



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 02:41 AM UTC

PDB ID : 9I80 / pdb\_00009i80  
Title : LecA in complex with a tolcapone derivative glycomimetic  
Authors : Varrot, A.  
Deposited on : 2025-02-03  
Resolution : 1.95 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

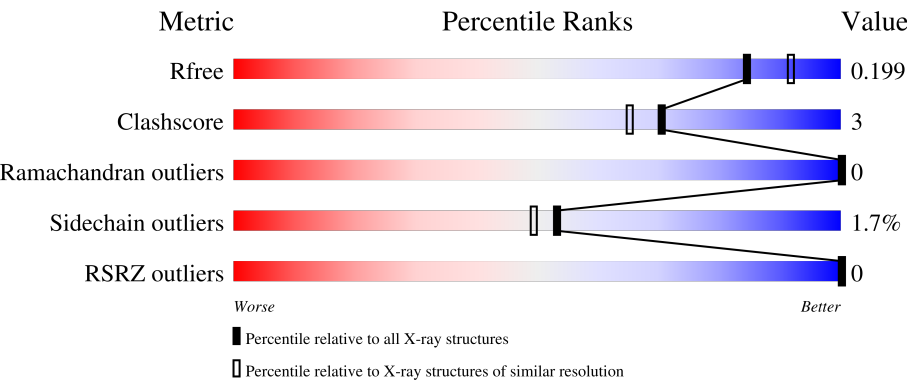
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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 <sub>free</sub>	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	121	<div><div></div><div>90%9%</div></div>
1	B	121	<div><div></div><div>93%7%</div></div>
1	C	121	<div><div></div><div>88%9%</div></div>
1	D	121	<div><div></div><div>89%10%</div></div>
1	E	121	<div><div></div><div>95%5%</div></div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	121	 88% 11% •
1	G	121	 88% 9% •
1	H	121	 83% 15% •

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8382 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PA-I galactophilic lectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	121	Total	C	N	O	S	0	1	0
			910	573	158	176	3			
1	B	121	Total	C	N	O	S	0	2	0
			919	577	160	179	3			
1	C	121	Total	C	N	O	S	0	1	0
			904	569	156	176	3			
1	D	121	Total	C	N	O	S	0	0	0
			897	565	155	174	3			
1	E	121	Total	C	N	O	S	0	0	0
			901	567	156	175	3			
1	F	121	Total	C	N	O	S	0	1	0
			910	573	158	176	3			
1	G	121	Total	C	N	O	S	0	0	0
			901	567	156	175	3			
1	H	121	Total	C	N	O	S	0	2	0
			914	577	158	176	3			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

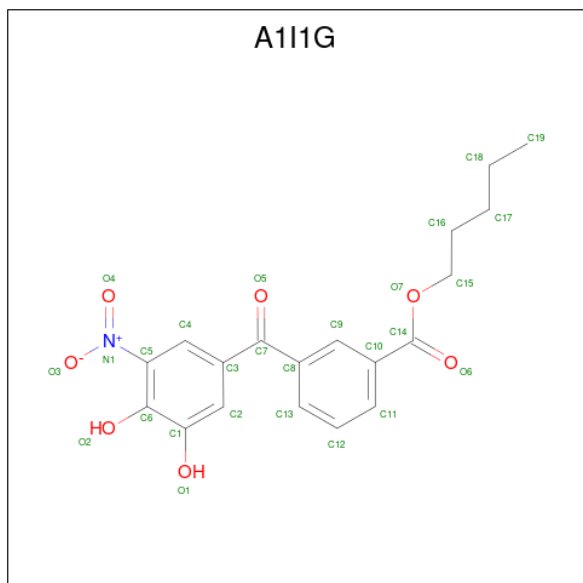
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		
2	E	1	Total	Ca	0	0
			1	1		
2	F	1	Total	Ca	0	0
			1	1		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Ca	0	0
			1	1		
2	H	1	Total	Ca	0	0
			1	1		

- Molecule 3 is pentyl 3-[3-nitro-4,5-bis(oxidanyl)phenyl]carbonylbenzoate (CCD ID: A1I1G) (formula: C<sub>19</sub>H<sub>19</sub>NO<sub>7</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			27	19	1	7		
3	B	1	Total	C	N	O	0	0
			27	19	1	7		
3	C	1	Total	C	N	O	0	0
			22	14	1	7		
3	D	1	Total	C	N	O	0	0
			27	19	1	7		
3	E	1	Total	C	N	O	0	0
			27	19	1	7		
3	F	1	Total	C	N	O	0	0
			27	19	1	7		
3	G	1	Total	C	N	O	0	0
			25	17	1	7		
3	H	1	Total	C	N	O	0	0
			25	17	1	7		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	138	Total 141	O 141	0	3
4	B	120	Total 123	O 123	0	3
4	C	135	Total 138	O 138	0	3
4	D	115	Total 117	O 117	0	2
4	E	107	Total 109	O 109	0	2
4	F	96	Total 96	O 96	0	0
4	G	91	Total 94	O 94	0	3
4	H	91	Total 93	O 93	0	2

### 3 Residue-property plots

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: PA-I galactophilic lectin

Chain A:  90% 9% .




- Molecule 1: PA-I galactophilic lectin

Chain B:  93% 7% .




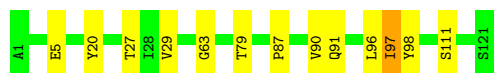
- Molecule 1: PA-I galactophilic lectin

Chain C:  88% 9% .



- Molecule 1: PA-I galactophilic lectin

Chain D:  89% 10% .




- Molecule 1: PA-I galactophilic lectin

Chain E:  95% 5% .

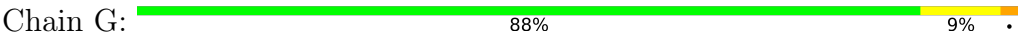


- Molecule 1: PA-I galactophilic lectin

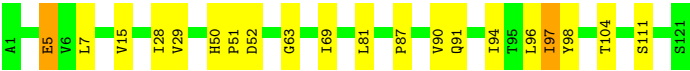
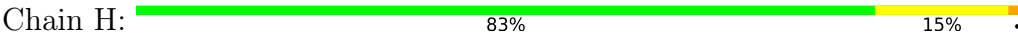
Chain F:  88% 11% .



• Molecule 1: PA-I galactophilic lectin



• Molecule 1: PA-I galactophilic lectin





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.21Å 81.21Å 165.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.13 – 1.95 47.13 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.13-1.95) 100.0 (47.13-1.95)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.52 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.166 , 0.203 0.161 , 0.199	Depositor DCC
$R_{free}$ test set	3915 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.2	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 30.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.115 for h,-k,-l	Xtriage
Reported twinning fraction	0.867 for H, K, L 0.133 for -K, -H, -L	Depositor
Outliers	0 of 77517 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8382	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	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 55.42 % 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 3.1707e-05.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, A1I1G

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.96	0/933	1.24	1/1273 (0.1%)
1	B	0.93	0/942	1.19	1/1286 (0.1%)
1	C	0.97	0/927	1.23	2/1267 (0.2%)
1	D	0.95	0/920	1.23	0/1257
1	E	0.94	0/924	1.27	0/1262
1	F	0.88	0/933	1.23	2/1273 (0.2%)
1	G	0.92	0/924	1.25	2/1262 (0.2%)
1	H	0.92	0/937	1.24	2/1279 (0.2%)
All	All	0.93	0/7440	1.23	10/10159 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	59	ASP	CA-CB-CG	6.62	119.22	112.60
1	C	48	ARG	NE-CZ-NH2	5.76	124.39	119.20
1	G	10	ASN	CB-CA-C	5.57	119.69	110.78
1	H	5	GLU	CB-CG-CD	5.51	121.96	112.60
1	H	104	THR	OG1-CB-CG2	5.42	120.15	109.30
1	F	40	GLN	N-CA-CB	-5.20	102.92	110.36
1	G	120	GLN	CB-CA-C	5.08	118.34	109.65
1	C	5	GLU	CB-CG-CD	5.05	121.19	112.60
1	A	48	ARG	NE-CZ-NH2	5.03	123.73	119.20
1	F	77	VAL	CB-CA-C	-5.03	106.66	111.44

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	A	910	0	873	10	0
1	B	919	0	875	6	0
1	C	904	0	861	8	0
1	D	897	0	855	8	0
1	E	901	0	861	4	0
1	F	910	0	873	8	0
1	G	901	0	861	8	0
1	H	914	0	877	11	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	27	0	0	1	0
3	B	27	0	0	0	0
3	C	22	0	0	0	0
3	D	27	0	0	0	0
3	E	27	0	0	0	0
3	F	27	0	0	0	0
3	G	25	0	0	1	0
3	H	25	0	0	0	0
4	A	141	0	0	0	0
4	B	123	0	0	0	0
4	C	138	0	0	0	0
4	D	117	0	0	0	0
4	E	109	0	0	0	0
4	F	96	0	0	0	0
4	G	94	0	0	0	0
4	H	93	0	0	1	0
All	All	8382	0	6936	49	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 (49) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:28:ILE:HG12	1:G:116:ILE:HG12	1.72	0.71
1:H:7[A]:LEU:HD23	1:H:111:SER:HB3	1.81	0.60
1:H:15:VAL:HG23	4:H:350:HOH:O	2.01	0.60
1:F:28:ILE:HG12	1:F:116:ILE:HG12	1.83	0.58
1:A:120:GLN:HG3	1:C:83:ARG:NH2	2.21	0.56
1:G:63:GLY:HA2	1:G:98:TYR:CZ	2.40	0.56
1:H:5:GLU:HG3	1:H:111:SER:HB2	1.87	0.54
1:G:45:GLN:HG3	1:G:79:THR:HG23	1.90	0.53
1:D:20:TYR:O	1:D:91:GLN:HG2	2.09	0.53
1:B:63:GLY:HA2	1:B:98:TYR:CZ	2.45	0.52
1:C:63:GLY:HA2	1:C:98:TYR:CZ	2.44	0.52
1:E:63:GLY:HA2	1:E:98:TYR:CZ	2.44	0.52
1:F:121:SER:O	1:G:1:ALA:N	2.38	0.51
1:F:96:LEU:C	1:F:97:ILE:HG13	2.36	0.51
1:H:87:PRO:HG2	1:H:90:VAL:HG21	1.93	0.51
1:F:63:GLY:HA2	1:F:98:TYR:CZ	2.46	0.50
1:F:1:ALA:N	1:G:121:SER:OXT	2.44	0.49
1:H:96:LEU:C	1:H:97:ILE:HG13	2.38	0.48
1:H:69:ILE:HG12	1:H:94:ILE:HG12	1.96	0.48
1:H:52:ASP:C	1:H:52:ASP:OD1	2.57	0.48
1:H:63:GLY:HA2	1:H:98:TYR:CZ	2.49	0.47
1:C:88:ASN:O	1:C:89:ASN:HB2	2.14	0.47
1:D:5:GLU:HG3	1:D:111:SER:HB2	1.97	0.47
1:H:50:HIS:CG	1:H:51:PRO:HD2	2.49	0.47
1:C:5:GLU:HG3	1:C:111:SER:HB2	1.97	0.47
1:C:27:THR:HG21	1:D:27:THR:HG21	1.96	0.47
1:A:41[B]:LYS:HE3	1:B:48:ARG:CZ	2.45	0.46
1:A:41[B]:LYS:HE3	1:B:48:ARG:NH2	2.30	0.46
1:A:96:LEU:C	1:A:97:ILE:HG13	2.40	0.46
1:D:96:LEU:C	1:D:97:ILE:HG13	2.41	0.45
1:G:96:LEU:C	1:G:97:ILE:HG13	2.43	0.44
1:F:69:ILE:HG12	1:F:94:ILE:HG12	2.00	0.43
1:A:79:THR:HG22	1:B:79:THR:HG22	2.00	0.43
1:D:63:GLY:HA2	1:D:98:TYR:CZ	2.53	0.43
1:C:96:LEU:C	1:C:97:ILE:HG13	2.43	0.43
1:C:79:THR:HG22	1:D:79:THR:HG22	2.01	0.42
1:D:87:PRO:HG2	1:D:90:VAL:HG21	2.01	0.42
1:E:48:ARG:HH12	1:F:41[A]:LYS:HE3	1.83	0.42
1:A:50:HIS:ND1	1:A:51:PRO:O	2.53	0.42
1:E:82:PHE:O	1:E:83:ARG:C	2.63	0.42
1:C:29:VAL:HG22	1:D:29:VAL:HG22	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:29:VAL:HG22	1:H:29:VAL:HG22	2.01	0.41
1:A:63:GLY:HA2	1:A:98:TYR:CZ	2.56	0.41
1:G:50:HIS:HE1	3:G:202:A1I1G:O5	2.03	0.41
1:A:27:THR:HG21	1:B:27:THR:HG21	2.02	0.41
1:A:29:VAL:HG22	1:B:29:VAL:HG22	2.01	0.41
1:E:27:THR:HG21	1:F:27:THR:HG21	2.02	0.41
1:H:28:ILE:HD12	1:H:81:LEU:HD12	2.03	0.41
1:A:50:HIS:HE1	3:A:202:A1I1G:O5	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	120/121 (99%)	116 (97%)	4 (3%)	0	100	100
1	B	121/121 (100%)	118 (98%)	3 (2%)	0	100	100
1	C	120/121 (99%)	115 (96%)	5 (4%)	0	100	100
1	D	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
1	E	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
1	F	120/121 (99%)	116 (97%)	4 (3%)	0	100	100
1	G	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
1	H	121/121 (100%)	117 (97%)	4 (3%)	0	100	100
All	All	959/968 (99%)	928 (97%)	31 (3%)	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	A	95/94 (101%)	94 (99%)	1 (1%)	65	64
1	B	96/94 (102%)	93 (97%)	3 (3%)	35	26
1	C	94/94 (100%)	91 (97%)	3 (3%)	34	25
1	D	93/94 (99%)	92 (99%)	1 (1%)	65	64
1	E	94/94 (100%)	94 (100%)	0	100	100
1	F	95/94 (101%)	94 (99%)	1 (1%)	65	64
1	G	94/94 (100%)	91 (97%)	3 (3%)	34	25
1	H	95/94 (101%)	93 (98%)	2 (2%)	47	41
All	All	756/752 (100%)	742 (98%)	14 (2%)	53	45

