A482LRD5
GGG	6	MET	-	initiating methionine	UNP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

- Molecule 2 is Imipenem (three-letter code: ID1) (formula: $C_{12}H_{19}N_3O_4S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	AAA	1	Total	C	H	N	O	S	3	0
			37	12	17	3	4	1		
2	BBB	1	Total	C	H	N	O	S	3	0
			37	12	17	3	4	1		
2	CCC	1	Total	C	H	N	O	S	3	0
			37	12	17	3	4	1		
2	DDD	1	Total	C	H	N	O	S	3	0
			37	12	17	3	4	1		
2	EEE	1	Total	C	H	N	O	S	3	0
			37	12	17	3	4	1		
2	FFF	1	Total	C	H	N	O	S	6	1
			74	24	34	6	8	2		
2	GGG	1	Total	C	H	N	O	S	6	1
			74	24	34	6	8	2		
2	HHH	1	Total	C	H	N	O	S	3	0
			37	12	17	3	4	1		

- Molecule 3 is 1-BUTANOL (three-letter code: 1BO) (formula: $C_4H_{10}O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	H	O	0	0
			15	4	10	1		
3	AAA	1	Total	C	H	O	0	0
			15	4	10	1		
3	BBB	1	Total	C	H	O	0	0
			15	4	10	1		
3	BBB	1	Total	C	H	O	0	0
			15	4	10	1		
3	BBB	1	Total	C	H	O	0	0
			15	4	10	1		
3	CCC	1	Total	C	H	O	0	0
			15	4	10	1		
3	EEE	1	Total	C	H	O	0	0
			15	4	10	1		
3	FFF	1	Total	C	H	O	0	0
			15	4	10	1		
3	GGG	1	Total	C	H	O	0	0
			15	4	10	1		
3	GGG	1	Total	C	H	O	0	0
			15	4	10	1		
3	HHH	1	Total	C	H	O	0	0
			15	4	10	1		
3	HHH	1	Total	C	H	O	0	0
			15	4	10	1		

- Molecule 4 is BROMIDE ION (three-letter code: BR) (formula: Br) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	2	Total Br 3 3	0	1
4	BBB	3	Total Br 5 5	0	2
4	CCC	2	Total Br 3 3	0	1
4	DDD	1	Total Br 1 1	0	0
4	EEE	1	Total Br 2 2	0	1
4	GGG	1	Total Br 2 2	0	1
4	HHH	2	Total Br 4 4	0	2

- Molecule 5 is water.

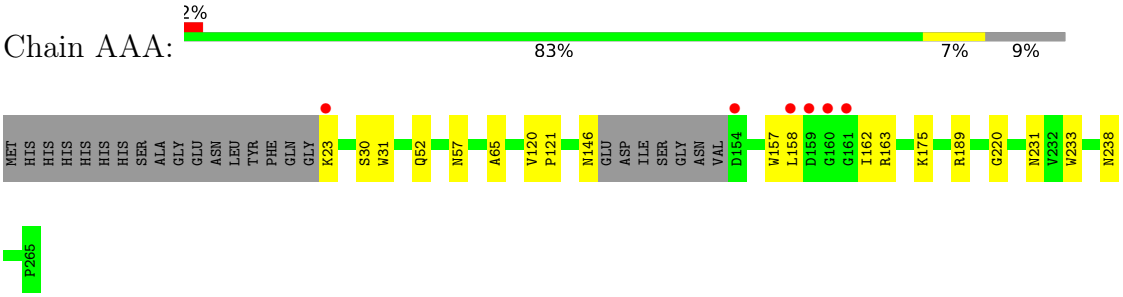
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	86	Total O 87 87	0	1
5	BBB	89	Total O 89 89	0	0
5	CCC	47	Total O 47 47	0	0
5	DDD	52	Total O 52 52	0	0
5	EEE	48	Total O 48 48	0	0
5	FFF	33	Total O 33 33	0	0
5	GGG	72	Total O 73 73	0	1
5	HHH	89	Total O 89 89	0	0

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.

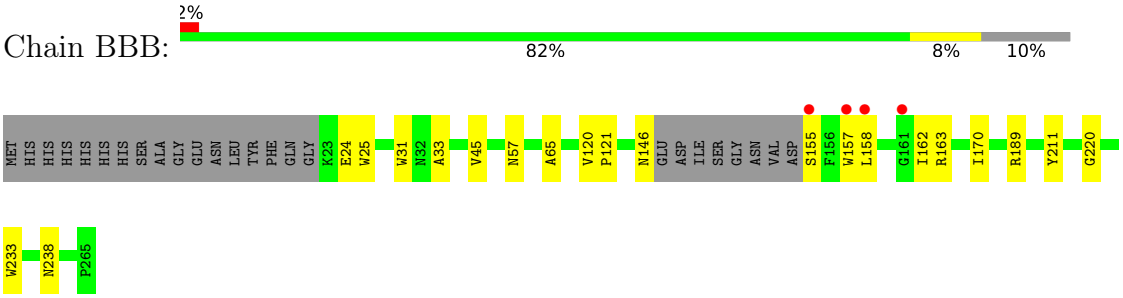
• Molecule 1: Beta-lactamase

Chain AAA:



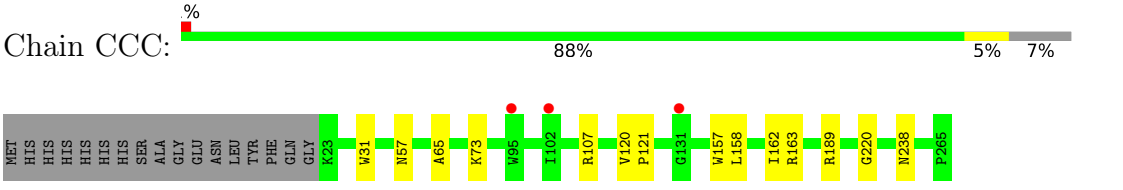
• Molecule 1: Beta-lactamase

Chain BBB:



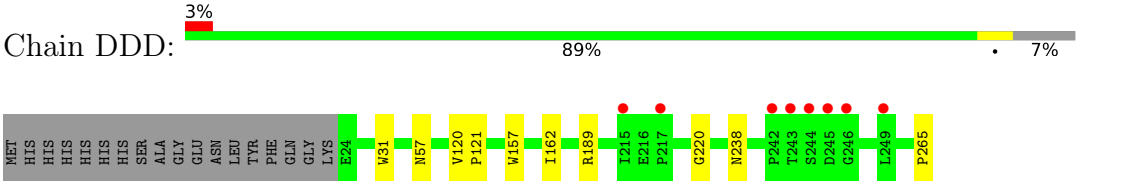
• Molecule 1: Beta-lactamase

Chain CCC:



• Molecule 1: Beta-lactamase

Chain DDD:

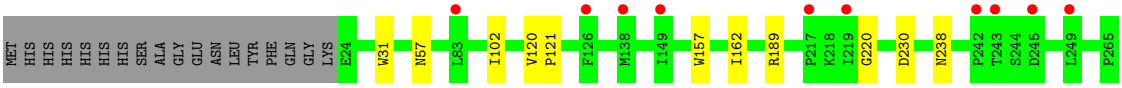


• Molecule 1: Beta-lactamase

Chain EEE:

• Molecule 1: Beta-lactamase

Chain FFF:



• Molecule 1: Beta-lactamase

Chain GGG:

• Molecule 1: Beta-lactamase

Chain HHH:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.40Å 161.93Å 107.78Å 90.00° 90.51° 90.00°	Depositor
Resolution (Å)	80.97 – 2.15 80.97 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.5 (80.97-2.15) 99.5 (80.97-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.210 , 0.250 0.216 , 0.253	Depositor DCC
R_{free} test set	5894 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	31.5	Xtriage
Anisotropy	0.824	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 51.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.105 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	32404	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: BR, ALY, 1BO, ID1

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	0.71	0/1976	0.81	0/2670
1	BBB	0.70	0/1968	0.81	0/2659
1	CCC	0.67	0/2038	0.79	0/2756
1	DDD	0.69	0/2018	0.79	1/2730 (0.0%)
1	EEE	0.67	0/2029	0.79	0/2745
1	FFF	0.67	0/2018	0.78	0/2730
1	GGG	0.69	0/2027	0.80	1/2741 (0.0%)
1	HHH	0.70	0/2018	0.80	1/2730 (0.0%)
All	All	0.69	0/16092	0.80	3/21761 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	HHH	265	PRO	CA-C-O	5.44	133.26	120.20
1	DDD	265	PRO	CA-C-O	5.31	132.95	120.20
1	GGG	163	ARG	NE-CZ-NH1	-5.14	117.73	120.30

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	1941	1911	1902	16	0
1	BBB	1933	1907	1898	20	0
1	CCC	2001	1963	1953	9	0
1	DDD	1982	1942	1934	5	0
1	EEE	1992	1950	1940	7	0
1	FFF	1982	1942	1934	7	0
1	GGG	1991	1955	1947	11	0
1	HHH	1982	1942	1934	6	0
2	AAA	20	17	0	1	0
2	BBB	20	17	0	6	0
2	CCC	20	17	0	2	0
2	DDD	20	17	0	0	0
2	EEE	20	17	0	1	0
2	FFF	40	34	0	2	0
2	GGG	40	34	0	3	0
2	HHH	20	17	0	3	0
3	AAA	10	20	20	4	0
3	BBB	15	30	30	2	0
3	CCC	5	10	10	0	0
3	EEE	5	10	10	0	0
3	FFF	5	10	10	0	0
3	GGG	10	20	20	1	0
3	HHH	10	20	20	0	0
4	AAA	3	0	0	0	0
4	BBB	5	0	0	5	0
4	CCC	3	0	0	2	0
4	DDD	1	0	0	0	0
4	EEE	2	0	0	2	0
4	GGG	2	0	0	0	0
4	HHH	4	0	0	4	0
5	AAA	87	0	0	2	0
5	BBB	89	0	0	2	0
5	CCC	47	0	0	0	0
5	DDD	52	0	0	0	0
5	EEE	48	0	0	1	0
5	FFF	33	0	0	0	0
5	GGG	73	0	0	1	0
5	HHH	89	0	0	0	0
All	All	16602	15802	15562	87	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.

All (87) 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)
2:HHH:301:ID1:C62	4:HHH:304[A]:BR:BR	2.58	1.06
5:AAA:480:HOH:O	4:HHH:305[A]:BR:BR	2.53	0.81
1:BBB:158:LEU:HD23	2:BBB:301:ID1:C31	2.12	0.80
1:BBB:158:LEU:HD23	2:BBB:301:ID1:O31	1.83	0.77
1:AAA:30:SER:HB2	1:BBB:33:ALA:HB1	1.68	0.74
1:AAA:233:TRP:HE1	3:AAA:302:1BO:H41	1.56	0.70
4:BBB:306[B]:BR:BR	5:BBB:484:HOH:O	2.64	0.69
1:BBB:155:SER:HA	1:BBB:158:LEU:HD13	1.75	0.68
1:HHH:189:ARG:HD2	4:HHH:305[B]:BR:BR	2.50	0.67
1:AAA:158:LEU:HD23	2:AAA:301:ID1:C31	2.25	0.66
2:FFF:301[B]:ID1:S21	2:FFF:301[B]:ID1:O31	2.52	0.66
1:BBB:189:ARG:HD2	4:BBB:306[B]:BR:BR	2.53	0.64
1:CCC:189:ARG:HD2	4:CCC:304[B]:BR:BR	2.55	0.61
4:CCC:304[A]:BR:BR	1:FFF:189:ARG:HD2	2.56	0.61
1:BBB:158:LEU:HG	2:BBB:301:ID1:O32	2.01	0.61
1:AAA:231:ASN:HD22	3:AAA:302:1BO:C4	2.15	0.59
2:HHH:301:ID1:S21	2:HHH:301:ID1:O31	2.61	0.59
1:CCC:158:LEU:HD21	2:CCC:301:ID1:C62	2.35	0.57
1:DDD:189:ARG:HD2	4:EEE:303[A]:BR:BR	2.60	0.57
1:EEE:189:ARG:HD2	4:EEE:303[B]:BR:BR	2.62	0.55
1:GGG:158:LEU:HD21	2:GGG:301[B]:ID1:C62	2.38	0.54
4:BBB:306[A]:BR:BR	1:GGG:189:ARG:HD2	2.63	0.53
1:EEE:158:LEU:HD21	2:EEE:301:ID1:C62	2.38	0.53
1:AAA:31:TRP:HB2	1:AAA:57:ASN:HB3	1.90	0.53
1:BBB:233:TRP:HE1	3:BBB:302:1BO:H32	1.74	0.52
4:BBB:306[A]:BR:BR	1:GGG:186:ARG:HA	2.64	0.52
1:GGG:250:ARG:NH2	2:GGG:301[B]:ID1:O32	2.36	0.51
1:AAA:175:LYS:NZ	5:AAA:402:HOH:O	2.42	0.50
1:CCC:31:TRP:HB2	1:CCC:57:ASN:HB3	1.94	0.50
1:EEE:31:TRP:HB2	1:EEE:57:ASN:HB3	1.94	0.49
1:FFF:31:TRP:HB2	1:FFF:57:ASN:HB3	1.95	0.48
1:HHH:31:TRP:HB2	1:HHH:57:ASN:HB3	1.94	0.48
1:BBB:31:TRP:HB2	1:BBB:57:ASN:HB3	1.95	0.48
1:CCC:107:ARG:NH2	1:FFF:230:ASP:OD1	2.47	0.48
1:GGG:31:TRP:HB2	1:GGG:57:ASN:HB3	1.96	0.48
2:GGG:301[A]:ID1:S21	2:GGG:301[A]:ID1:O32	2.71	0.48
1:DDD:157:TRP:HA	1:DDD:162:ILE:CG2	2.45	0.47
1:FFF:157:TRP:HA	1:FFF:162:ILE:CG2	2.44	0.47
1:AAA:189:ARG:HD2	4:HHH:305[A]:BR:BR	2.70	0.47
1:AAA:231:ASN:HD22	3:AAA:302:1BO:H41	1.80	0.47
1:CCC:73:ALY:HH31	2:CCC:301:ID1:C62	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FFF:102:ILE:HD11	2:FFF:301[A]:ID1:N26	2.29	0.47
2:HHH:301:ID1:O62	2:HHH:301:ID1:C1	2.62	0.46
1:AAA:220:GLY:O	1:AAA:238:ASN:HA	2.16	0.46
1:BBB:65:ALA:HB1	1:BBB:163:ARG:HB3	1.98	0.46
1:AAA:65:ALA:HB1	1:AAA:163:ARG:HB3	1.98	0.45
1:AAA:157:TRP:HA	1:AAA:162:ILE:CG2	2.46	0.45
1:DDD:31:TRP:HB2	1:DDD:57:ASN:HB3	1.97	0.45
1:BBB:233:TRP:HE1	3:BBB:302:1BO:C3	2.29	0.45
1:EEE:157:TRP:HA	1:EEE:162:ILE:CG2	2.47	0.45
1:HHH:157:TRP:HA	1:HHH:162:ILE:CG2	2.47	0.45
1:BBB:157:TRP:HA	1:BBB:162:ILE:CG2	2.46	0.45
1:BBB:158:LEU:CD2	2:BBB:301:ID1:C31	2.90	0.45
1:CCC:157:TRP:HA	1:CCC:162:ILE:CG2	2.47	0.45
1:GGG:157:TRP:HA	1:GGG:162:ILE:CG2	2.47	0.45
1:GGG:231:ASN:HD22	3:GGG:302:1BO:H41	1.80	0.45
1:CCC:120:VAL:N	1:CCC:121:PRO:CD	2.81	0.44
1:BBB:158:LEU:CG	2:BBB:301:ID1:O32	2.65	0.44
1:DDD:220:GLY:O	1:DDD:238:ASN:HA	2.18	0.44
2:BBB:301:ID1:C61	4:BBB:307[A]:BR:BR	3.21	0.43
1:CCC:220:GLY:O	1:CCC:238:ASN:HA	2.18	0.43
1:BBB:146:ASN:ND2	1:BBB:163:ARG:HB2	2.33	0.43
1:FFF:220:GLY:O	1:FFF:238:ASN:HA	2.18	0.43
1:HHH:120:VAL:N	1:HHH:121:PRO:CD	2.82	0.43
1:FFF:120:VAL:N	1:FFF:121:PRO:CD	2.82	0.43
1:GGG:220:GLY:O	1:GGG:238:ASN:HA	2.18	0.43
1:EEE:220:GLY:O	1:EEE:238:ASN:HA	2.18	0.43
1:EEE:120:VAL:N	1:EEE:121:PRO:CD	2.82	0.42
1:BBB:220:GLY:O	1:BBB:238:ASN:HA	2.19	0.42
1:HHH:220:GLY:O	1:HHH:238:ASN:HA	2.18	0.42
1:DDD:120:VAL:N	1:DDD:121:PRO:CD	2.82	0.42
1:BBB:211:TYR:OH	5:BBB:401:HOH:O	2.20	0.42
1:BBB:120:VAL:N	1:BBB:121:PRO:CD	2.83	0.42
1:AAA:157:TRP:CE2	1:AAA:158:LEU:HD11	2.55	0.42
1:GGG:120:VAL:N	1:GGG:121:PRO:CD	2.83	0.42
1:AAA:23:LYS:NZ	1:AAA:52:GLN:HE21	2.17	0.42
1:BBB:45:VAL:HG12	1:BBB:170:ILE:HD12	2.02	0.42
1:AAA:120:VAL:N	1:AAA:121:PRO:CD	2.83	0.41
1:GGG:51:LYS:HE3	5:GGG:450:HOH:O	2.20	0.41
1:GGG:163:ARG:HH21	1:GGG:163:ARG:HG2	1.85	0.41
1:AAA:146:ASN:ND2	1:AAA:163:ARG:HB2	2.35	0.41
1:BBB:157:TRP:NE1	1:BBB:158:LEU:HD11	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EEE:123:TYR:HB3	5:EEE:411:HOH:O	2.21	0.41
1:BBB:24:GLU:HG3	1:BBB:25:TRP:N	2.34	0.41
1:AAA:233:TRP:HE1	3:AAA:302:1BO:C4	2.31	0.40
1:HHH:65:ALA:HB1	1:HHH:163:ARG:HB3	2.03	0.40
1:CCC:65:ALA:HB1	1:CCC:163:ARG:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
1	BBB	230/260 (88%)	226 (98%)	4 (2%)	0	100	100
1	CCC	241/260 (93%)	236 (98%)	5 (2%)	0	100	100
1	DDD	239/260 (92%)	234 (98%)	5 (2%)	0	100	100
1	EEE	240/260 (92%)	235 (98%)	5 (2%)	0	100	100
1	FFF	239/260 (92%)	234 (98%)	5 (2%)	0	100	100
1	GGG	240/260 (92%)	235 (98%)	5 (2%)	0	100	100
1	HHH	239/260 (92%)	233 (98%)	6 (2%)	0	100	100
All	All	1899/2080 (91%)	1860 (98%)	39 (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	205/225 (91%)	205 (100%)	0	100	100
1	BBB	204/225 (91%)	204 (100%)	0	100	100
1	CCC	212/225 (94%)	212 (100%)	0	100	100
1	DDD	210/225 (93%)	210 (100%)	0	100	100
1	EEE	211/225 (94%)	211 (100%)	0	100	100
1	FFF	210/225 (93%)	210 (100%)	0	100	100
1	GGG	211/225 (94%)	210 (100%)	1 (0%)	88	92
1	HHH	210/225 (93%)	210 (100%)	0	100	100
All	All	1673/1800 (93%)	1672 (100%)	1 (0%)	93	96

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

Mol	Chain	Res	Type
1	GGG	101	ASP

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)

8 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	ALY	AAA	73	1	10,11,12	0.37	0	7,12,14	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	ALY	CCC	73	1	10,11,12	0.39	0	7,12,14	0.43	0
1	ALY	EEE	73	1	10,11,12	0.37	0	7,12,14	0.34	0
1	ALY	FFF	73	1	10,11,12	0.47	0	7,12,14	0.41	0
1	ALY	HHH	73	1	10,11,12	0.39	0	7,12,14	0.51	0
1	ALY	BBB	73	1	10,11,12	0.33	0	7,12,14	0.35	0
1	ALY	GGG	73	1	10,11,12	0.39	0	7,12,14	0.35	0
1	ALY	DDD	73	1	10,11,12	0.34	0	7,12,14	0.39	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	ALY	AAA	73	1	-	0/9/10/12	-
1	ALY	CCC	73	1	-	0/9/10/12	-
1	ALY	EEE	73	1	-	0/9/10/12	-
1	ALY	FFF	73	1	-	0/9/10/12	-
1	ALY	HHH	73	1	-	0/9/10/12	-
1	ALY	BBB	73	1	-	0/9/10/12	-
1	ALY	GGG	73	1	-	0/9/10/12	-
1	ALY	DDD	73	1	-	1/9/10/12	-

