



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 20, 2024 – 10:25 pm GMT

PDB ID : 7O5N  
Title : Crystal Structure of a Class D carbapenemase complexed with Avibactam  
Authors : Zhou, Q.; Zhang, Z.; He, Y.; Jin, Y.  
Deposited on : 2021-04-09  
Resolution : 1.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

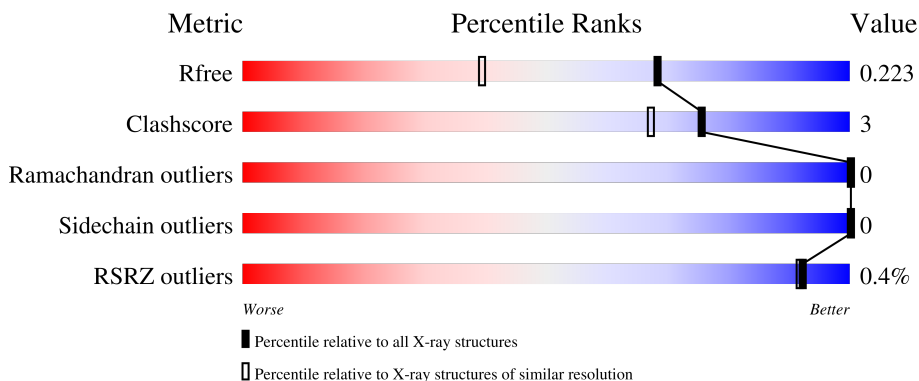
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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

Mol	Chain	Length	Quality of chain
1	AAA	260	 88% 5% 7%
1	BBB	260	 88% 5% 7%
1	CCC	260	 87% 6% 7%
1	DDD	260	 89% 7%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	1BO	AAA	402	-	-	X	-
4	CL	AAA	405[B]	-	-	X	-
4	CL	BBB	305[B]	-	-	X	-
4	CL	CCC	305[B]	-	-	X	-
4	CL	DDD	303[B]	-	-	X	-

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 16886 atoms, of which 8024 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Beta-lactamase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	AAA	243	4003	1285	1985	355	369	9	46	4	0
1	BBB	242	3979	1279	1973	352	367	8	46	4	0
1	CCC	242	3979	1279	1973	352	367	8	46	4	0
1	DDD	242	3988	1282	1975	355	367	9	47	4	0

There are 68 discrepancies between the modelled and reference sequences:

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

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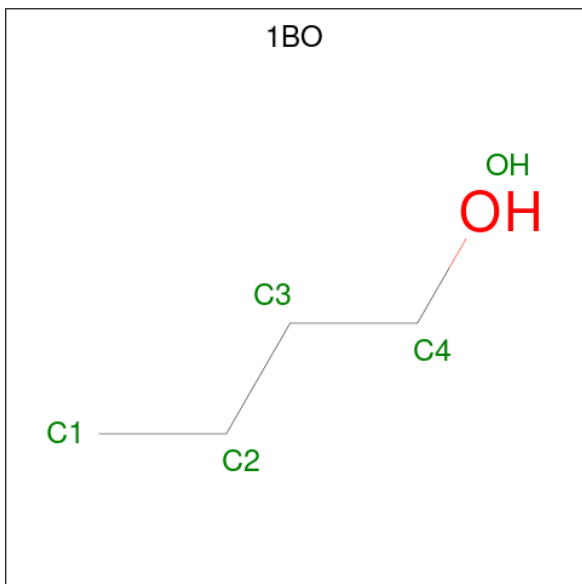
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	10	HIS	-	expression tag	UNP Q6XEC0
BBB	11	HIS	-	expression tag	UNP Q6XEC0
BBB	12	HIS	-	expression tag	UNP Q6XEC0
BBB	13	SER	-	expression tag	UNP Q6XEC0
BBB	14	ALA	-	expression tag	UNP Q6XEC0
BBB	15	GLY	-	expression tag	UNP Q6XEC0
BBB	16	GLU	-	expression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

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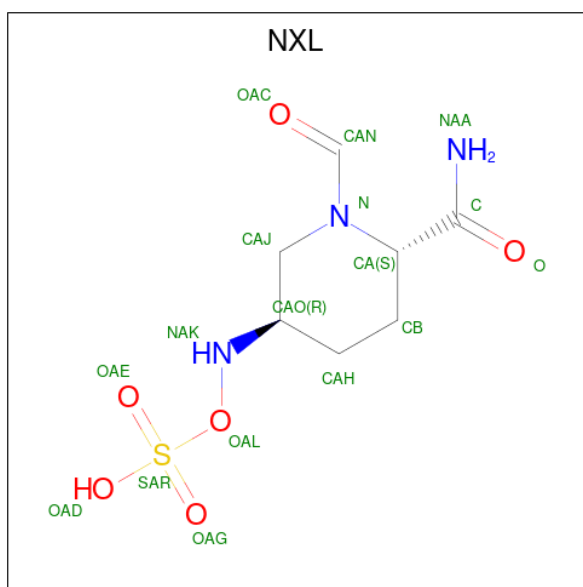
Chain	Residue	Modelled	Actual	Comment	Reference
DDD	18	LEU	-	expression tag	UNP Q6XEC0
DDD	19	TYR	-	expression tag	UNP Q6XEC0
DDD	20	PHE	-	expression tag	UNP Q6XEC0
DDD	21	GLN	-	expression tag	UNP Q6XEC0
DDD	22	GLY	-	expression tag	UNP Q6XEC0

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



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

- Molecule 3 is (2S,5R)-1-formyl-5-[(sulfooxy)amino]piperidine-2-carboxamide (three-letter code: NXL) (formula: C<sub>7</sub>H<sub>13</sub>N<sub>3</sub>O<sub>6</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			S
3	AAA	1	28	7	11	3	6	1	0	0
3	BBB	1	28	7	11	3	6	1	0	0
3	CCC	1	28	7	11	3	6	1	0	0
3	DDD	1	28	7	11	3	6	1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	AAA	3	5	5	0	2
4	BBB	1	2	2	0	1
4	CCC	3	5	5	0	2
4	DDD	1	2	2	0	1

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	AAA	185	185	185	0	0
6	BBB	144	145	145	0	1
6	CCC	192	192	192	0	0
6	DDD	170	172	172	0	2



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

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

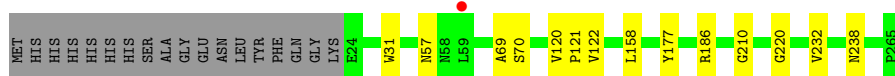
- Molecule 1: Beta-lactamase

Chain AAA: 



- Molecule 1: Beta-lactamase

Chain BBB: 



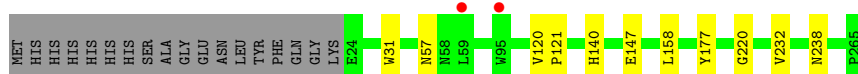
- Molecule 1: Beta-lactamase

Chain CCC: 



- Molecule 1: Beta-lactamase

Chain DDD: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.75Å 107.96Å 125.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.14 – 1.60 73.04 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (73.14-1.60) 99.9 (73.04-1.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.93 (at 1.60Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.188 , 0.216 0.194 , 0.223	Depositor DCC
$R_{free}$ test set	7895 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.2	Xtrriage
Anisotropy	0.728	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 48.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	16886	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.04 % 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 1.2117e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, GOL, 1BO, NXL

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	0/2067	0.82	0/2793
1	BBB	0.70	0/2058	0.82	0/2783
1	CCC	0.70	0/2058	0.82	0/2783
1	DDD	0.71	0/2063	0.81	0/2789
All	All	0.71	0/8246	0.82	0/11148