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	ILE
1	B	91[A]	GLN
1	B	91[B]	GLN
1	B	97	ILE
1	C	88	ASN
1	C	97	ILE
1	C	121	SER
1	D	97	ILE
1	F	97	ILE
1	G	97	ILE
1	G	120	GLN
1	G	121	SER
1	H	91	GLN
1	H	97	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	53	GLN
1	C	91	GLN
1	E	91	GLN
1	E	115	ASN
1	G	14	GLN
1	G	78	ASN
1	G	88	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	$\# Z  > 2$
3	A1I1G	E	202	2	28,28,28	0.60	0	33,38,38	0.82	1 (3%)
3	A1I1G	F	202	2	28,28,28	1.02	1 (3%)	33,38,38	1.03	1 (3%)
3	A1I1G	G	202	2	26,26,28	0.91	1 (3%)	31,36,38	1.28	2 (6%)
3	A1I1G	B	202	2	28,28,28	0.94	2 (7%)	33,38,38	1.37	5 (15%)
3	A1I1G	A	202	2	28,28,28	1.04	1 (3%)	33,38,38	1.22	3 (9%)
3	A1I1G	D	202	2	28,28,28	0.88	0	33,38,38	1.20	3 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	A1I1G	C	202	2	23,23,28	0.83	0	28,33,38	0.74	0
3	A1I1G	H	202	2	26,26,28	0.87	0	31,36,38	0.84	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
3	A1I1G	E	202	2	-	2/20/22/22	0/2/2/2
3	A1I1G	F	202	2	-	1/20/22/22	0/2/2/2
3	A1I1G	G	202	2	-	3/18/20/22	0/2/2/2
3	A1I1G	B	202	2	-	4/20/22/22	0/2/2/2
3	A1I1G	A	202	2	-	5/20/22/22	0/2/2/2
3	A1I1G	D	202	2	-	2/20/22/22	0/2/2/2
3	A1I1G	C	202	2	-	3/14/16/22	0/2/2/2
3	A1I1G	H	202	2	-	1/18/20/22	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	202	A1I1G	O7-C14	-2.66	1.27	1.33
3	B	202	A1I1G	O1-C1	2.51	1.41	1.36
3	B	202	A1I1G	C2-C3	2.47	1.43	1.39
3	A	202	A1I1G	O1-C1	2.42	1.41	1.36
3	G	202	A1I1G	O7-C14	-2.17	1.28	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	202	A1I1G	C2-C1-C6	-4.19	117.54	120.45
3	A	202	A1I1G	O5-C7-C8	-3.40	114.71	120.15
3	G	202	A1I1G	O5-C7-C8	-3.18	115.06	120.15
3	D	202	A1I1G	O5-C7-C8	-2.95	115.43	120.15
3	B	202	A1I1G	O1-C1-C2	2.85	127.15	119.45
3	A	202	A1I1G	C2-C1-C6	-2.82	118.49	120.45
3	D	202	A1I1G	C11-C10-C9	2.72	122.39	119.25
3	G	202	A1I1G	O7-C15-C16	-2.70	98.70	108.87
3	B	202	A1I1G	C3-C2-C1	2.69	122.43	120.09
3	B	202	A1I1G	O5-C7-C8	-2.61	115.97	120.15
3	F	202	A1I1G	O7-C15-C16	2.50	117.25	108.61

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	202	A1I1G	O1-C1-C2	2.43	126.01	119.45
3	E	202	A1I1G	O1-C1-C2	2.20	125.39	119.45
3	D	202	A1I1G	C10-C9-C8	-2.12	117.97	120.43
3	B	202	A1I1G	O2-C6-C5	2.00	123.56	120.89

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	202	A1I1G	O7-C15-C16-C17
3	D	202	A1I1G	O7-C15-C16-C17
3	B	202	A1I1G	O6-C14-O7-C15
3	G	202	A1I1G	O7-C15-C16-C17
3	A	202	A1I1G	O7-C15-C16-C17
3	B	202	A1I1G	C10-C14-O7-C15
3	A	202	A1I1G	C15-C16-C17-C18
3	D	202	A1I1G	C15-C16-C17-C18
3	F	202	A1I1G	C16-C17-C18-C19
3	A	202	A1I1G	C16-C17-C18-C19
3	B	202	A1I1G	C15-C16-C17-C18
3	A	202	A1I1G	O6-C14-O7-C15
3	C	202	A1I1G	C3-C7-C8-C9
3	G	202	A1I1G	C3-C7-C8-C13
3	C	202	A1I1G	O5-C7-C8-C9
3	E	202	A1I1G	O5-C7-C8-C13
3	G	202	A1I1G	O5-C7-C8-C13
3	A	202	A1I1G	C3-C7-C8-C13
3	C	202	A1I1G	C3-C7-C8-C13
3	E	202	A1I1G	O5-C7-C8-C9
3	B	202	A1I1G	C16-C17-C18-C19

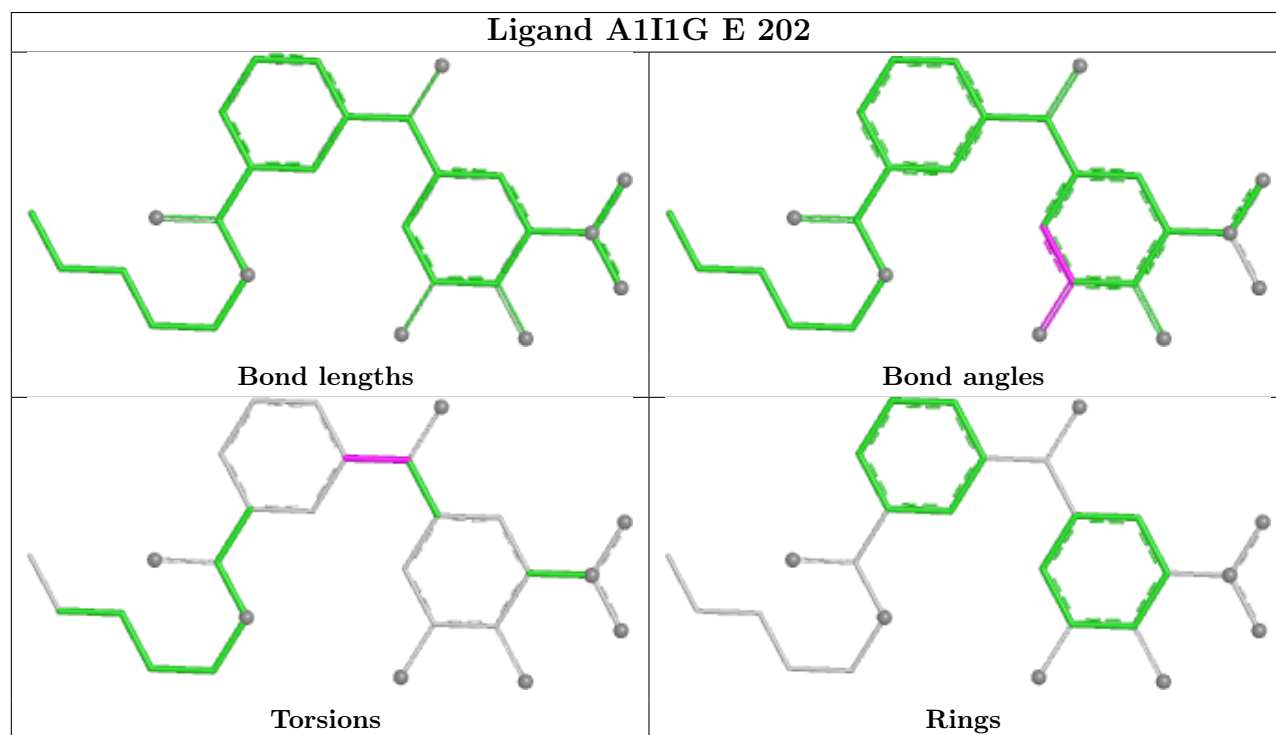
There are no ring outliers.