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	DDD	73	ALY	CG-CD-CE-NZ

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	CCC	73	ALY	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 42 ligands modelled in this entry, 20 are monoatomic - leaving 22 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	ID1	FFF	301[B]	1	15,20,20	0.97	1 (6%)	10,26,26	0.98	1 (10%)
3	1BO	BBB	303	-	4,4,4	0.35	0	3,3,3	0.17	0
2	ID1	BBB	301	1	15,20,20	1.05	2 (13%)	10,26,26	1.59	2 (20%)
3	1BO	AAA	303	-	4,4,4	0.36	0	3,3,3	0.31	0
2	ID1	AAA	301	1	15,20,20	1.25	2 (13%)	10,26,26	1.24	0
2	ID1	FFF	301[A]	1	15,20,20	0.96	2 (13%)	10,26,26	2.04	3 (30%)
3	1BO	EEE	302	-	4,4,4	0.11	0	3,3,3	0.17	0
3	1BO	GGG	303	-	4,4,4	0.23	0	3,3,3	0.14	0
2	ID1	CCC	301	1	15,20,20	0.91	1 (6%)	10,26,26	2.11	4 (40%)
3	1BO	GGG	302	-	4,4,4	0.19	0	3,3,3	0.37	0
3	1BO	FFF	302	-	4,4,4	0.23	0	3,3,3	0.13	0
2	ID1	GGG	301[B]	1,4	15,20,20	0.94	1 (6%)	10,26,26	1.86	3 (30%)
2	ID1	DDD	301	1	15,20,20	1.15	2 (13%)	10,26,26	1.70	3 (30%)
3	1BO	BBB	304	-	4,4,4	0.43	0	3,3,3	0.42	0
3	1BO	BBB	302	-	4,4,4	0.40	0	3,3,3	0.84	0
3	1BO	AAA	302	-	4,4,4	0.56	0	3,3,3	0.28	0
2	ID1	HHH	301	1	15,20,20	1.39	2 (13%)	10,26,26	2.11	5 (50%)
3	1BO	CCC	302	-	4,4,4	0.29	0	3,3,3	0.30	0
3	1BO	HHH	303	-	4,4,4	0.24	0	3,3,3	0.30	0
2	ID1	EEE	301	1	15,20,20	1.09	1 (6%)	10,26,26	1.89	4 (40%)
2	ID1	GGG	301[A]	1	15,20,20	1.77	2 (13%)	10,26,26	0.85	0
3	1BO	HHH	302	-	4,4,4	0.63	0	3,3,3	0.33	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
2	ID1	FFF	301[B]	1	-	7/17/32/32	0/1/1/1
3	1BO	BBB	303	-	-	1/2/2/2	-
2	ID1	BBB	301	1	-	7/17/32/32	0/1/1/1
3	1BO	AAA	303	-	-	2/2/2/2	-
2	ID1	AAA	301	1	-	4/17/32/32	0/1/1/1
2	ID1	FFF	301[A]	1	-	3/17/32/32	0/1/1/1
3	1BO	EEE	302	-	-	2/2/2/2	-
3	1BO	GGG	303	-	-	1/2/2/2	-
2	ID1	CCC	301	1	-	6/17/32/32	0/1/1/1
3	1BO	GGG	302	-	-	0/2/2/2	-
3	1BO	FFF	302	-	-	1/2/2/2	-
2	ID1	GGG	301[B]	1,4	-	4/17/32/32	0/1/1/1
2	ID1	DDD	301	1	-	4/17/32/32	0/1/1/1
3	1BO	BBB	304	-	-	0/2/2/2	-
3	1BO	BBB	302	-	-	1/2/2/2	-
3	1BO	AAA	302	-	-	1/2/2/2	-
2	ID1	HHH	301	1	-	4/17/32/32	0/1/1/1
3	1BO	CCC	302	-	-	2/2/2/2	-
3	1BO	HHH	303	-	-	1/2/2/2	-
2	ID1	EEE	301	1	-	3/17/32/32	0/1/1/1
2	ID1	GGG	301[A]	1	-	9/17/32/32	0/1/1/1
3	1BO	HHH	302	-	-	1/2/2/2	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	GGG	301[A]	ID1	C2-S21	4.93	1.88	1.83
2	GGG	301[A]	ID1	O32-C31	-3.66	1.19	1.30
2	HHH	301	ID1	O32-C31	-3.49	1.20	1.30
2	FFF	301[B]	ID1	O32-C31	-3.31	1.20	1.30
2	AAA	301	ID1	O32-C31	-3.28	1.21	1.30
2	GGG	301[B]	ID1	O32-C31	-3.14	1.21	1.30
2	AAA	301	ID1	C2-S21	3.01	1.86	1.83
2	HHH	301	ID1	C22-S21	2.99	1.85	1.81
2	DDD	301	ID1	C2-S21	2.83	1.86	1.83
2	DDD	301	ID1	O32-C31	-2.77	1.22	1.30
2	FFF	301[A]	ID1	C2-S21	2.48	1.85	1.83
2	BBB	301	ID1	O32-C31	-2.43	1.23	1.30
2	BBB	301	ID1	C2-S21	2.36	1.85	1.83
2	EEE	301	ID1	O32-C31	-2.33	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	FFF	301[A]	ID1	O32-C31	-2.31	1.23	1.30
2	CCC	301	ID1	O32-C31	-2.29	1.23	1.30

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	CCC	301	ID1	C6-C5-N4	-4.97	102.43	112.00
2	HHH	301	ID1	C22-C23-N24	4.16	113.99	110.78
2	FFF	301[A]	ID1	C6-C5-N4	-3.90	104.50	112.00
2	GGG	301[B]	ID1	C22-C23-N24	-3.89	107.77	110.78
2	EEE	301	ID1	C2-C3-C31	3.64	132.13	124.62
2	DDD	301	ID1	C6-C5-N4	-3.43	105.40	112.00
2	BBB	301	ID1	C23-N24-C25	3.39	121.46	117.22
2	FFF	301[A]	ID1	C23-N24-C25	3.13	121.13	117.22
2	BBB	301	ID1	C22-C23-N24	3.12	113.19	110.78
2	HHH	301	ID1	O62-C61-C62	-3.05	100.71	109.74
2	EEE	301	ID1	C6-C5-N4	-3.02	106.19	112.00
2	GGG	301[B]	ID1	C23-N24-C25	2.48	120.32	117.22
2	CCC	301	ID1	C2-C3-C31	2.42	129.62	124.62
2	FFF	301[B]	ID1	C2-C3-C31	-2.35	119.77	124.62
2	GGG	301[B]	ID1	C1-C2-C3	2.34	102.50	100.31
2	DDD	301	ID1	C22-C23-N24	-2.33	108.98	110.78
2	HHH	301	ID1	C1-C2-C3	-2.30	98.15	100.31
2	EEE	301	ID1	C23-N24-C25	2.29	120.08	117.22
2	FFF	301[A]	ID1	C2-C3-C31	2.23	129.22	124.62
2	HHH	301	ID1	C6-C5-N4	2.21	116.25	112.00
2	DDD	301	ID1	C23-N24-C25	2.19	119.96	117.22
2	CCC	301	ID1	C23-N24-C25	2.16	119.92	117.22
2	EEE	301	ID1	O7-C7-C6	-2.09	119.94	125.23
2	HHH	301	ID1	C2-C3-C31	-2.06	120.36	124.62
2	CCC	301	ID1	C1-C2-C3	2.05	102.22	100.31

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	301	ID1	C1-C5-C6-C7
2	AAA	301	ID1	S21-C22-C23-N24
2	AAA	301	ID1	C22-C23-N24-C25
2	BBB	301	ID1	C3-C2-S21-C22
2	BBB	301	ID1	C1-C5-C6-C7
2	BBB	301	ID1	C7-C6-C61-C62

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Mol	Chain	Res	Type	Atoms
2	BBB	301	ID1	S21-C22-C23-N24
2	CCC	301	ID1	C1-C5-C6-C7
2	CCC	301	ID1	C7-C6-C61-C62
2	CCC	301	ID1	C5-C6-C61-O62
2	CCC	301	ID1	C23-C22-S21-C2
2	CCC	301	ID1	S21-C22-C23-N24
2	DDD	301	ID1	C1-C2-S21-C22
2	DDD	301	ID1	C1-C5-C6-C7
2	DDD	301	ID1	C23-C22-S21-C2
2	DDD	301	ID1	S21-C22-C23-N24
2	EEE	301	ID1	C1-C5-C6-C7
2	EEE	301	ID1	C23-C22-S21-C2
2	EEE	301	ID1	S21-C22-C23-N24
2	FFF	301[A]	ID1	C1-C2-S21-C22
2	FFF	301[A]	ID1	S21-C22-C23-N24
2	FFF	301[B]	ID1	C7-C6-C61-O62
2	FFF	301[B]	ID1	C7-C6-C61-C62
2	FFF	301[B]	ID1	C5-C6-C61-O62
2	FFF	301[B]	ID1	C5-C6-C61-C62
2	FFF	301[B]	ID1	C23-C22-S21-C2
2	GGG	301[A]	ID1	C1-C5-C6-C7
2	GGG	301[A]	ID1	C7-C6-C61-O62
2	GGG	301[A]	ID1	C7-C6-C61-C62
2	GGG	301[A]	ID1	C5-C6-C61-O62
2	GGG	301[A]	ID1	C5-C6-C61-C62
2	GGG	301[B]	ID1	C23-C22-S21-C2
2	GGG	301[B]	ID1	S21-C22-C23-N24
2	HHH	301	ID1	C3-C2-S21-C22
2	HHH	301	ID1	C1-C5-C6-C7
2	HHH	301	ID1	C23-C22-S21-C2
3	GGG	303	1BO	C1-C2-C3-C4
3	HHH	302	1BO	C1-C2-C3-C4
3	BBB	302	1BO	C2-C3-C4-OH
3	BBB	303	1BO	C2-C3-C4-OH
3	EEE	302	1BO	C2-C3-C4-OH
3	CCC	302	1BO	C1-C2-C3-C4
3	CCC	302	1BO	C2-C3-C4-OH
3	FFF	302	1BO	C2-C3-C4-OH
2	CCC	301	ID1	C7-C6-C61-O62
3	AAA	303	1BO	C1-C2-C3-C4
2	FFF	301[B]	ID1	C22-C23-N24-C25
2	FFF	301[A]	ID1	C1-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
2	FFF	301[B]	ID1	C1-C5-C6-C7
2	GGG	301[B]	ID1	C1-C5-C6-C7
3	AAA	302	1BO	C1-C2-C3-C4
2	HHH	301	ID1	C22-C23-N24-C25
2	GGG	301[A]	ID1	C2-C3-C31-O32
2	BBB	301	ID1	C23-C22-S21-C2
2	GGG	301[A]	ID1	C1-C5-C6-C61
2	AAA	301	ID1	N4-C3-C31-O32
2	GGG	301[A]	ID1	N4-C3-C31-O32
2	BBB	301	ID1	C5-C6-C7-O7
2	GGG	301[A]	ID1	C5-C6-C7-O7
2	GGG	301[B]	ID1	C1-C2-S21-C22
2	BBB	301	ID1	C7-C6-C61-O62
3	AAA	303	1BO	C2-C3-C4-OH
3	HHH	303	1BO	C1-C2-C3-C4
3	EEE	302	1BO	C1-C2-C3-C4

There are no ring outliers.

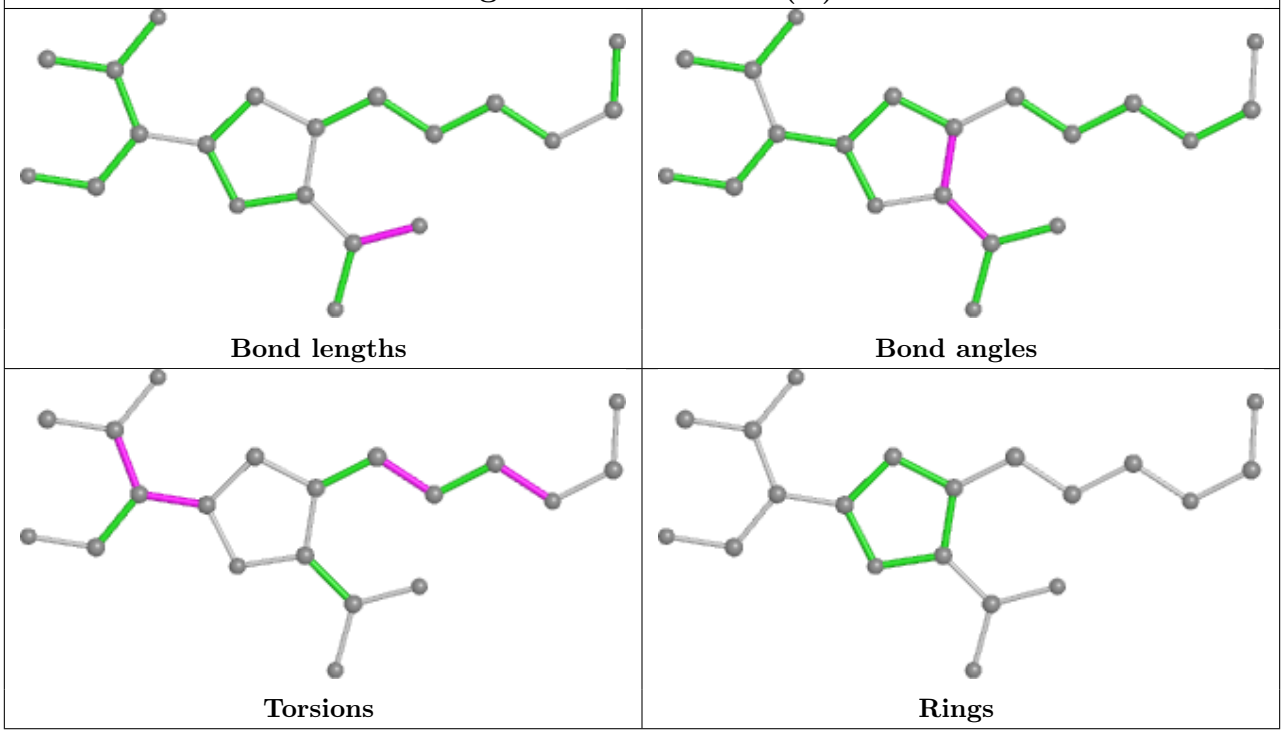
12 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	FFF	301[B]	ID1	1	0
2	BBB	301	ID1	6	0
2	AAA	301	ID1	1	0
2	FFF	301[A]	ID1	1	0
2	CCC	301	ID1	2	0
3	GGG	302	1BO	1	0
2	GGG	301[B]	ID1	2	0
3	BBB	302	1BO	2	0
3	AAA	302	1BO	4	0
2	HHH	301	ID1	3	0
2	EEE	301	ID1	1	0
2	GGG	301[A]	ID1	1	0

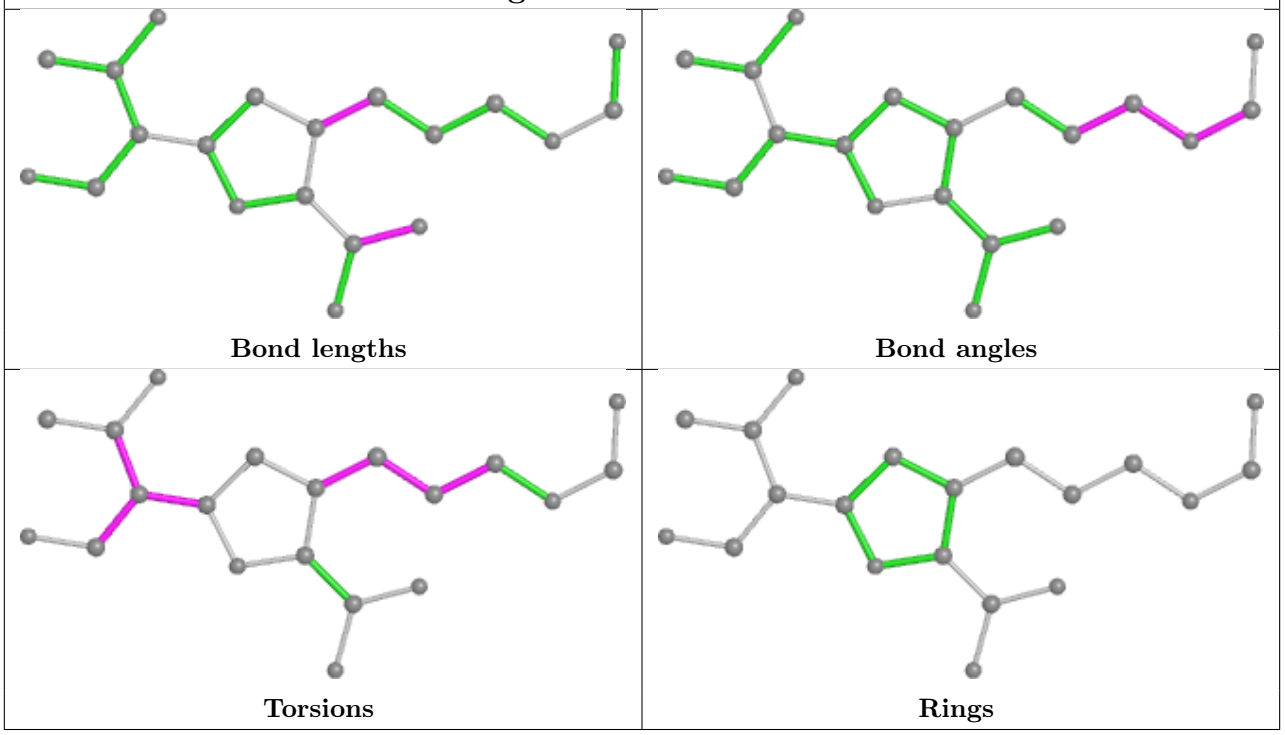
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

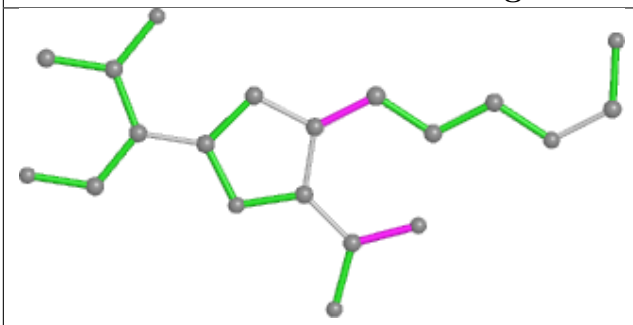
Ligand ID1 FFF 301 (B)