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	2018	1985	1974	12	0
1	BBB	2006	1973	1964	13	0
1	CCC	2006	1973	1964	11	0
1	DDD	2013	1975	1963	8	0
2	AAA	10	20	20	7	0
2	BBB	10	20	20	2	0
2	CCC	5	10	10	1	0
3	AAA	17	11	11	0	0
3	BBB	17	11	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	CCC	17	11	11	0	0
3	DDD	17	11	11	0	0
4	AAA	5	0	0	5	0
4	BBB	2	0	0	4	0
4	CCC	5	0	0	5	0
4	DDD	2	0	0	3	0
5	BBB	6	8	8	1	0
5	CCC	6	8	8	0	0
5	DDD	6	8	8	0	0
6	AAA	185	0	0	4	0
6	BBB	145	0	0	2	0
6	CCC	192	0	0	0	0
6	DDD	172	0	0	1	0
All	All	8862	8024	7983	50	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 (50) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:158[B]:LEU:HD21	4:BBB:305[B]:CL:CL	1.07	1.59
1:DDD:158:LEU:HD21	4:DDD:303[B]:CL:CL	1.04	1.58
1:CCC:158[B]:LEU:HD21	4:CCC:305[B]:CL:CL	1.50	1.48
1:DDD:158:LEU:CD2	4:DDD:303[B]:CL:CL	1.97	1.46
1:BBB:158[B]:LEU:CD2	4:BBB:305[B]:CL:CL	2.03	1.41
1:AAA:158:LEU:HD21	4:AAA:405[B]:CL:CL	1.90	1.08
1:CCC:158[B]:LEU:CD2	4:CCC:305[B]:CL:CL	2.42	1.04
4:AAA:406[A]:CL:CL	6:BBB:538:HOH:O	2.39	0.76
4:CCC:306[A]:CL:CL	6:DDD:560:HOH:O	2.44	0.73
4:AAA:406[B]:CL:CL	6:AAA:674:HOH:O	2.46	0.70
2:BBB:302:1BO:H12	6:BBB:543:HOH:O	1.94	0.66
1:AAA:158:LEU:CD2	4:AAA:405[B]:CL:CL	2.76	0.65
1:DDD:158:LEU:CG	4:DDD:303[B]:CL:CL	2.80	0.65
1:AAA:230:ASP:OD1	6:AAA:501:HOH:O	2.14	0.65
1:BBB:158[B]:LEU:CG	4:BBB:305[B]:CL:CL	2.86	0.59
1:AAA:31:TRP:HB2	1:AAA:57:ASN:HB3	1.86	0.57
1:CCC:31:TRP:HB2	1:CCC:57:ASN:HB3	1.89	0.55
1:DDD:31:TRP:HB2	1:DDD:57:ASN:HB3	1.90	0.54
1:AAA:184:SER:CB	2:AAA:401:1BO:H31	2.39	0.53
1:AAA:220:GLY:O	1:AAA:238:ASN:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:96:ASP:H	2:AAA:402:1BO:H13	1.75	0.51
1:CCC:220:GLY:O	1:CCC:238:ASN:HA	2.11	0.51
1:BBB:69:ALA:HA	1:BBB:158[B]:LEU:HD23	1.94	0.48
1:DDD:140[A]:HIS:CD2	1:DDD:147:GLU:OE1	2.67	0.47
1:DDD:120:VAL:N	1:DDD:121:PRO:HD2	2.30	0.47
1:DDD:177:TYR:CZ	1:DDD:232[B]:VAL:HG21	2.51	0.46
1:BBB:70:SER:HB2	1:BBB:210:GLY:HA2	1.98	0.45
1:BBB:186:ARG:HD3	2:BBB:302:1BO:H32	1.97	0.45
1:CCC:157:TRP:CD1	1:CCC:158[B]:LEU:HG	2.52	0.45
1:AAA:95:TRP:HA	2:AAA:402:1BO:H11	1.98	0.45
2:AAA:402:1BO:C1	6:AAA:618:HOH:O	2.64	0.45
1:AAA:96:ASP:H	2:AAA:402:1BO:C1	2.31	0.44
1:AAA:73:LYS:NZ	4:AAA:405[A]:CL:CL	2.81	0.43
1:BBB:120:VAL:N	1:BBB:121:PRO:HD2	2.32	0.43
1:CCC:120:VAL:N	1:CCC:121:PRO:HD2	2.33	0.43
1:BBB:158[B]:LEU:HD11	4:BBB:305[B]:CL:CL	2.55	0.43
1:CCC:177:TYR:CZ	1:CCC:232[B]:VAL:HG21	2.53	0.43
1:AAA:177:TYR:CZ	1:AAA:232[B]:VAL:HG21	2.54	0.43
1:AAA:186:ARG:HD3	2:AAA:401:1BO:H22	2.01	0.43
1:CCC:184:SER:CB	2:CCC:302:1BO:H31	2.49	0.42
1:CCC:134:ARG:O	1:CCC:138:MET:HG2	2.20	0.42
1:BBB:31:TRP:HB2	1:BBB:57:ASN:HB3	2.00	0.42
1:DDD:220:GLY:O	1:DDD:238:ASN:HA	2.20	0.42
1:BBB:122:VAL:HG22	5:BBB:301:GOL:H31	2.02	0.42
2:AAA:402:1BO:H11	6:AAA:618:HOH:O	2.20	0.41
1:BBB:220:GLY:O	1:BBB:238:ASN:HA	2.20	0.41
1:CCC:189:ARG:HD2	4:CCC:306[B]:CL:CL	2.57	0.41
1:CCC:73:LYS:NZ	4:CCC:305[A]:CL:CL	2.85	0.41
1:BBB:177:TYR:CZ	1:BBB:232[B]:VAL:HG21	2.56	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	245/260 (94%)	240 (98%)	5 (2%)	0	100	100
1	BBB	244/260 (94%)	239 (98%)	5 (2%)	0	100	100
1	CCC	244/260 (94%)	239 (98%)	5 (2%)	0	100	100
1	DDD	244/260 (94%)	240 (98%)	4 (2%)	0	100	100
All	All	977/1040 (94%)	958 (98%)	19 (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	216/226 (96%)	216 (100%)	0	100	100
1	BBB	215/226 (95%)	215 (100%)	0	100	100
1	CCC	215/226 (95%)	215 (100%)	0	100	100
1	DDD	215/226 (95%)	215 (100%)	0	100	100
All	All	861/904 (95%)	861 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 14 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	1BO	AAA	402	-	4,4,4	0.12	0	3,3,3	0.12	0
2	1BO	BBB	303	-	4,4,4	0.13	0	3,3,3	0.10	0
2	1BO	AAA	401	-	4,4,4	0.14	0	3,3,3	0.08	0
3	NXL	AAA	403	1	14,17,17	0.68	0	17,24,24	1.83	5 (29%)
2	1BO	CCC	302	-	4,4,4	0.22	0	3,3,3	0.24	0
3	NXL	DDD	302	1	14,17,17	0.60	0	17,24,24	1.55	2 (11%)
3	NXL	CCC	303	1	14,17,17	0.52	0	17,24,24	2.11	7 (41%)
3	NXL	BBB	304	1	14,17,17	0.93	1 (7%)	17,24,24	1.33	2 (11%)
5	GOL	BBB	301	-	5,5,5	0.10	0	5,5,5	0.25	0
2	1BO	BBB	302	-	4,4,4	0.25	0	3,3,3	0.26	0
5	GOL	DDD	301	-	5,5,5	0.15	0	5,5,5	0.32	0
5	GOL	CCC	301	-	5,5,5	0.13	0	5,5,5	0.31	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	1BO	AAA	402	-	-	1/2/2/2	-
2	1BO	BBB	303	-	-	2/2/2/2	-
2	1BO	AAA	401	-	-	1/2/2/2	-
3	NXL	AAA	403	1	-	2/5/25/25	0/1/1/1
2	1BO	CCC	302	-	-	2/2/2/2	-
3	NXL	DDD	302	1	-	2/5/25/25	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NXL	CCC	303	1	-	2/5/25/25	0/1/1/1
3	NXL	BBB	304	1	-	2/5/25/25	0/1/1/1
5	GOL	BBB	301	-	-	2/4/4/4	-
2	1BO	BBB	302	-	-	1/2/2/2	-
5	GOL	DDD	301	-	-	2/4/4/4	-
5	GOL	CCC	301	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BBB	304	NXL	O-C	-2.18	1.19	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	CCC	303	NXL	OAL-SAR-OAE	4.12	116.36	103.29
3	AAA	403	NXL	OAL-SAR-OAG	3.40	114.08	103.29
3	CCC	303	NXL	CB-CA-N	-3.35	105.46	110.31
3	DDD	302	NXL	O-C-CA	3.27	126.10	120.26
3	AAA	403	NXL	CAO-CAJ-N	-3.26	105.52	110.11
3	CCC	303	NXL	CAO-CAJ-N	-3.25	105.54	110.11
3	BBB	304	NXL	CB-CA-N	-3.23	105.64	110.31
3	DDD	302	NXL	OAL-SAR-OAG	3.10	113.14	103.29
3	CCC	303	NXL	O-C-CA	3.04	125.69	120.26
3	AAA	403	NXL	CA-C-NAA	-2.62	110.18	116.55
3	AAA	403	NXL	OAL-SAR-OAE	-2.52	95.31	103.29
3	AAA	403	NXL	O-C-CA	2.45	124.63	120.26
3	CCC	303	NXL	OAL-SAR-OAG	-2.35	95.84	103.29
3	CCC	303	NXL	CA-C-NAA	-2.27	111.04	116.55
3	CCC	303	NXL	CAH-CAO-CAJ	-2.18	106.87	109.71
3	BBB	304	NXL	CAO-CAJ-N	-2.11	107.15	110.11

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	BBB	304	NXL	O-C-CA-CB
3	BBB	304	NXL	NAA-C-CA-CB
3	DDD	302	NXL	NAA-C-CA-CB
5	BBB	301	GOL	C1-C2-C3-O3

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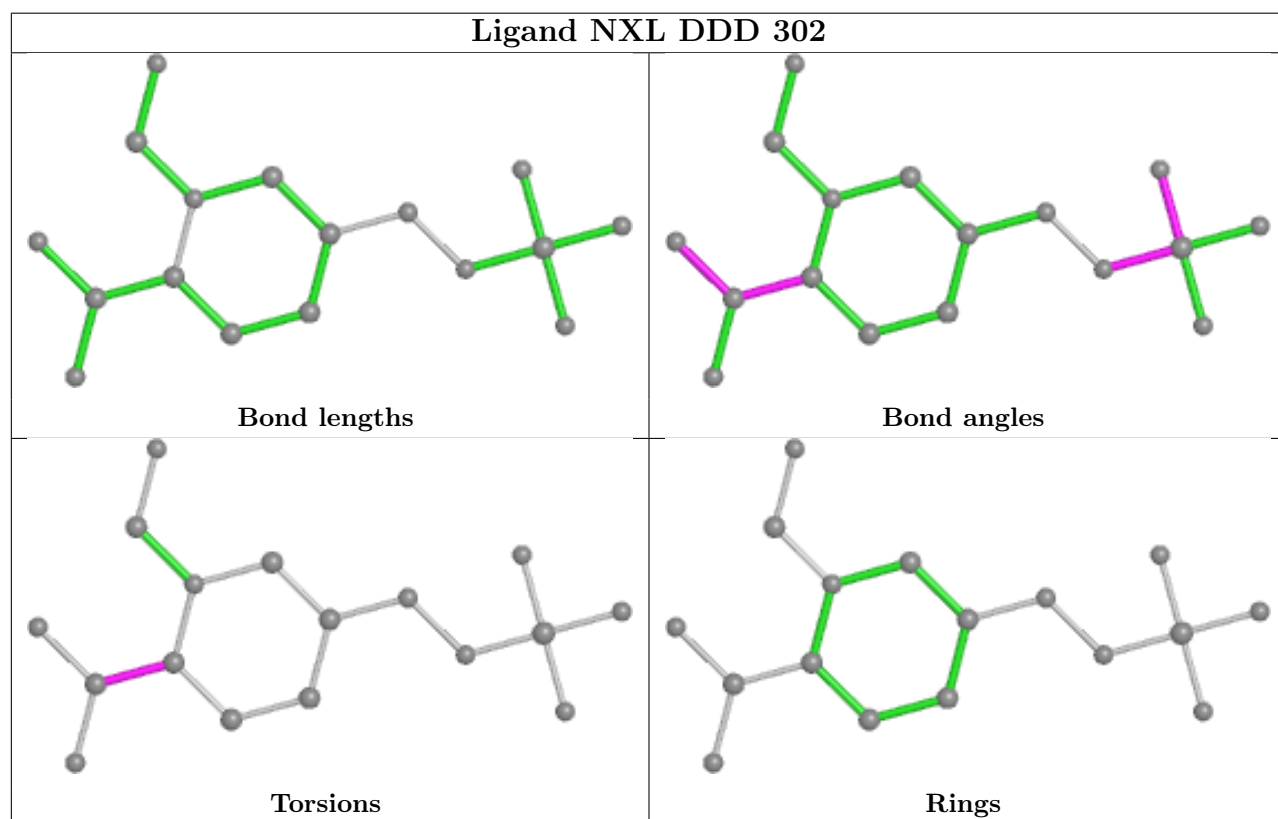
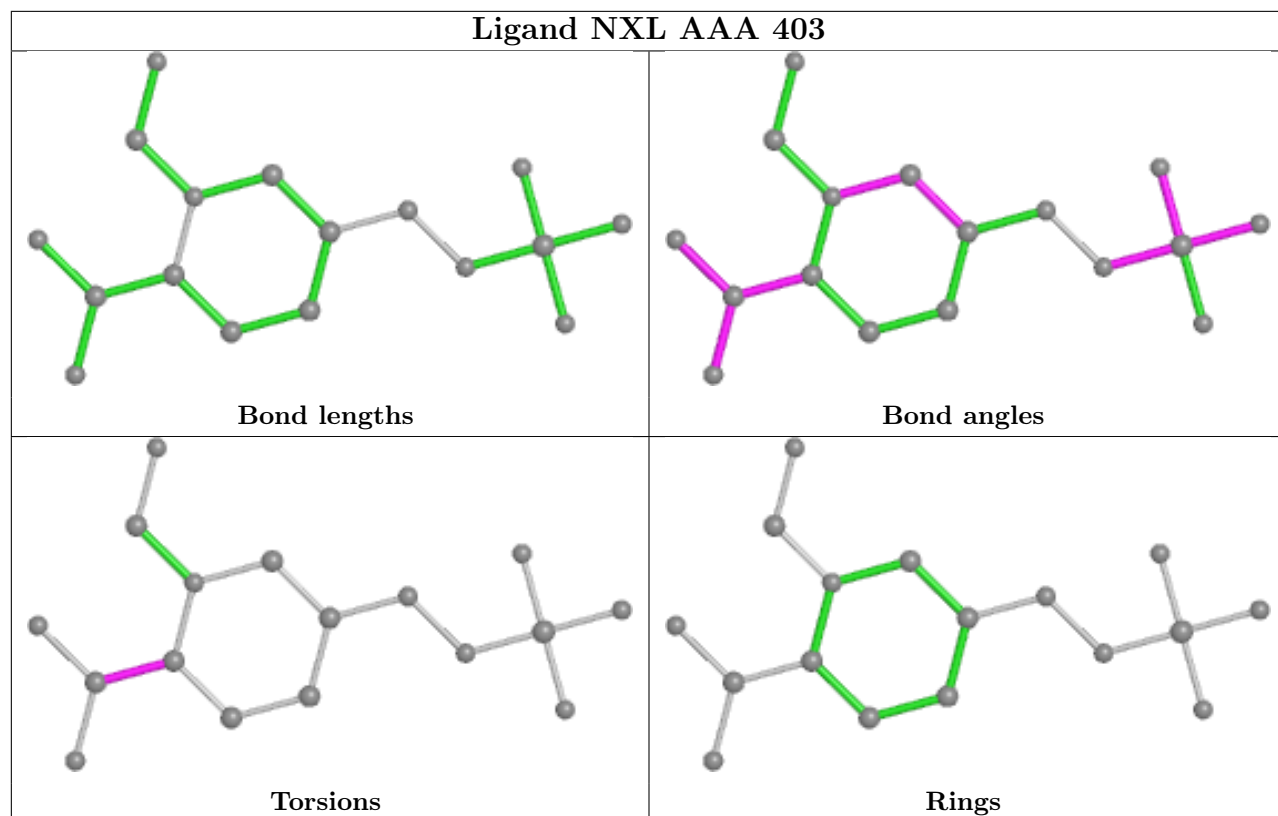
Mol	Chain	Res	Type	Atoms
5	CCC	301	GOL	C1-C2-C3-O3
5	DDD	301	GOL	C1-C2-C3-O3
5	CCC	301	GOL	O2-C2-C3-O3
3	AAA	403	NXL	NAA-C-CA-CB
3	CCC	303	NXL	NAA-C-CA-CB
3	AAA	403	NXL	O-C-CA-CB
3	CCC	303	NXL	O-C-CA-CB
3	DDD	302	NXL	O-C-CA-CB
5	DDD	301	GOL	O2-C2-C3-O3
5	BBB	301	GOL	O2-C2-C3-O3
2	CCC	302	1BO	C1-C2-C3-C4
2	BBB	302	1BO	C2-C3-C4-OH
2	CCC	302	1BO	C2-C3-C4-OH
2	AAA	402	1BO	C2-C3-C4-OH
2	BBB	303	1BO	C2-C3-C4-OH
2	AAA	401	1BO	C1-C2-C3-C4
2	BBB	303	1BO	C1-C2-C3-C4