2 monomers are involved in 2 short contacts:

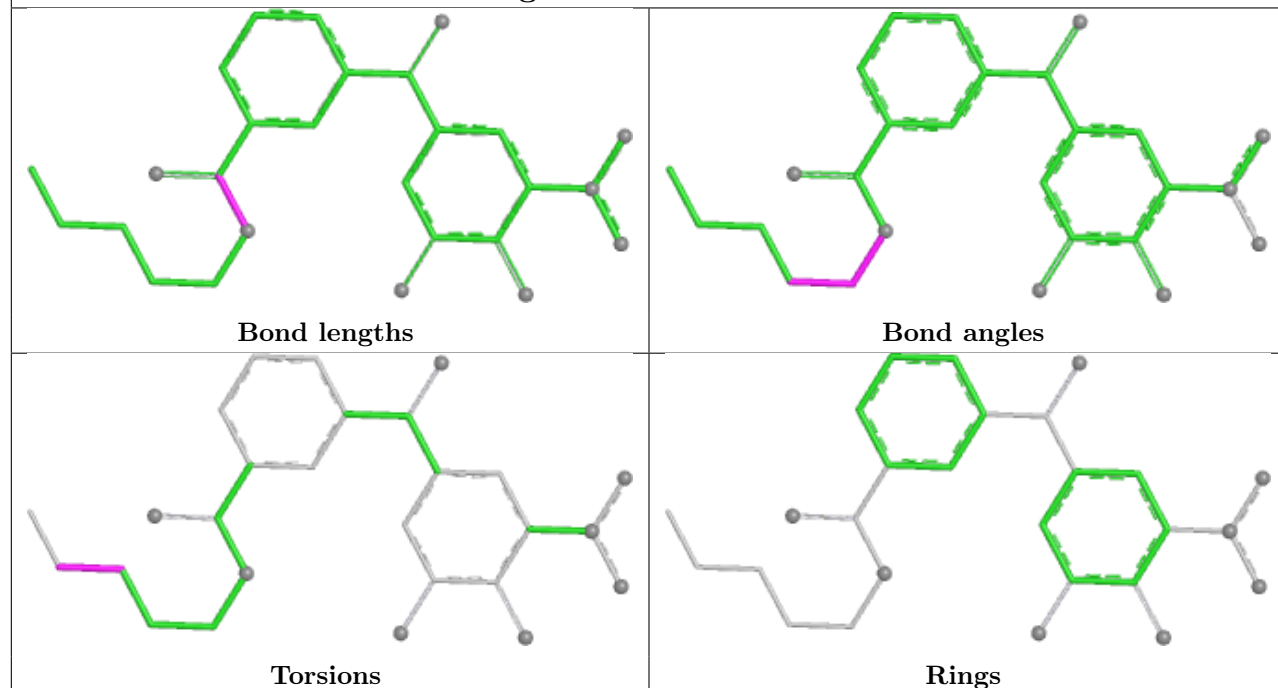
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	202	A1I1G	1	0
3	A	202	A1I1G	1	0

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

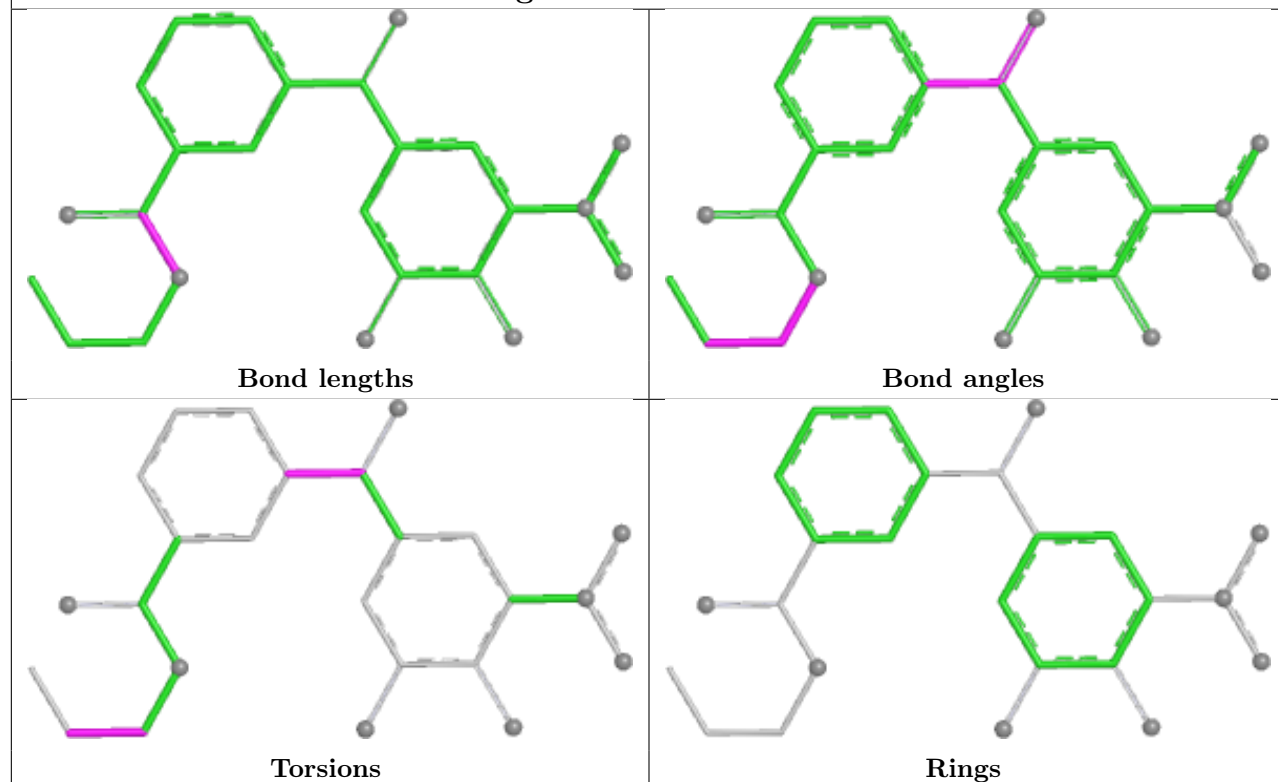
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



