



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 10:04 AM UTC

PDB ID : 8AQI / pdb_00008aqi
Title : NanoLuc luciferase with bound coelenteramide in surface allosteric site
Authors : Nemergut, M.; Marek, M.
Deposited on : 2022-08-12
Resolution : 1.99 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

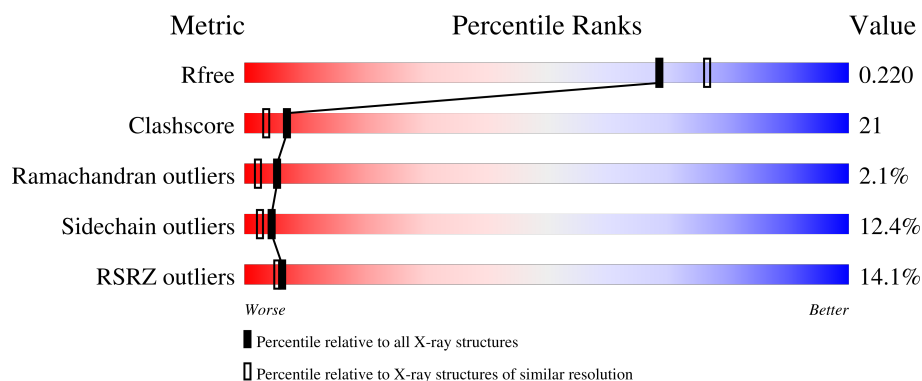
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	181	9% 50% 35% 9% 6%
1	B	181	15% 35% 40% 18% 5%
1	C	181	17% 46% 38% 9% 6%
1	D	181	14% 53% 34% 7% 5%
1	E	181	15% 52% 34% 8% 5%

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Mol	Chain	Length	Quality of chain
1	F	181	
1	G	181	
1	H	181	

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	CEI	A	201	-	X	X	-
3	CL	B	204	-	-	X	-
4	PG4	B	201	-	-	X	-
4	PG4	F	201	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11291 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 NanoLuc luciferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	1	0
			1360	877	229	250	4			
1	B	172	Total	C	N	O	S	0	0	0
			1357	875	227	251	4			
1	C	171	Total	C	N	O	S	0	0	0
			1349	871	225	249	4			
1	D	172	Total	C	N	O	S	0	0	0
			1357	875	227	251	4			
1	E	172	Total	C	N	O	S	0	0	0
			1357	875	227	251	4			
1	F	171	Total	C	N	O	S	0	0	0
			1349	871	225	249	4			
1	G	171	Total	C	N	O	S	0	0	0
			1349	871	225	249	4			
1	H	171	Total	C	N	O	S	0	1	0
			1357	876	226	250	5			

There are 224 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP Q9GV45
A	-10	HIS	-	expression tag	UNP Q9GV45
A	-9	HIS	-	expression tag	UNP Q9GV45
A	-8	HIS	-	expression tag	UNP Q9GV45
A	-7	HIS	-	expression tag	UNP Q9GV45
A	-6	HIS	-	expression tag	UNP Q9GV45
A	-5	HIS	-	expression tag	UNP Q9GV45
A	-4	SER	-	expression tag	UNP Q9GV45
A	-3	ASP	-	expression tag	UNP Q9GV45
A	-2	ASN	-	expression tag	UNP Q9GV45
A	-1	MET	-	expression tag	UNP Q9GV45
A	0	VAL	-	expression tag	UNP Q9GV45
A	4	GLU	ALA	engineered mutation	UNP Q9GV45

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Chain	Residue	Modelled	Actual	Comment	Reference
A	11	ARG	GLN	engineered mutation	UNP Q9GV45
A	18	LEU	GLN	engineered mutation	UNP Q9GV45
A	27	VAL	LEU	engineered mutation	UNP Q9GV45
A	33	ASN	ALA	engineered mutation	UNP Q9GV45
A	43	ARG	LYS	engineered mutation	UNP Q9GV45
A	44	ILE	VAL	engineered mutation	UNP Q9GV45
A	54	ILE	ALA	engineered mutation	UNP Q9GV45
A	68	ASP	PHE	engineered mutation	UNP Q9GV45
A	72	GLN	LEU	engineered mutation	UNP Q9GV45
A	75	LYS	MET	engineered mutation	UNP Q9GV45
A	90	VAL	ILE	engineered mutation	UNP Q9GV45
A	115	GLU	PRO	engineered mutation	UNP Q9GV45
A	124	LYS	GLN	engineered mutation	UNP Q9GV45
A	138	ILE	TYR	engineered mutation	UNP Q9GV45
A	166	ARG	ASN	engineered mutation	UNP Q9GV45
B	-11	MET	-	initiating methionine	UNP Q9GV45
B	-10	HIS	-	expression tag	UNP Q9GV45
B	-9	HIS	-	expression tag	UNP Q9GV45
B	-8	HIS	-	expression tag	UNP Q9GV45
B	-7	HIS	-	expression tag	UNP Q9GV45
B	-6	HIS	-	expression tag	UNP Q9GV45
B	-5	HIS	-	expression tag	UNP Q9GV45
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B	-3	ASP	-	expression tag	UNP Q9GV45
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B	-1	MET	-	expression tag	UNP Q9GV45
B	0	VAL	-	expression tag	UNP Q9GV45
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B	54	ILE	ALA	engineered mutation	UNP Q9GV45
B	68	ASP	PHE	engineered mutation	UNP Q9GV45
B	72	GLN	LEU	engineered mutation	UNP Q9GV45
B	75	LYS	MET	engineered mutation	UNP Q9GV45
B	90	VAL	ILE	engineered mutation	UNP Q9GV45
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B	124	LYS	GLN	engineered mutation	UNP Q9GV45
B	138	ILE	TYR	engineered mutation	UNP Q9GV45

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Chain	Residue	Modelled	Actual	Comment	Reference
B	166	ARG	ASN	engineered mutation	UNP Q9GV45
C	-11	MET	-	initiating methionine	UNP Q9GV45
C	-10	HIS	-	expression tag	UNP Q9GV45
C	-9	HIS	-	expression tag	UNP Q9GV45
C	-8	HIS	-	expression tag	UNP Q9GV45
C	-7	HIS	-	expression tag	UNP Q9GV45
C	-6	HIS	-	expression tag	UNP Q9GV45
C	-5	HIS	-	expression tag	UNP Q9GV45
C	-4	SER	-	expression tag	UNP Q9GV45
C	-3	ASP	-	expression tag	UNP Q9GV45
C	-2	ASN	-	expression tag	UNP Q9GV45
C	-1	MET	-	expression tag	UNP Q9GV45
C	0	VAL	-	expression tag	UNP Q9GV45
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C	18	LEU	GLN	engineered mutation	UNP Q9GV45
C	27	VAL	LEU	engineered mutation	UNP Q9GV45
C	33	ASN	ALA	engineered mutation	UNP Q9GV45
C	43	ARG	LYS	engineered mutation	UNP Q9GV45
C	44	ILE	VAL	engineered mutation	UNP Q9GV45
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C	68	ASP	PHE	engineered mutation	UNP Q9GV45
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C	124	LYS	GLN	engineered mutation	UNP Q9GV45
C	138	ILE	TYR	engineered mutation	UNP Q9GV45
C	166	ARG	ASN	engineered mutation	UNP Q9GV45
D	-11	MET	-	initiating methionine	UNP Q9GV45
D	-10	HIS	-	expression tag	UNP Q9GV45
D	-9	HIS	-	expression tag	UNP Q9GV45
D	-8	HIS	-	expression tag	UNP Q9GV45
D	-7	HIS	-	expression tag	UNP Q9GV45
D	-6	HIS	-	expression tag	UNP Q9GV45
D	-5	HIS	-	expression tag	UNP Q9GV45
D	-4	SER	-	expression tag	UNP Q9GV45
D	-3	ASP	-	expression tag	UNP Q9GV45
D	-2	ASN	-	expression tag	UNP Q9GV45
D	-1	MET	-	expression tag	UNP Q9GV45
D	0	VAL	-	expression tag	UNP Q9GV45
D	4	GLU	ALA	engineered mutation	UNP Q9GV45

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D	18	LEU	GLN	engineered mutation	UNP Q9GV45
D	27	VAL	LEU	engineered mutation	UNP Q9GV45
D	33	ASN	ALA	engineered mutation	UNP Q9GV45
D	43	ARG	LYS	engineered mutation	UNP Q9GV45
D	44	ILE	VAL	engineered mutation	UNP Q9GV45
D	54	ILE	ALA	engineered mutation	UNP Q9GV45
D	68	ASP	PHE	engineered mutation	UNP Q9GV45
D	72	GLN	LEU	engineered mutation	UNP Q9GV45
D	75	LYS	MET	engineered mutation	UNP Q9GV45
D	90	VAL	ILE	engineered mutation	UNP Q9GV45
D	115	GLU	PRO	engineered mutation	UNP Q9GV45
D	124	LYS	GLN	engineered mutation	UNP Q9GV45
D	138	ILE	TYR	engineered mutation	UNP Q9GV45
D	166	ARG	ASN	engineered mutation	UNP Q9GV45
E	-11	MET	-	initiating methionine	UNP Q9GV45
E	-10	HIS	-	expression tag	UNP Q9GV45
E	-9	HIS	-	expression tag	UNP Q9GV45
E	-8	HIS	-	expression tag	UNP Q9GV45
E	-7	HIS	-	expression tag	UNP Q9GV45
E	-6	HIS	-	expression tag	UNP Q9GV45
E	-5	HIS	-	expression tag	UNP Q9GV45
E	-4	SER	-	expression tag	UNP Q9GV45
E	-3	ASP	-	expression tag	UNP Q9GV45
E	-2	ASN	-	expression tag	UNP Q9GV45
E	-1	MET	-	expression tag	UNP Q9GV45
E	0	VAL	-	expression tag	UNP Q9GV45
E	4	GLU	ALA	engineered mutation	UNP Q9GV45
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E	27	VAL	LEU	engineered mutation	UNP Q9GV45
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E	43	ARG	LYS	engineered mutation	UNP Q9GV45
E	44	ILE	VAL	engineered mutation	UNP Q9GV45
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E	75	LYS	MET	engineered mutation	UNP Q9GV45
E	90	VAL	ILE	engineered mutation	UNP Q9GV45
E	115	GLU	PRO	engineered mutation	UNP Q9GV45
E	124	LYS	GLN	engineered mutation	UNP Q9GV45
E	138	ILE	TYR	engineered mutation	UNP Q9GV45