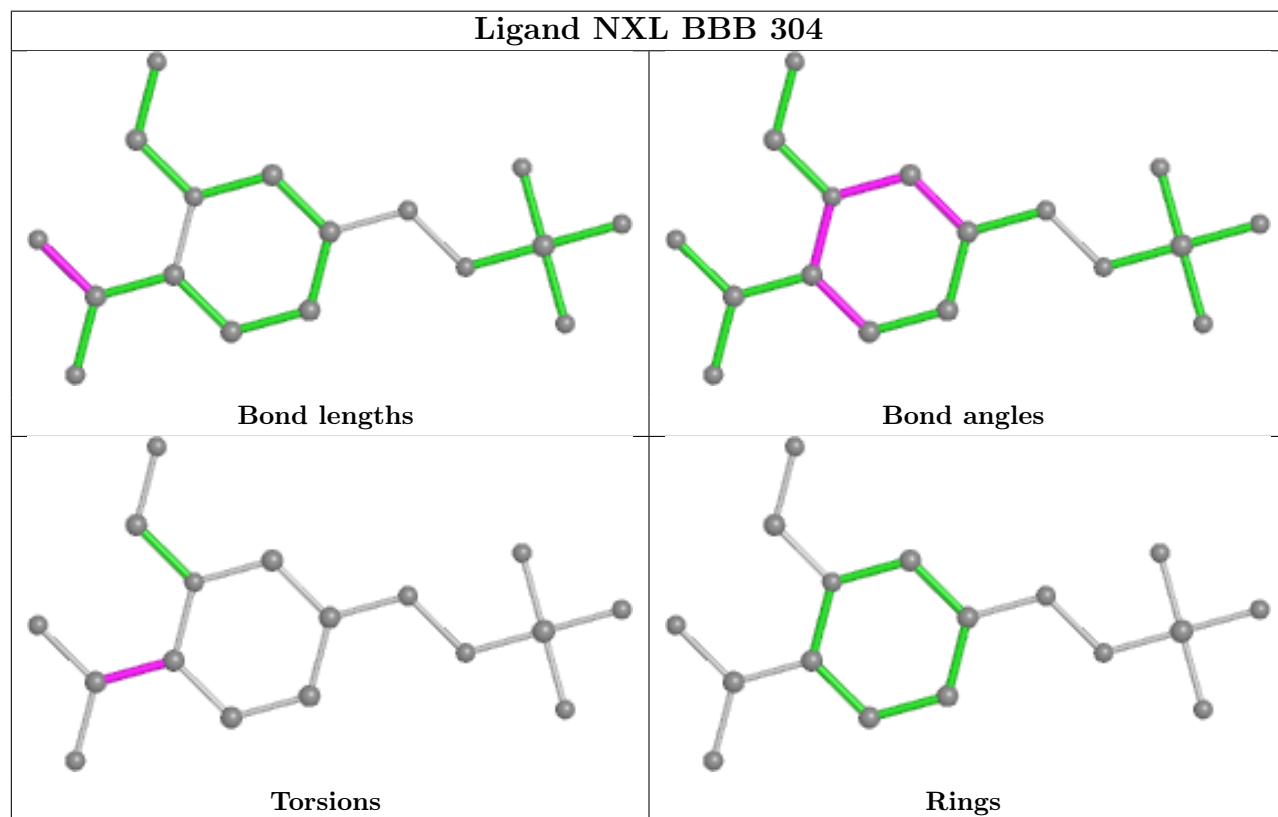
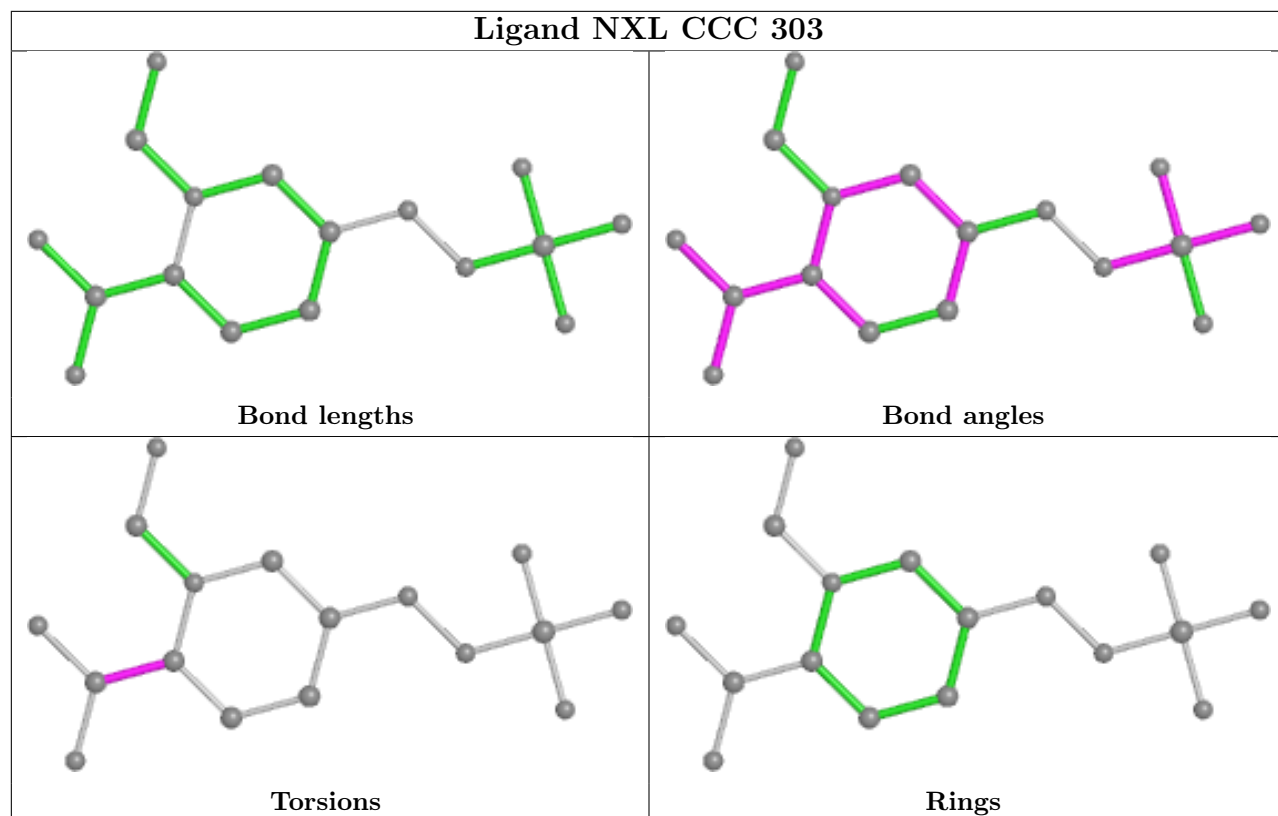
There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	402	1BO	5	0
2	AAA	401	1BO	2	0
2	CCC	302	1BO	1	0
5	BBB	301	GOL	1	0
2	BBB	302	1BO	2	0

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





## 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	AAA	243/260 (93%)	-0.34	1 (0%) 92   92	22, 31, 45, 71	24 (9%)
1	BBB	242/260 (93%)	-0.28	1 (0%) 92   92	23, 35, 58, 78	2 (0%)
1	CCC	242/260 (93%)	-0.37	0 100   100	21, 31, 47, 59	1 (0%)
1	DDD	242/260 (93%)	-0.39	2 (0%) 86   86	22, 33, 54, 70	2 (0%)
All	All	969/1040 (93%)	-0.35	4 (0%) 92   92	21, 33, 52, 78	29 (2%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	59	LEU	2.5
1	AAA	23	LYS	2.4
1	BBB	59	LEU	2.2
1	DDD	95	TRP	2.1