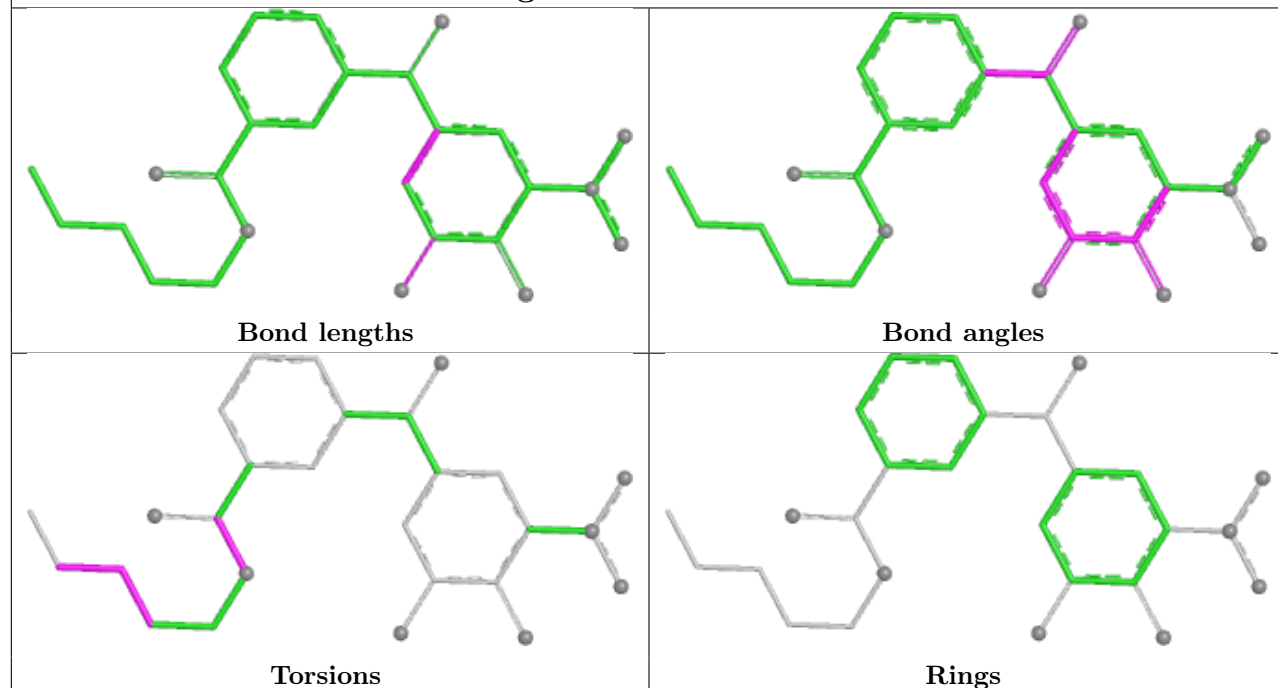
## Ligand A1I1G F 202



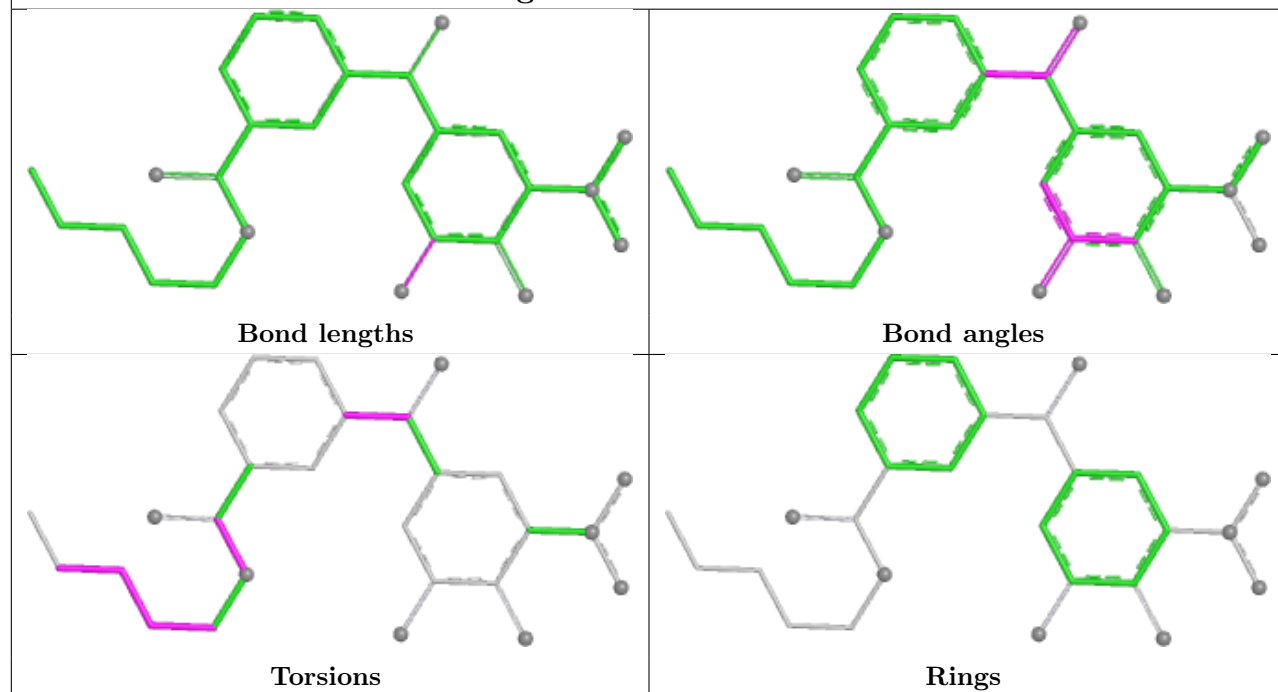
## Ligand A1I1G G 202



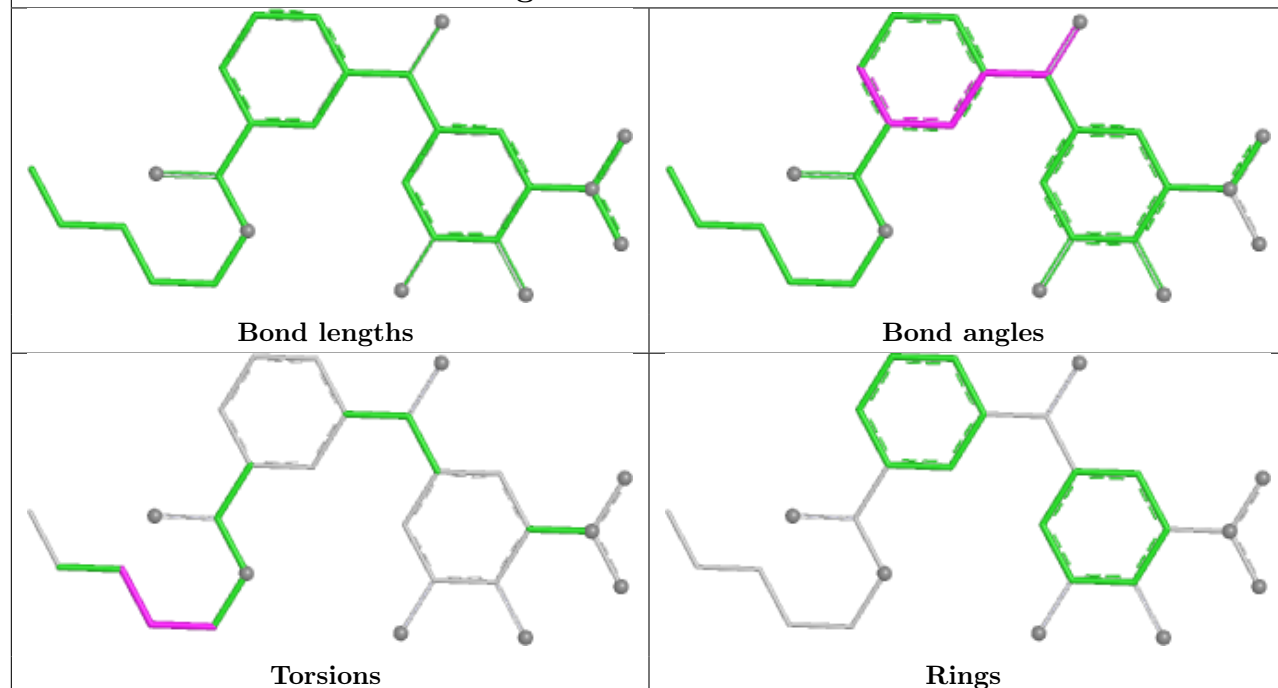
## Ligand A1I1G B 202



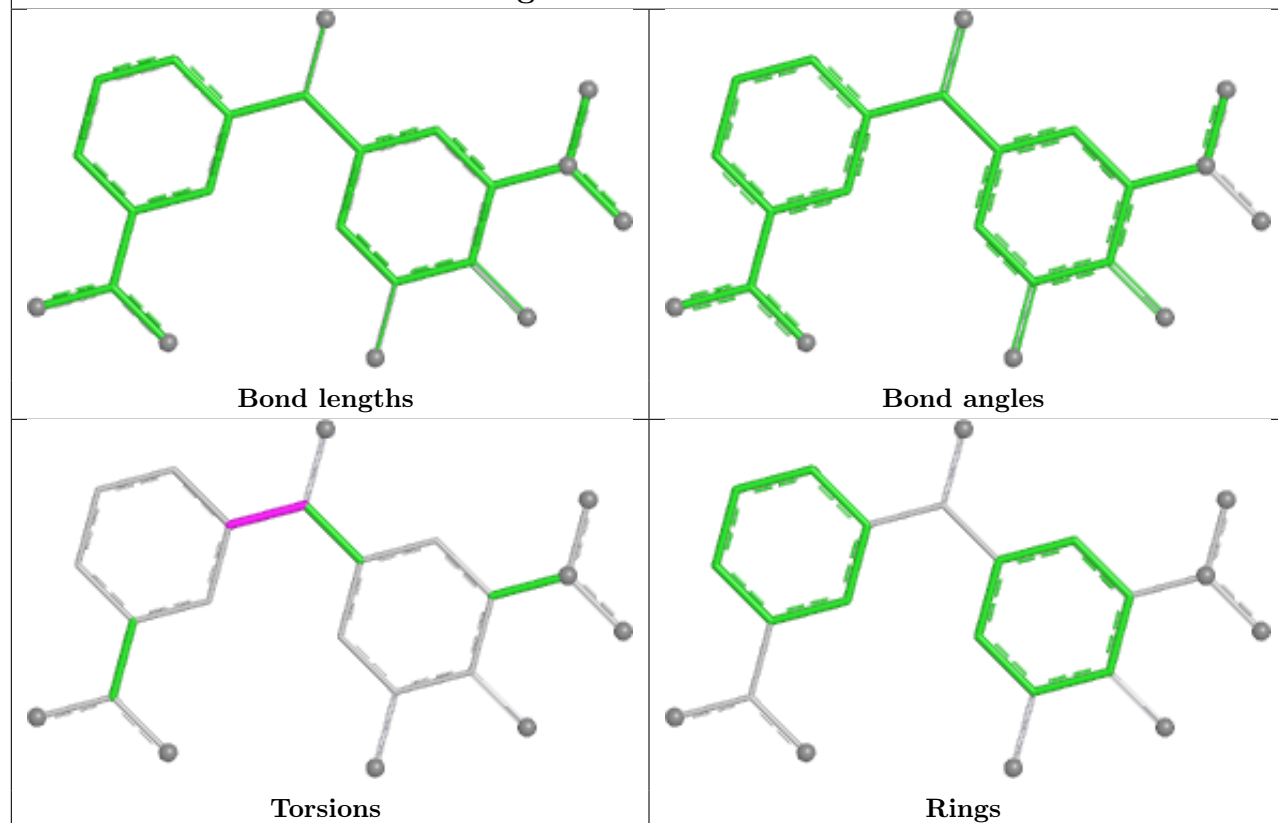
## Ligand A1I1G A 202

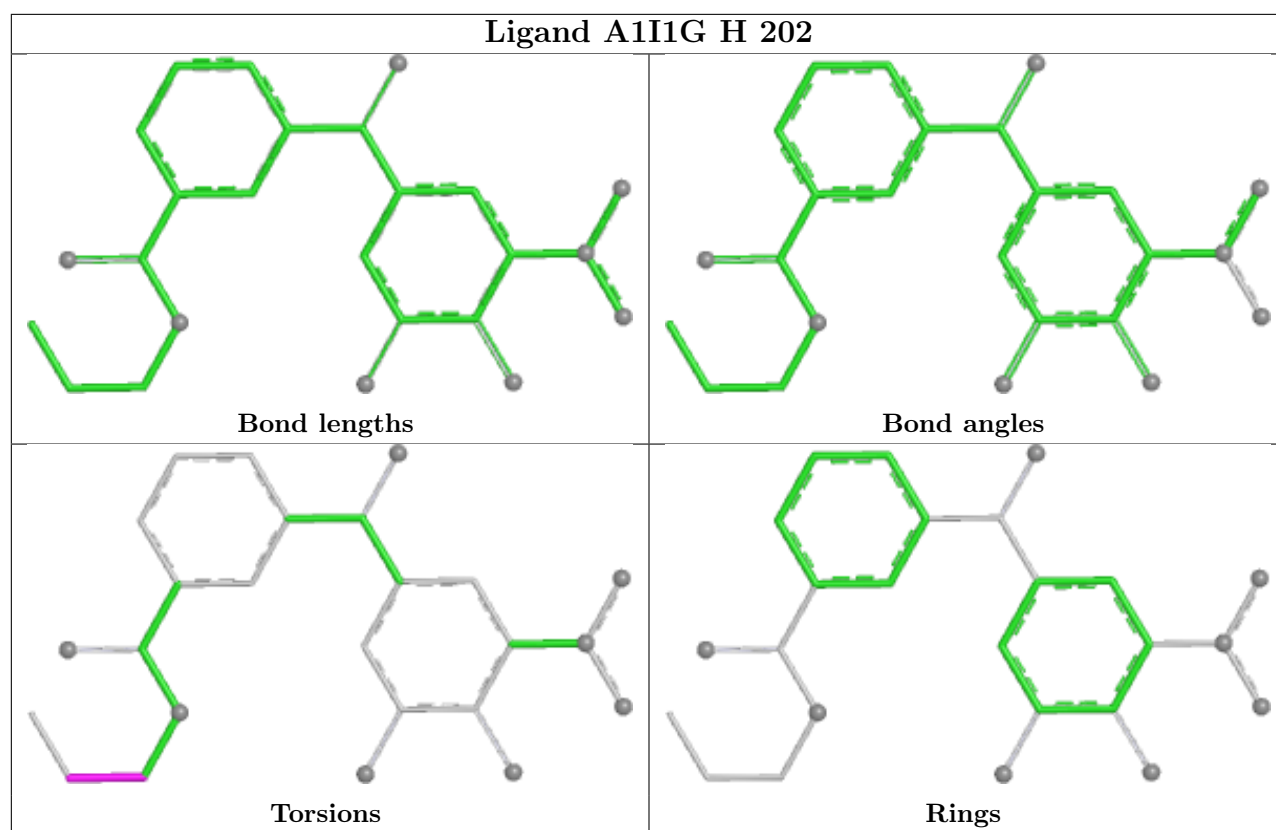


## Ligand A1I1G D 202



## Ligand A1I1G C 202





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	121/121 (100%)	-1.33	0 100 100	18, 27, 38, 48	1 (0%)
1	B	121/121 (100%)	-1.31	0 100 100	16, 28, 41, 60	2 (1%)
1	C	121/121 (100%)	-1.34	0 100 100	17, 25, 34, 46	1 (0%)
1	D	121/121 (100%)	-1.35	0 100 100	22, 28, 41, 57	0
1	E	121/121 (100%)	-1.25	0 100 100	23, 30, 40, 50	0
1	F	121/121 (100%)	-1.27	0 100 100	16, 32, 42, 57	1 (0%)
1	G	121/121 (100%)	-1.28	0 100 100	22, 31, 43, 53	0
1	H	121/121 (100%)	-1.28	0 100 100	15, 30, 44, 59	2 (1%)
All	All	968/968 (100%)	-1.30	0 100 100	15, 29, 42, 60	7 (0%)

There are no RSRZ outliers to report.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