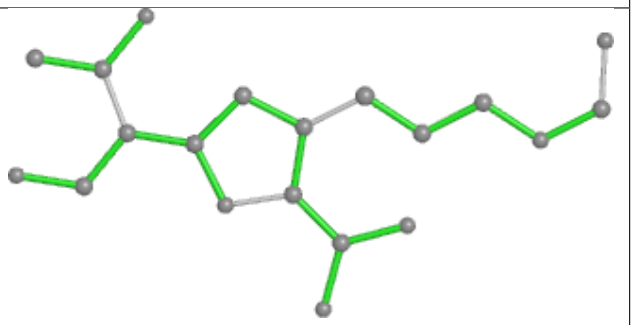
Ligand ID1 BBB 301



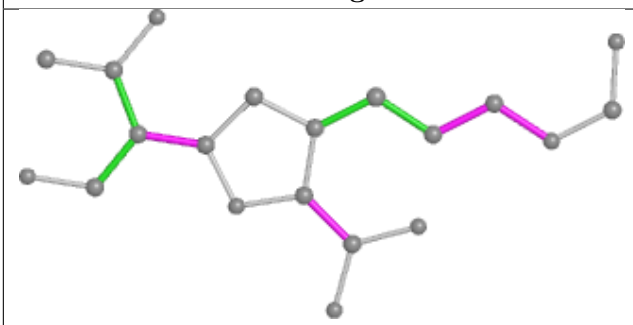
Ligand ID1 AAA 301



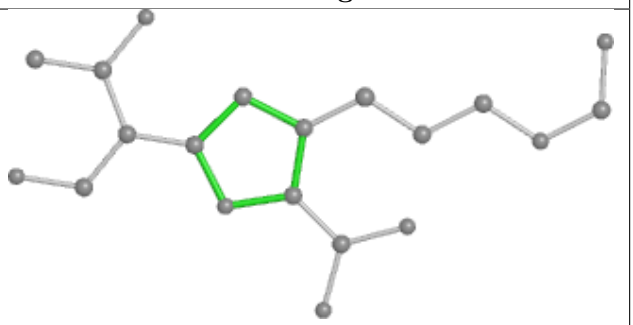
Bond lengths



Bond angles

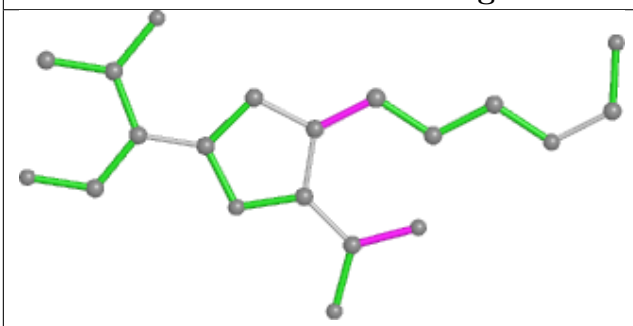


Torsions

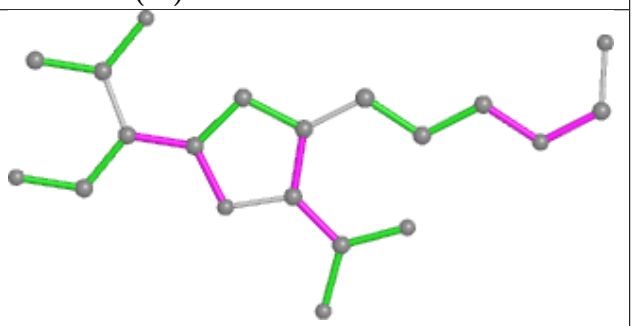


Rings

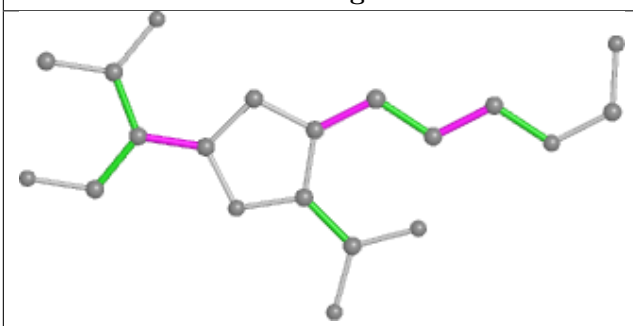
Ligand ID1 FFF 301 (A)



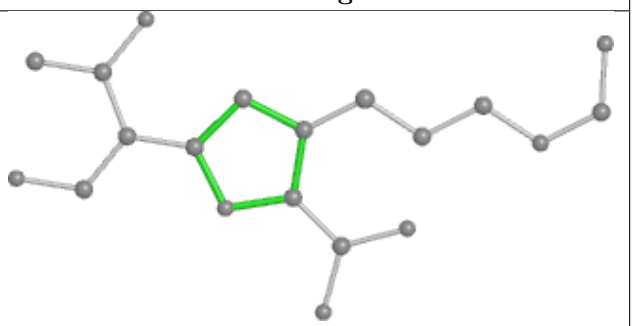
Bond lengths



Bond angles

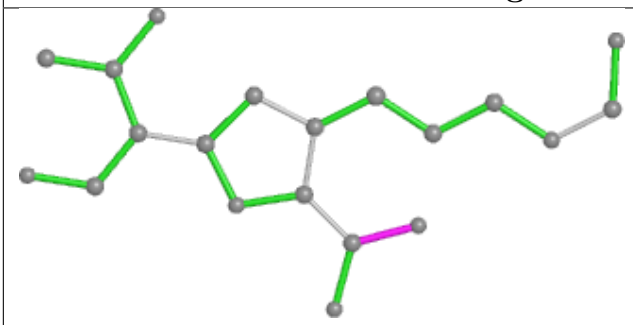


Torsions

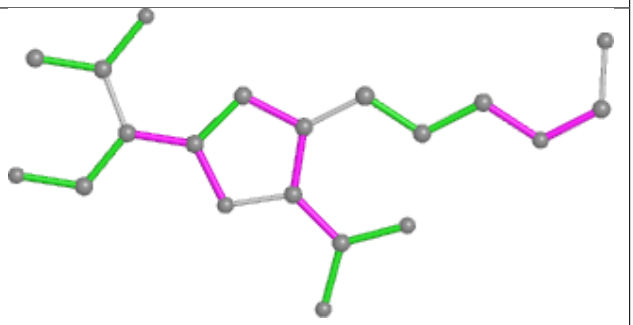


Rings

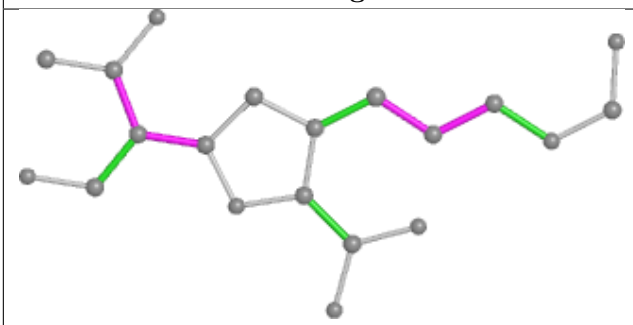
Ligand ID1 CCC 301



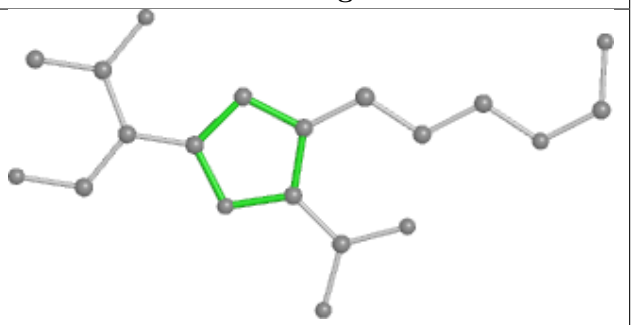
Bond lengths



Bond angles

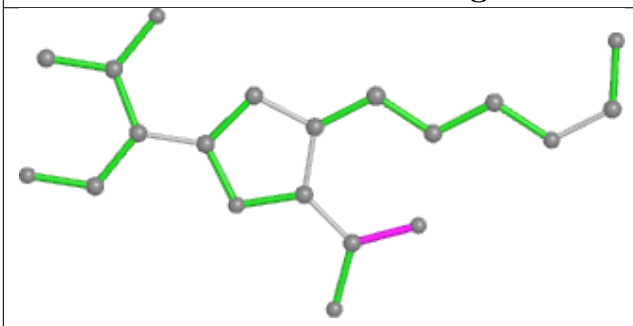


Torsions

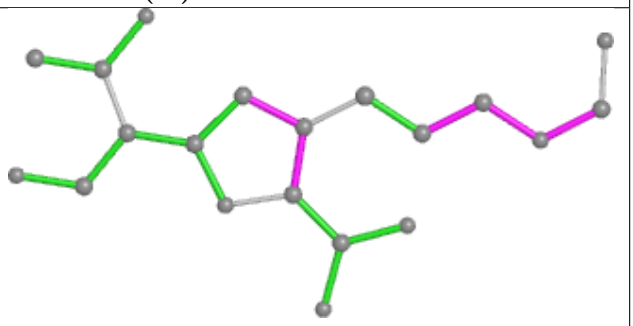


Rings

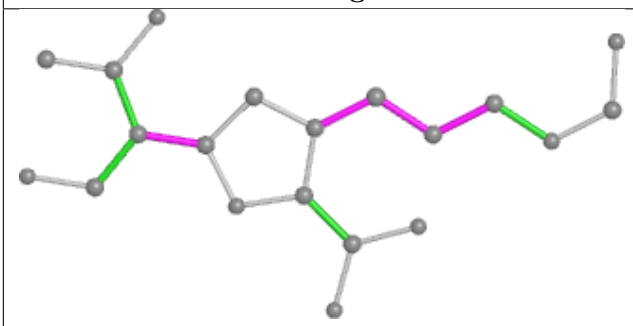
Ligand ID1 GGG 301 (B)



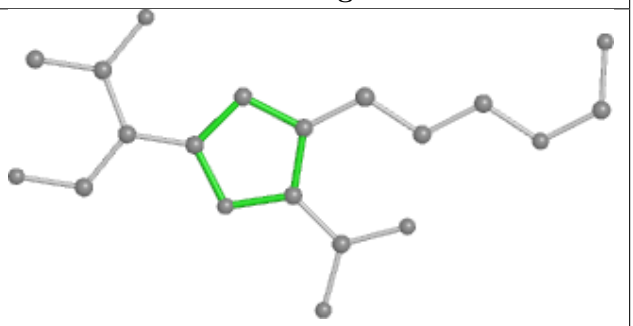
Bond lengths



Bond angles

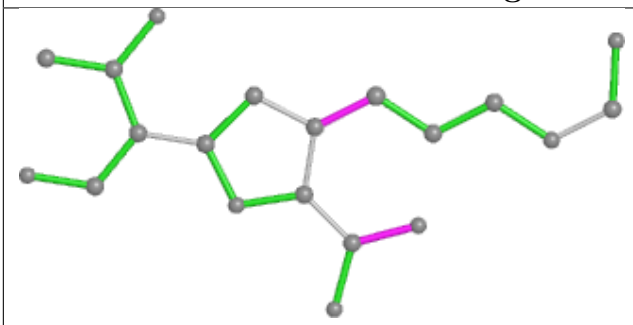


Torsions

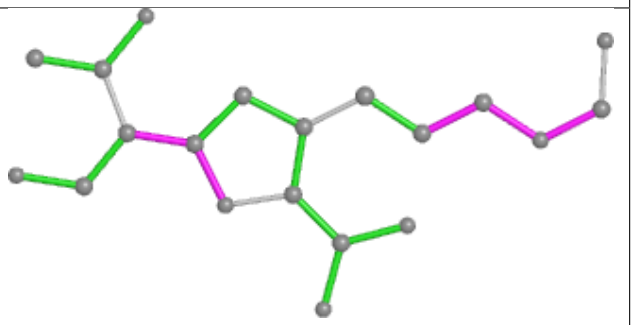


Rings

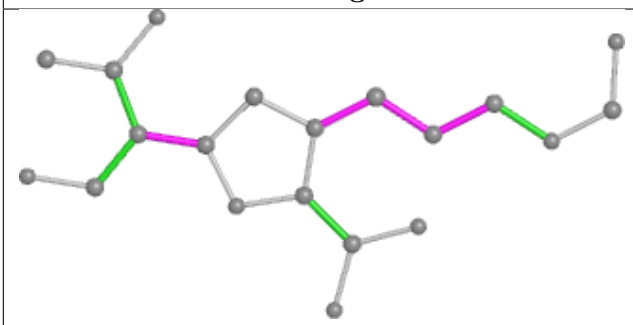
Ligand ID1 DDD 301



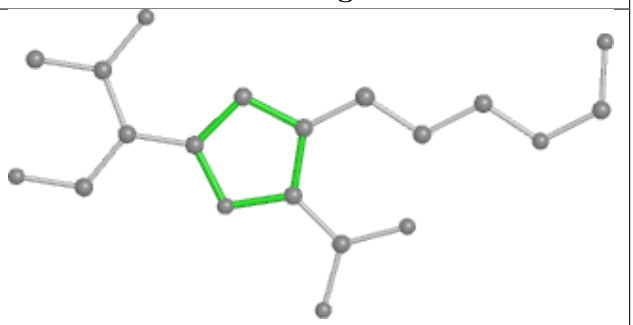
Bond lengths



Bond angles

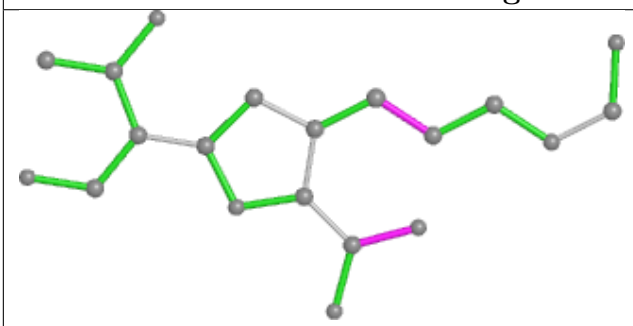


Torsions

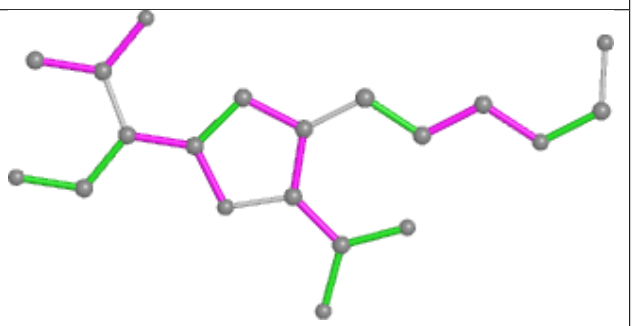


Rings

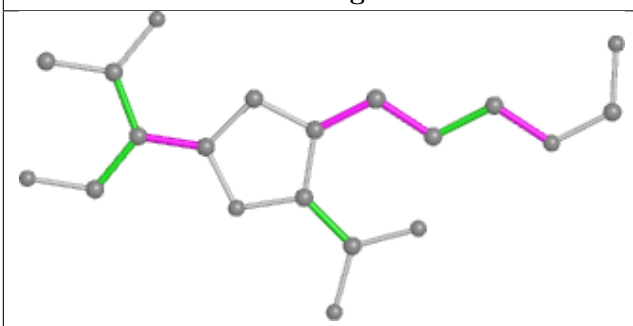
Ligand ID1 HHH 301



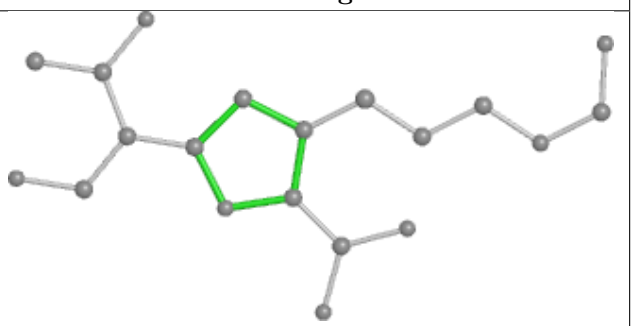
Bond lengths



Bond angles

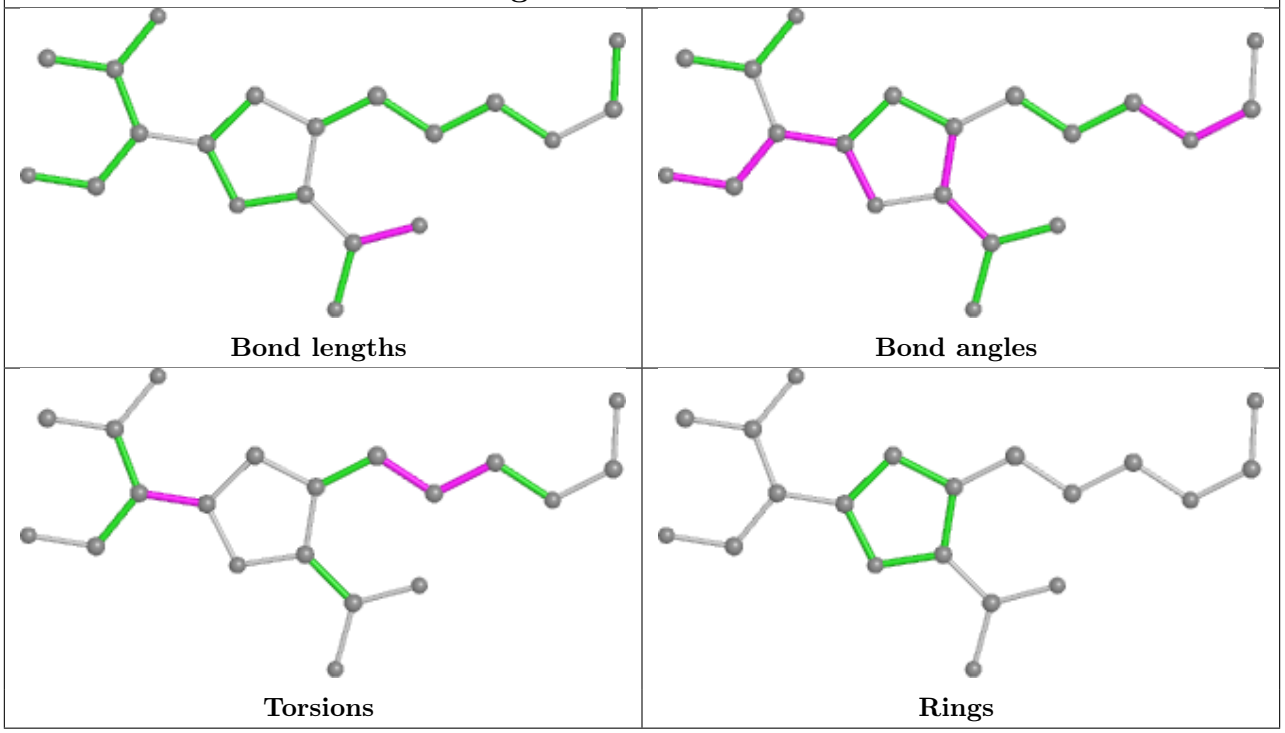


Torsions

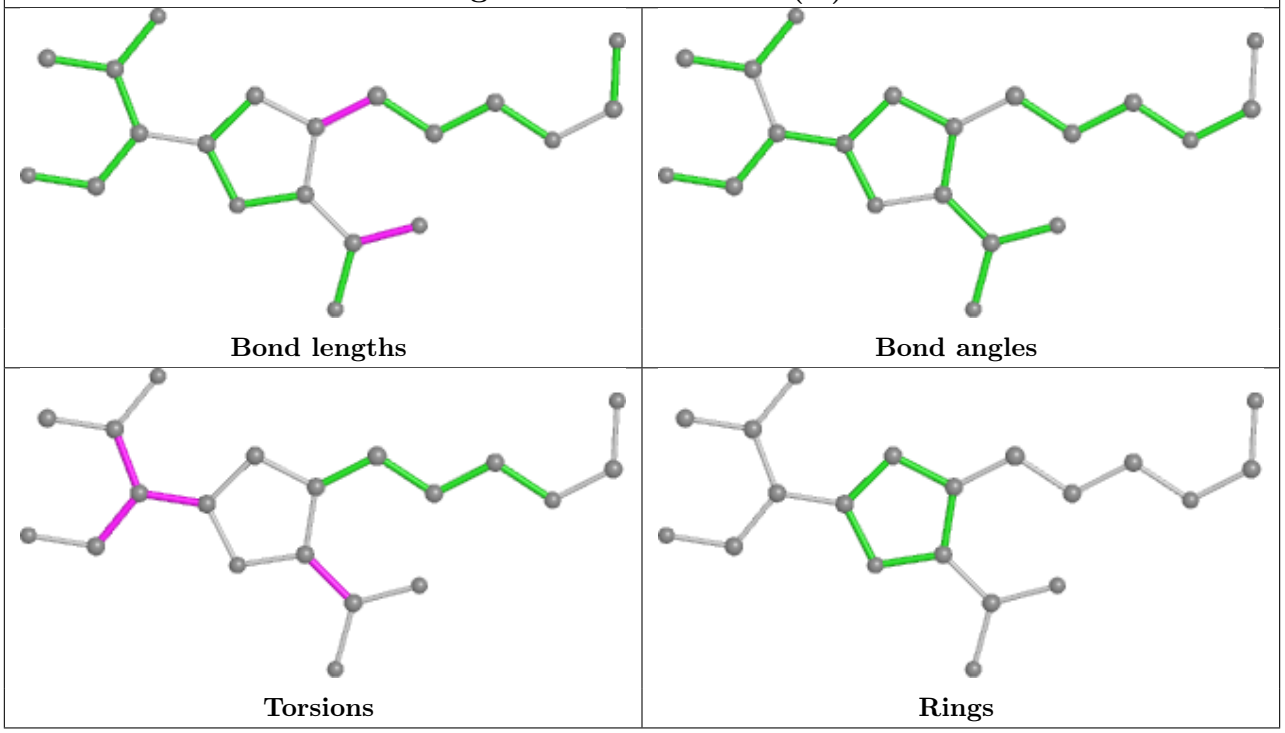


Rings

Ligand ID1 EEE 301



Ligand ID1 GGG 301 (A)