### 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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

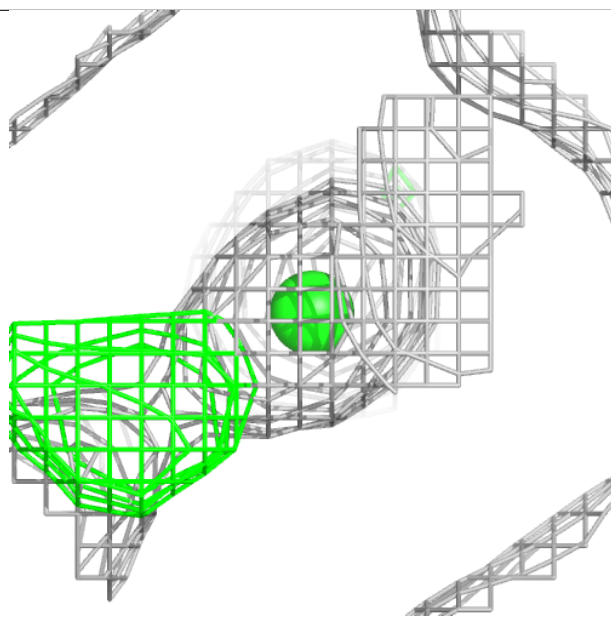
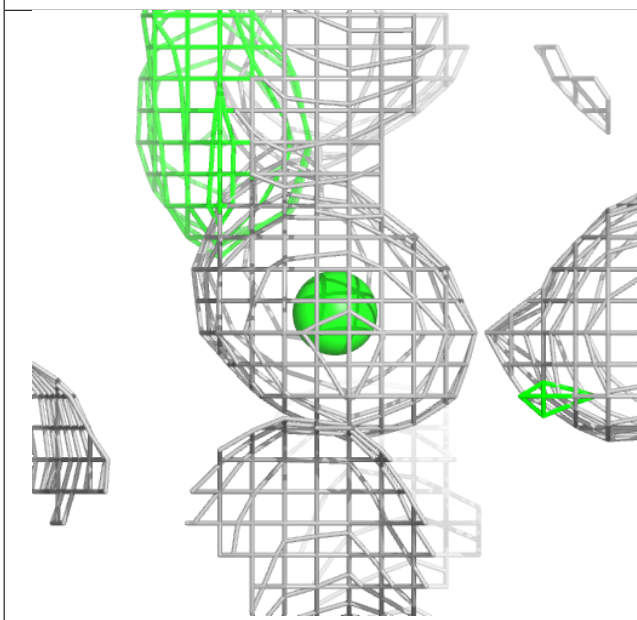
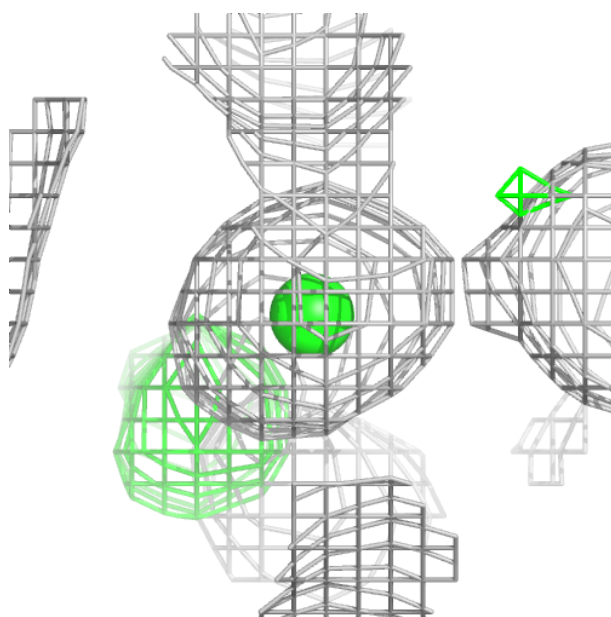
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	1BO	BBB	303	5/5	0.72	0.20	50,52,55,56	15
2	1BO	BBB	302	5/5	0.81	0.15	39,47,50,51	15
2	1BO	CCC	302	5/5	0.84	0.15	42,46,47,48	9
5	GOL	BBB	301	6/6	0.89	0.12	43,49,55,56	14
2	1BO	AAA	401	5/5	0.90	0.11	42,48,50,50	9
5	GOL	DDD	301	6/6	0.90	0.15	43,48,52,52	14
4	CL	CCC	306[B]	1/1	0.92	0.08	38,38,38,38	1
2	1BO	AAA	402	5/5	0.92	0.10	31,42,45,45	0
5	GOL	CCC	301	6/6	0.92	0.13	37,45,49,49	5
4	CL	CCC	306[A]	1/1	0.92	0.08	37,37,37,37	1
4	CL	AAA	405[B]	1/1	0.94	0.17	39,39,39,39	1
4	CL	AAA	405[A]	1/1	0.94	0.17	38,38,38,38	1
3	NXL	DDD	302	17/17	0.95	0.10	26,33,47,51	8
4	CL	CCC	305[A]	1/1	0.95	0.16	37,37,37,37	1
4	CL	CCC	305[B]	1/1	0.95	0.16	38,38,38,38	1
3	NXL	BBB	304	17/17	0.95	0.11	27,36,53,57	28
4	CL	AAA	406[B]	1/1	0.96	0.08	37,37,37,37	1
4	CL	BBB	305[A]	1/1	0.96	0.10	41,41,41,41	1
4	CL	BBB	305[B]	1/1	0.96	0.10	36,36,36,36	1
3	NXL	AAA	403	17/17	0.96	0.12	25,31,43,45	5
4	CL	AAA	406[A]	1/1	0.96	0.08	40,40,40,40	1
3	NXL	CCC	303	17/17	0.97	0.13	23,33,44,44	7
4	CL	DDD	303[A]	1/1	0.97	0.08	40,40,40,40	1
4	CL	DDD	303[B]	1/1	0.97	0.08	31,31,31,31	1
4	CL	CCC	304	1/1	0.99	0.08	27,27,27,27	0
4	CL	AAA	404	1/1	0.99	0.10	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.

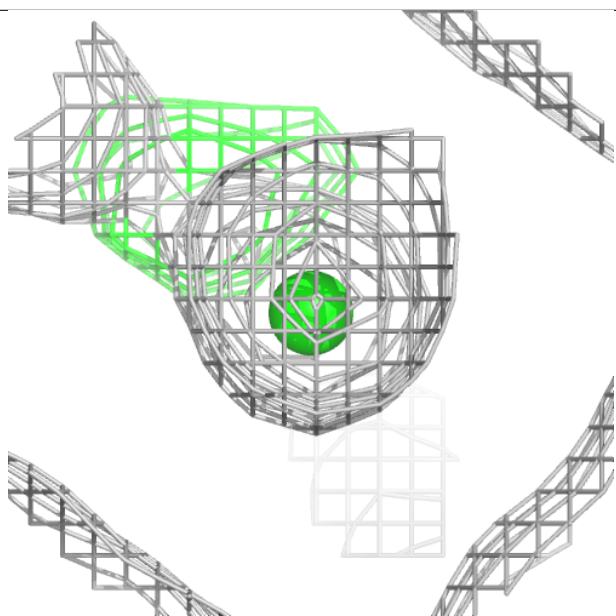
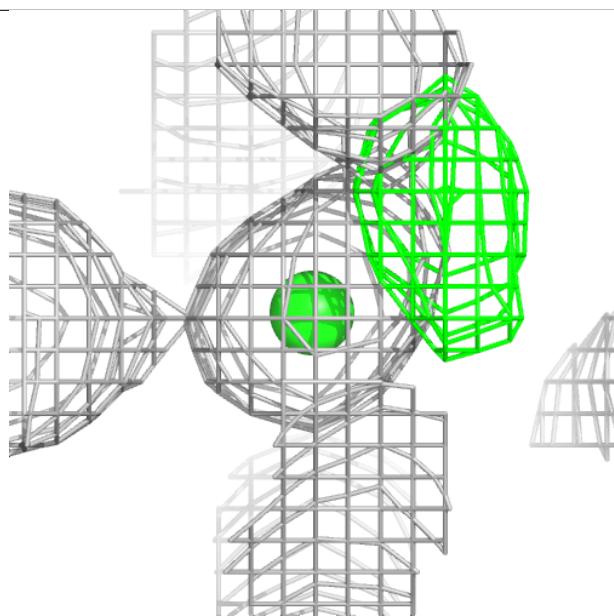
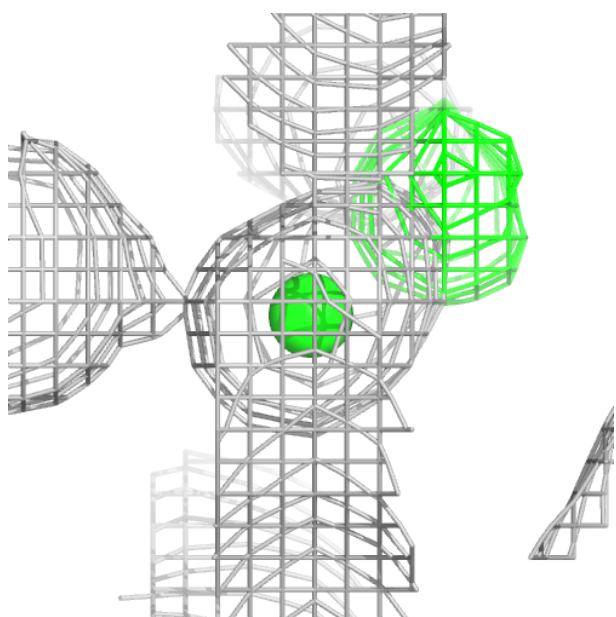
**Electron density around CL CCC 306 (B):**

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



**Electron density around CL CCC 306 (A):**

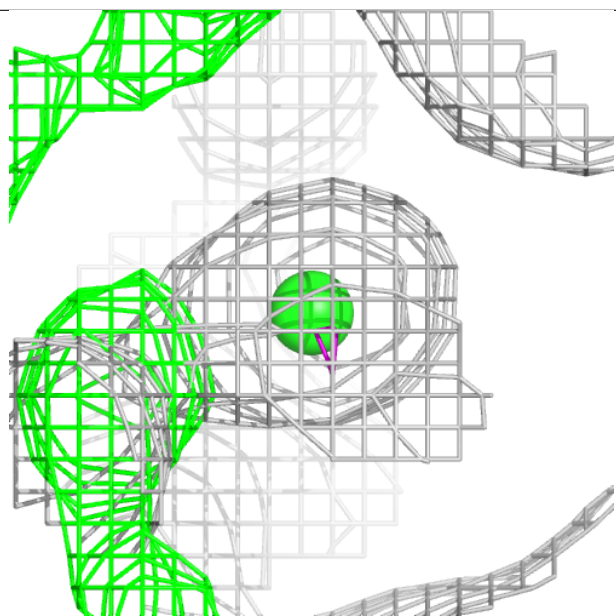
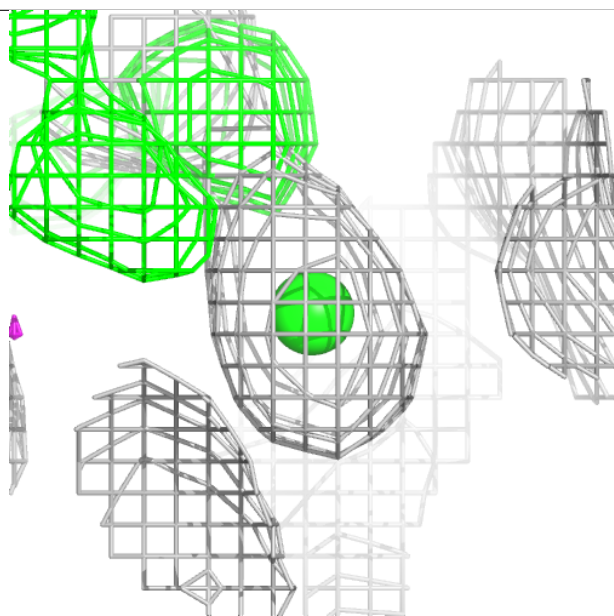
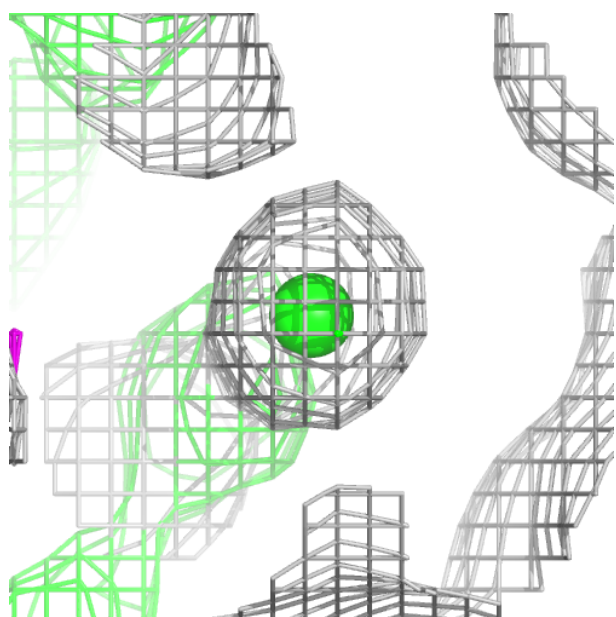
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