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

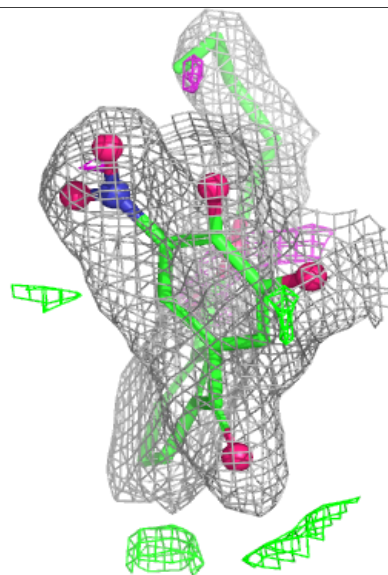
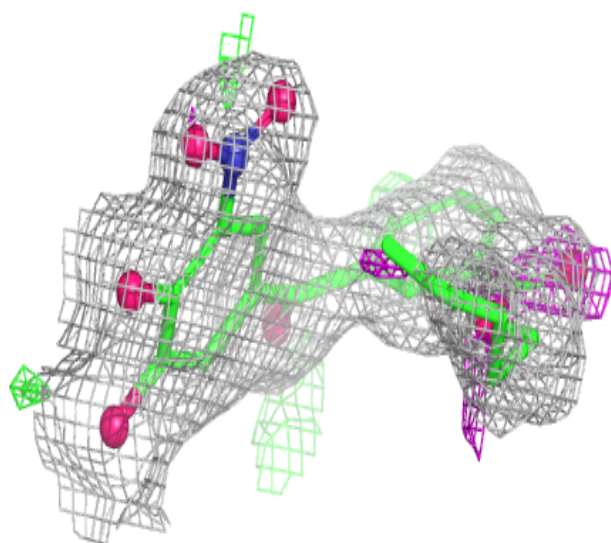
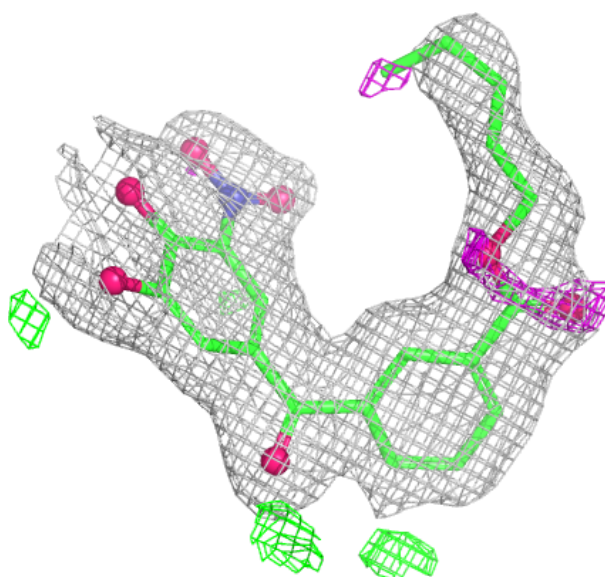
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	A1I1G	D	202	27/27	0.98	0.04	23,28,32,33	0
3	A1I1G	G	202	25/27	0.98	0.04	21,27,30,30	0
3	A1I1G	C	202	22/27	0.99	0.04	22,31,48,54	0
3	A1I1G	A	202	27/27	0.99	0.04	22,27,32,33	0
3	A1I1G	E	202	27/27	0.99	0.03	22,35,43,46	0
3	A1I1G	F	202	27/27	0.99	0.03	23,27,33,37	0
3	A1I1G	B	202	27/27	0.99	0.04	25,36,48,55	0
3	A1I1G	H	202	25/27	0.99	0.04	21,27,32,36	0
2	CA	A	201	1/1	1.00	0.01	28,28,28,28	0
2	CA	B	201	1/1	1.00	0.01	27,27,27,27	0
2	CA	C	201	1/1	1.00	0.01	25,25,25,25	0
2	CA	D	201	1/1	1.00	0.01	32,32,32,32	0
2	CA	E	201	1/1	1.00	0.02	29,29,29,29	0
2	CA	F	201	1/1	1.00	0.02	28,28,28,28	0
2	CA	G	201	1/1	1.00	0.01	31,31,31,31	0
2	CA	H	201	1/1	1.00	0.01	27,27,27,27	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.



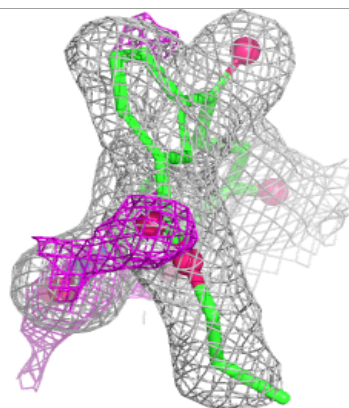
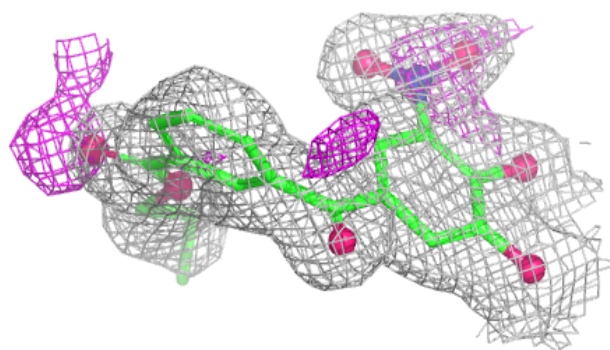
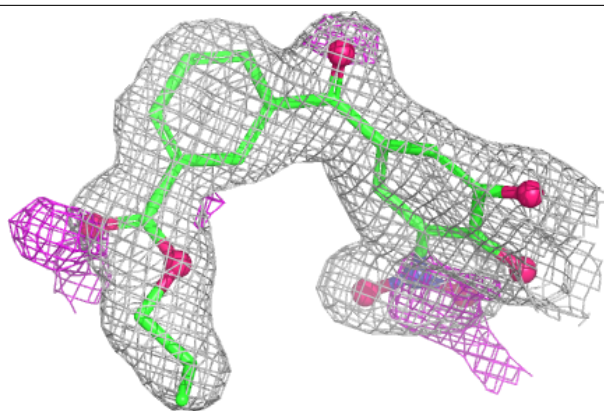
**Electron density around A1I1G D 202:**

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

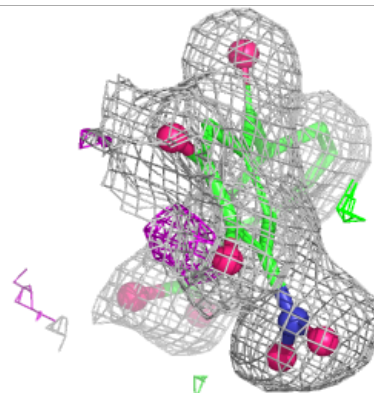
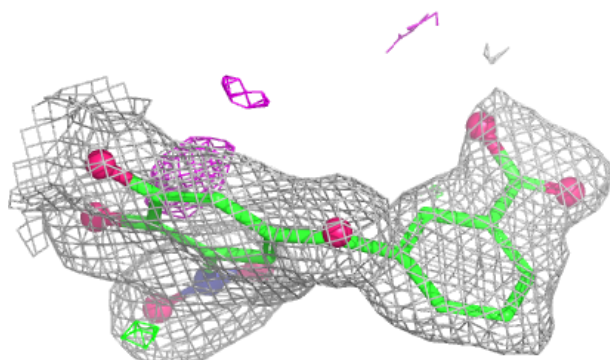
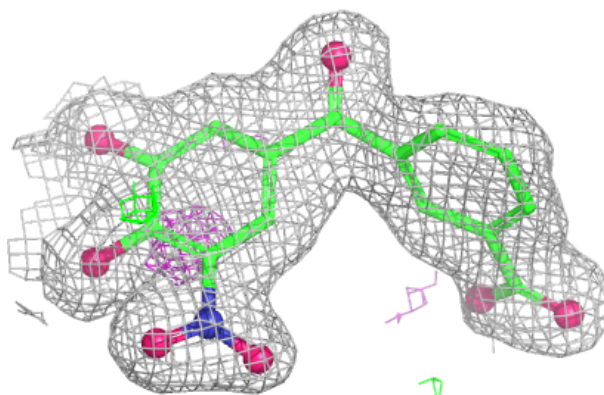


**Electron density around A1I1G G 202:**

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

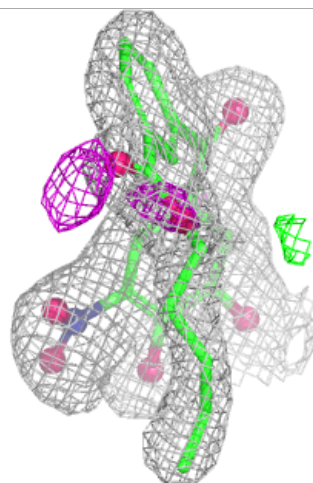
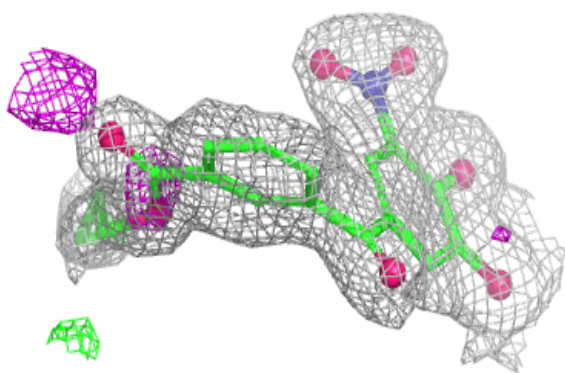
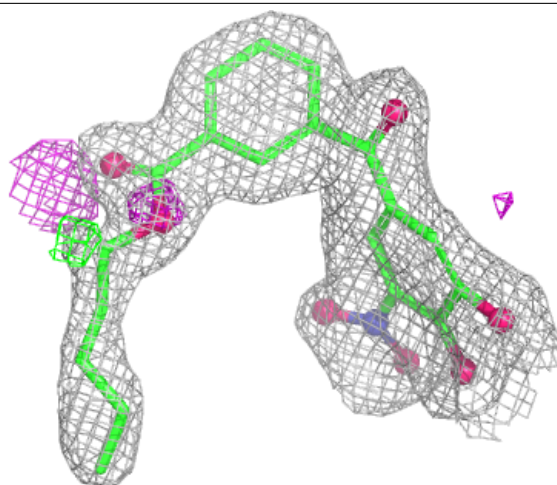
**Electron density around A1I1G C 202:**

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



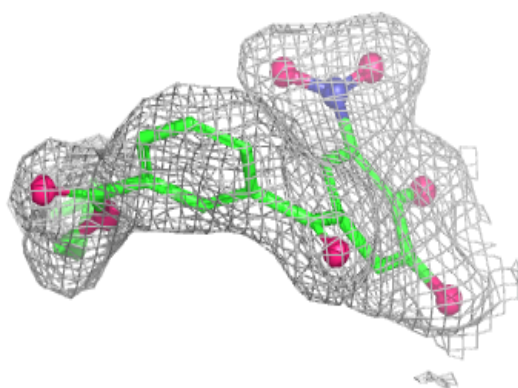
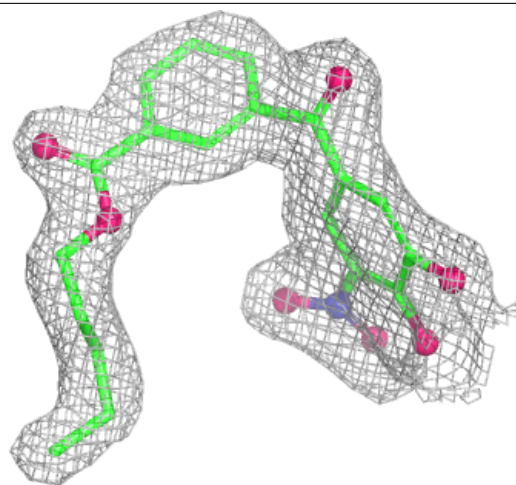
**Electron density around A1I1G A 202:**