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Chain	Residue	Modelled	Actual	Comment	Reference
E	166	ARG	ASN	engineered mutation	UNP Q9GV45
F	-11	MET	-	initiating methionine	UNP Q9GV45
F	-10	HIS	-	expression tag	UNP Q9GV45
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F	-8	HIS	-	expression tag	UNP Q9GV45
F	-7	HIS	-	expression tag	UNP Q9GV45
F	-6	HIS	-	expression tag	UNP Q9GV45
F	-5	HIS	-	expression tag	UNP Q9GV45
F	-4	SER	-	expression tag	UNP Q9GV45
F	-3	ASP	-	expression tag	UNP Q9GV45
F	-2	ASN	-	expression tag	UNP Q9GV45
F	-1	MET	-	expression tag	UNP Q9GV45
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F	11	ARG	GLN	engineered mutation	UNP Q9GV45
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F	72	GLN	LEU	engineered mutation	UNP Q9GV45
F	75	LYS	MET	engineered mutation	UNP Q9GV45
F	90	VAL	ILE	engineered mutation	UNP Q9GV45
F	115	GLU	PRO	engineered mutation	UNP Q9GV45
F	124	LYS	GLN	engineered mutation	UNP Q9GV45
F	138	ILE	TYR	engineered mutation	UNP Q9GV45
F	166	ARG	ASN	engineered mutation	UNP Q9GV45
G	-11	MET	-	initiating methionine	UNP Q9GV45
G	-10	HIS	-	expression tag	UNP Q9GV45
G	-9	HIS	-	expression tag	UNP Q9GV45
G	-8	HIS	-	expression tag	UNP Q9GV45
G	-7	HIS	-	expression tag	UNP Q9GV45
G	-6	HIS	-	expression tag	UNP Q9GV45
G	-5	HIS	-	expression tag	UNP Q9GV45
G	-4	SER	-	expression tag	UNP Q9GV45
G	-3	ASP	-	expression tag	UNP Q9GV45
G	-2	ASN	-	expression tag	UNP Q9GV45
G	-1	MET	-	expression tag	UNP Q9GV45
G	0	VAL	-	expression tag	UNP Q9GV45
G	4	GLU	ALA	engineered mutation	UNP Q9GV45

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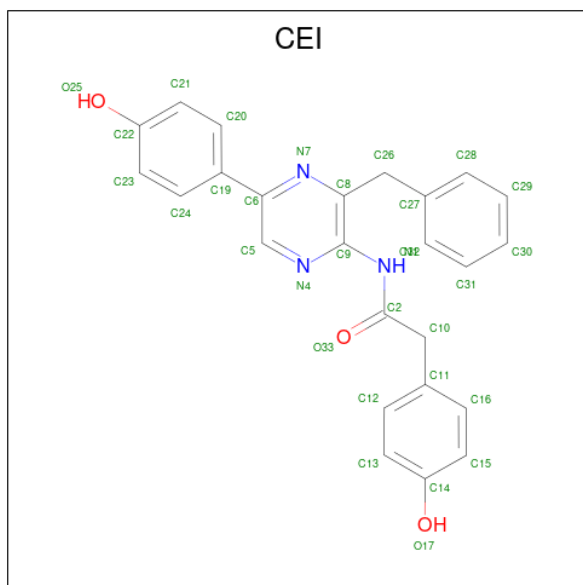
Chain	Residue	Modelled	Actual	Comment	Reference
G	11	ARG	GLN	engineered mutation	UNP Q9GV45
G	18	LEU	GLN	engineered mutation	UNP Q9GV45
G	27	VAL	LEU	engineered mutation	UNP Q9GV45
G	33	ASN	ALA	engineered mutation	UNP Q9GV45
G	43	ARG	LYS	engineered mutation	UNP Q9GV45
G	44	ILE	VAL	engineered mutation	UNP Q9GV45
G	54	ILE	ALA	engineered mutation	UNP Q9GV45
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G	124	LYS	GLN	engineered mutation	UNP Q9GV45
G	138	ILE	TYR	engineered mutation	UNP Q9GV45
G	166	ARG	ASN	engineered mutation	UNP Q9GV45
H	-11	MET	-	initiating methionine	UNP Q9GV45
H	-10	HIS	-	expression tag	UNP Q9GV45
H	-9	HIS	-	expression tag	UNP Q9GV45
H	-8	HIS	-	expression tag	UNP Q9GV45
H	-7	HIS	-	expression tag	UNP Q9GV45
H	-6	HIS	-	expression tag	UNP Q9GV45
H	-5	HIS	-	expression tag	UNP Q9GV45
H	-4	SER	-	expression tag	UNP Q9GV45
H	-3	ASP	-	expression tag	UNP Q9GV45
H	-2	ASN	-	expression tag	UNP Q9GV45
H	-1	MET	-	expression tag	UNP Q9GV45
H	0	VAL	-	expression tag	UNP Q9GV45
H	4	GLU	ALA	engineered mutation	UNP Q9GV45
H	11	ARG	GLN	engineered mutation	UNP Q9GV45
H	18	LEU	GLN	engineered mutation	UNP Q9GV45
H	27	VAL	LEU	engineered mutation	UNP Q9GV45
H	33	ASN	ALA	engineered mutation	UNP Q9GV45
H	43	ARG	LYS	engineered mutation	UNP Q9GV45
H	44	ILE	VAL	engineered mutation	UNP Q9GV45
H	54	ILE	ALA	engineered mutation	UNP Q9GV45
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H	90	VAL	ILE	engineered mutation	UNP Q9GV45
H	115	GLU	PRO	engineered mutation	UNP Q9GV45
H	124	LYS	GLN	engineered mutation	UNP Q9GV45
H	138	ILE	TYR	engineered mutation	UNP Q9GV45

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Chain	Residue	Modelled	Actual	Comment	Reference
H	166	ARG	ASN	engineered mutation	UNP Q9GV45

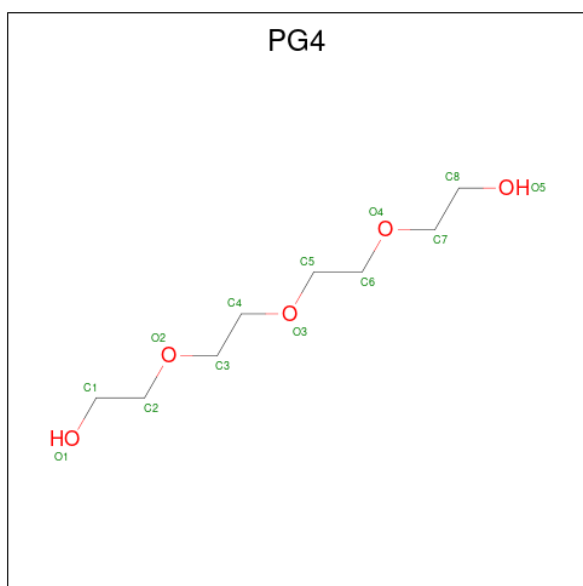
- Molecule 2 is N-[3-BENZYL-5-(4-HYDROXYPHENYL)PYRAZIN-2-YL]-2-(4-HYDROXYPHENYL)ACETAMIDE (CCD ID: CEI) (formula: C₂₅H₂₁N₃O₃) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	2	Total	Cl	0	0
			2	2		
3	G	1	Total	Cl	0	0
			1	1		
3	H	2	Total	Cl	0	0
			2	2		

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			13	8	5		
4	C	1	Total	C	O	0	0
			13	8	5		
4	F	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	55	Total	O	0	0
			55	55		
5	B	40	Total	O	0	0
			40	40		
5	C	37	Total	O	0	0
			37	37		

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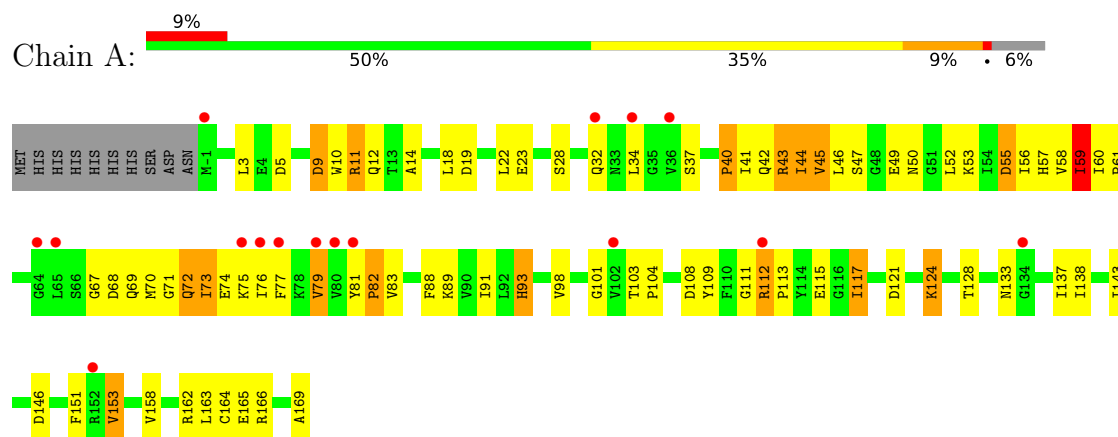
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	30	Total 30	O 30	0	0
5	E	37	Total 37	O 37	0	0
5	F	42	Total 42	O 42	0	0
5	G	49	Total 49	O 49	0	0
5	H	50	Total 50	O 50	0	0