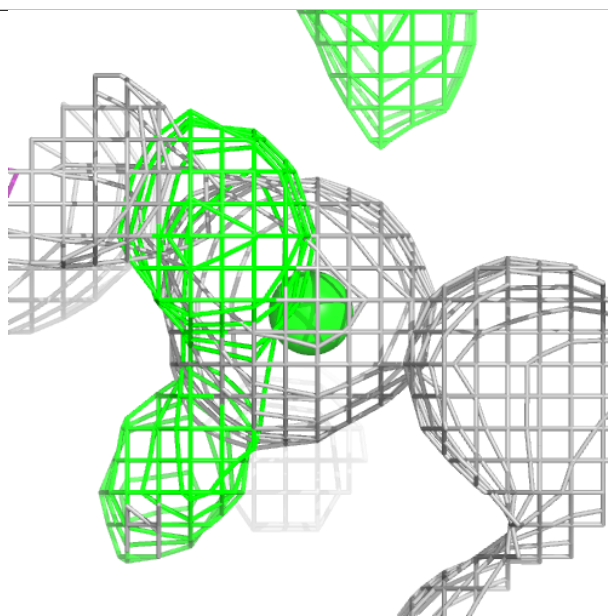
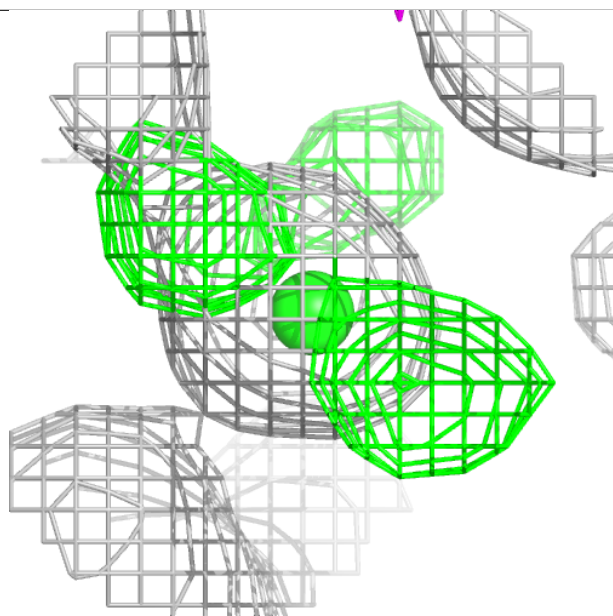
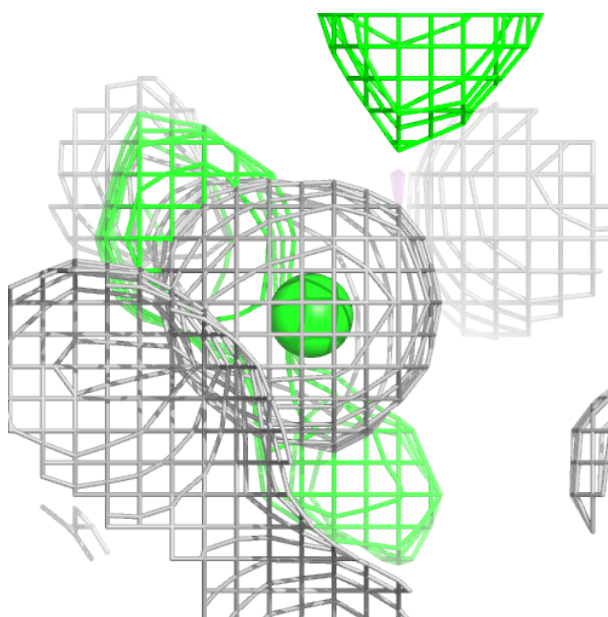
**Electron density around CL AAA 405 (B):**

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and green (positive)



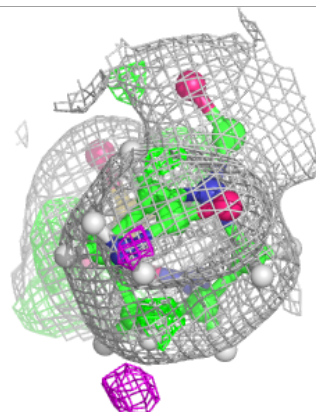
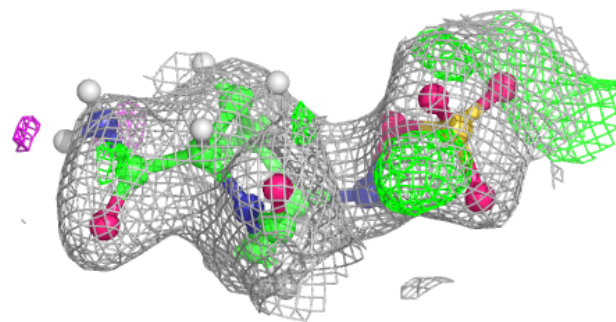
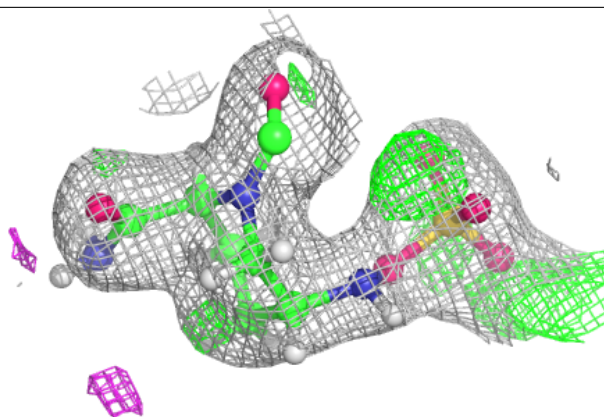
**Electron density around CL AAA 405 (A):**

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and green (positive)



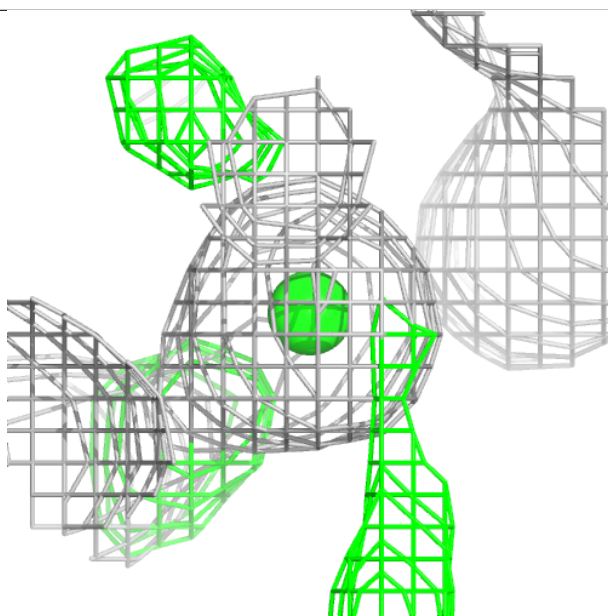
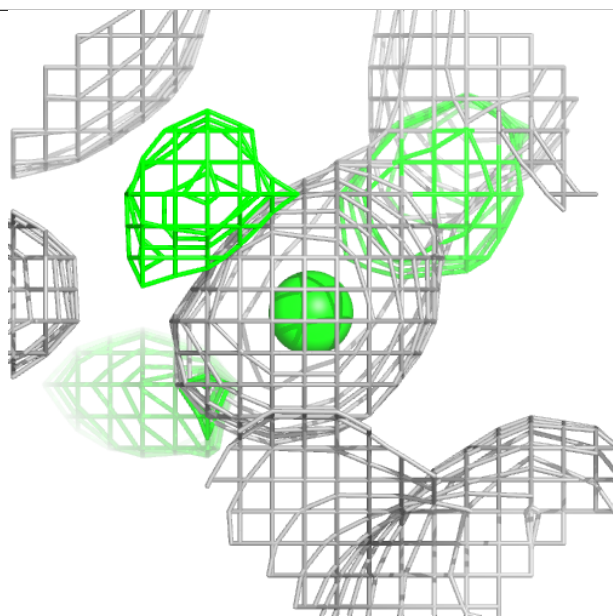
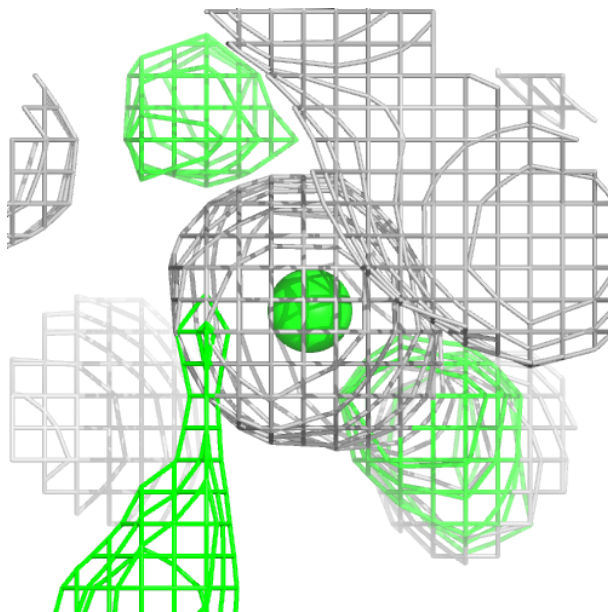
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and green (positive)



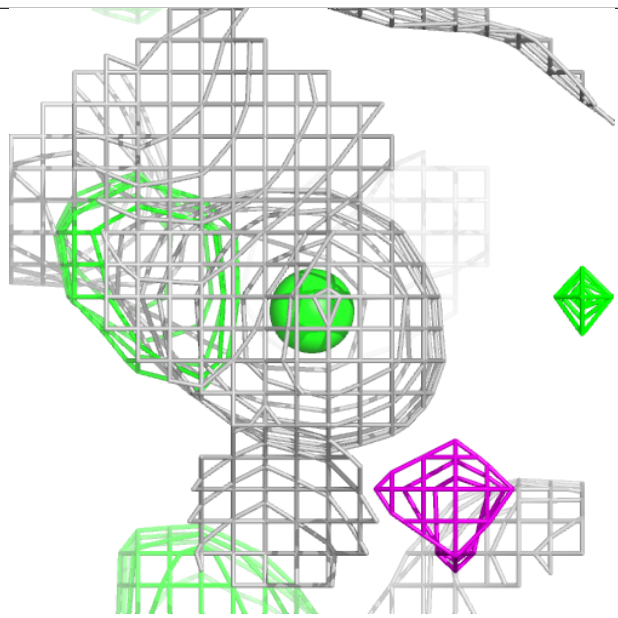
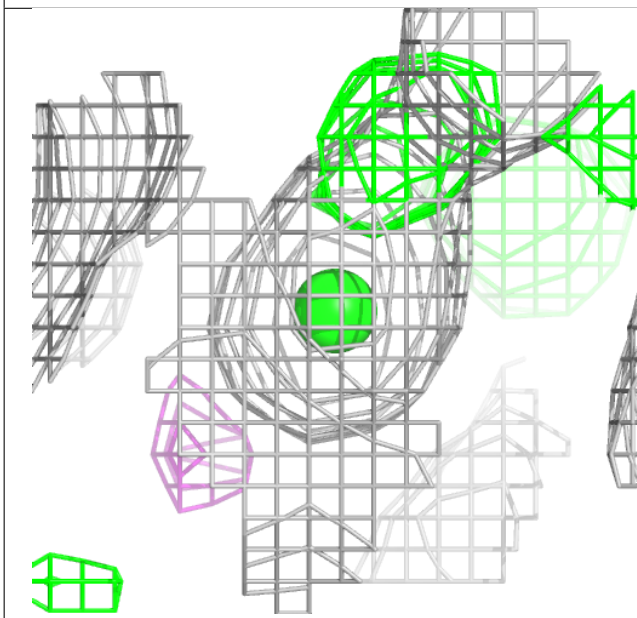
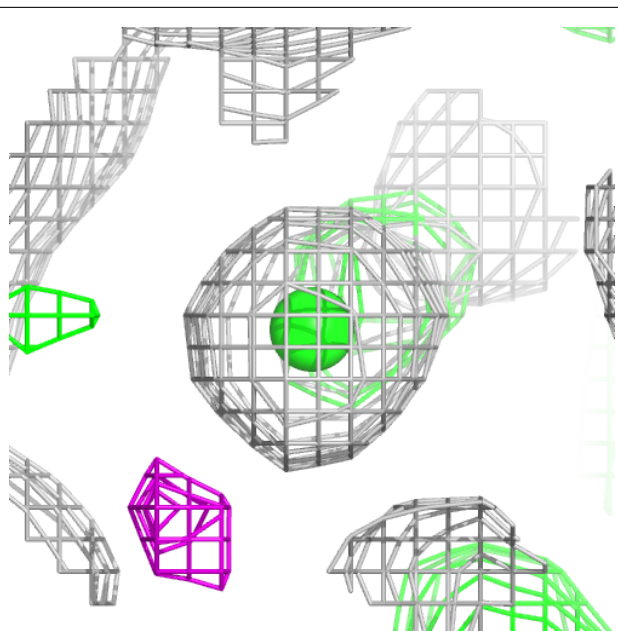
**Electron density around CL CCC 305 (A):**

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and green (positive)