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



**Electron density around A1I1G E 202:**

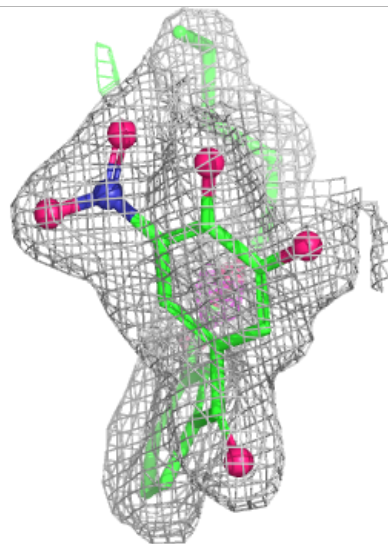
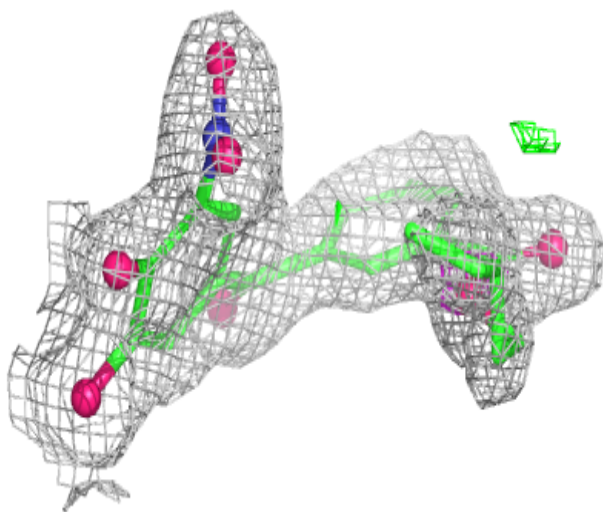
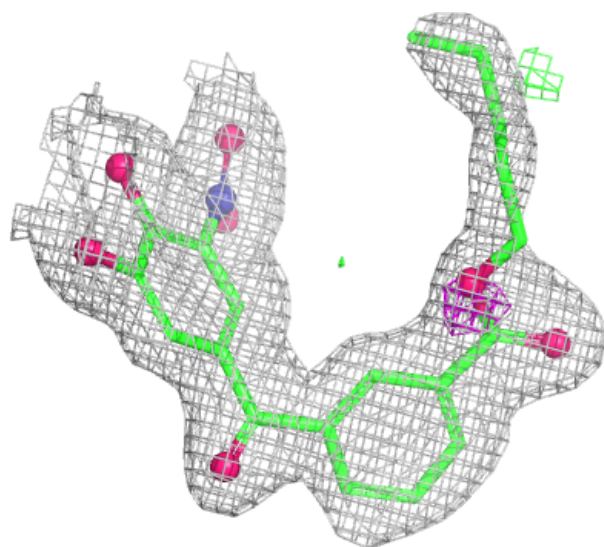
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





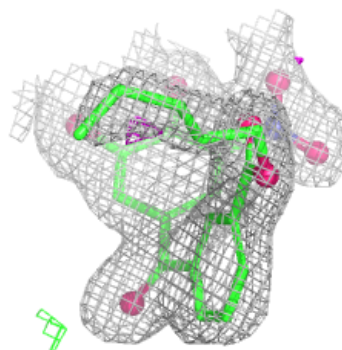
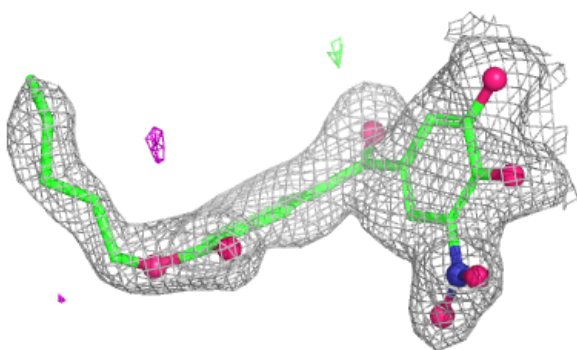
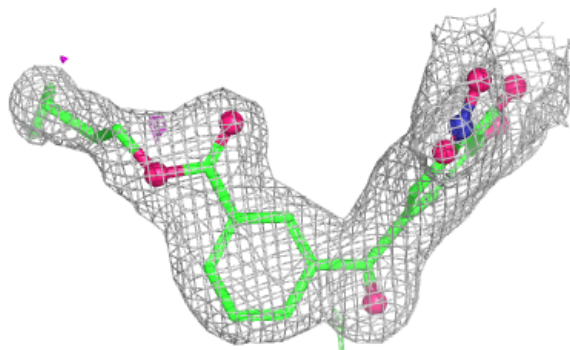
**Electron density around A1I1G F 202:**

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

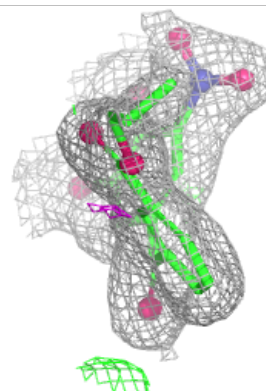
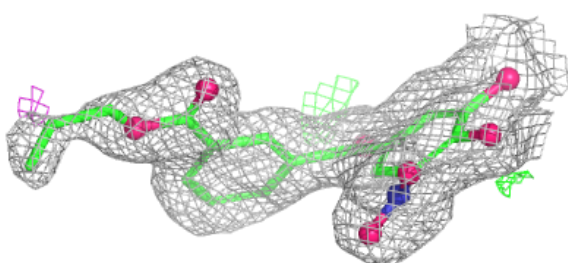
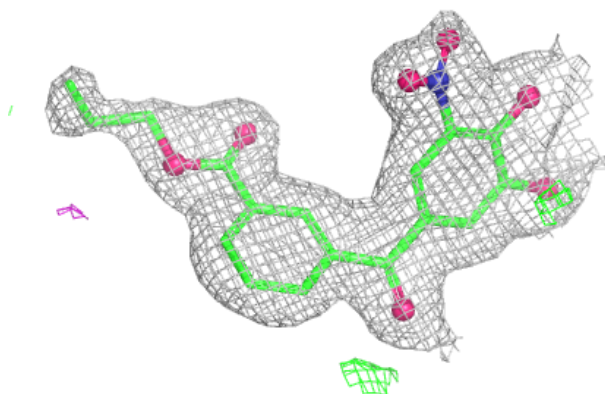


**Electron density around A1I1G B 202:**

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

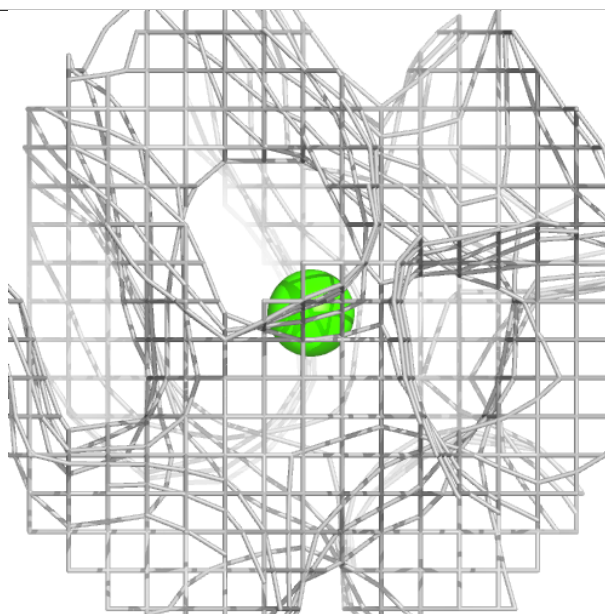
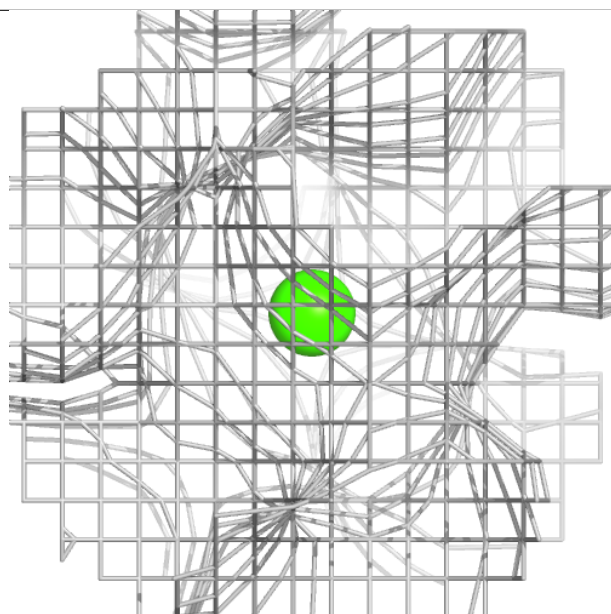
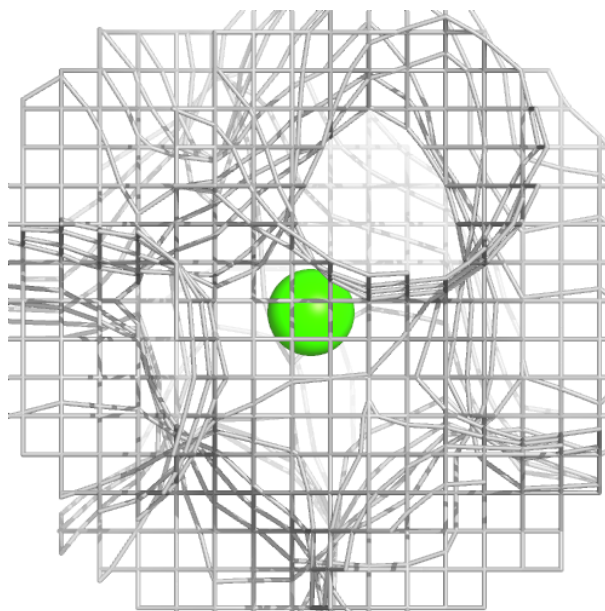
**Electron density around A1I1G H 202:**

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



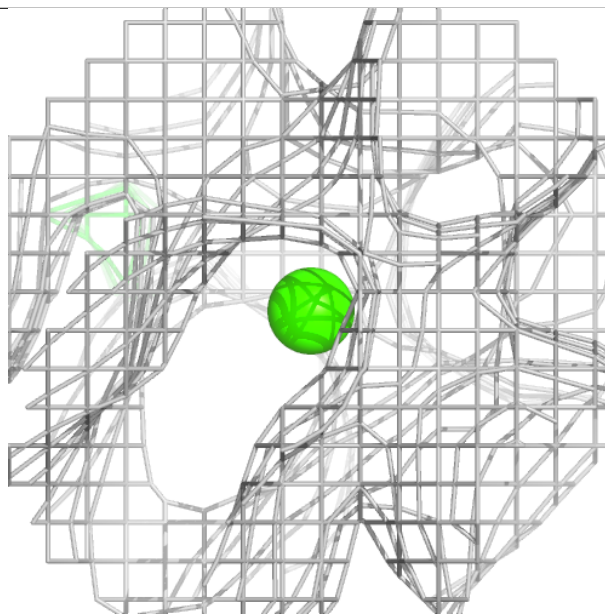
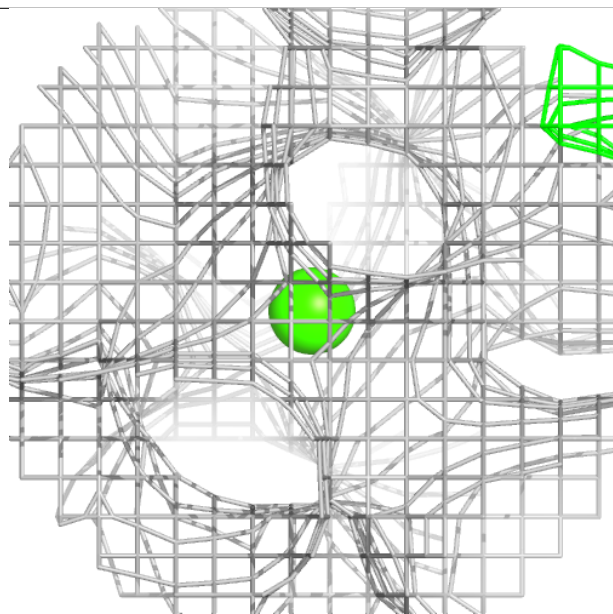
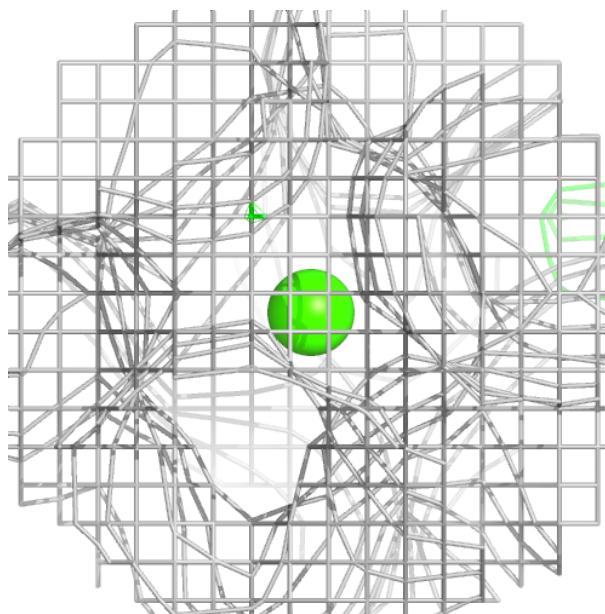
**Electron density around CA A 201:**