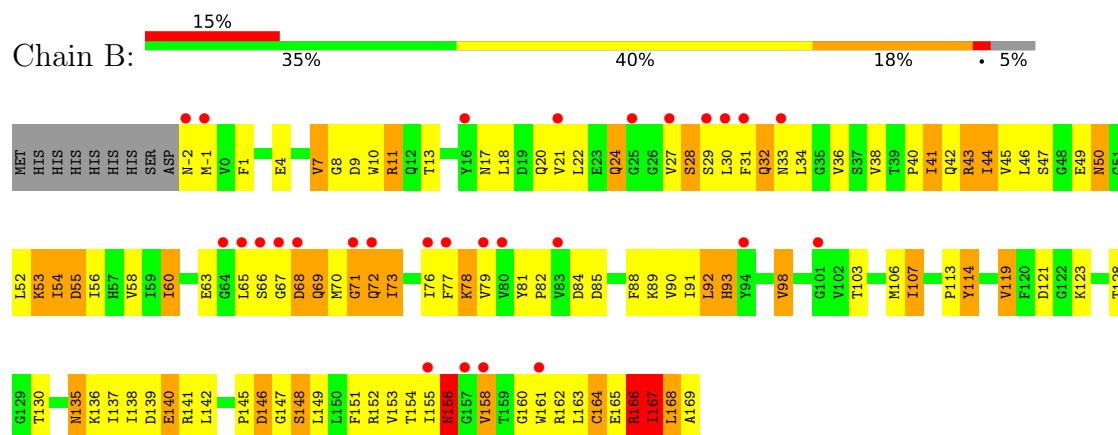
3 Residue-property plots [i](#)

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.

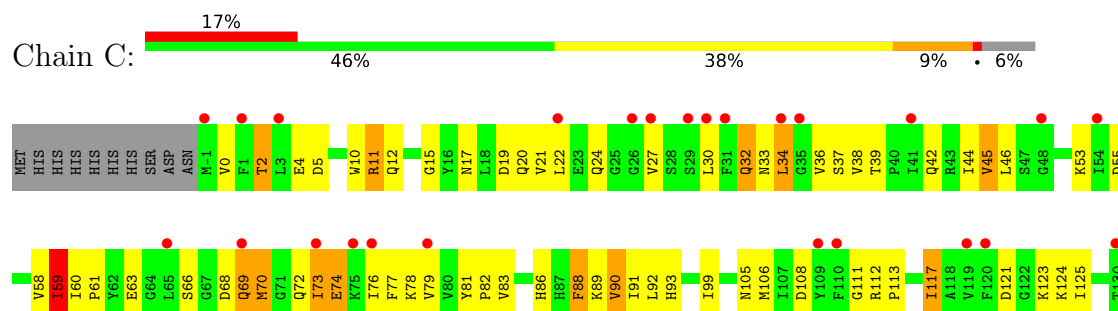
• Molecule 1: NanoLuc luciferase



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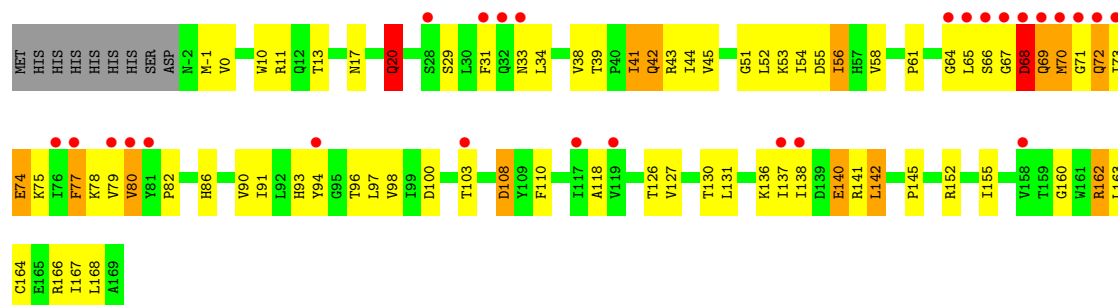


• Molecule 1: NanoLuc luciferase

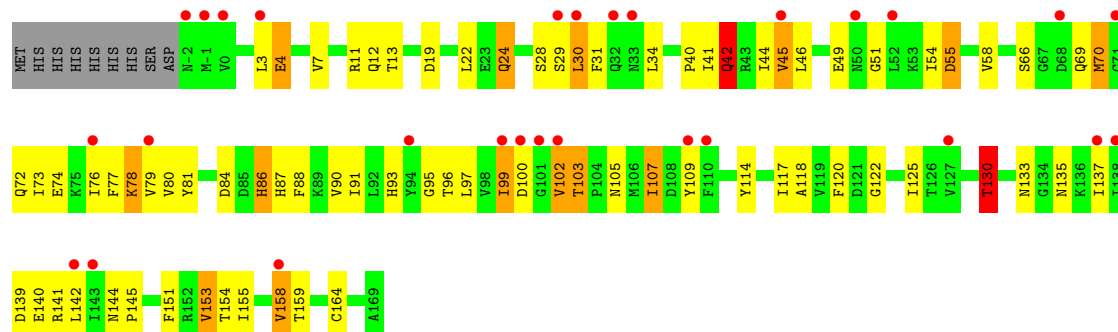




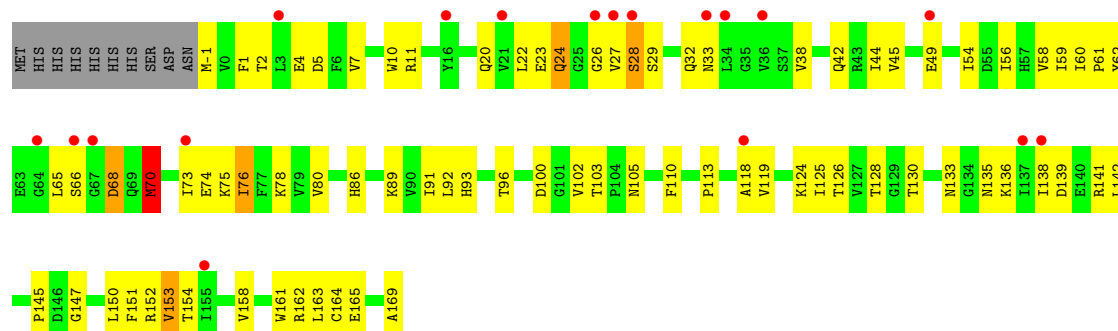
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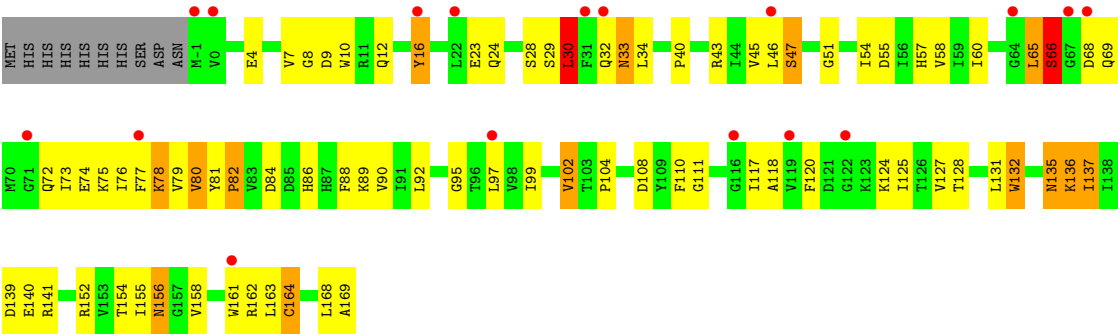


• Molecule 1: NanoLuc luciferase

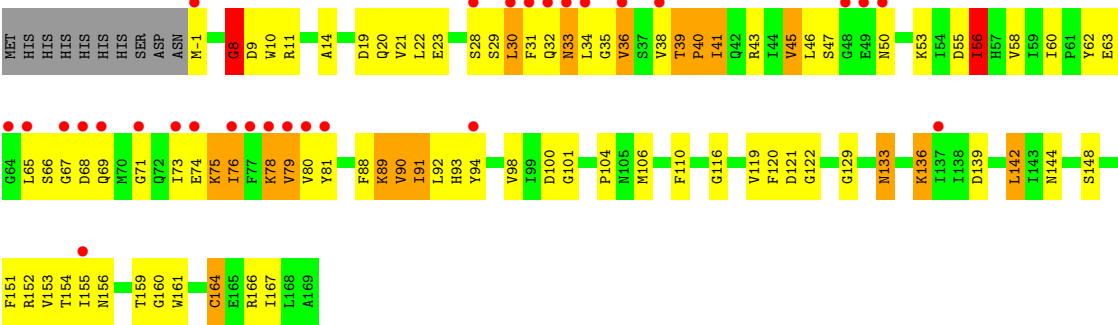


• Molecule 1: NanoLuc luciferase





● Molecule 1: NanoLuc luciferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	86.98Å 87.28Å 191.52Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	44.35 – 1.99 44.35 – 1.99	Depositor EDS
% Data completeness (in resolution range)	98.2 (44.35-1.99) 99.1 (44.35-1.99)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.188 , 0.207 0.201 , 0.220	Depositor DCC
R_{free} test set	4977 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.029 for k,h,-l 0.011 for -k,-h,-l 0.005 for -h,-k,l	Xtriage
Reported twinning fraction	0.485 for H, K, L 0.166 for -h,-k,l 0.180 for -K, -H, -L 0.169 for K, H, -L	Depositor
Outliers	0 of 96946 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11291	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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 48.06 % 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 9.0845e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CEI, CL, PG4