5.7 Other polymers

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^{th} 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	235/260 (90%)	-0.05	6 (2%) 56 64	22, 32, 64, 116	7 (2%)
1	BBB	234/260 (90%)	-0.09	4 (1%) 70 76	22, 33, 63, 105	6 (2%)
1	CCC	242/260 (93%)	0.12	3 (1%) 79 83	27, 47, 78, 92	22 (9%)
1	DDD	241/260 (92%)	0.11	8 (3%) 46 55	27, 47, 84, 125	16 (6%)
1	EEE	241/260 (92%)	-0.01	1 (0%) 92 94	26, 45, 76, 97	17 (7%)
1	FFF	241/260 (92%)	0.25	10 (4%) 37 46	28, 53, 88, 112	22 (9%)
1	GGG	242/260 (93%)	-0.01	2 (0%) 86 89	23, 41, 67, 85	11 (4%)
1	HHH	241/260 (92%)	-0.11	0 100 100	23, 38, 63, 82	10 (4%)
All	All	1917/2080 (92%)	0.03	34 (1%) 68 75	22, 42, 78, 125	111 (5%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	158	LEU	7.7
1	AAA	158	LEU	6.8
1	DDD	246	GLY	4.3
1	BBB	155	SER	4.1
1	AAA	159	ASP	3.8
1	DDD	245	ASP	3.6
1	CCC	102	ILE	3.3
1	DDD	242	PRO	3.2
1	CCC	95	TRP	3.2
1	FFF	243	THR	3.1
1	AAA	161	GLY	3.0
1	DDD	217	PRO	2.9
1	FFF	219	ILE	2.8
1	FFF	245	ASP	2.8
1	FFF	83	LEU	2.7
1	GGG	39	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	FFF	126	PHE	2.7
1	DDD	243	THR	2.7
1	FFF	138	MET	2.6
1	BBB	161	GLY	2.6
1	FFF	217	PRO	2.5
1	BBB	157	TRP	2.4
1	FFF	249	LEU	2.4
1	FFF	149	ILE	2.3
1	CCC	131	GLY	2.2
1	AAA	154	ASP	2.2
1	FFF	242	PRO	2.2
1	DDD	249	LEU	2.1
1	GGG	29	LYS	2.1
1	DDD	244	SER	2.1
1	DDD	215	ILE	2.1
1	EEE	246	GLY	2.1
1	AAA	160	GLY	2.0
1	AAA	23	LYS	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^{th} 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	ALY	CCC	73	12/13	0.95	0.11	38,43,48,50	0
1	ALY	FFF	73	12/13	0.95	0.12	34,38,58,58	0
1	ALY	DDD	73	12/13	0.96	0.11	34,39,46,47	0
1	ALY	BBB	73	12/13	0.96	0.12	21,26,35,36	0
1	ALY	EEE	73	12/13	0.97	0.11	33,43,49,51	0
1	ALY	AAA	73	12/13	0.97	0.12	18,25,33,34	0
1	ALY	GGG	73	12/13	0.97	0.13	24,28,34,35	0
1	ALY	HHH	73	12/13	0.97	0.12	23,27,29,29	0

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^{th} 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
3	1BO	BBB	304	5/5	0.80	0.20	41,44,45,46	15
3	1BO	HHH	302	5/5	0.82	0.15	33,35,36,36	15
3	1BO	GGG	303	5/5	0.83	0.24	42,43,45,46	15
2	ID1	EEE	301	20/20	0.84	0.20	42,48,53,55	36
3	1BO	AAA	302	5/5	0.85	0.17	34,35,35,36	15
2	ID1	CCC	301	20/20	0.85	0.21	41,48,60,62	35
2	ID1	FFF	301[A]	20/20	0.86	0.25	35,51,57,57	37
2	ID1	FFF	301[B]	20/20	0.86	0.25	42,48,51,54	37
3	1BO	CCC	302	5/5	0.87	0.17	39,40,45,47	15
3	1BO	FFF	302	5/5	0.87	0.33	51,52,53,53	15
3	1BO	HHH	303	5/5	0.87	0.17	35,36,40,40	15
2	ID1	HHH	301	20/20	0.89	0.18	38,47,58,59	27
3	1BO	AAA	303	5/5	0.89	0.15	43,48,50,51	15
2	ID1	DDD	301	20/20	0.90	0.24	49,54,62,62	35
3	1BO	BBB	302	5/5	0.90	0.20	32,34,35,36	15
3	1BO	GGG	302	5/5	0.91	0.18	40,42,44,45	15
2	ID1	BBB	301	20/20	0.91	0.15	34,44,48,51	23
4	BR	HHH	304[A]	1/1	0.91	0.10	43,43,43,43	1
4	BR	HHH	304[B]	1/1	0.91	0.10	45,45,45,45	1
2	ID1	GGG	301[A]	20/20	0.92	0.18	33,36,43,46	37
2	ID1	GGG	301[B]	20/20	0.92	0.18	28,33,36,37	37
2	ID1	AAA	301	20/20	0.92	0.13	30,44,50,65	20
3	1BO	BBB	303	5/5	0.93	0.15	34,41,43,43	13
3	1BO	EEE	302	5/5	0.94	0.18	37,38,39,39	15
4	BR	AAA	305[A]	1/1	0.96	0.13	44,44,44,44	1
4	BR	AAA	305[B]	1/1	0.96	0.13	36,36,36,36	1
4	BR	BBB	307[A]	1/1	0.97	0.13	42,42,42,42	1
4	BR	BBB	307[B]	1/1	0.97	0.13	41,41,41,41	1
4	BR	CCC	304[A]	1/1	0.97	0.09	40,40,40,40	1
4	BR	CCC	304[B]	1/1	0.97	0.09	39,39,39,39	1
4	BR	GGG	304[A]	1/1	0.97	0.09	61,61,61,61	1
4	BR	GGG	304[B]	1/1	0.97	0.09	45,45,45,45	1
4	BR	BBB	306[A]	1/1	0.97	0.11	38,38,38,38	1
4	BR	BBB	306[B]	1/1	0.97	0.11	41,41,41,41	1
4	BR	HHH	305[A]	1/1	0.97	0.07	38,38,38,38	1
4	BR	HHH	305[B]	1/1	0.97	0.07	38,38,38,38	1
4	BR	EEE	303[A]	1/1	0.98	0.09	36,36,36,36	1

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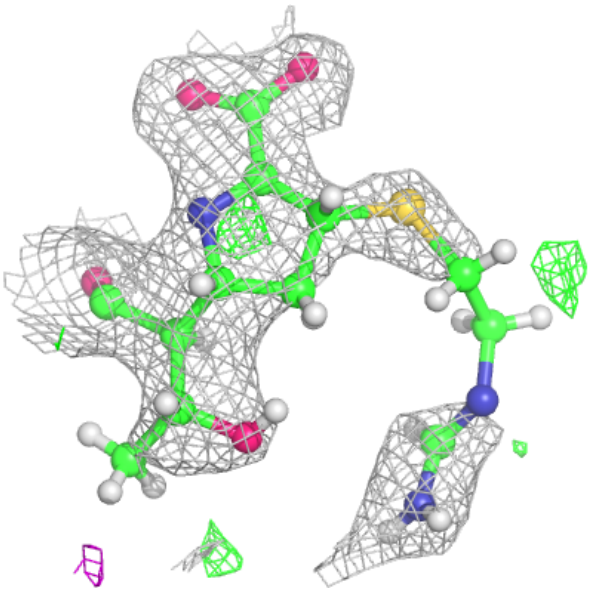
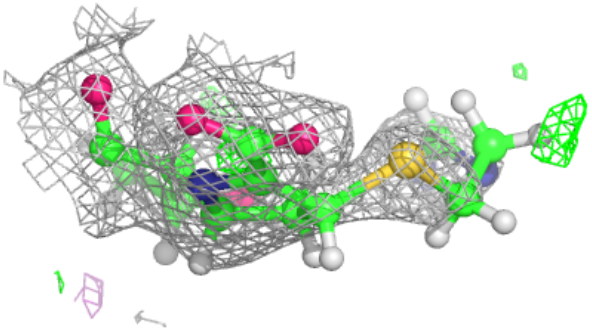
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BR	EEE	303[B]	1/1	0.98	0.09	40,40,40,40	1
4	BR	CCC	303	1/1	0.98	0.10	37,37,37,37	1
4	BR	DDD	302	1/1	0.98	0.11	38,38,38,38	1
4	BR	AAA	304	1/1	0.99	0.11	35,35,35,35	0
4	BR	BBB	305	1/1	0.99	0.11	36,36,36,36	0

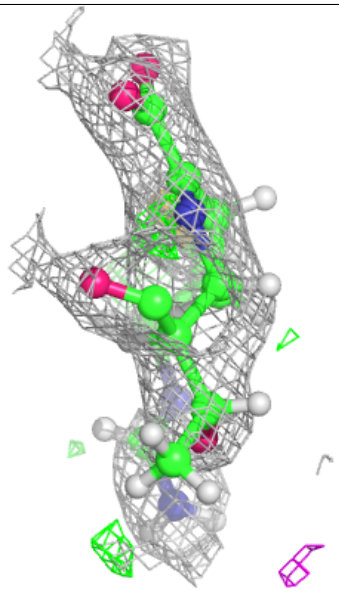
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ID1 EEE 301:

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

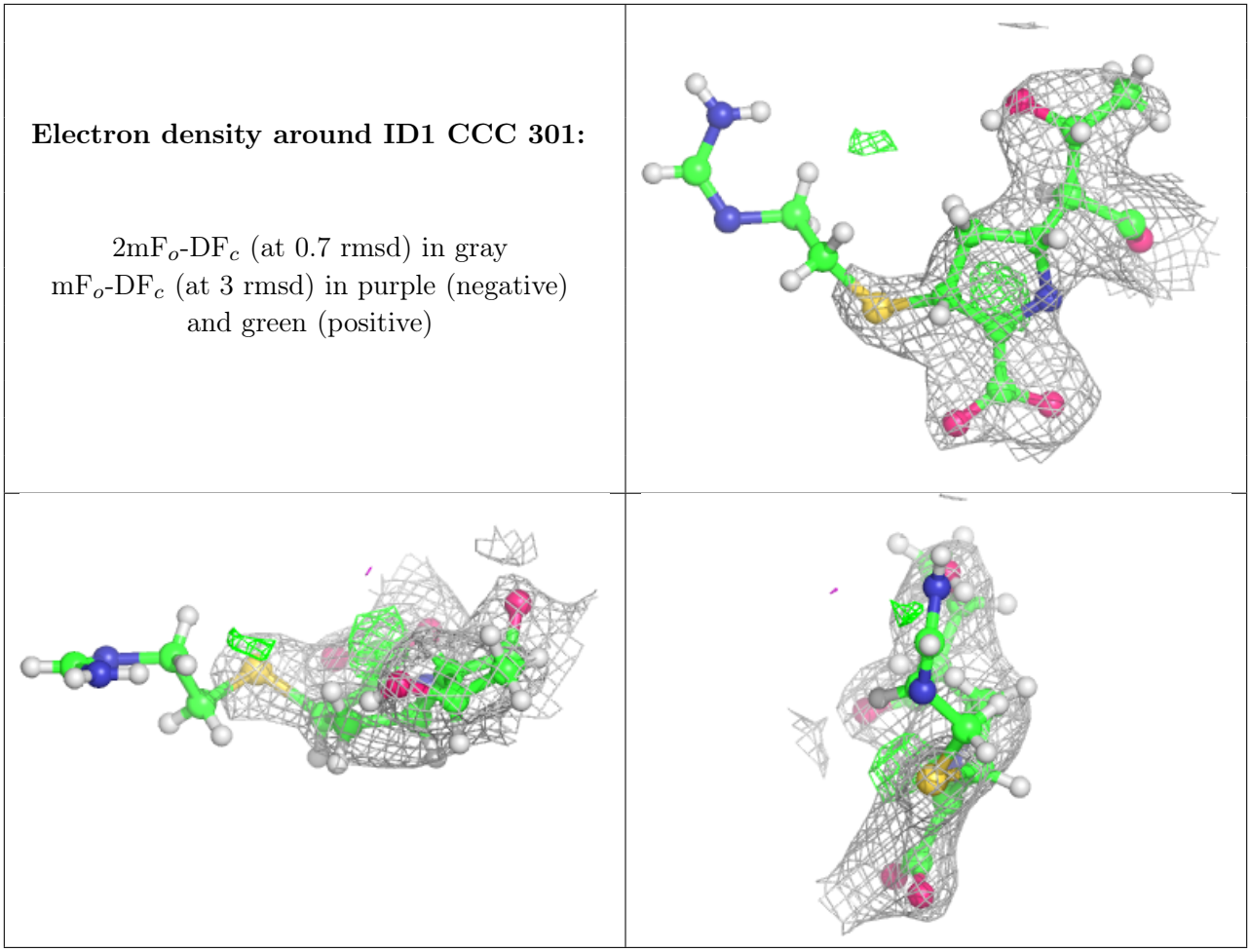






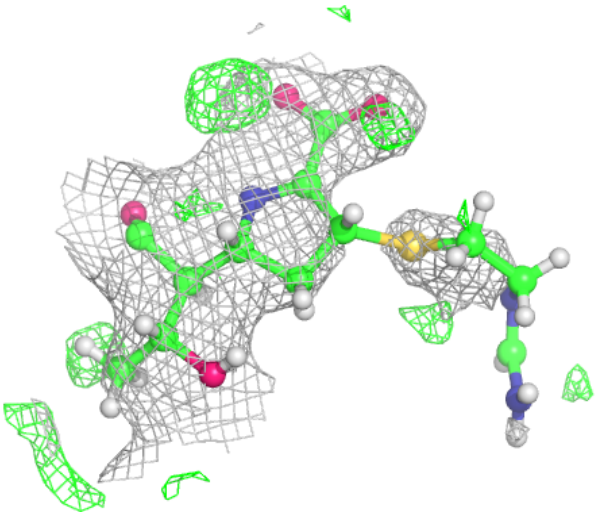
Electron density around ID1 CCC 301:

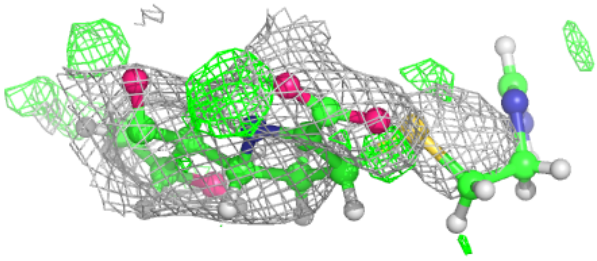
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

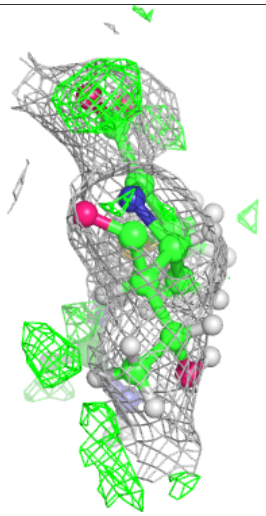


Electron density around ID1 FFF 301 (A):

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

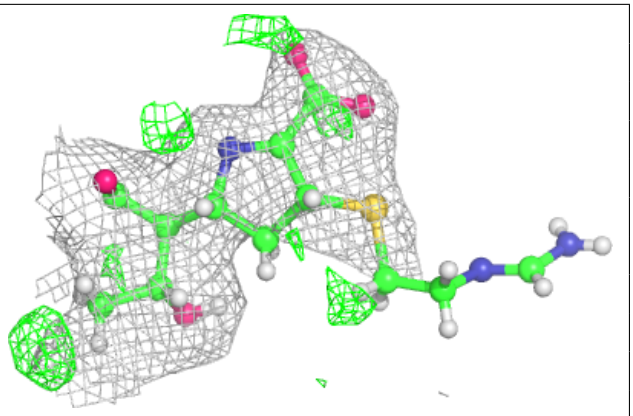


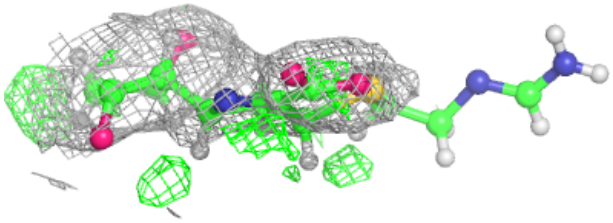


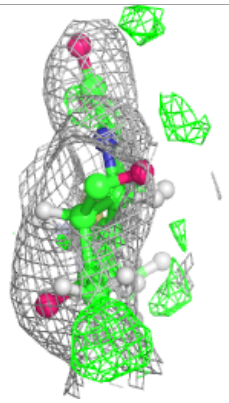


Electron density around ID1 FFF 301 (B):

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

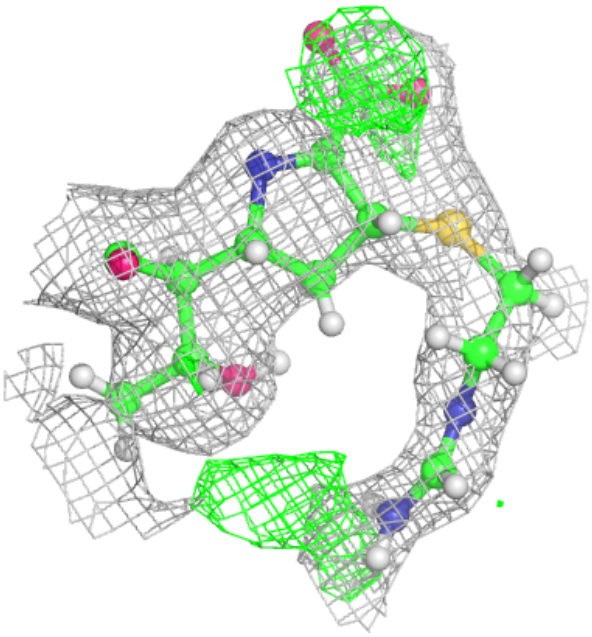


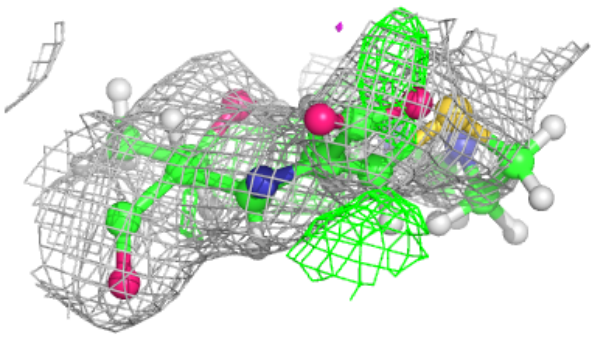


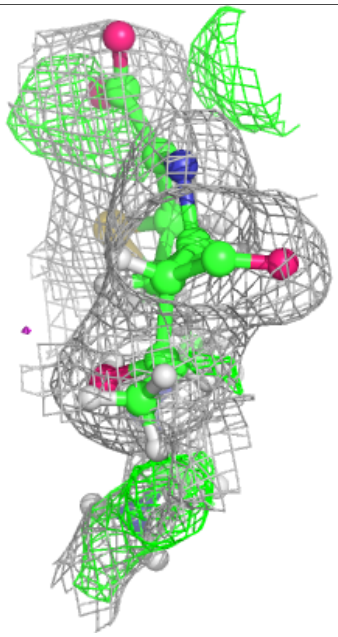


Electron density around ID1 HHH 301:

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

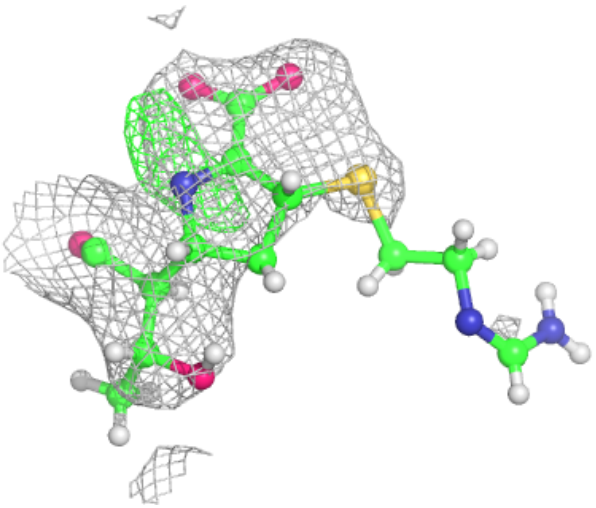


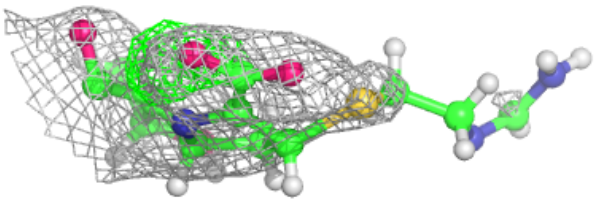


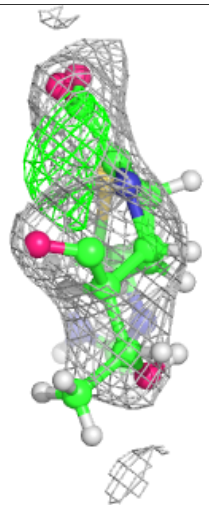


Electron density around ID1 DDD 301:

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

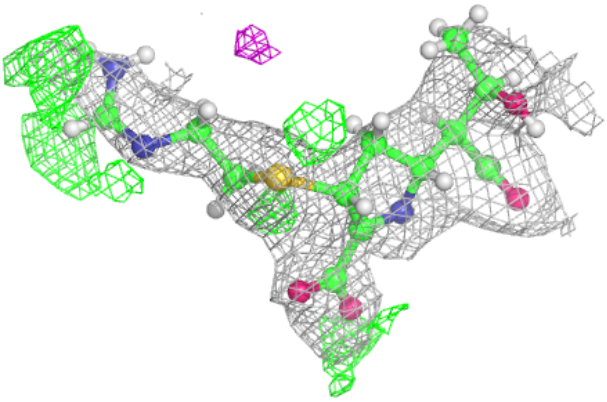


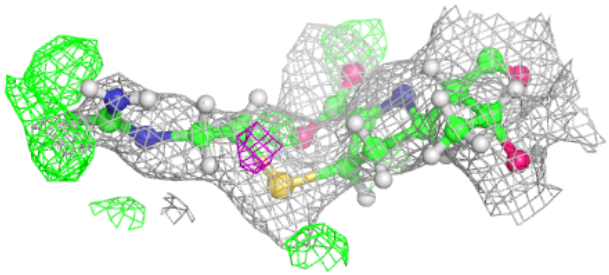


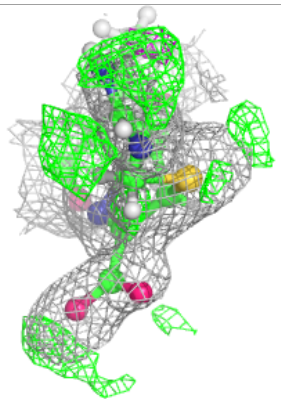


Electron density around ID1 BBB 301:

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

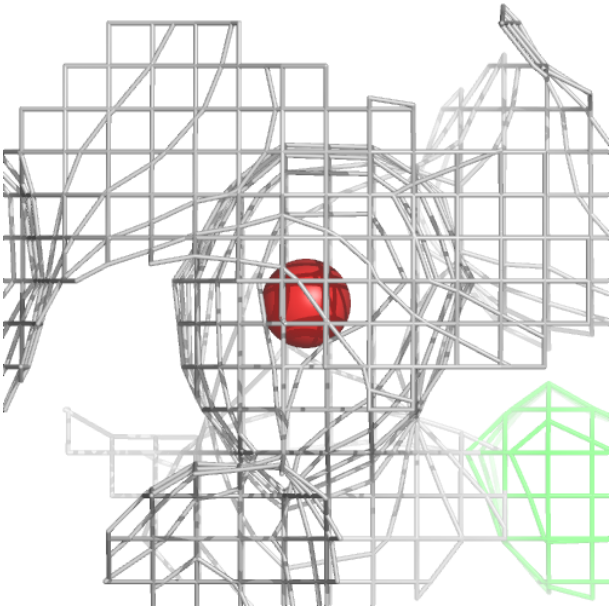


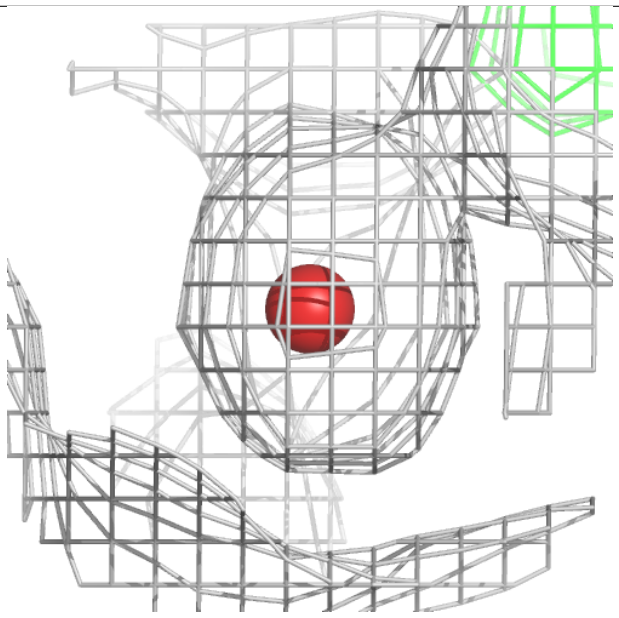


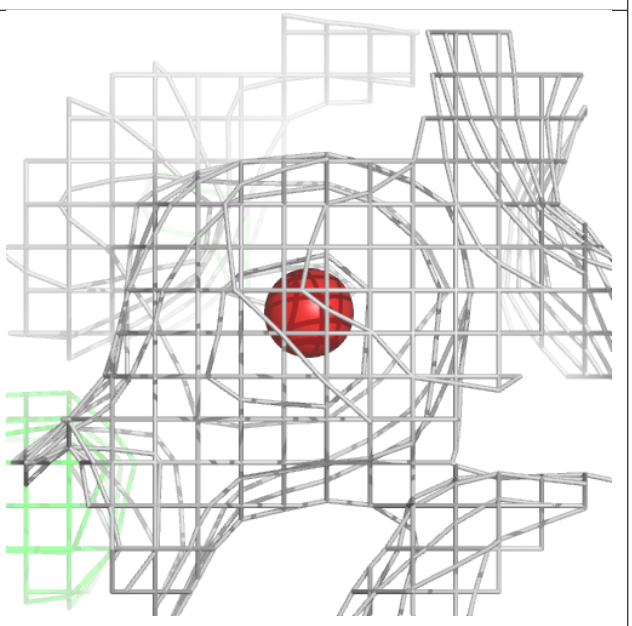


Electron density around BR HHH 304 (A):

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

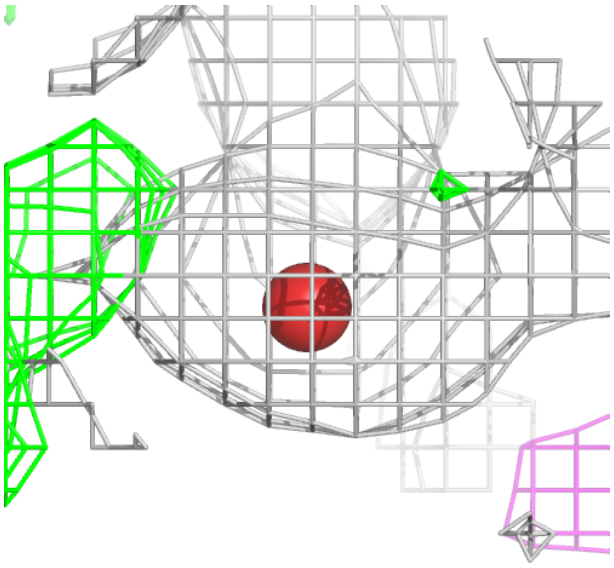


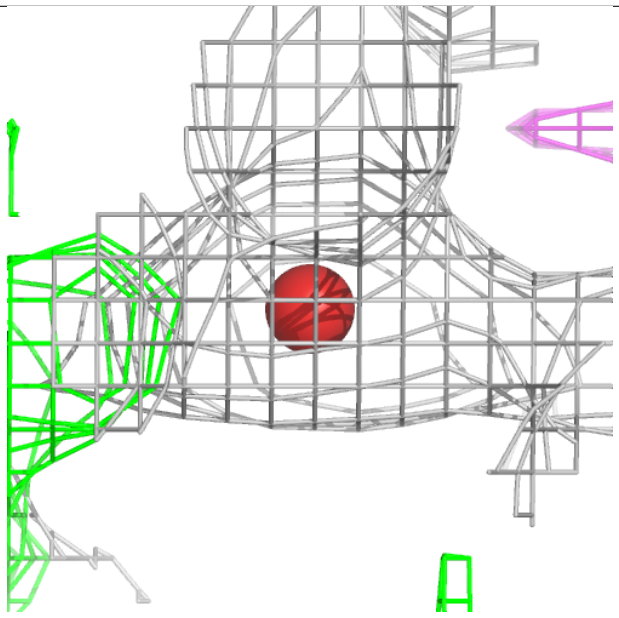


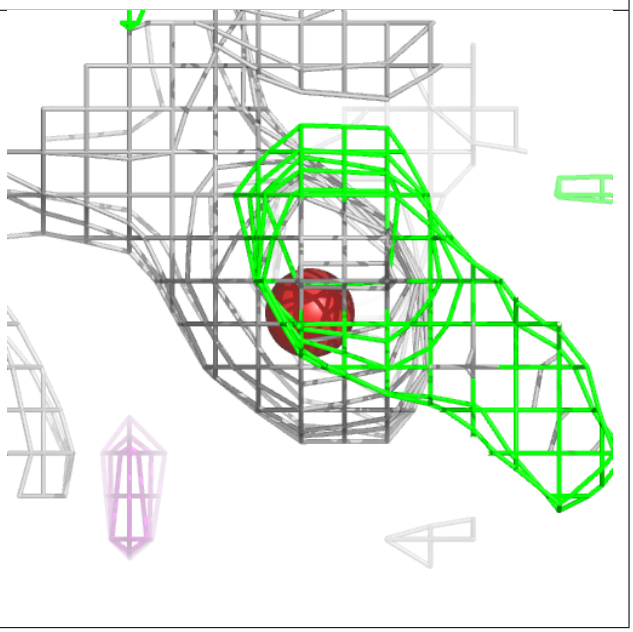


Electron density around BR HHH 304 (B):

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

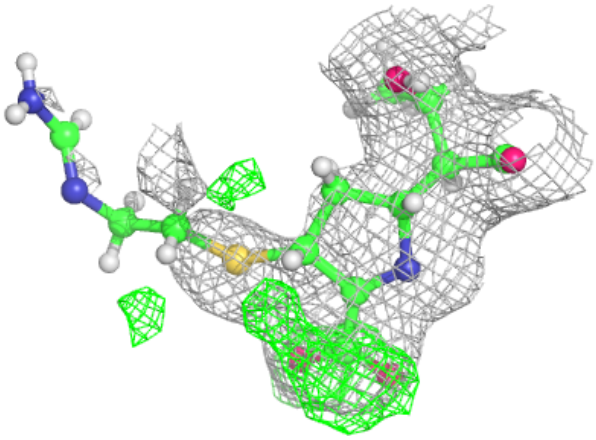


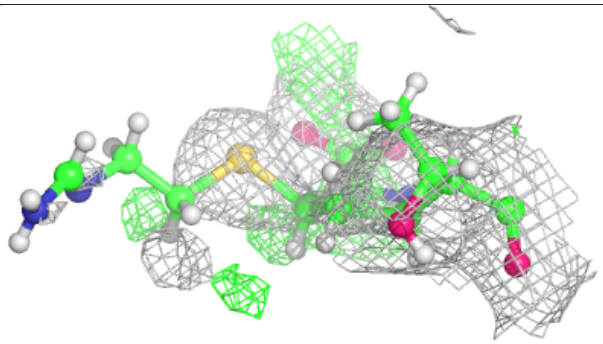


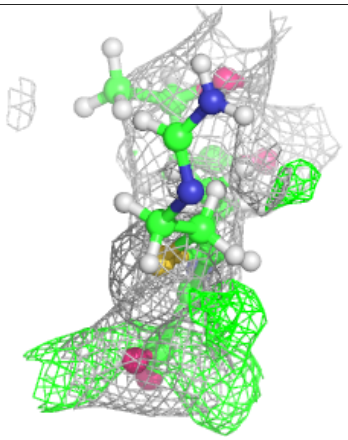


Electron density around ID1 GGG 301 (A):

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

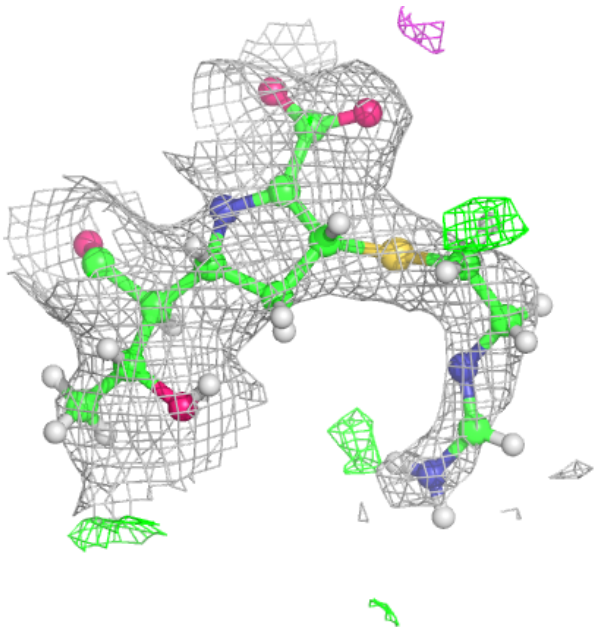


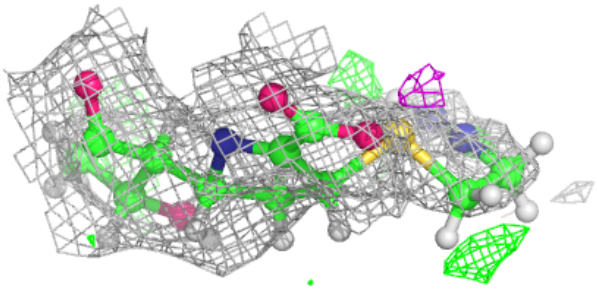


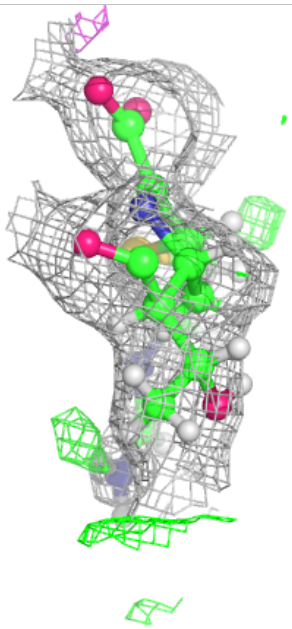


Electron density around ID1 GGG 301 (B):

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

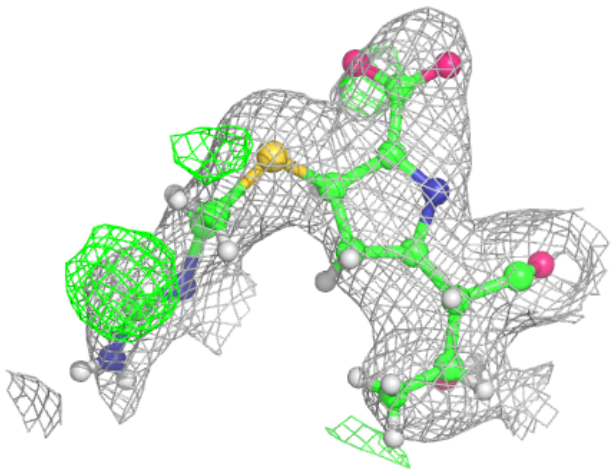


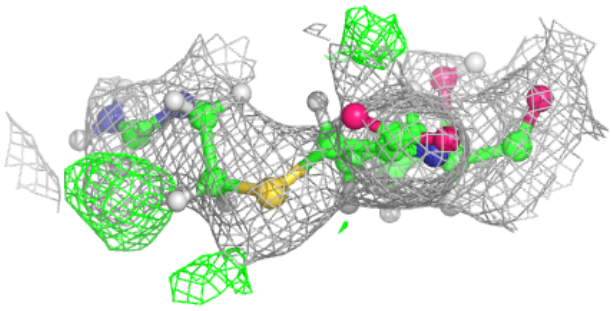


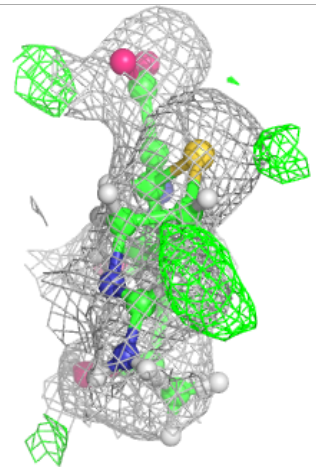


Electron density around ID1 AAA 301:

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

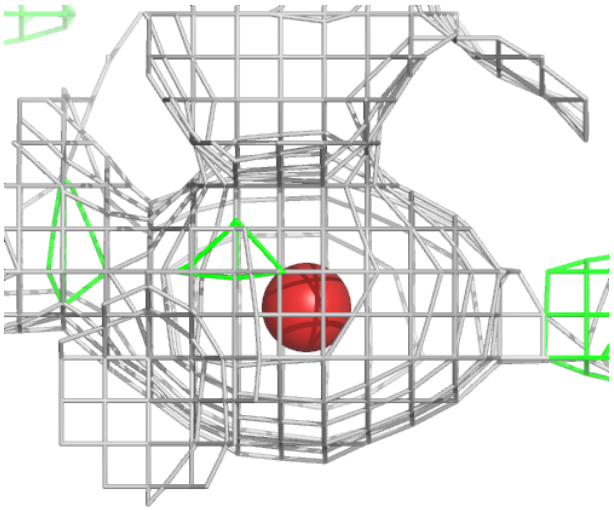


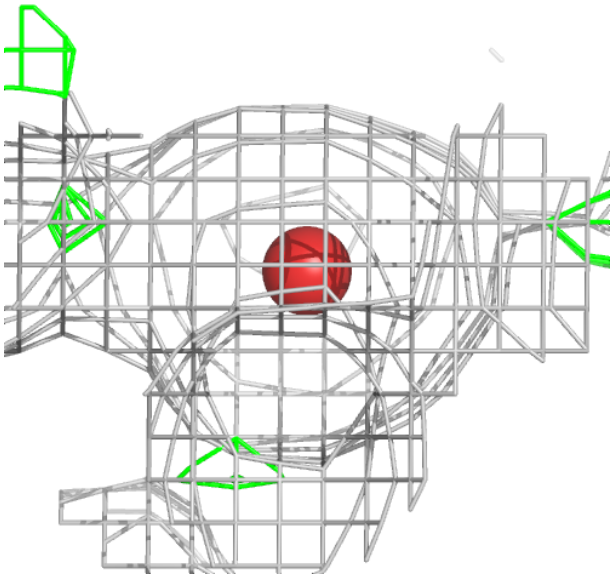


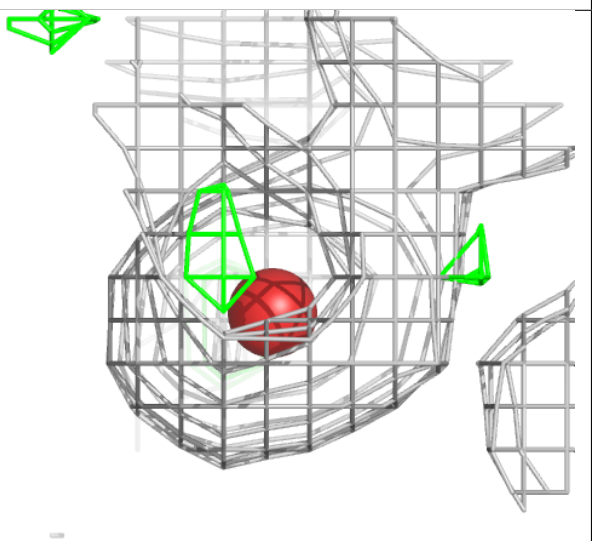


Electron density around BR AAA 305 (A):