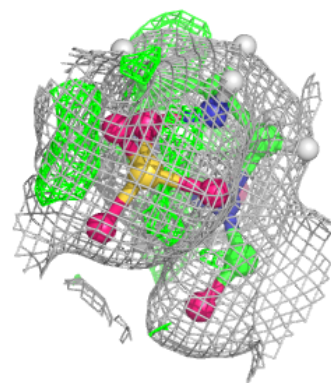
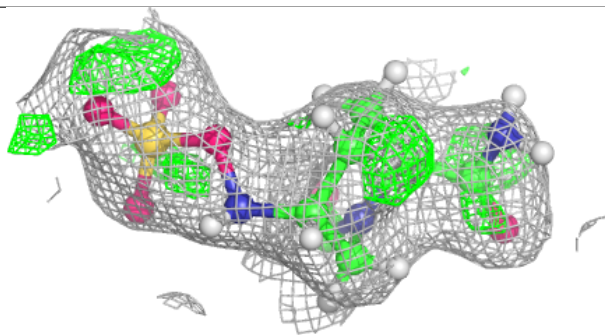
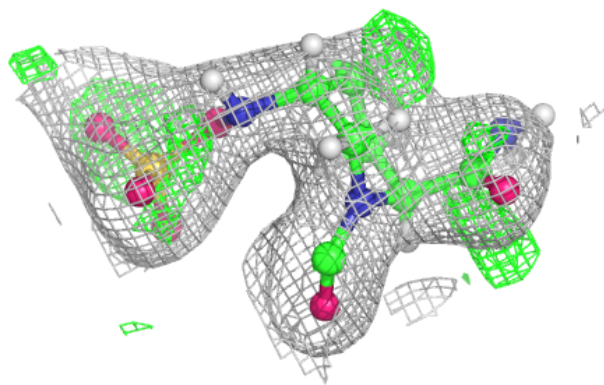
**Electron density around CL CCC 305 (B):**

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and green (positive)



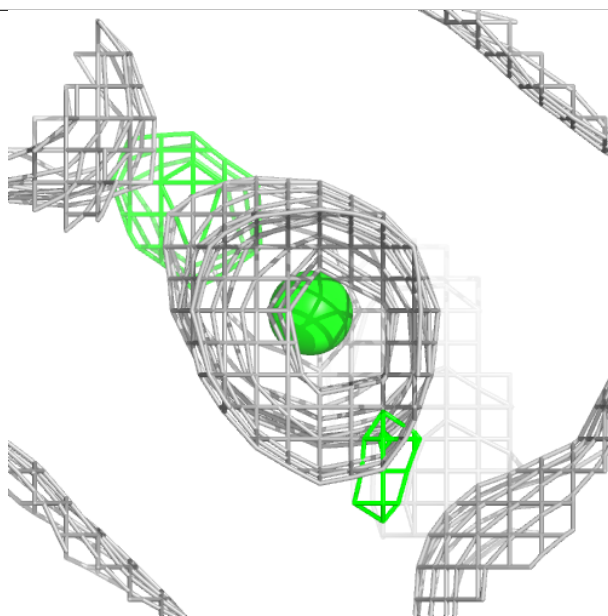
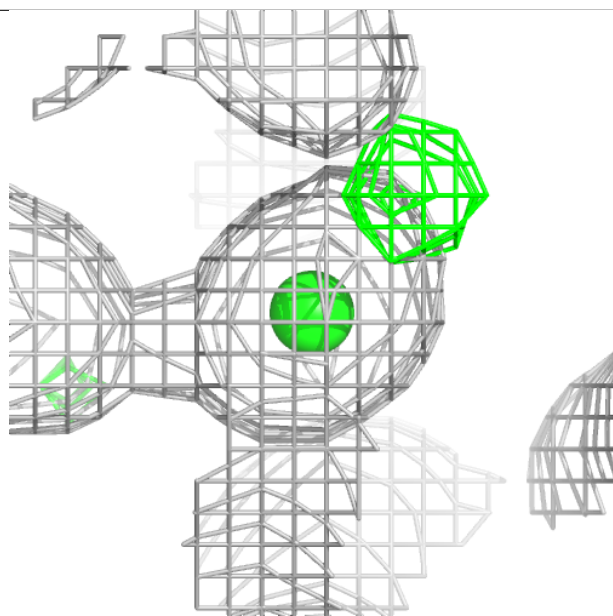
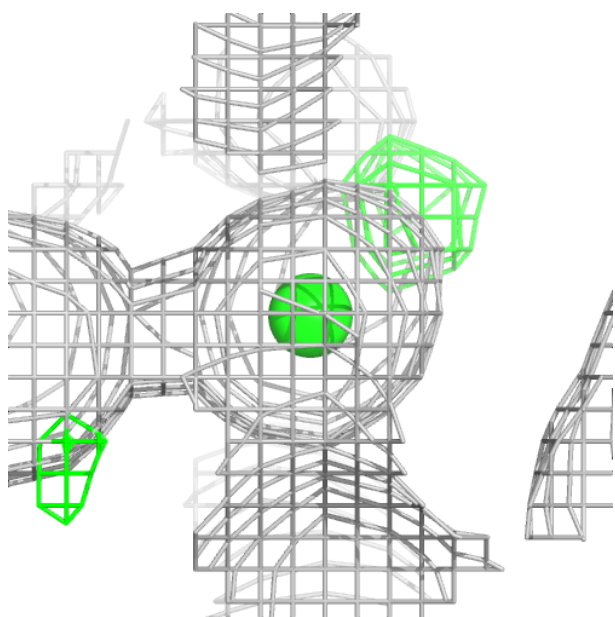
**Electron density around NXL BBB 304:**

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and green (positive)



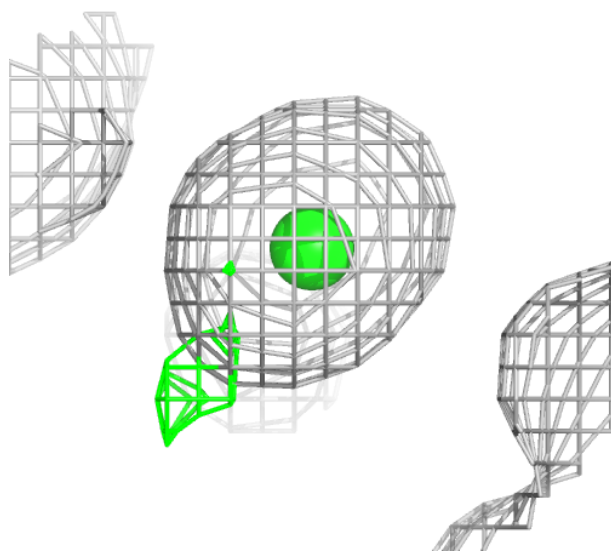
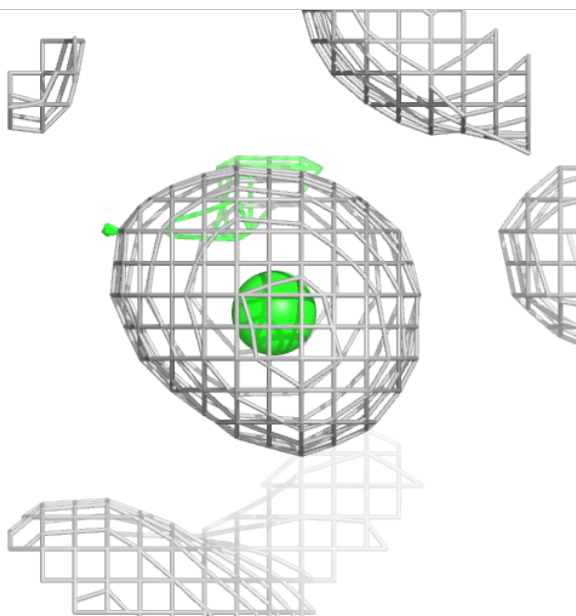
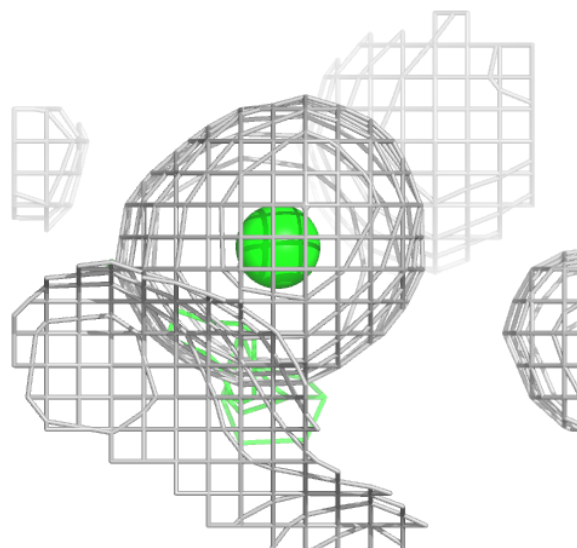
**Electron density around CL AAA 406 (B):**

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



**Electron density around CL BBB 305 (A):**

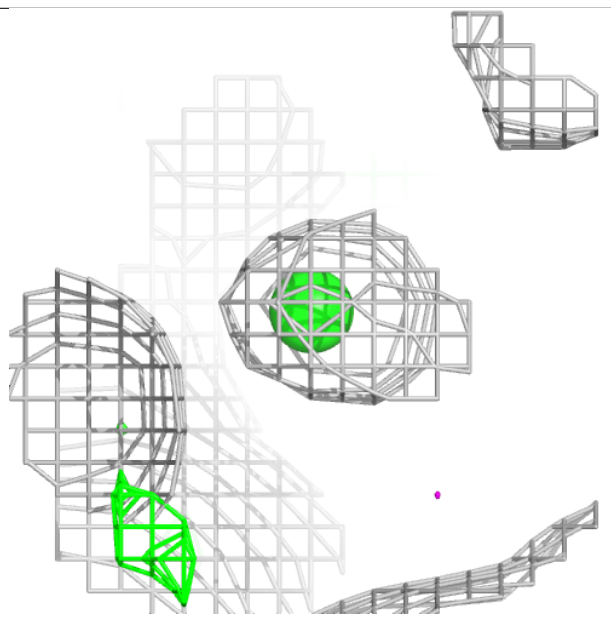
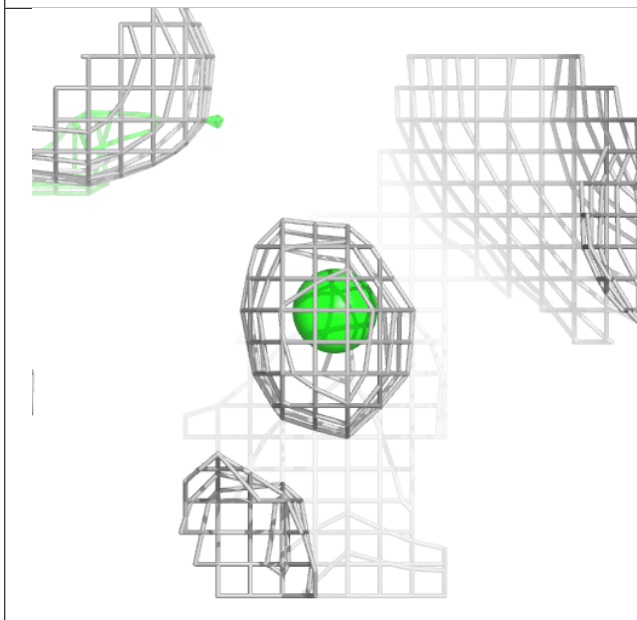
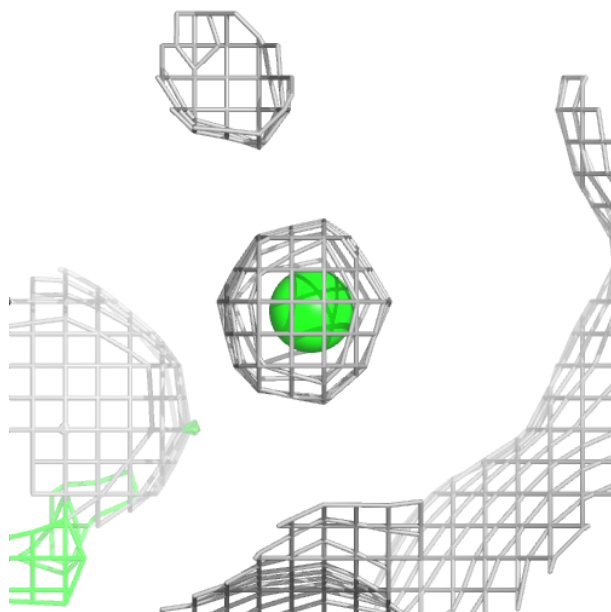
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