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	1.45	9/1389 (0.6%)	1.68	15/1884 (0.8%)
1	B	1.49	18/1386 (1.3%)	1.72	22/1881 (1.2%)
1	C	1.37	9/1378 (0.7%)	1.62	17/1870 (0.9%)
1	D	1.43	8/1386 (0.6%)	1.66	14/1881 (0.7%)
1	E	1.29	5/1386 (0.4%)	1.60	13/1881 (0.7%)
1	F	1.41	9/1378 (0.7%)	1.65	12/1870 (0.6%)
1	G	1.41	9/1378 (0.7%)	1.68	13/1870 (0.7%)
1	H	1.35	7/1386 (0.5%)	1.76	24/1880 (1.3%)
All	All	1.40	74/11067 (0.7%)	1.67	130/15017 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
1	D	0	2
1	E	0	1
1	F	0	1
1	H	0	2
All	All	0	10

The worst 5 of 74 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	7	VAL	C-O	9.84	1.33	1.24
1	A	47	SER	C-O	9.63	1.34	1.24
1	B	165	GLU	C-O	8.99	1.34	1.23
1	D	42	GLN	C-O	8.86	1.34	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	82	PRO	C-O	-8.55	1.14	1.23

The worst 5 of 130 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	85	ASP	CA-CB-CG	10.85	123.45	112.60
1	C	11	ARG	CB-CA-C	9.68	125.67	109.80
1	H	14	ALA	CA-C-N	8.91	128.83	122.33
1	H	14	ALA	C-N-CA	8.91	128.83	122.33
1	G	108	ASP	CA-CB-CG	8.40	121.00	112.60

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	GLY	Peptide
1	A	40	PRO	Mainchain
1	A	9	ASP	Mainchain
1	B	67	GLY	Peptide
1	D	67	GLY	Peptide

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	1360	0	1365	60	0
1	B	1357	0	1359	100	0
1	C	1349	0	1353	55	0
1	D	1357	0	1359	45	0
1	E	1357	0	1359	54	0
1	F	1349	0	1353	48	0
1	G	1349	0	1353	49	0
1	H	1357	0	1363	59	0
2	A	31	0	20	32	0
2	G	31	0	20	7	0
3	A	2	0	0	1	0
3	B	3	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	1	0
3	F	2	0	0	1	0
3	G	1	0	0	0	0
3	H	2	0	0	0	0
4	B	13	0	18	12	0
4	C	13	0	18	6	0
4	F	13	0	18	7	0
5	A	55	0	0	3	0
5	B	40	0	0	1	0
5	C	37	0	0	5	0
5	D	30	0	0	1	0
5	E	37	0	0	2	0
5	F	42	0	0	1	0
5	G	49	0	0	0	0
5	H	50	0	0	4	0
All	All	11291	0	10958	459	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 21.

The worst 5 of 459 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:F:89:LYS:HZ2	4:F:201:PG4:H72	0.96	1.08
1:B:89:LYS:NZ	4:B:201:PG4:H22	1.70	1.07
1:F:89:LYS:NZ	4:F:201:PG4:H72	1.69	1.06
1:G:169:ALA:HB2	1:H:41:ILE:HD11	1.40	1.04
1:H:34:LEU:HD22	1:H:36:VAL:HG23	1.46	0.96

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	A	170/181 (94%)	157 (92%)	9 (5%)	4 (2%)	4	2
1	B	170/181 (94%)	152 (89%)	12 (7%)	6 (4%)	3	1
1	C	169/181 (93%)	154 (91%)	13 (8%)	2 (1%)	10	6
1	D	170/181 (94%)	149 (88%)	16 (9%)	5 (3%)	3	1
1	E	170/181 (94%)	153 (90%)	15 (9%)	2 (1%)	10	6
1	F	169/181 (93%)	144 (85%)	19 (11%)	6 (4%)	2	1
1	G	169/181 (93%)	158 (94%)	10 (6%)	1 (1%)	21	17
1	H	169/181 (93%)	152 (90%)	15 (9%)	2 (1%)	10	6
All	All	1356/1448 (94%)	1219 (90%)	109 (8%)	28 (2%)	5	2

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	32	GLN
1	B	69	GLN
1	C	70	MET
1	B	65	LEU
1	B	71	GLY

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	149/158 (94%)	132 (89%)	17 (11%)	5	3
1	B	149/158 (94%)	123 (83%)	26 (17%)	2	1
1	C	148/158 (94%)	125 (84%)	23 (16%)	2	1
1	D	149/158 (94%)	131 (88%)	18 (12%)	5	3
1	E	149/158 (94%)	137 (92%)	12 (8%)	11	7
1	F	148/158 (94%)	136 (92%)	12 (8%)	11	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	148/158 (94%)	130 (88%)	18 (12%)	5	3
1	H	149/158 (94%)	127 (85%)	22 (15%)	3	1
All	All	1189/1264 (94%)	1041 (88%)	148 (12%)	4	2

5 of 148 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	65	LEU
1	H	93	HIS
1	G	78	LYS
1	H	33	ASN
1	C	34	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	33	ASN
1	E	86	HIS
1	G	33	ASN
1	E	33	ASN
1	E	156	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 20 ligands modelled in this entry, 15 are monoatomic - leaving 5 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	CEI	G	201	-	33,34,34	2.44	11 (33%)	42,46,46	3.66	13 (30%)
2	CEI	A	201	-	33,34,34	1.88	10 (30%)	42,46,46	3.34	20 (47%)
4	PG4	C	201	-	12,12,12	1.03	0	11,11,11	0.95	0
4	PG4	F	201	-	12,12,12	0.89	1 (8%)	11,11,11	1.35	1 (9%)
4	PG4	B	201	-	12,12,12	0.88	1 (8%)	11,11,11	0.96	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	CEI	G	201	-	-	5/16/16/16	0/4/4/4
2	CEI	A	201	-	-	10/16/16/16	0/4/4/4
4	PG4	C	201	-	-	4/10/10/10	-
4	PG4	F	201	-	-	6/10/10/10	-
4	PG4	B	201	-	-	6/10/10/10	-

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	201	CEI	C2-N1	7.38	1.51	1.35
2	G	201	CEI	C9-N1	6.43	1.53	1.39
2	A	201	CEI	O33-C2	-6.10	1.11	1.23
2	G	201	CEI	O33-C2	-4.41	1.14	1.23
2	G	201	CEI	C10-C2	3.56	1.59	1.52

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	201	CEI	C10-C2-N1	12.82	138.71	114.73
2	A	201	CEI	O33-C2-N1	-9.47	106.66	123.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	201	CEI	C11-C10-C2	9.01	139.20	112.33
2	G	201	CEI	C8-C9-N1	8.94	130.03	118.48
2	A	201	CEI	C8-C9-N1	8.87	129.95	118.48