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



**Electron density around CA B 201:**

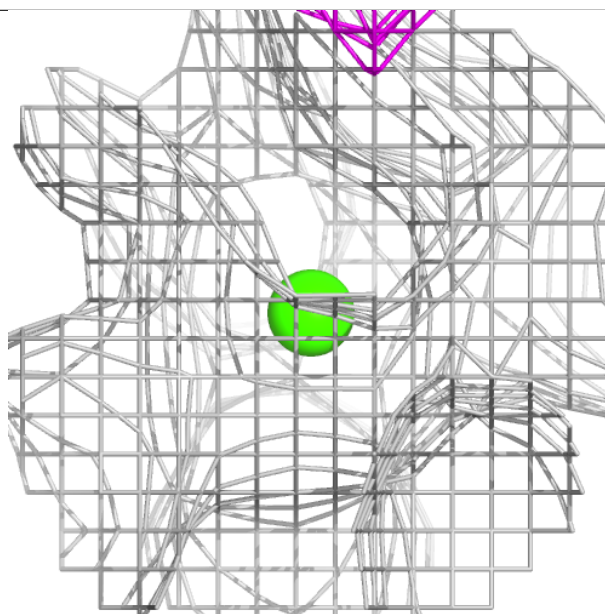
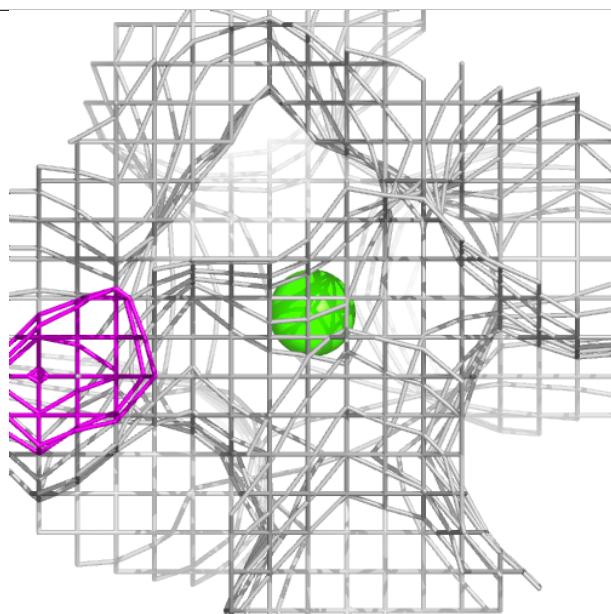
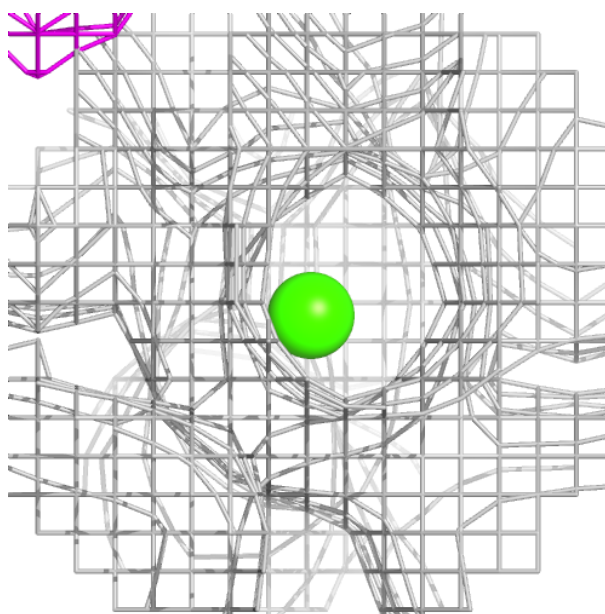
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





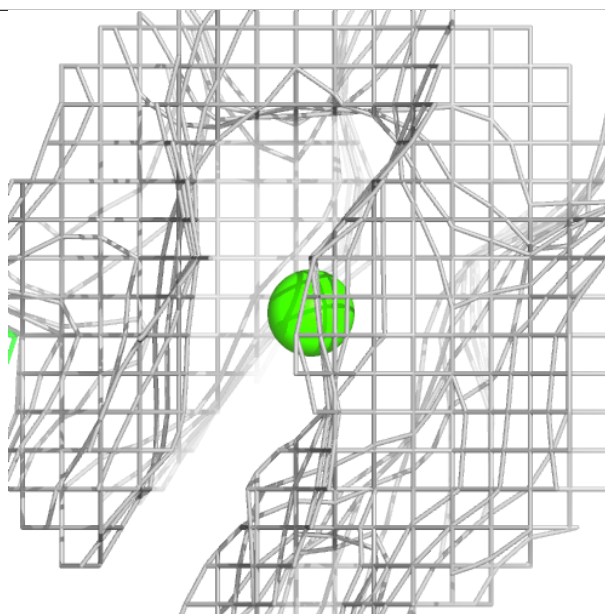
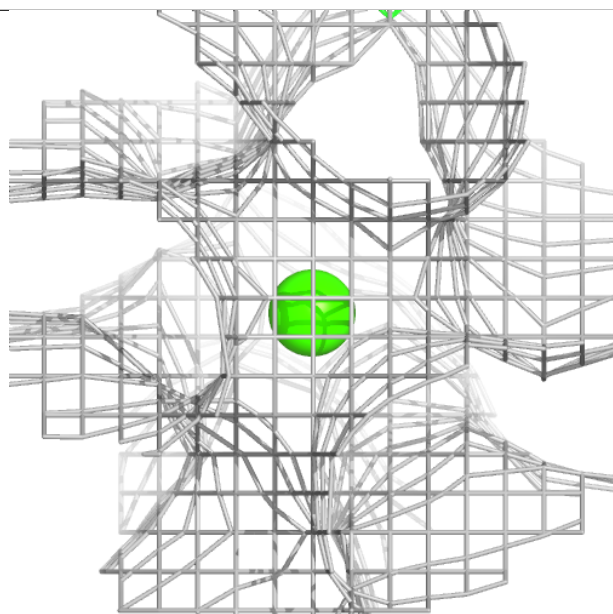
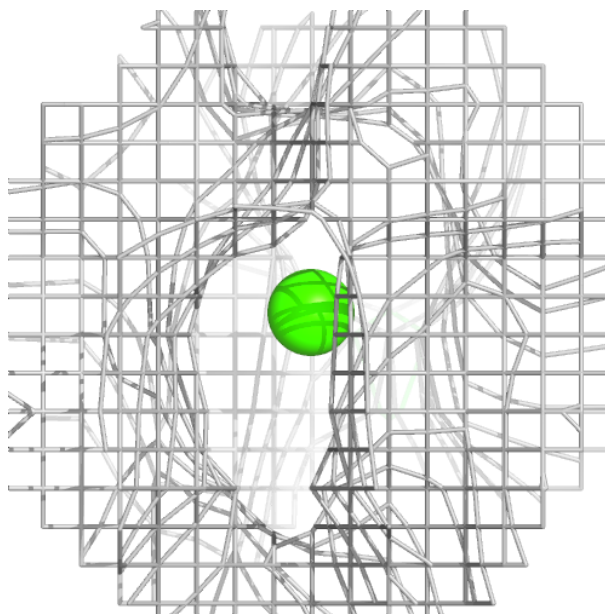
**Electron density around CA C 201:**

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



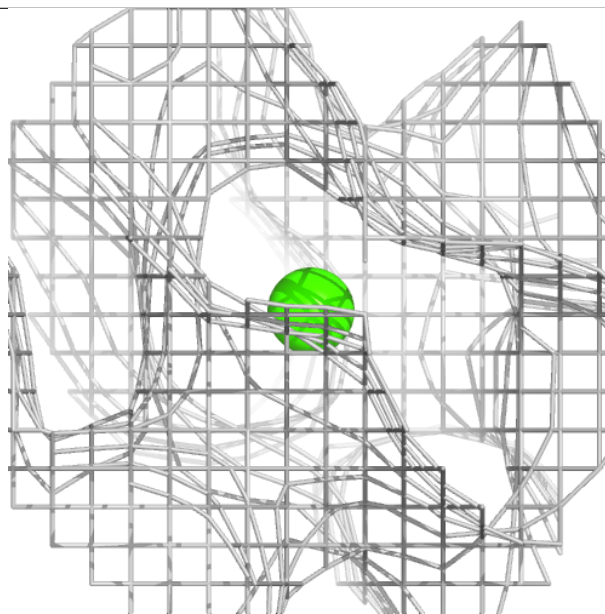
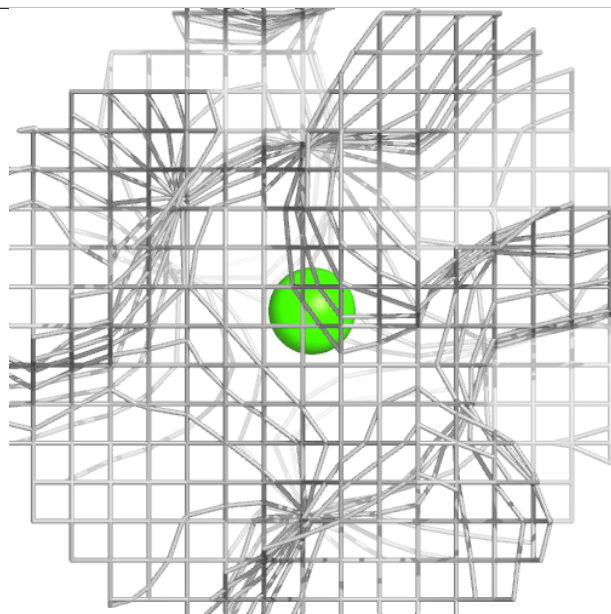
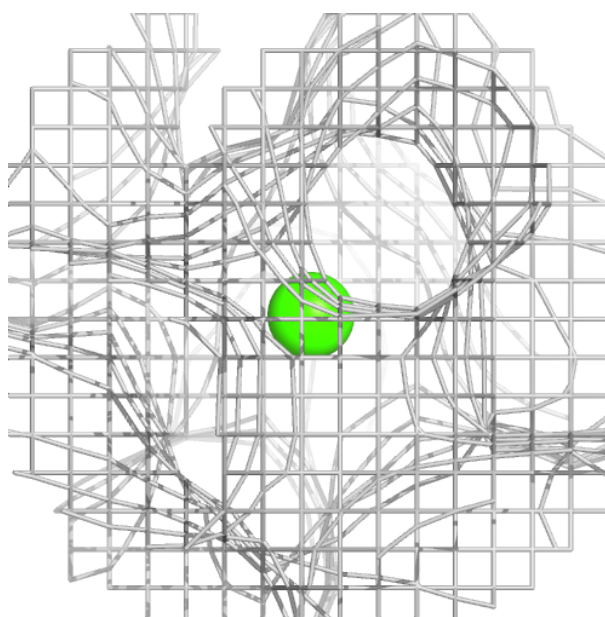
**Electron density around CA D 201:**