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

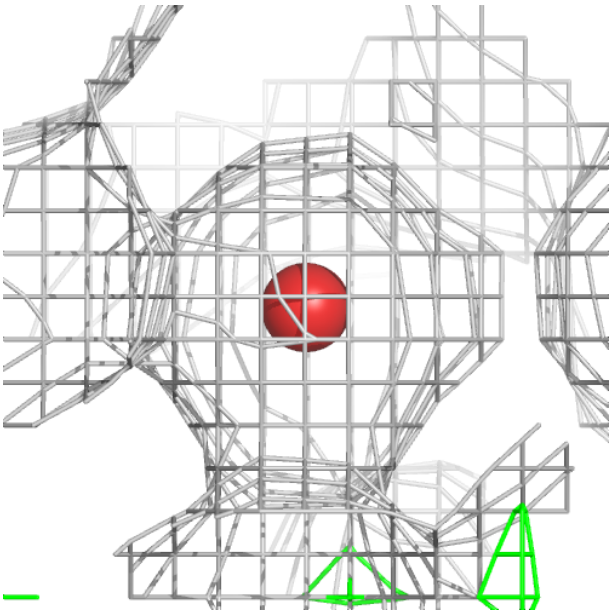


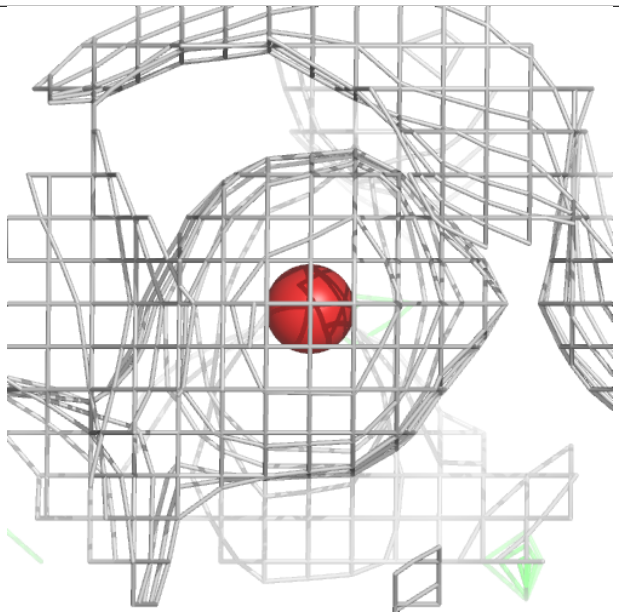


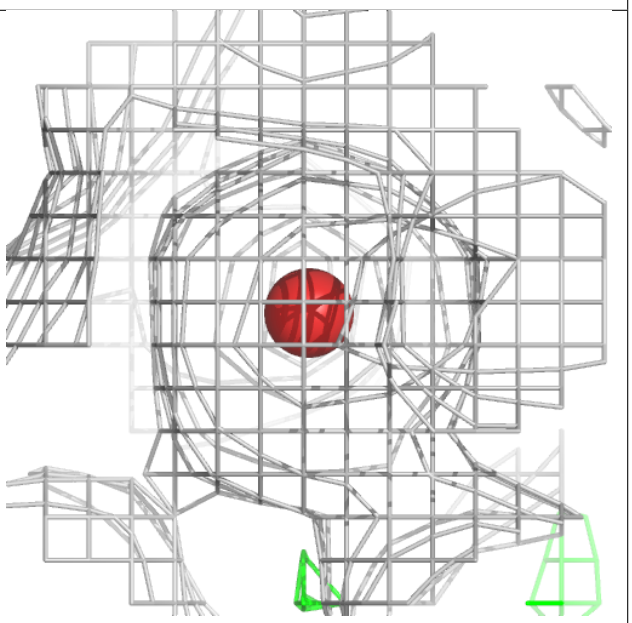


Electron density around BR AAA 305 (B):

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

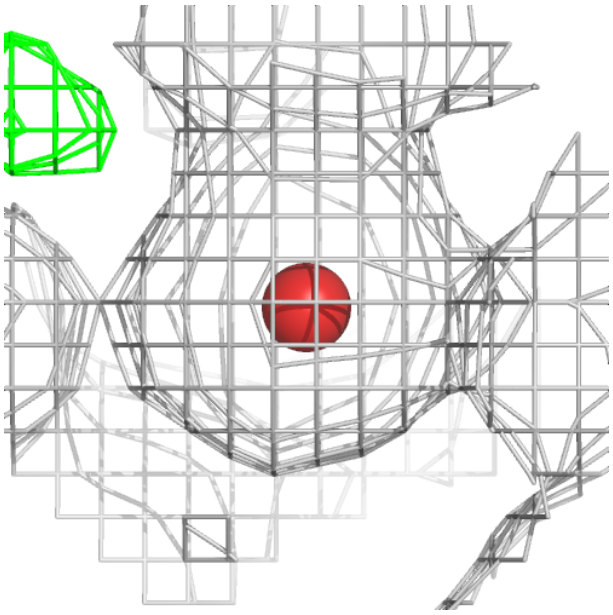


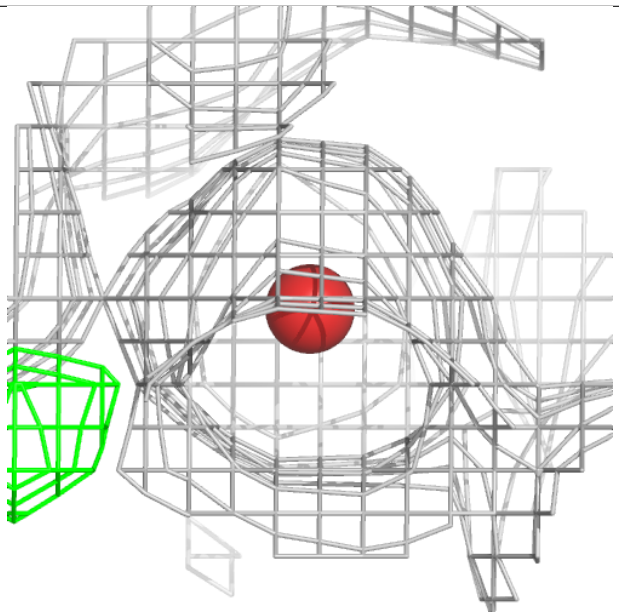


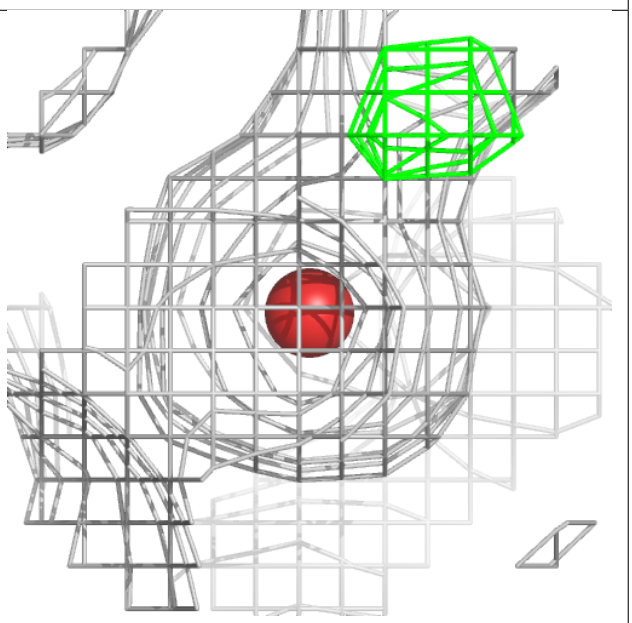


Electron density around BR BBB 307 (A):

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

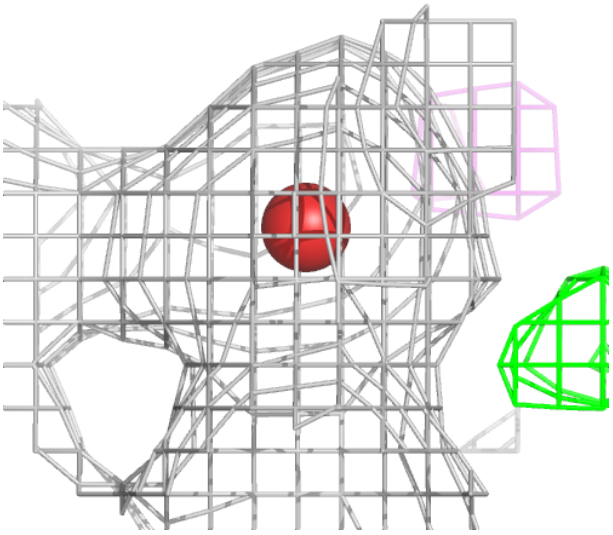


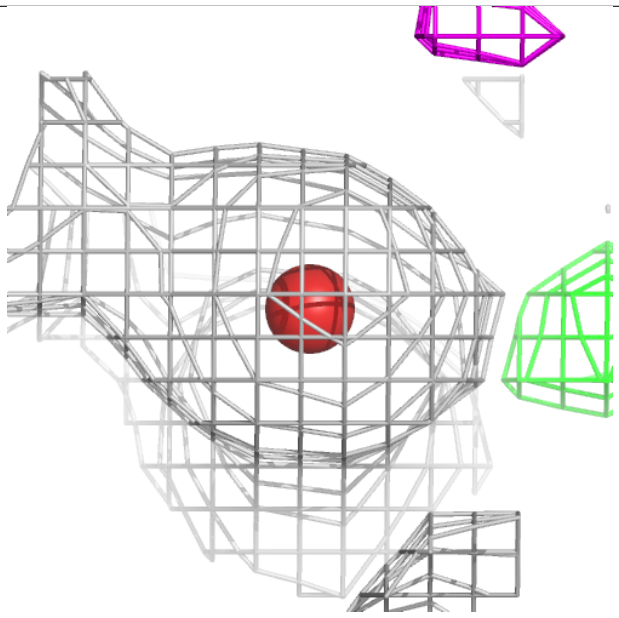


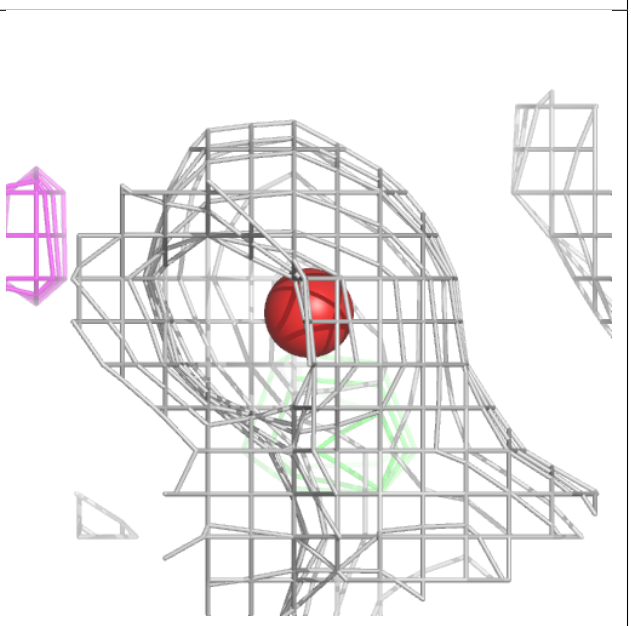


Electron density around BR BBB 307 (B):

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

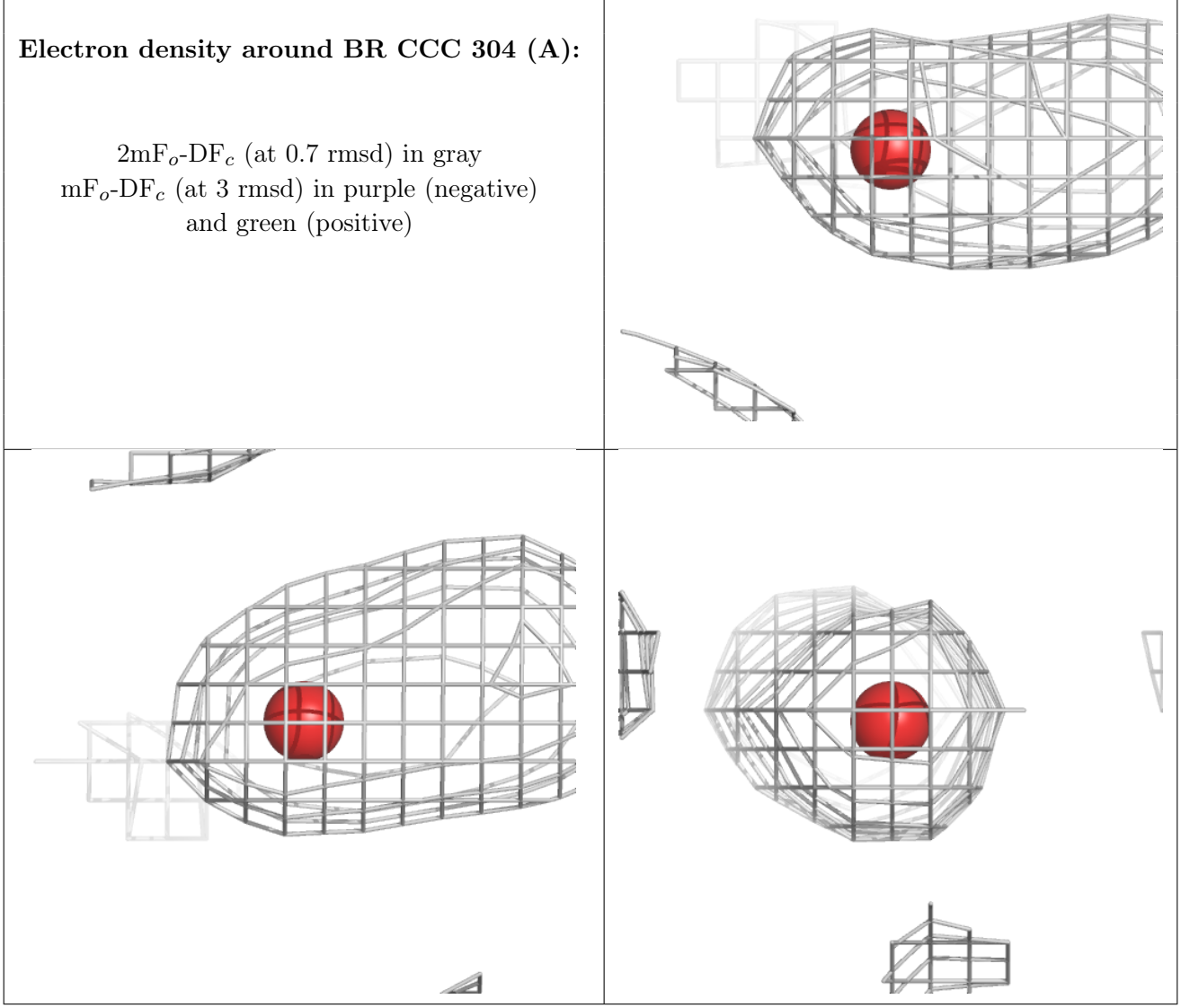






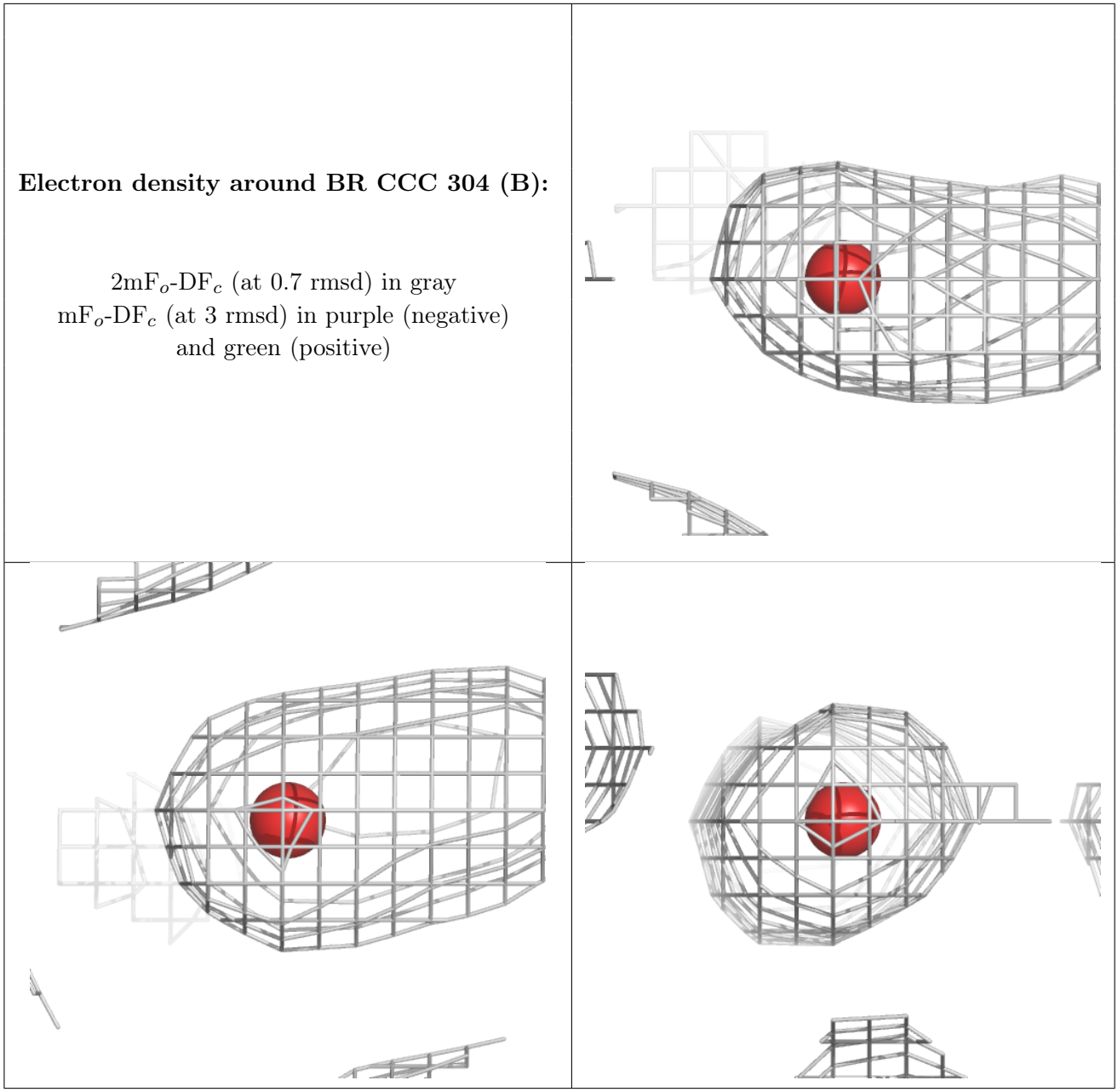
Electron density around BR CCC 304 (A):

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



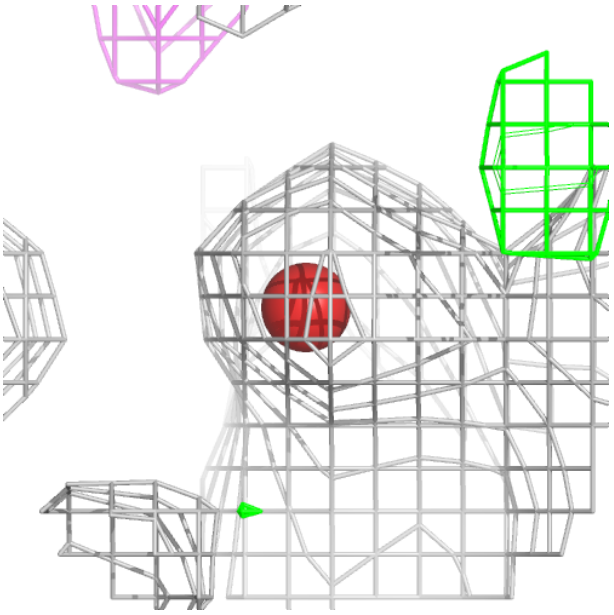
Electron density around BR CCC 304 (B):

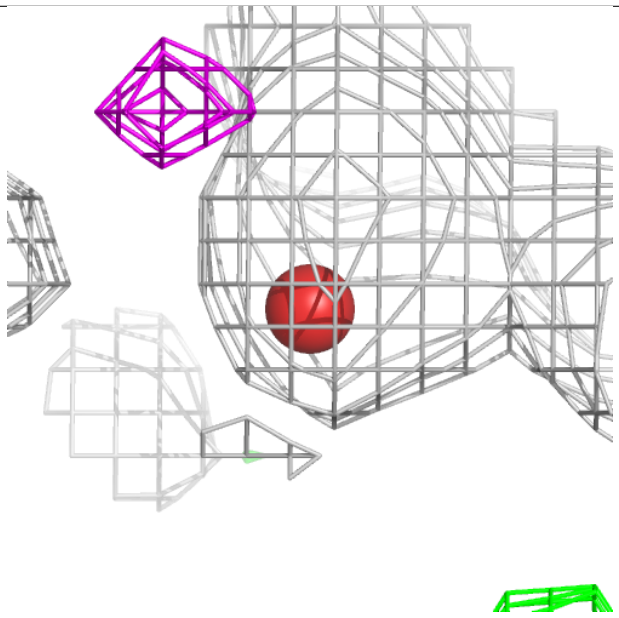
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

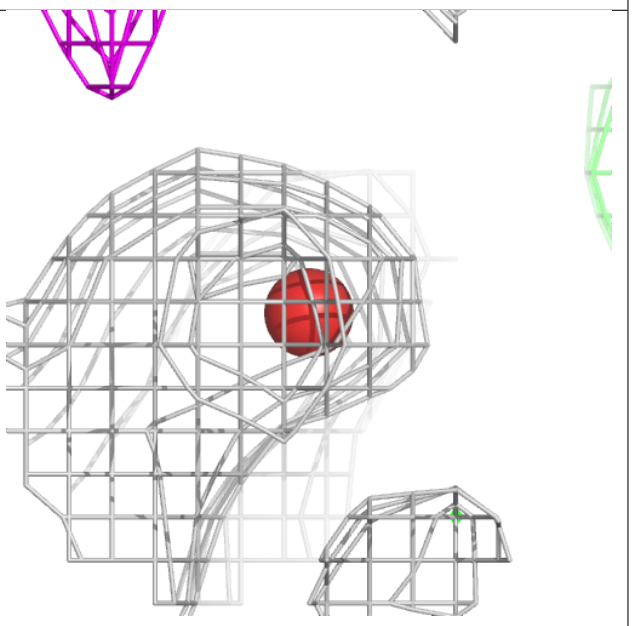


Electron density around BR GGG 304 (A):