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

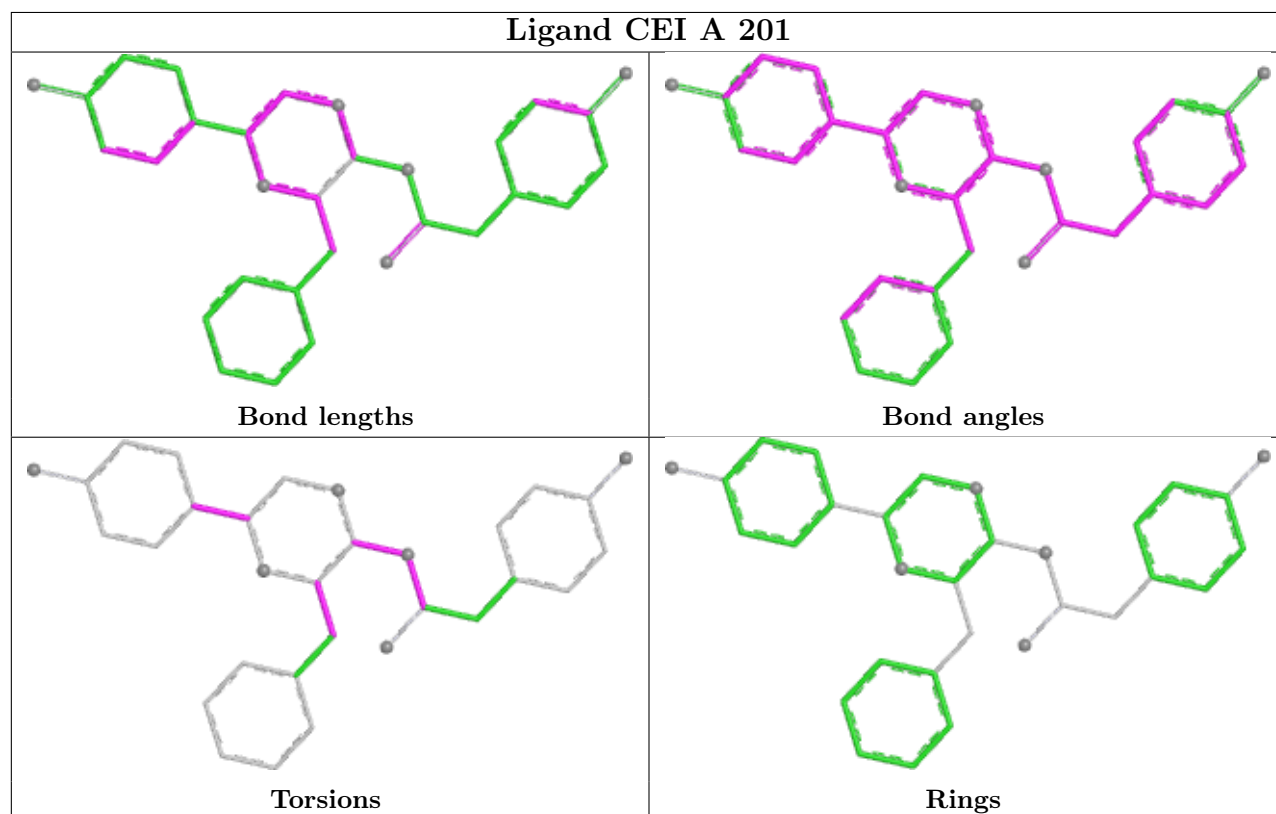
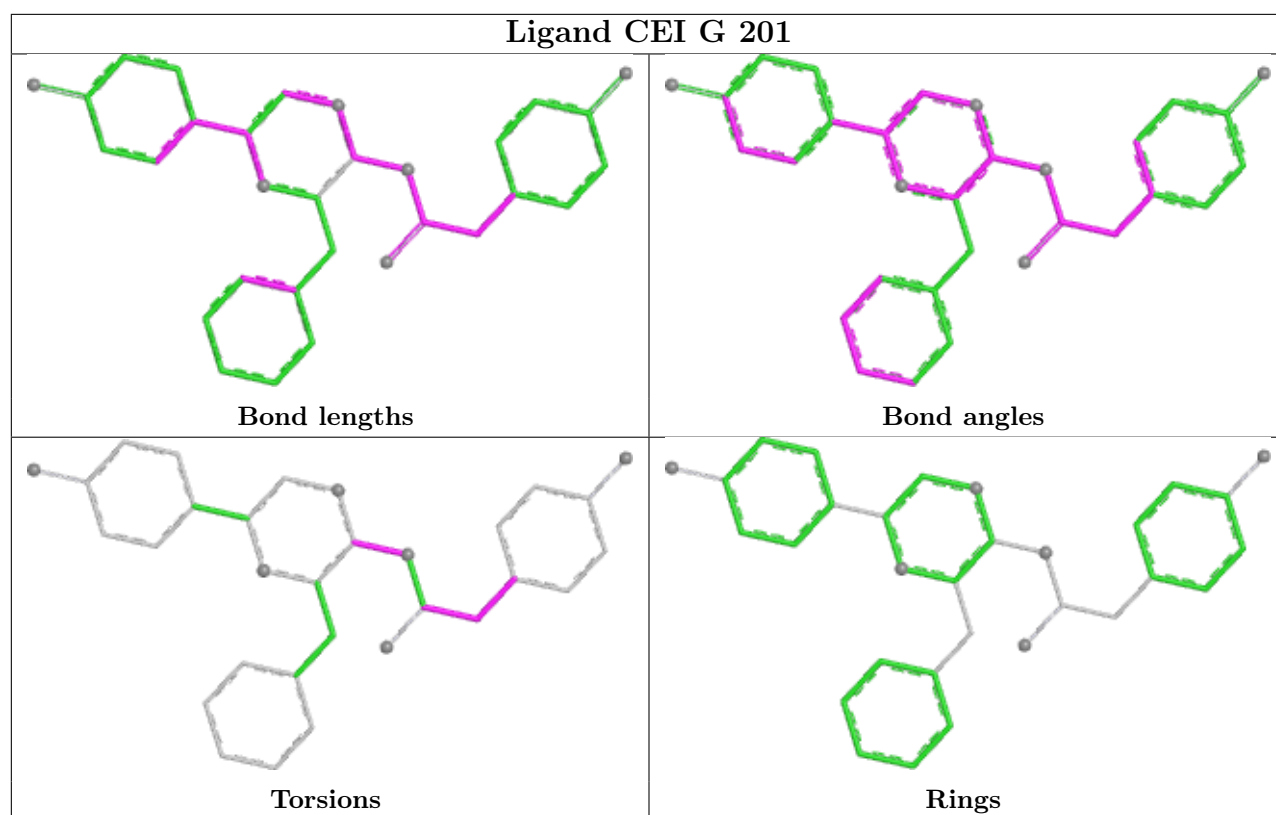
Mol	Chain	Res	Type	Atoms
2	A	201	CEI	C8-C9-N1-C2
2	A	201	CEI	N4-C9-N1-C2
2	A	201	CEI	C20-C19-C6-C5
4	C	201	PG4	C5-C6-O4-C7
4	C	201	PG4	C4-C3-O2-C2

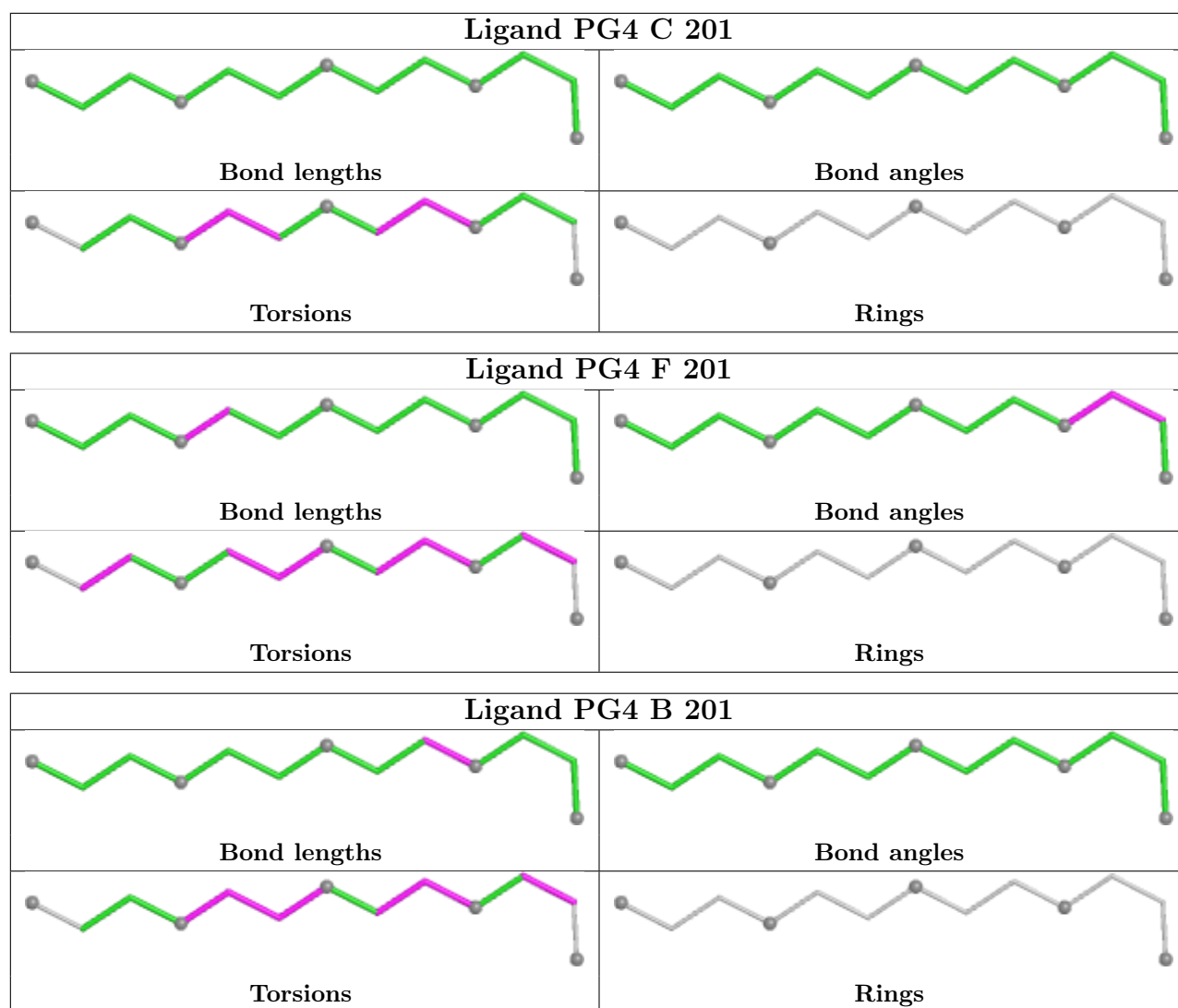
There are no ring outliers.