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



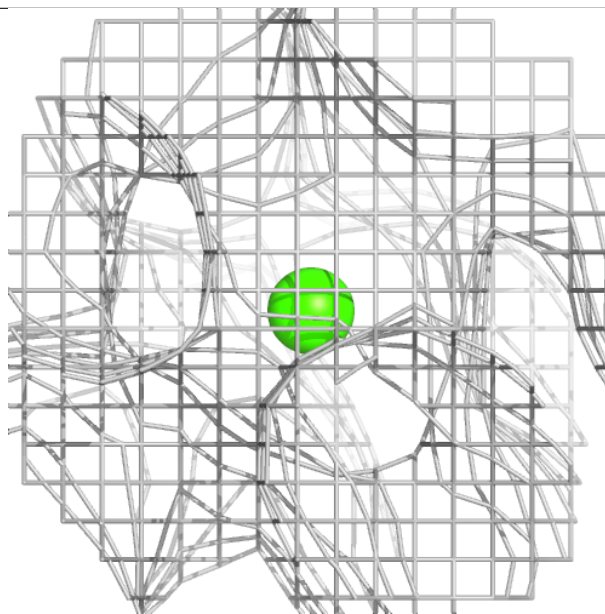
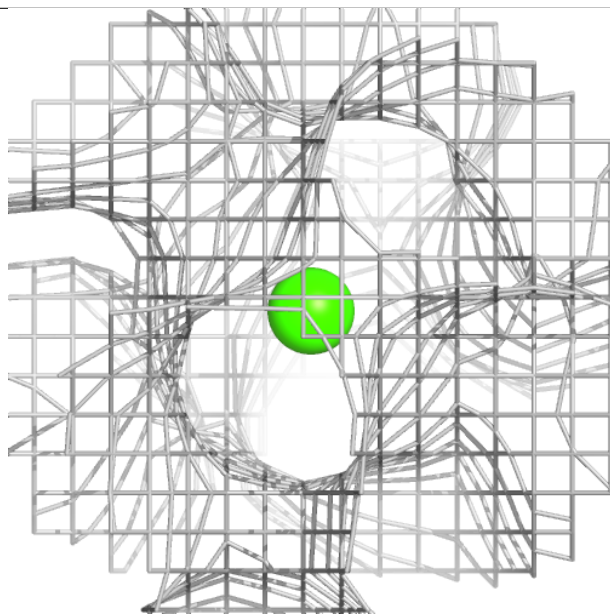
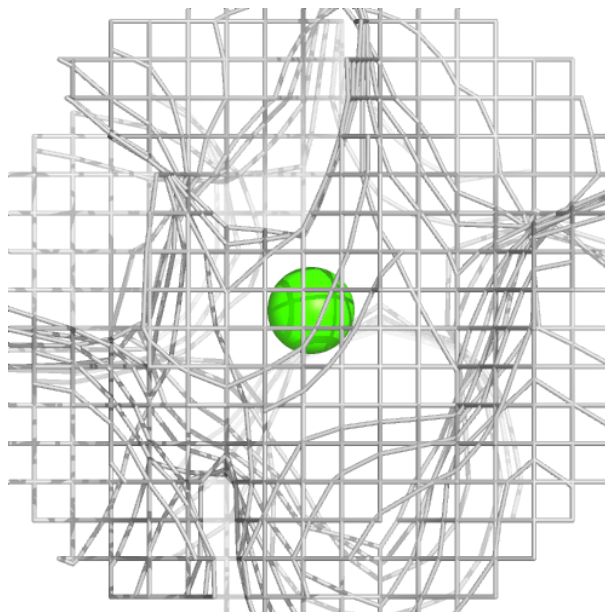
**Electron density around CA E 201:**

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



**Electron density around CA F 201:**

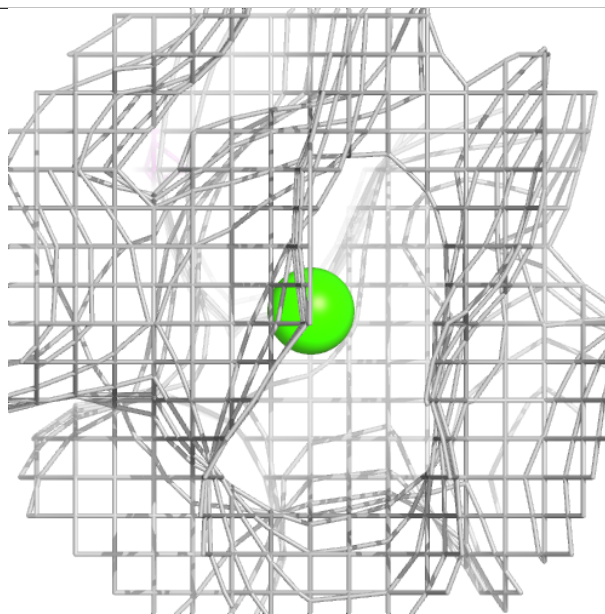
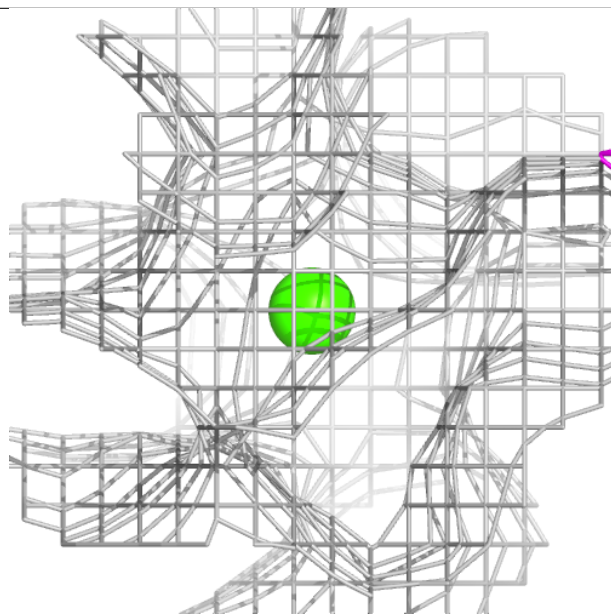
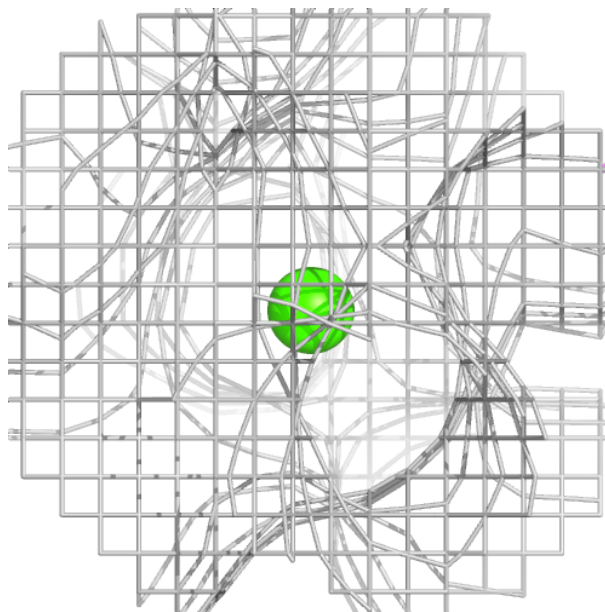
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





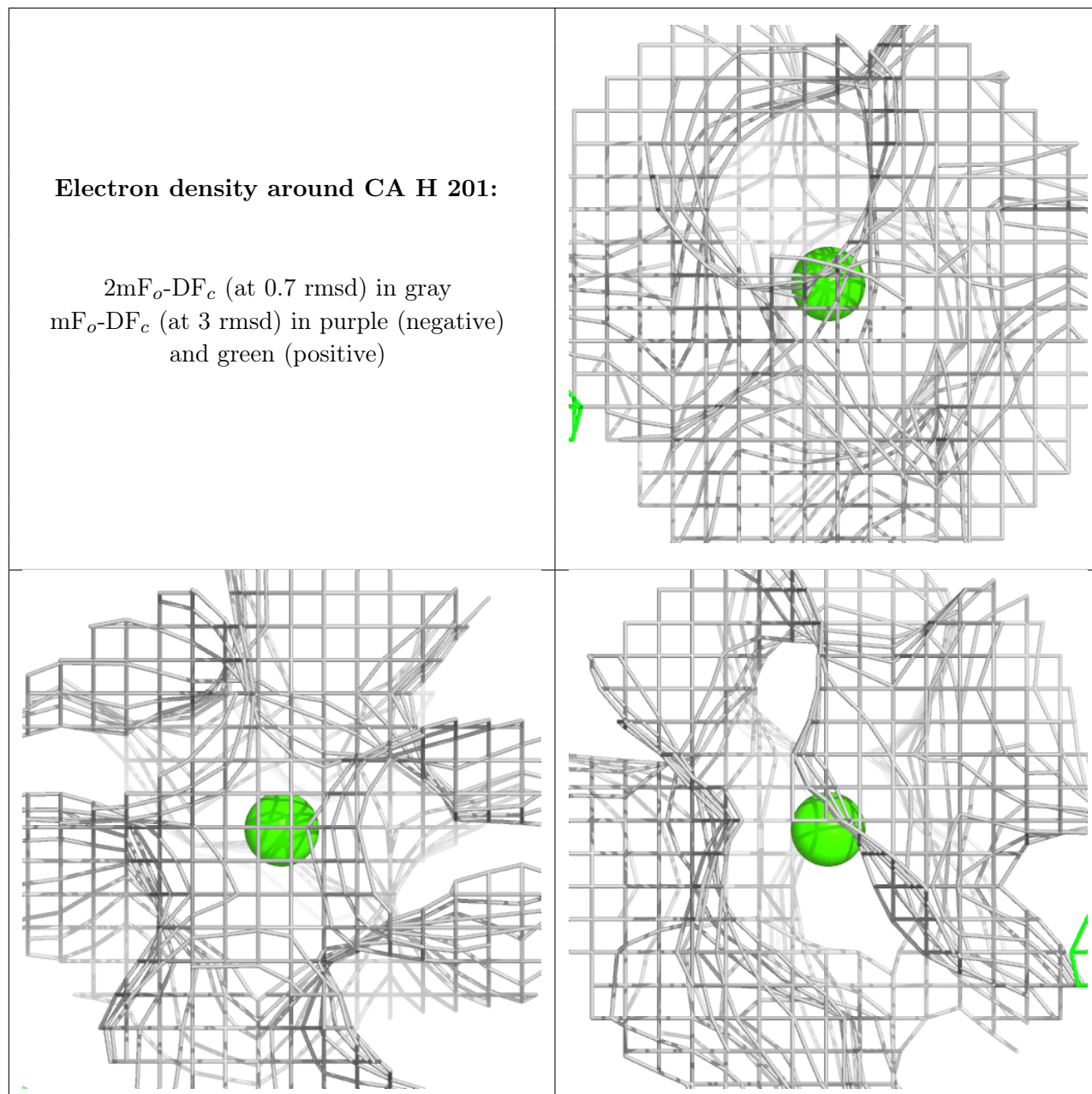
**Electron density around CA G 201:**

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



**Electron density around CA H 201:**

$2mF_o-DF_c$  (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.