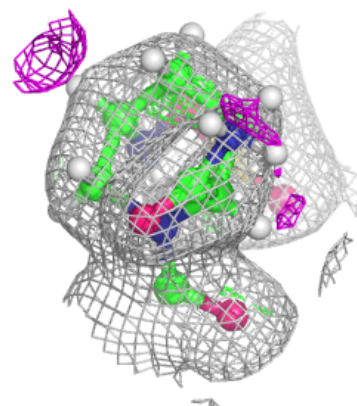
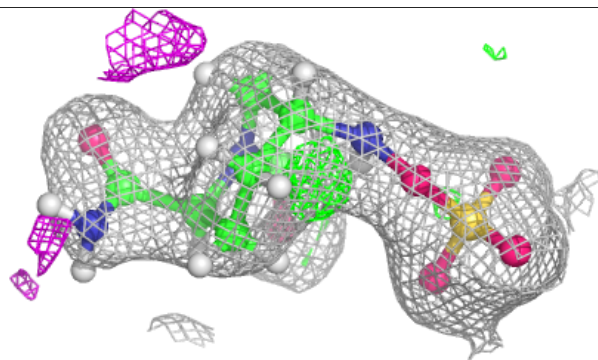
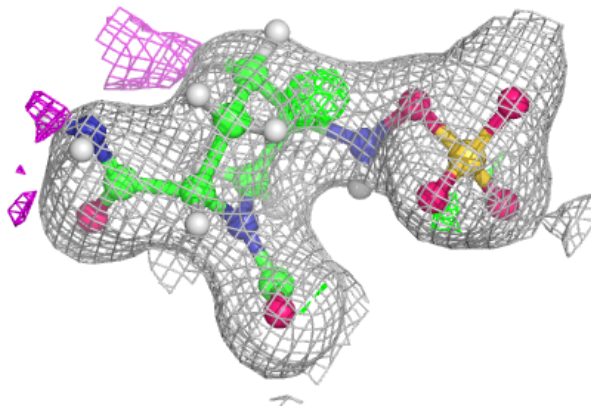
**Electron density around CL BBB 305 (B):**

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



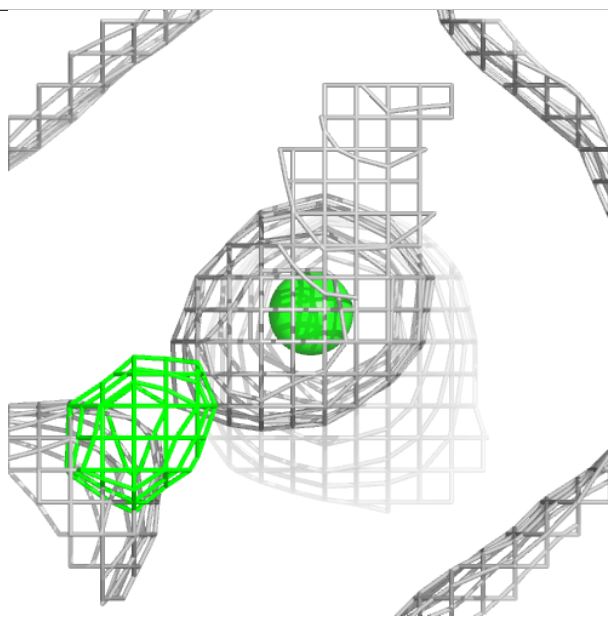
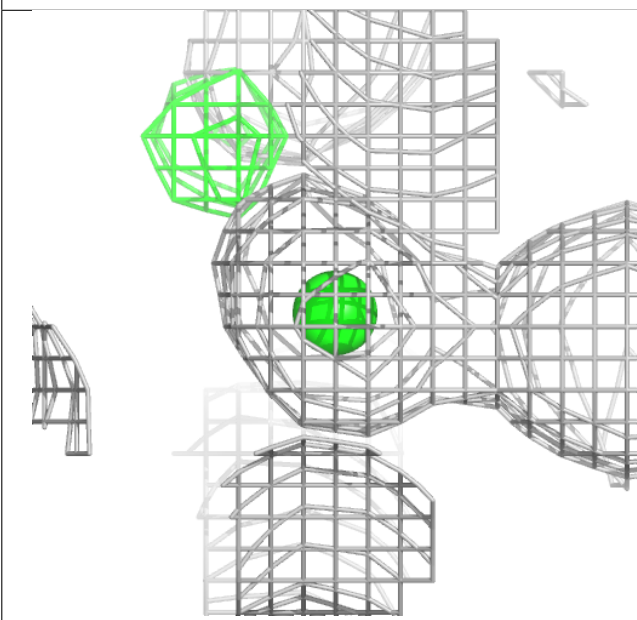
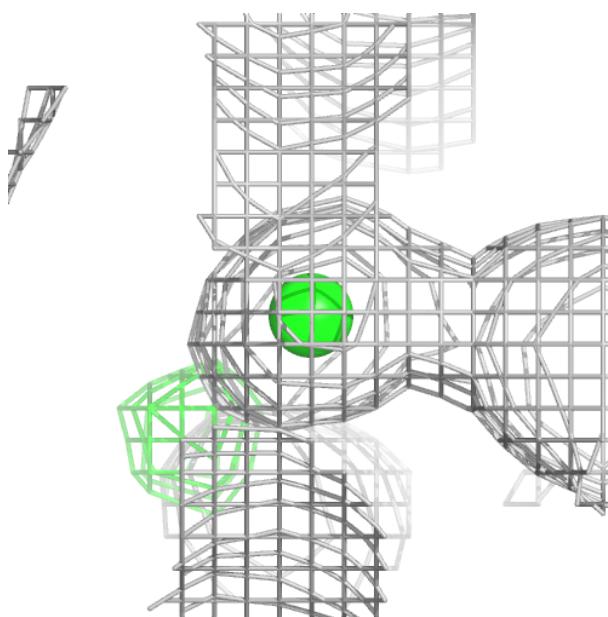
**Electron density around NXL AAA 403:**

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



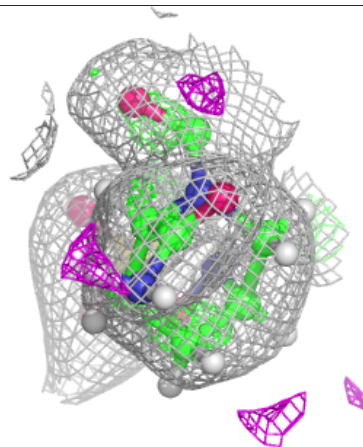
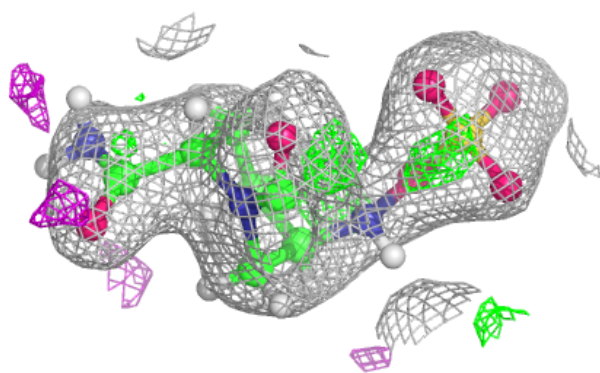
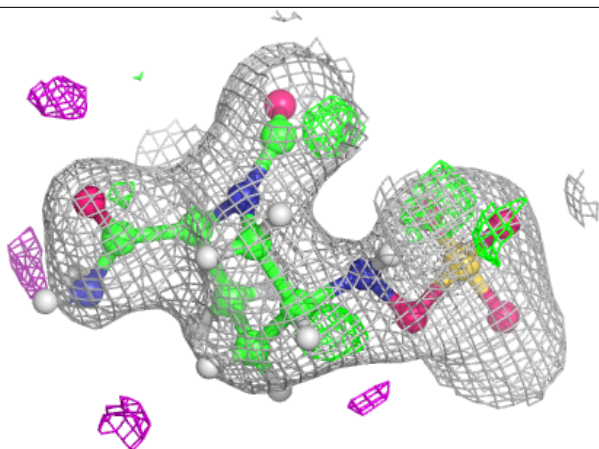
**Electron density around CL AAA 406 (A):**

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



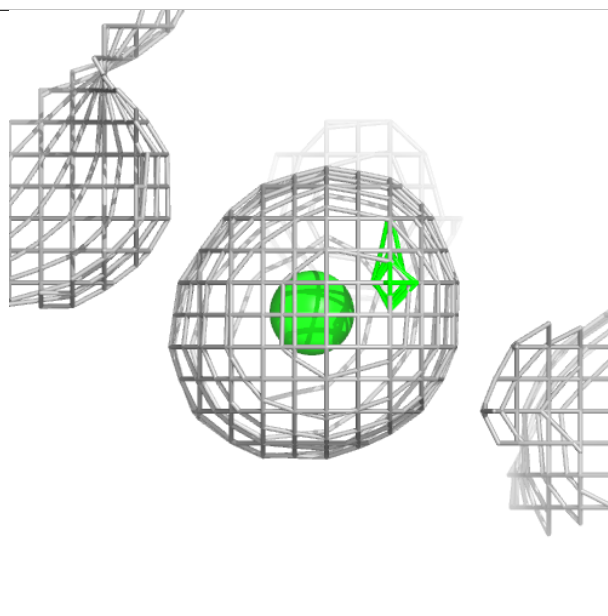
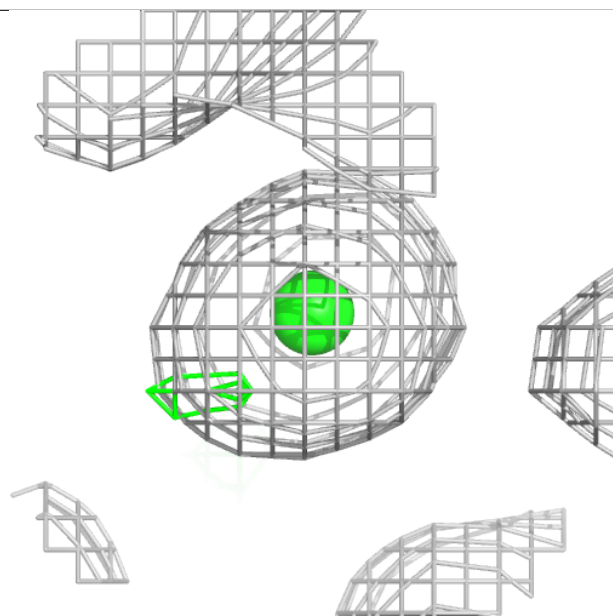
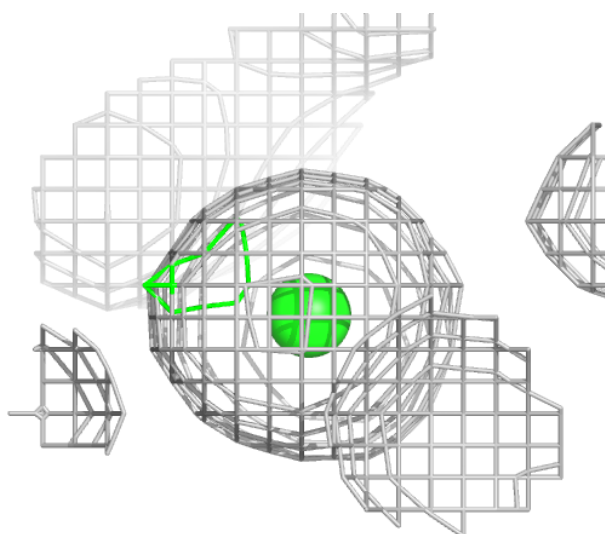
**Electron density around NXL CCC 303:**