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

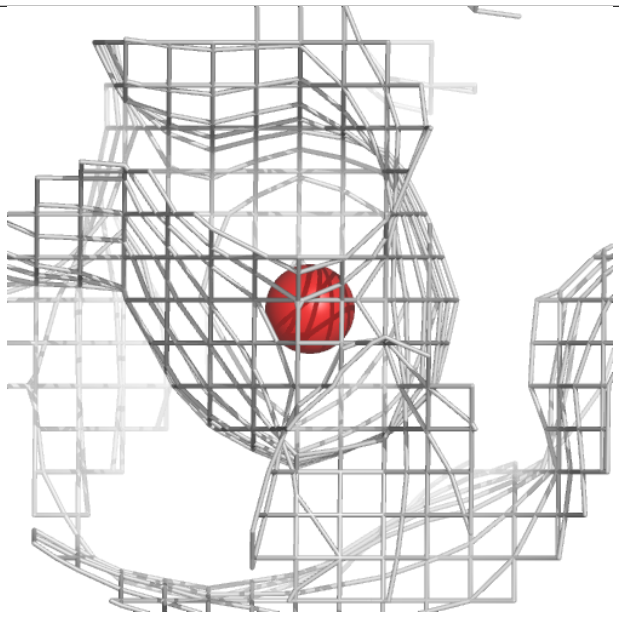


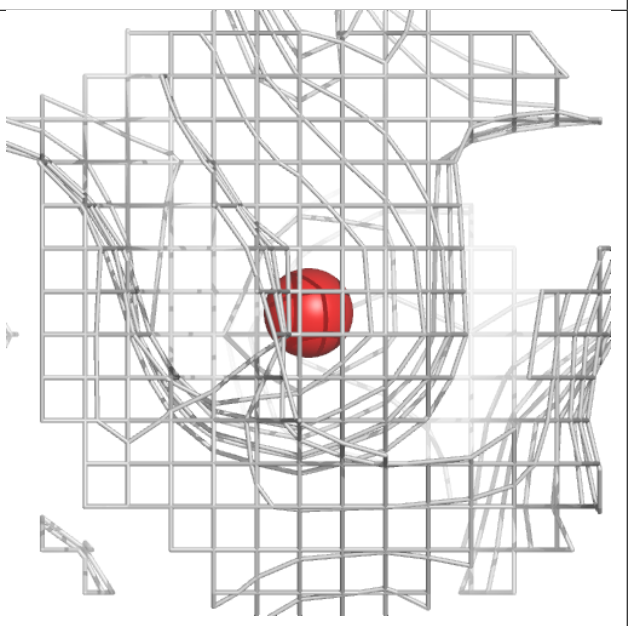




Electron density around BR GGG 304 (B):

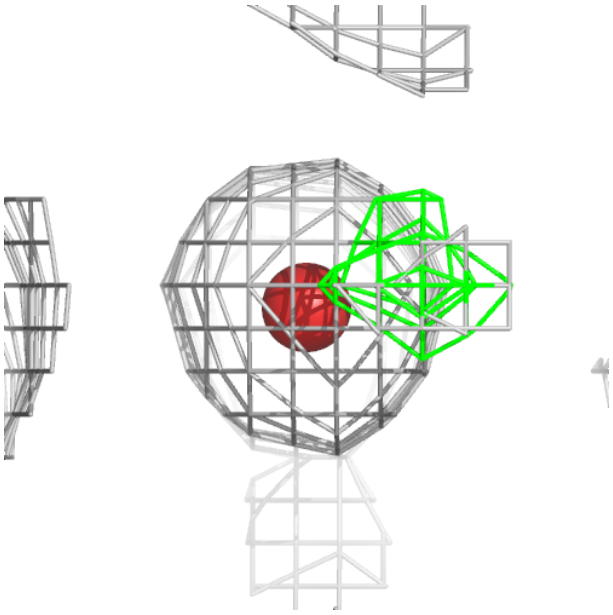
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

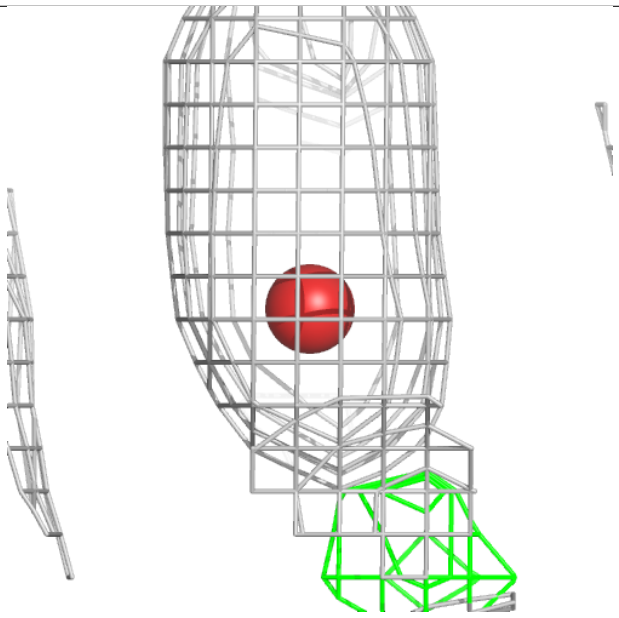


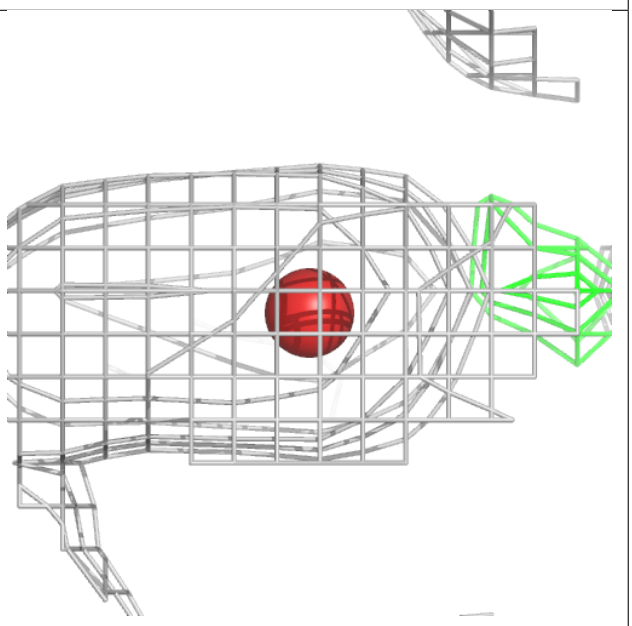


Electron density around BR BBB 306 (A):

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

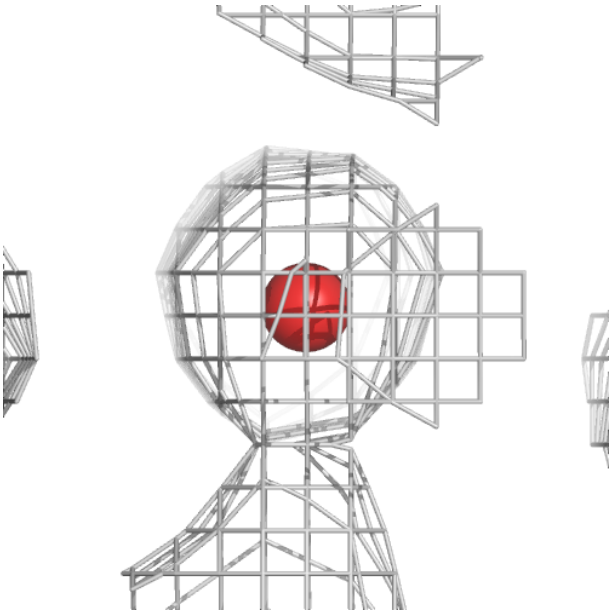


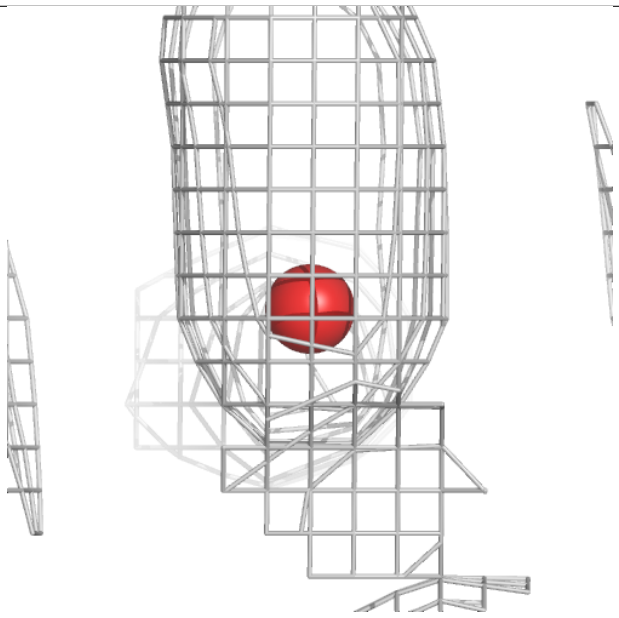


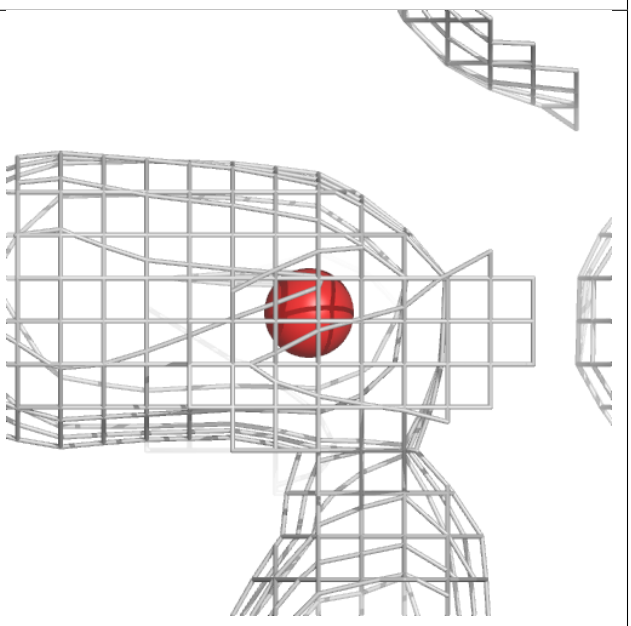


Electron density around BR BBB 306 (B):

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

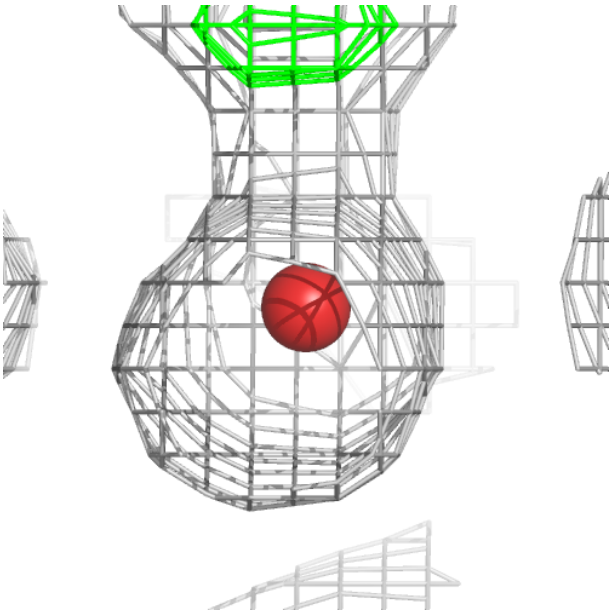


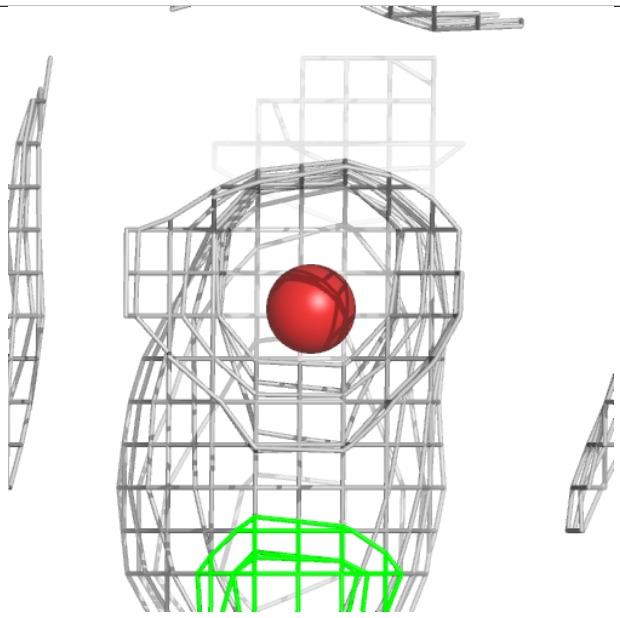


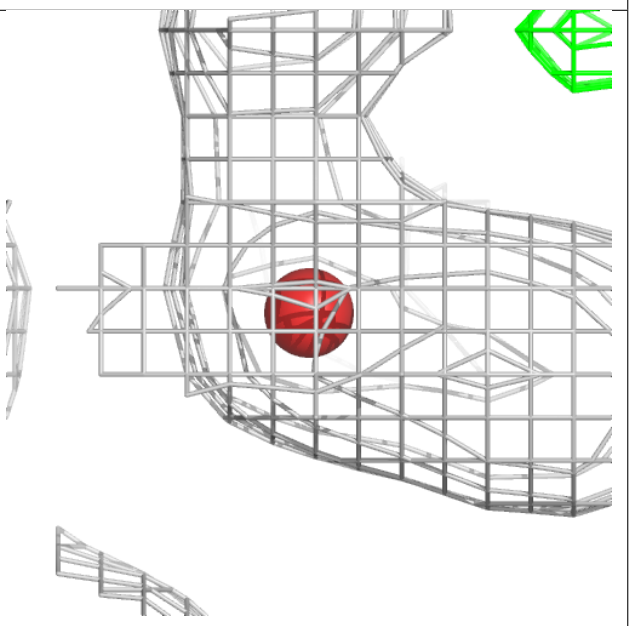


Electron density around BR HHH 305 (A):

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

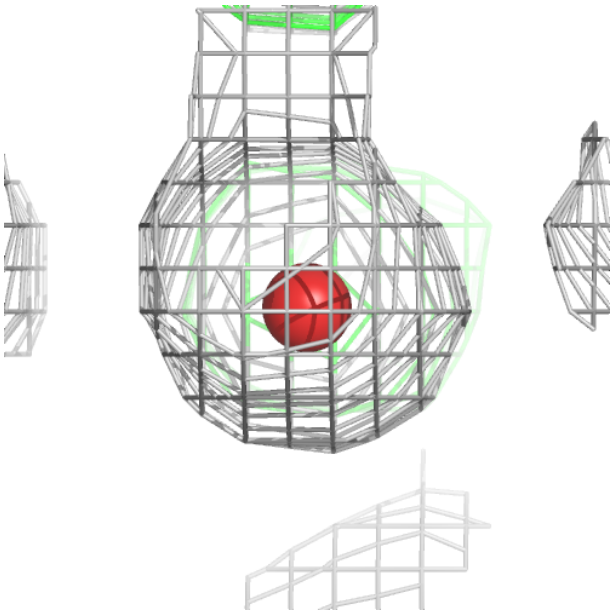


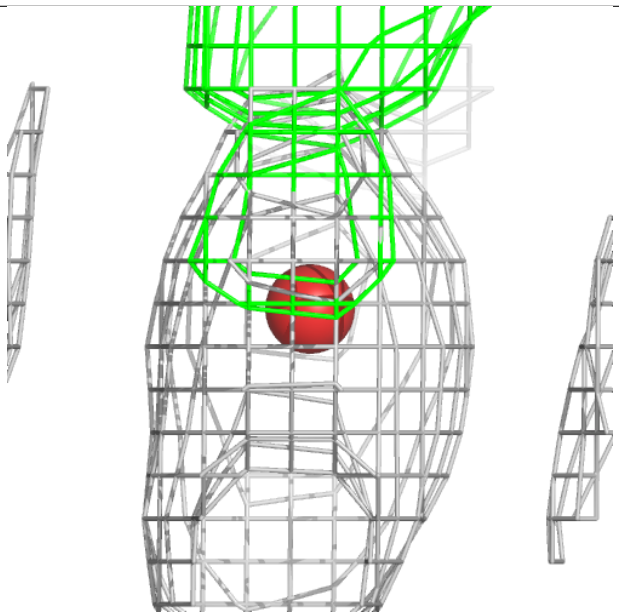


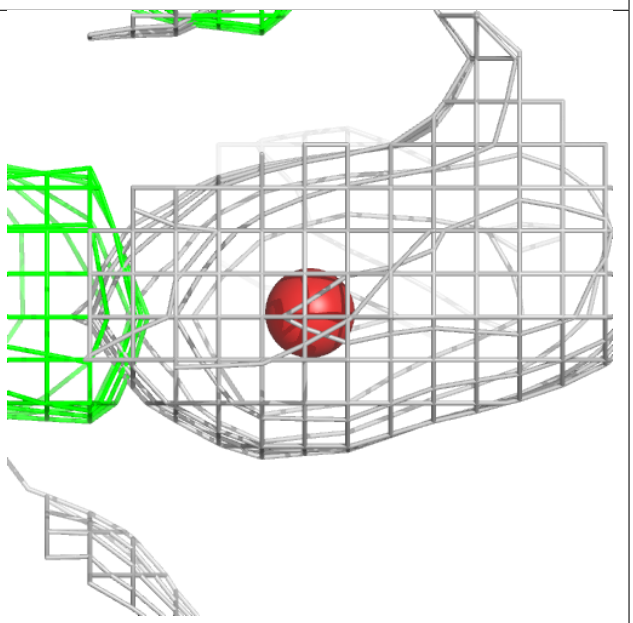


Electron density around BR HHH 305 (B):

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

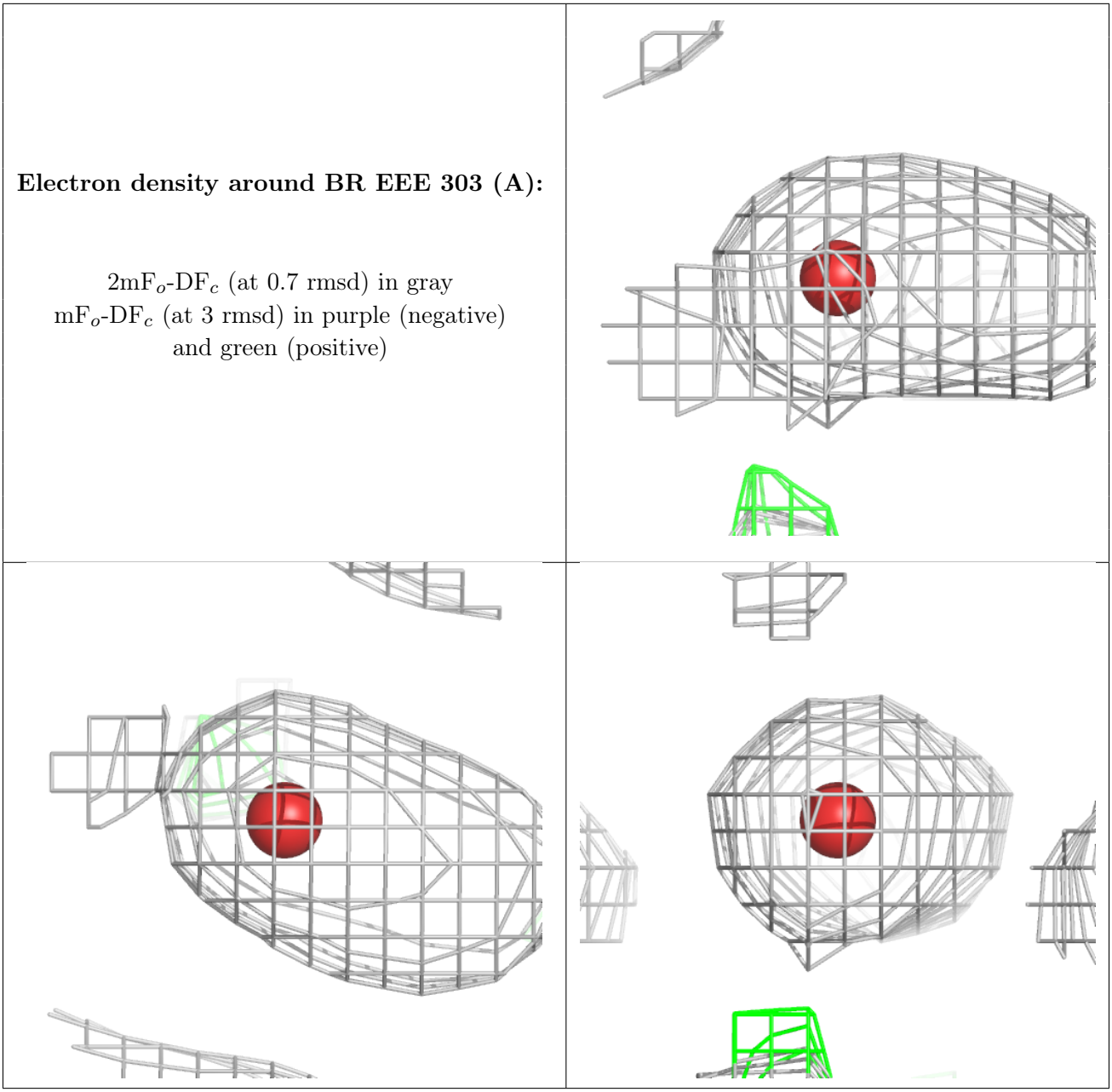






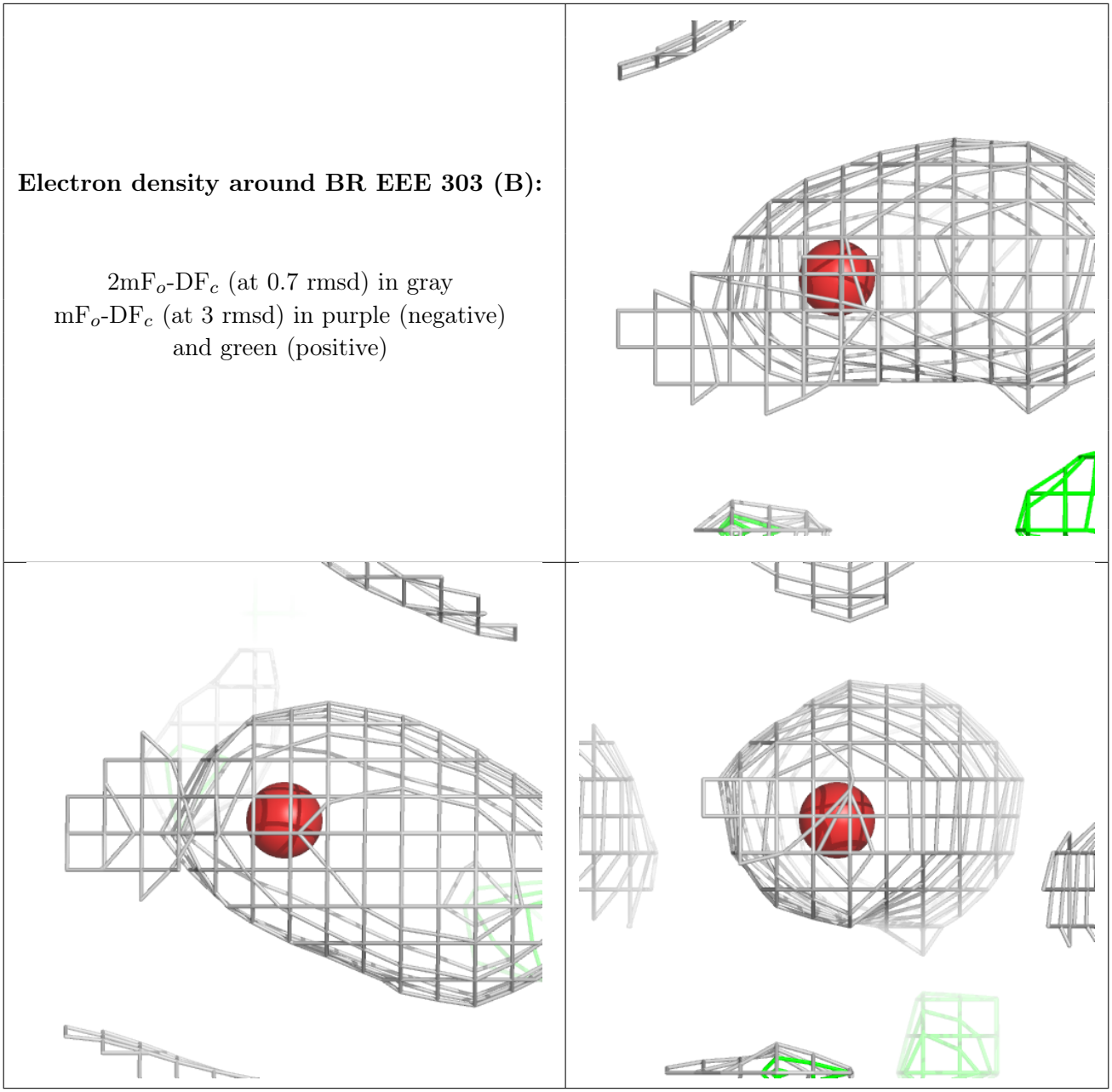
Electron density around BR EEE 303 (A):

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



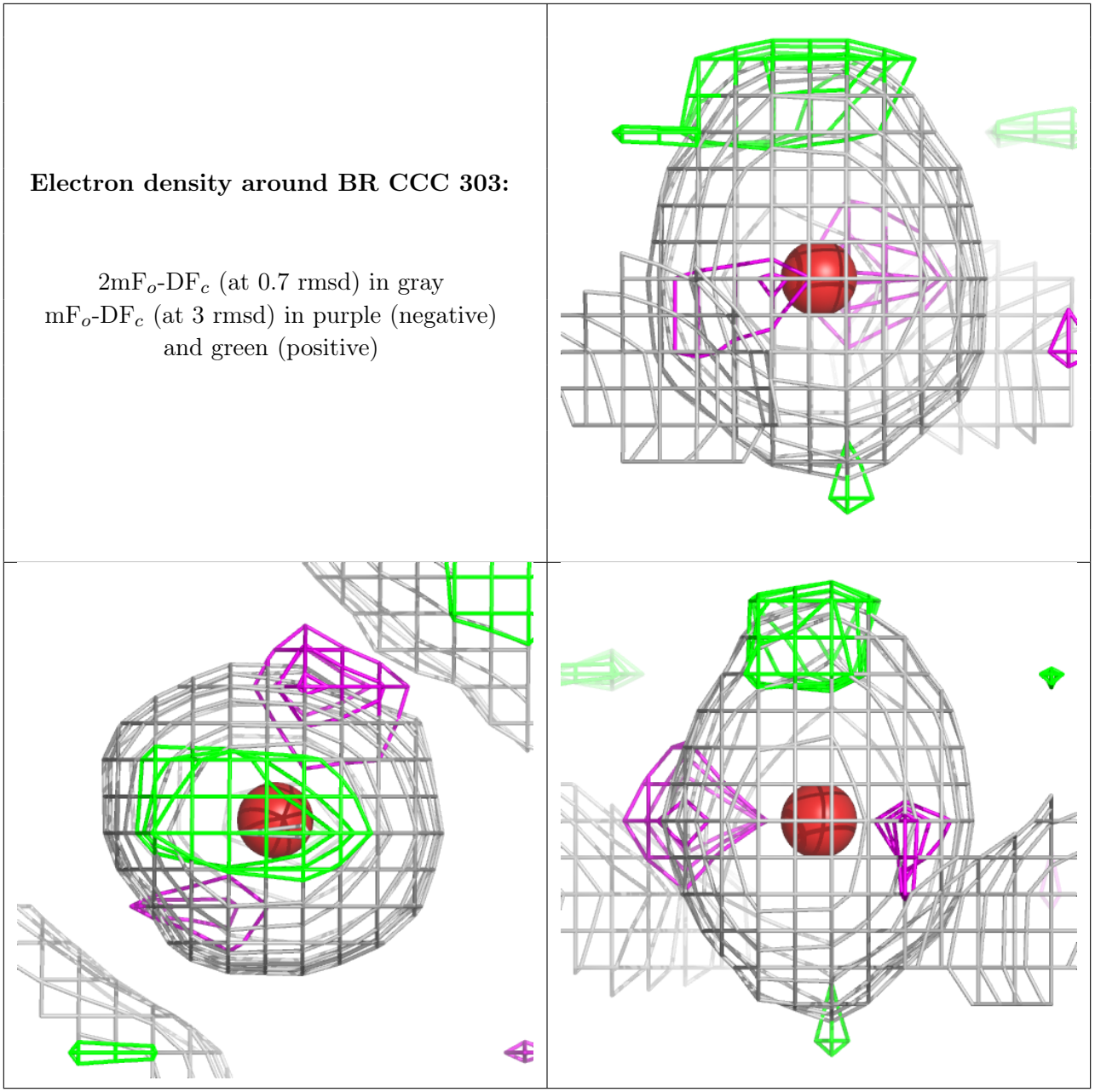
Electron density around BR EEE 303 (B):

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



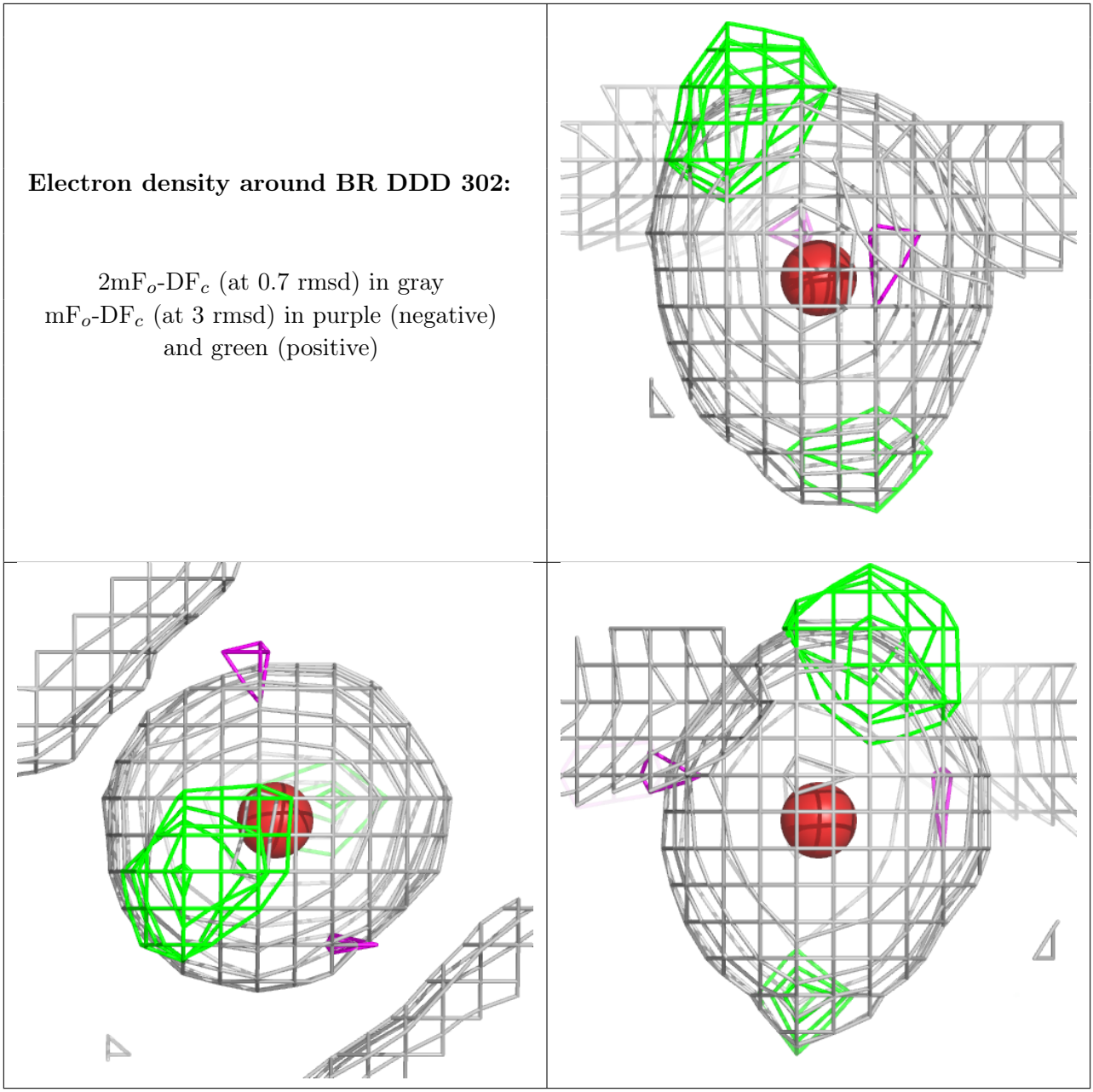
Electron density around BR CCC 303:

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



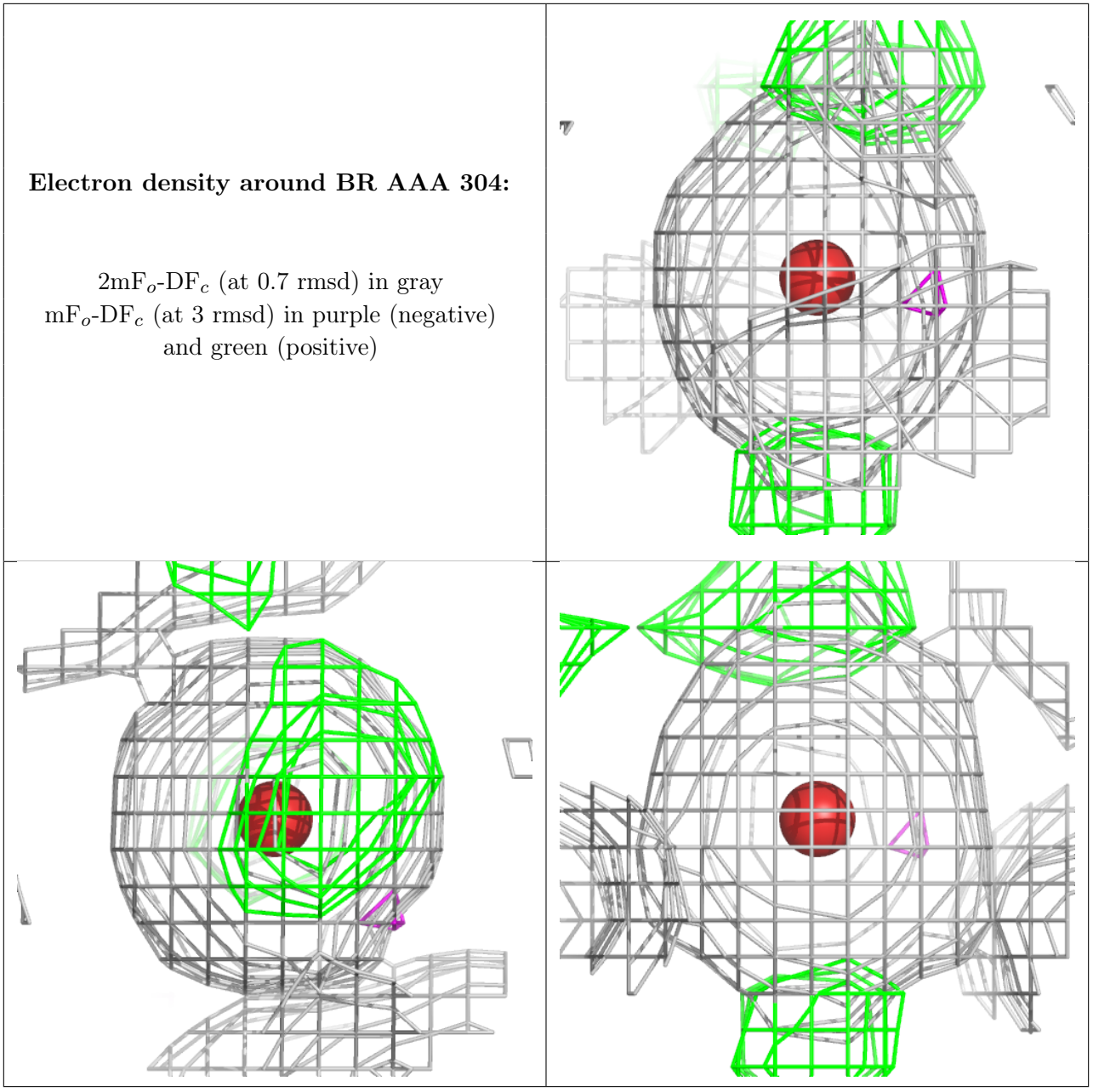
Electron density around BR DDD 302:

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



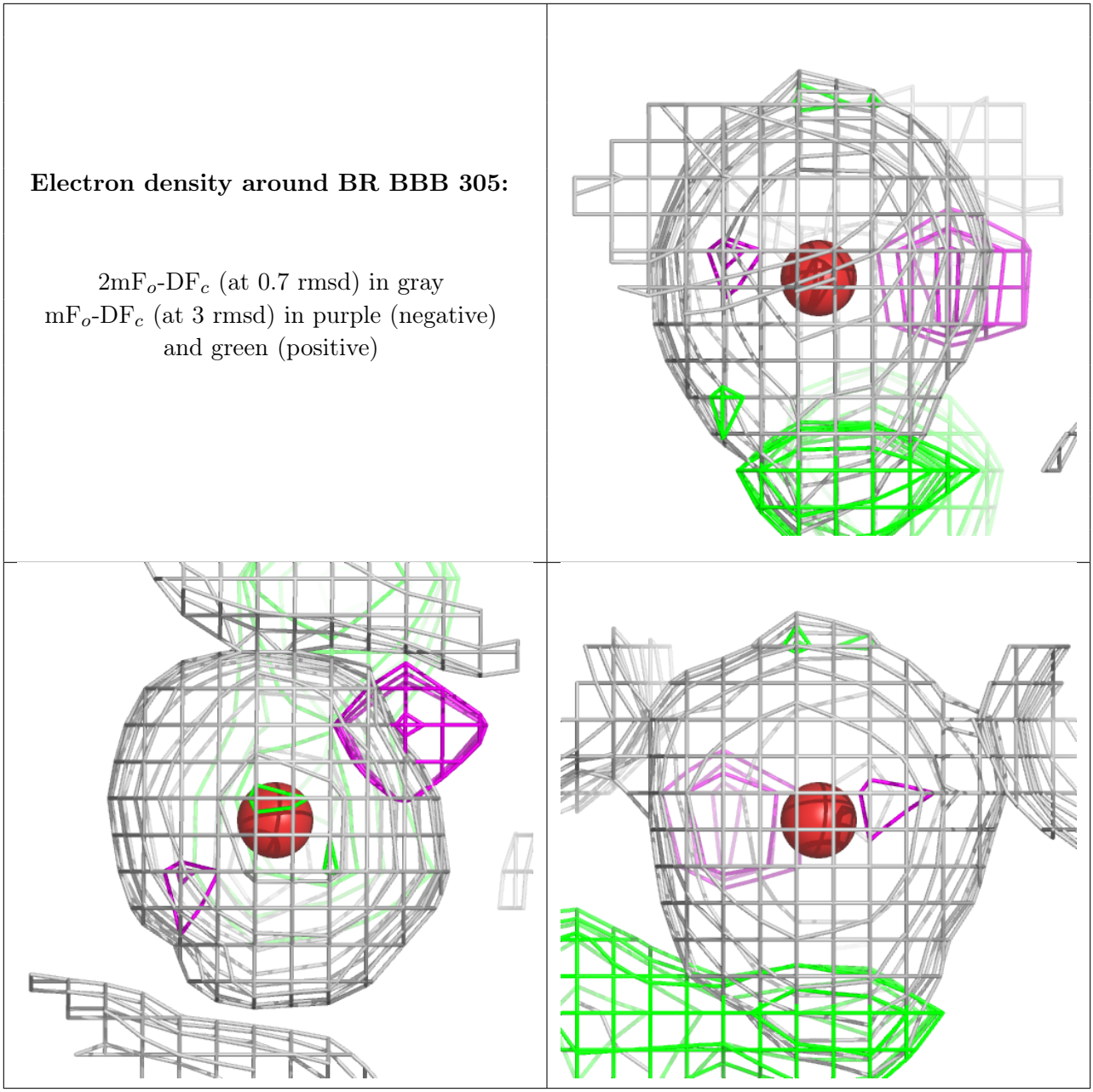
Electron density around BR AAA 304:

$2mF_o$-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)



6.5 Other polymers

There are no such residues in this entry.