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



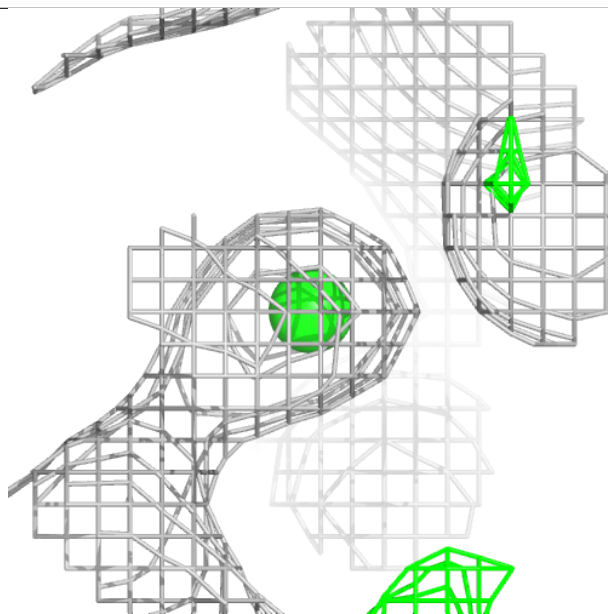
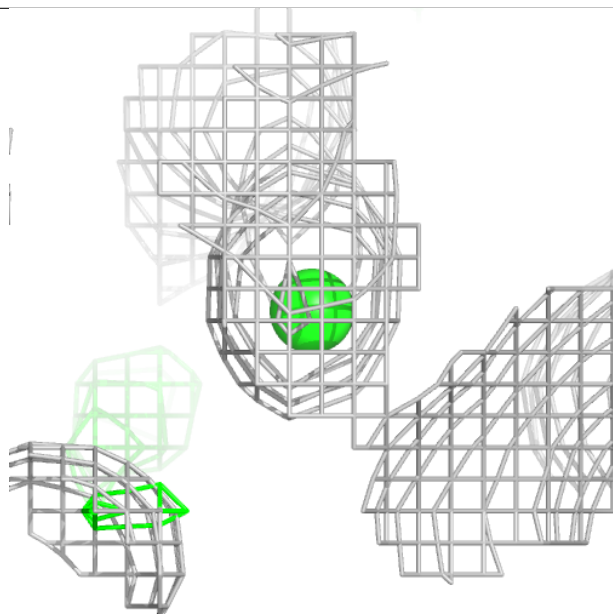
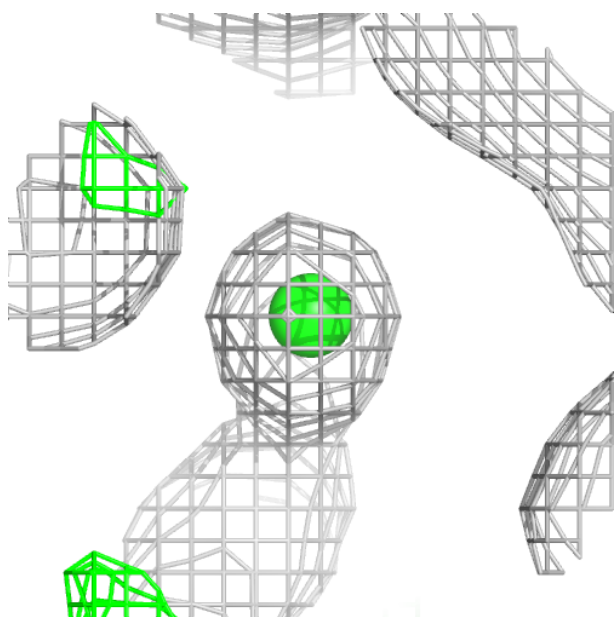
**Electron density around CL DDD 303 (A):**

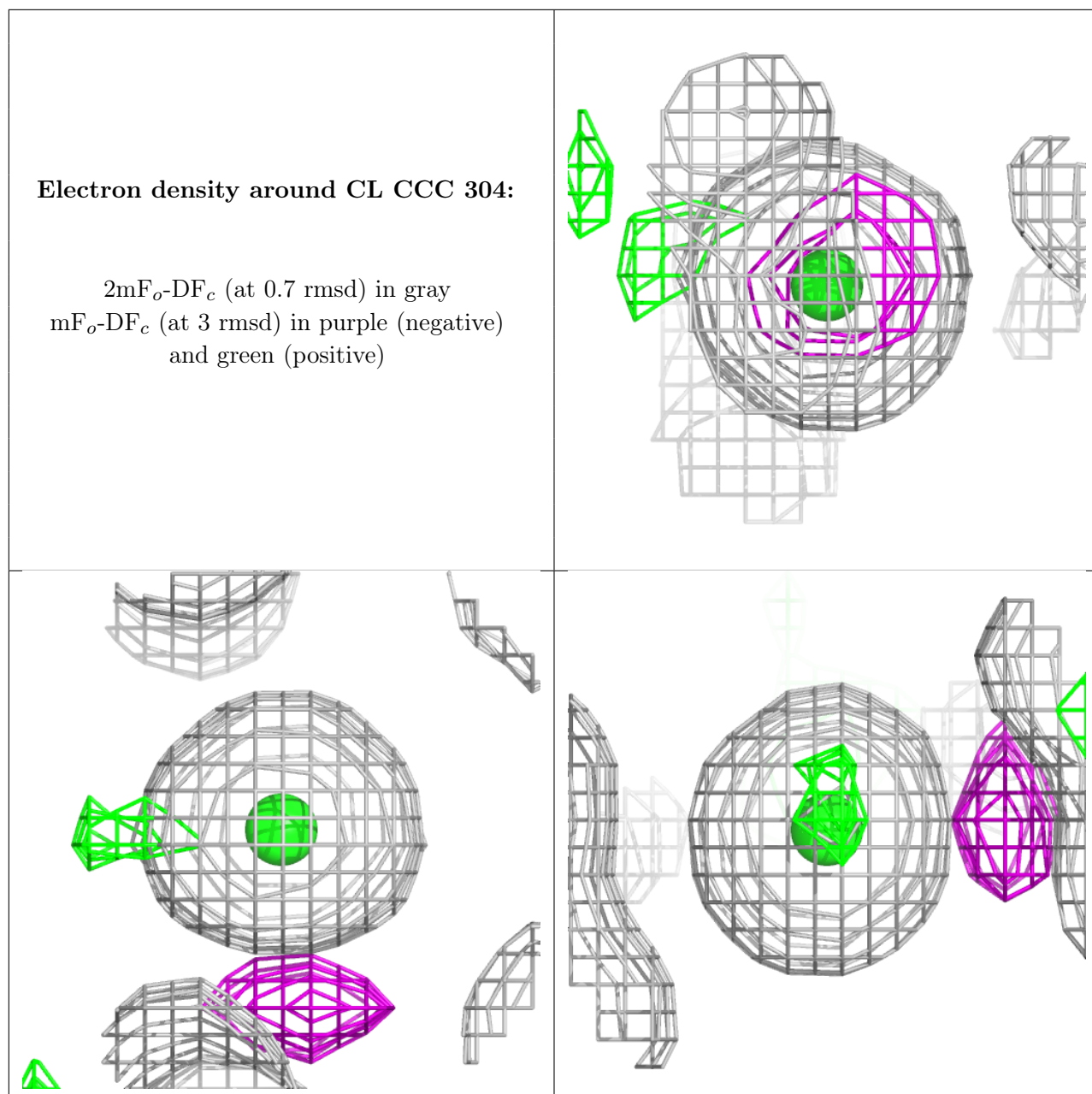
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

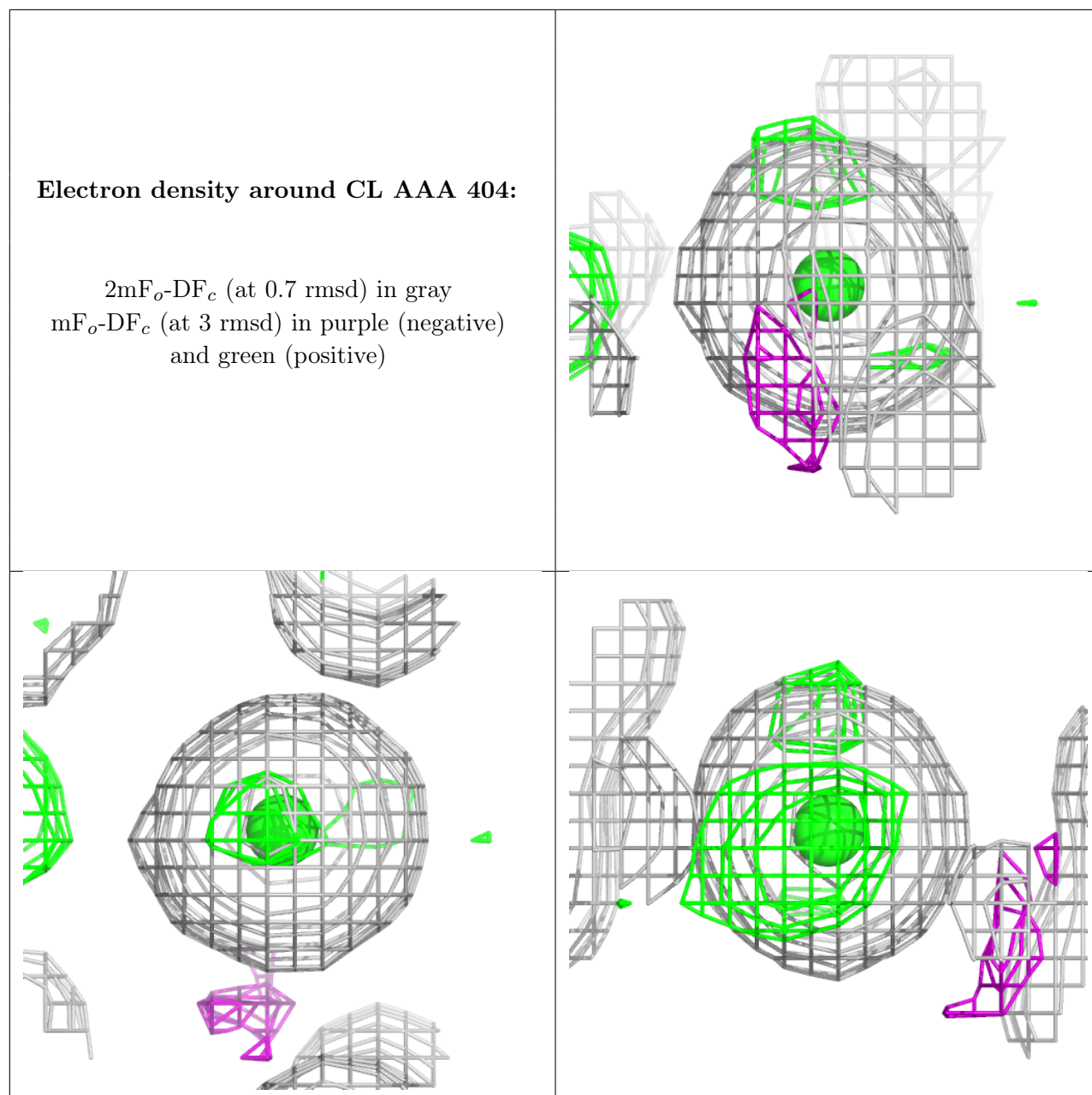


**Electron density around CL DDD 303 (B):**

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







## 6.5 Other polymers ⓘ

There are no such residues in this entry.