5 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	201	CEI	7	0
2	A	201	CEI	32	0
4	C	201	PG4	6	0
4	F	201	PG4	7	0
4	B	201	PG4	12	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	171/181 (94%)	0.88	16 (9%) 14 13	17, 32, 57, 74	1 (0%)
1	B	172/181 (95%)	1.03	28 (16%) 4 4	20, 35, 61, 103	0
1	C	171/181 (94%)	1.12	31 (18%) 3 3	20, 37, 61, 74	0
1	D	172/181 (95%)	1.24	26 (15%) 5 5	19, 38, 61, 70	0
1	E	172/181 (95%)	1.18	28 (16%) 4 4	23, 41, 57, 73	0
1	F	171/181 (94%)	1.05	18 (10%) 11 10	20, 36, 54, 67	0
1	G	171/181 (94%)	0.92	17 (9%) 13 11	19, 34, 50, 67	0
1	H	171/181 (94%)	1.15	29 (16%) 4 4	17, 33, 61, 79	1 (0%)
All	All	1371/1448 (94%)	1.07	193 (14%) 6 5	17, 36, 59, 103	2 (0%)

The worst 5 of 193 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	79	VAL	6.5
1	H	-1[A]	MET	6.2
1	B	67	GLY	5.4
1	C	76	ILE	5.2
1	D	71	GLY	5.2

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 ⓘ

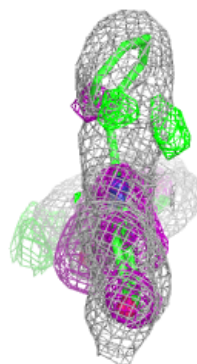
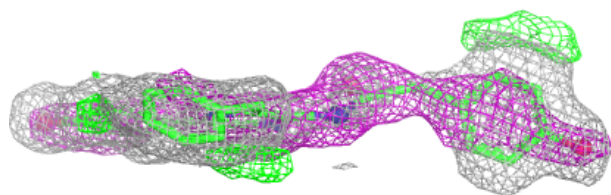
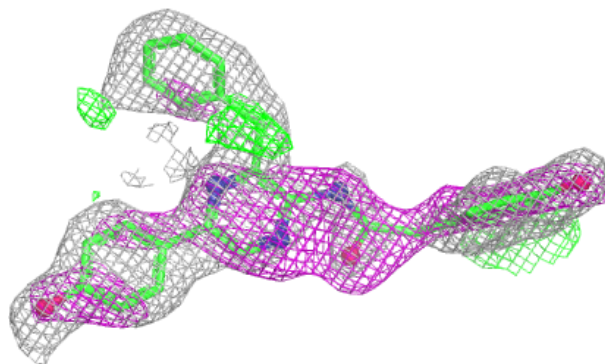
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CEI	G	201	31/31	0.74	0.14	15,17,28,28	0
2	CEI	A	201	31/31	0.77	0.13	15,17,28,28	0
4	PG4	F	201	13/13	0.89	0.10	22,25,28,29	0
4	PG4	B	201	13/13	0.90	0.10	23,27,28,29	0
3	CL	H	201	1/1	0.90	0.14	32,32,32,32	0
4	PG4	C	201	13/13	0.91	0.09	22,23,27,27	0
3	CL	F	203	1/1	0.93	0.12	33,33,33,33	0
3	CL	D	201	1/1	0.94	0.10	31,31,31,31	0
3	CL	B	203	1/1	0.95	0.07	35,35,35,35	0
3	CL	B	202	1/1	0.97	0.05	26,26,26,26	0
3	CL	G	202	1/1	0.97	0.11	31,31,31,31	0
3	CL	E	201	1/1	0.98	0.08	34,34,34,34	0
3	CL	E	202	1/1	0.98	0.13	32,32,32,32	0
3	CL	B	204	1/1	0.98	0.11	32,32,32,32	0
3	CL	A	203	1/1	0.98	0.12	31,31,31,31	0
3	CL	A	202	1/1	0.99	0.03	29,29,29,29	0
3	CL	H	202	1/1	0.99	0.12	30,30,30,30	0
3	CL	F	202	1/1	0.99	0.04	27,27,27,27	1
3	CL	D	202	1/1	0.99	0.03	32,32,32,32	0
3	CL	C	202	1/1	0.99	0.06	33,33,33,33	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.

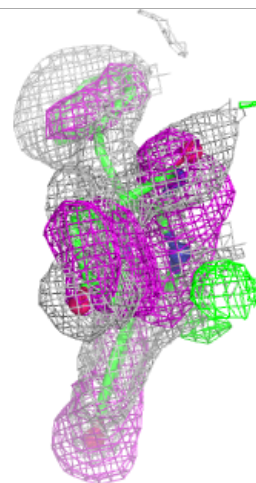
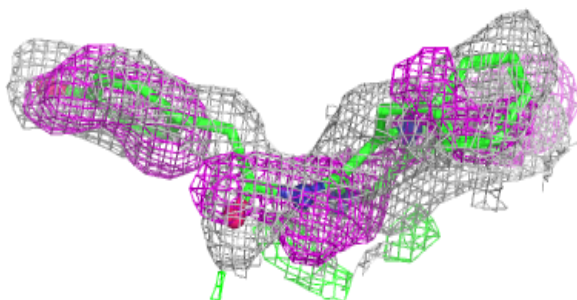
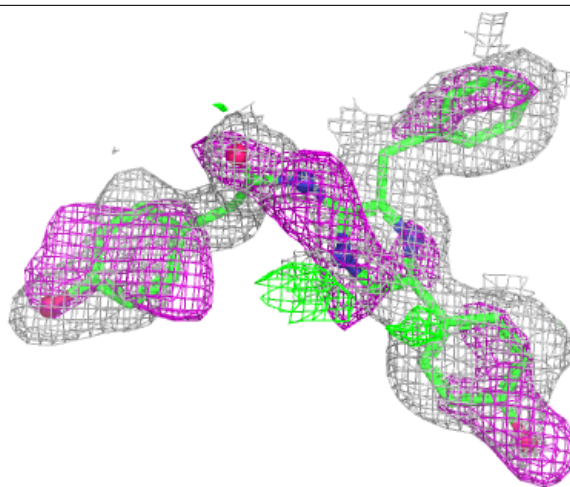
Electron density around CEI G 201:

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



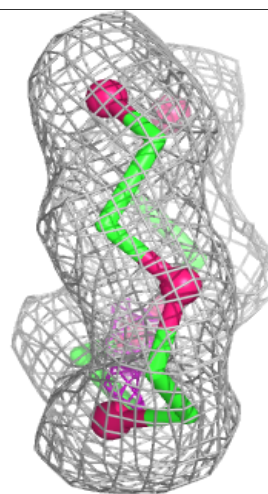
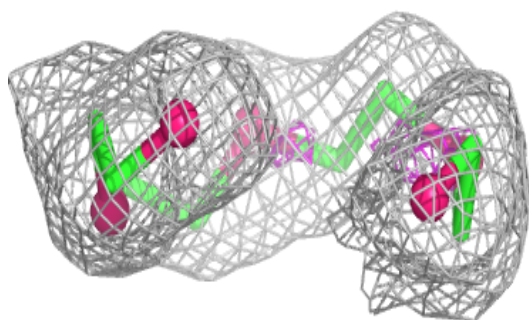
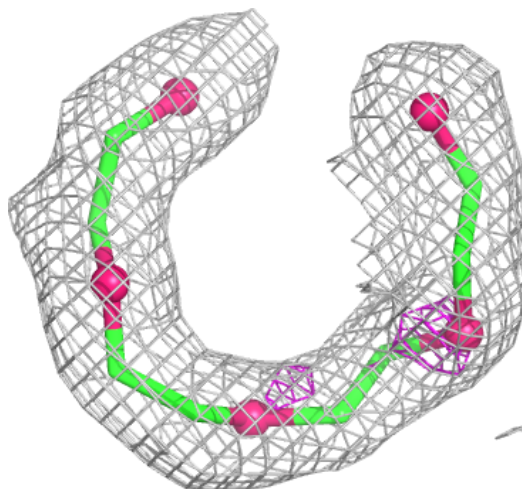
Electron density around CEI A 201:

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



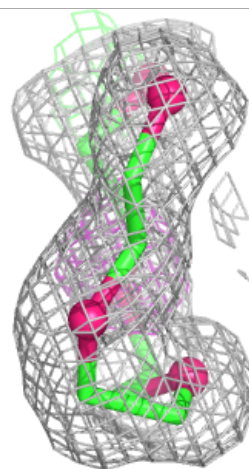
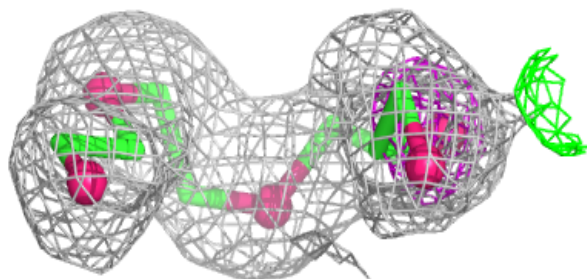
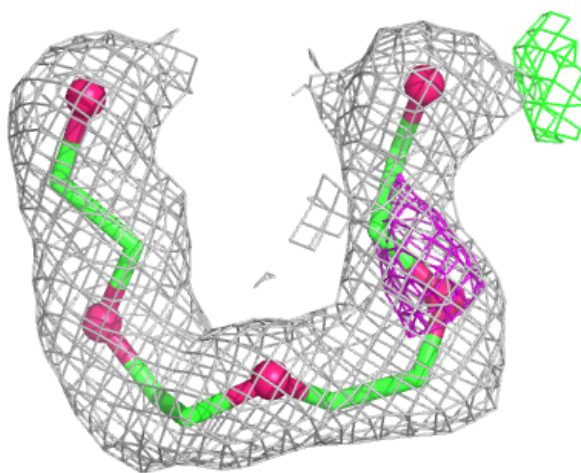
Electron density around PG4 F 201:

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



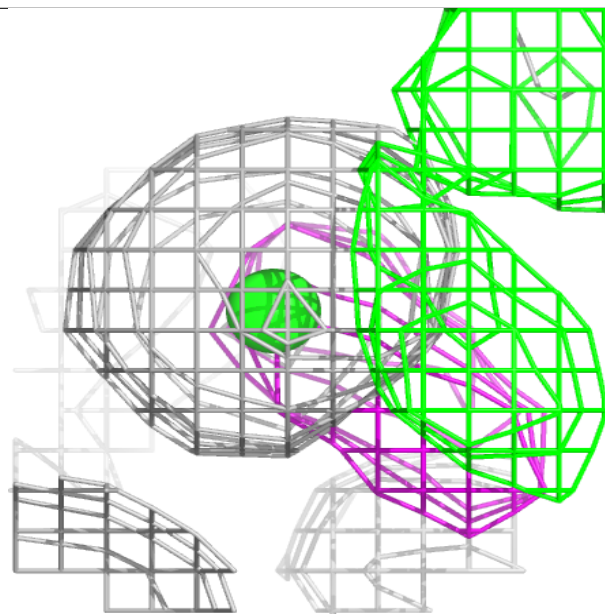
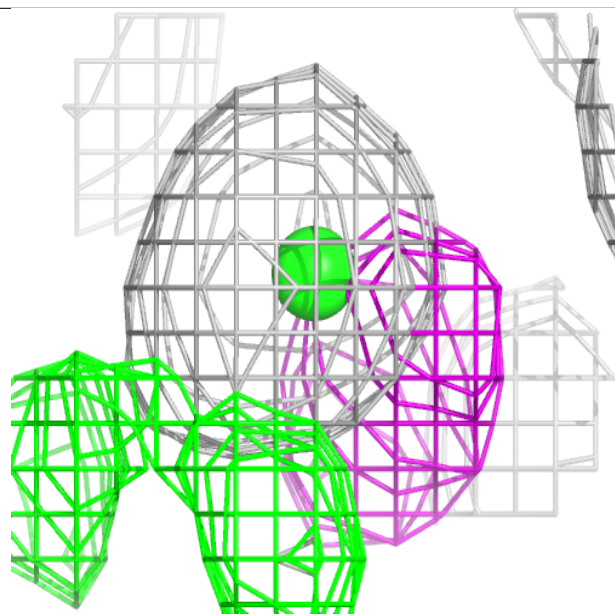
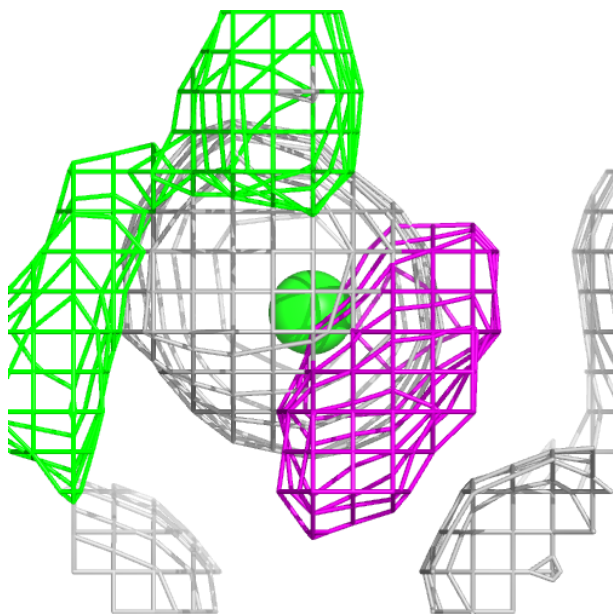
Electron density around PG4 B 201:

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



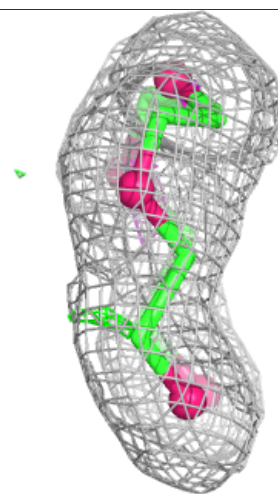
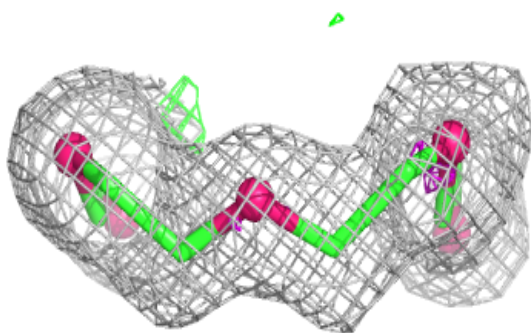
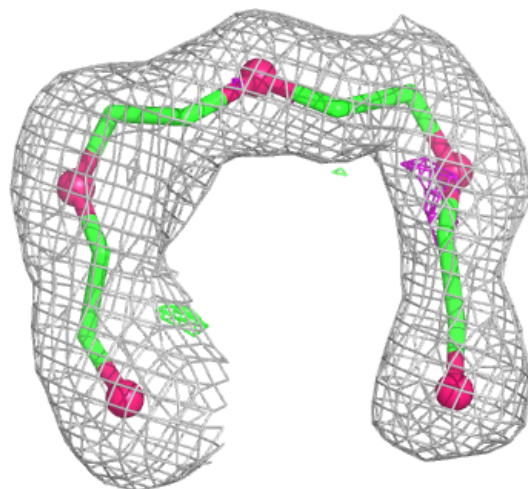
Electron density around CL H 201:

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



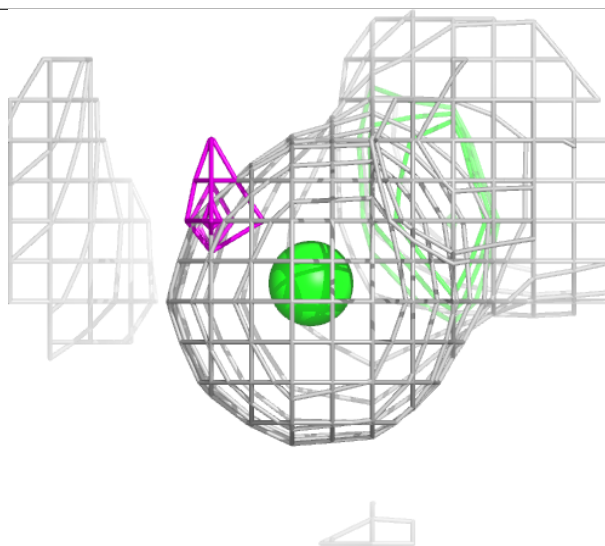
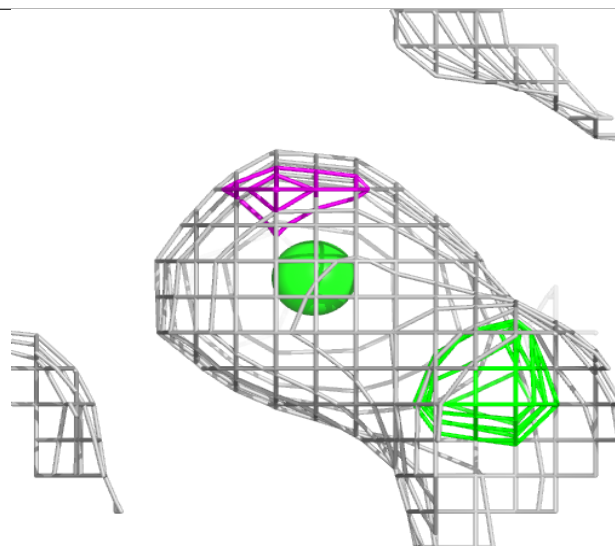
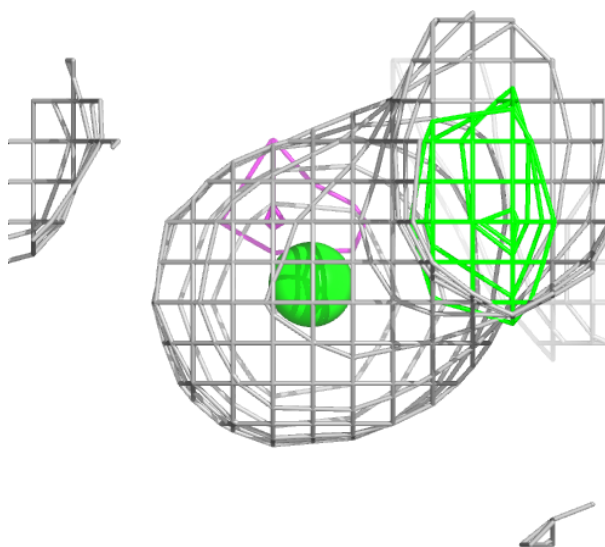
Electron density around PG4 C 201:

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



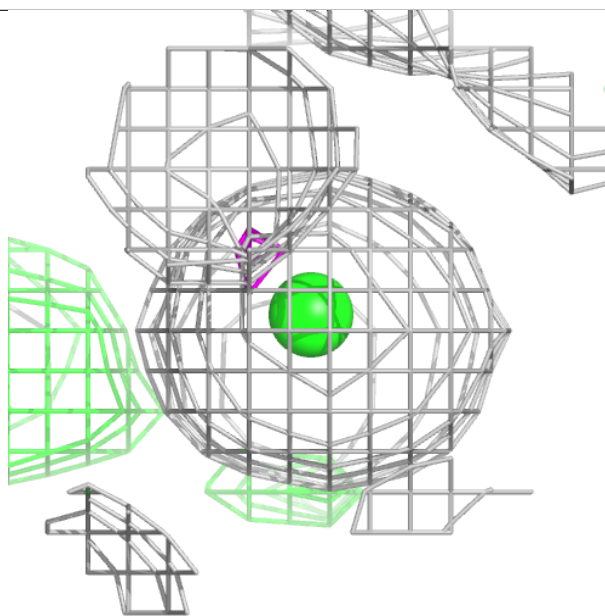
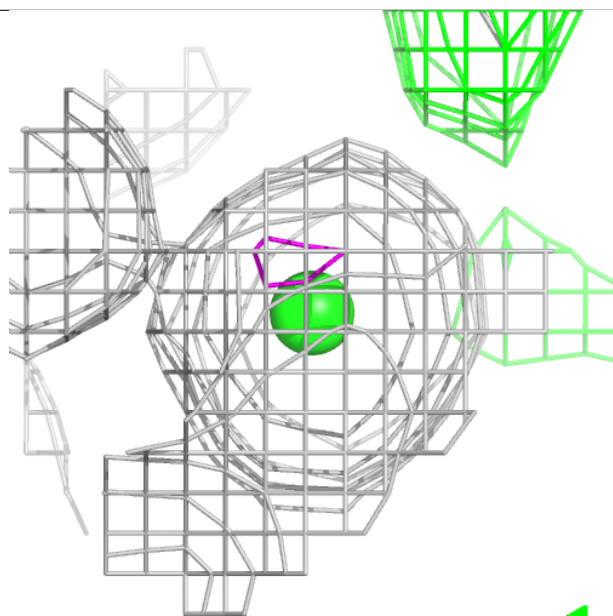
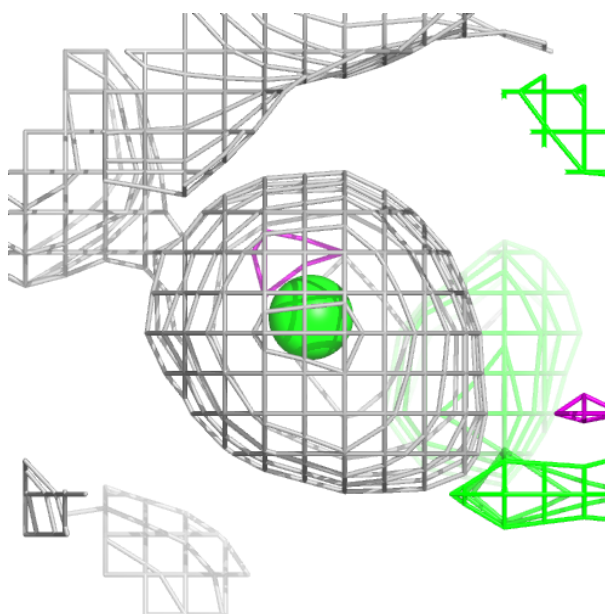
Electron density around CL F 203:

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



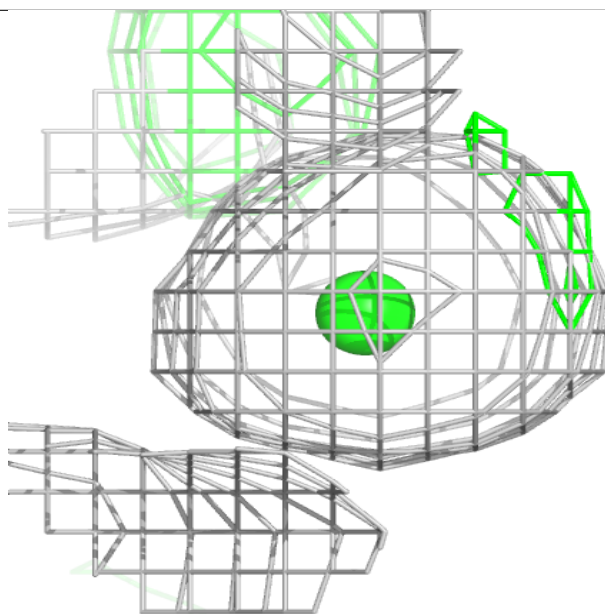
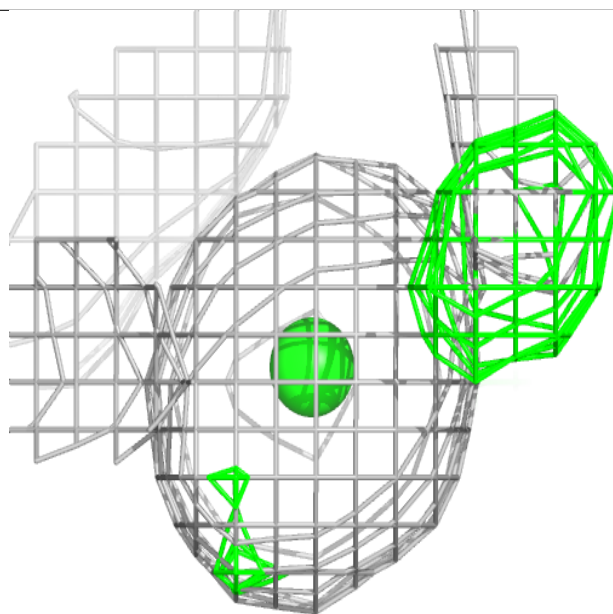
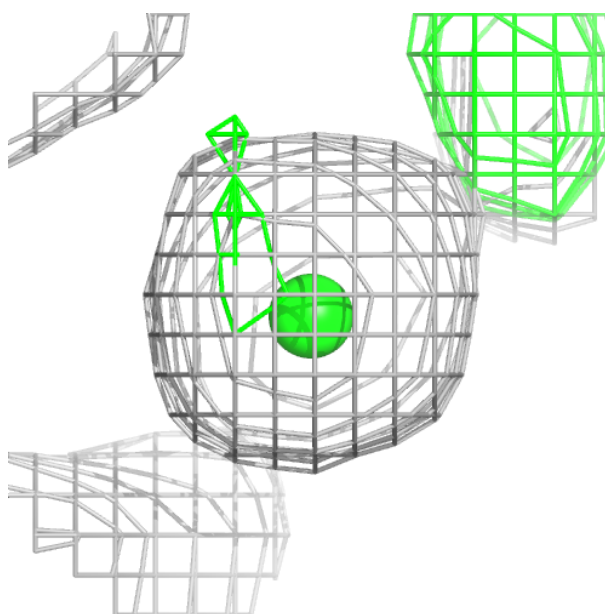
Electron density around CL D 201:

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



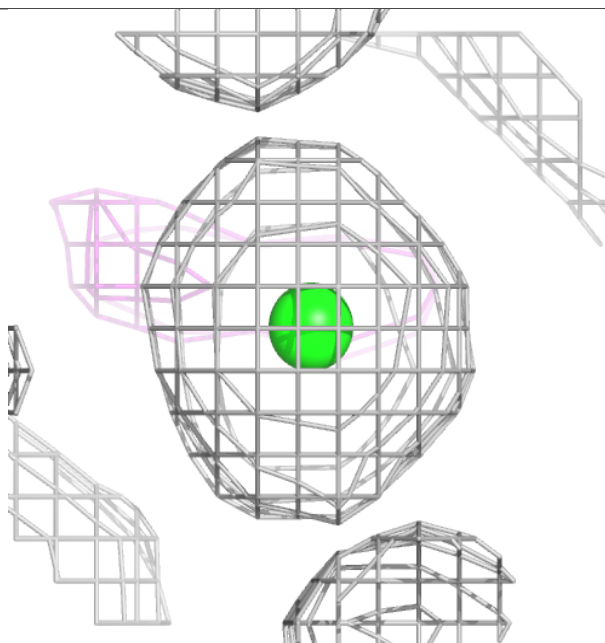
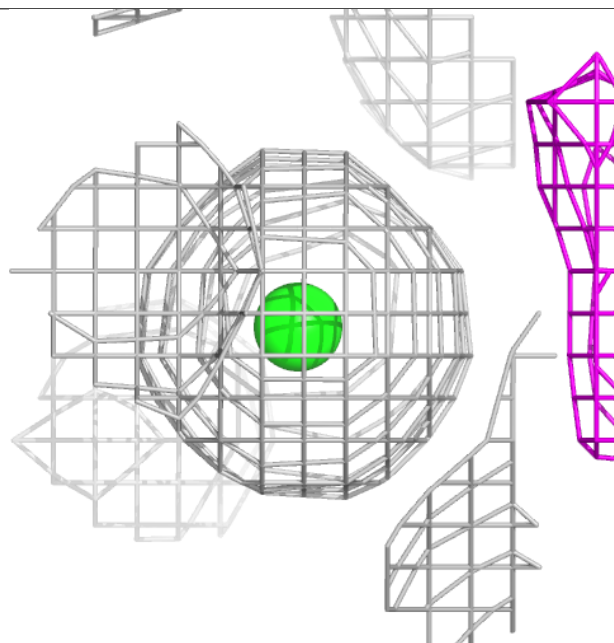
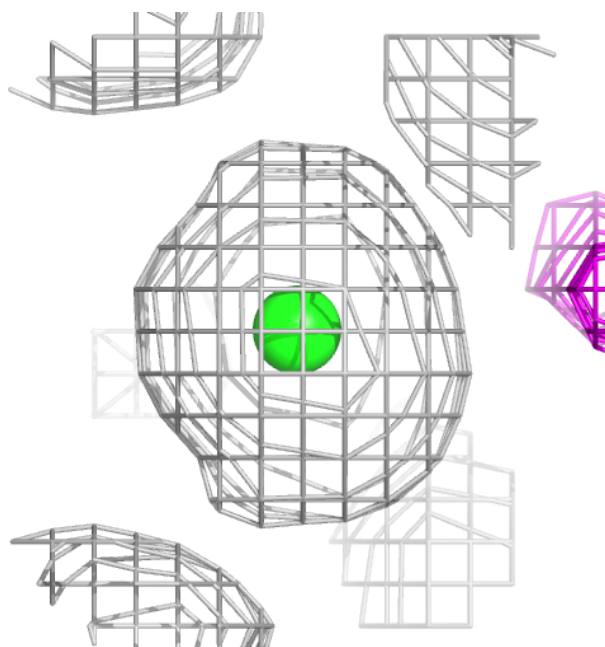
Electron density around CL B 203:

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



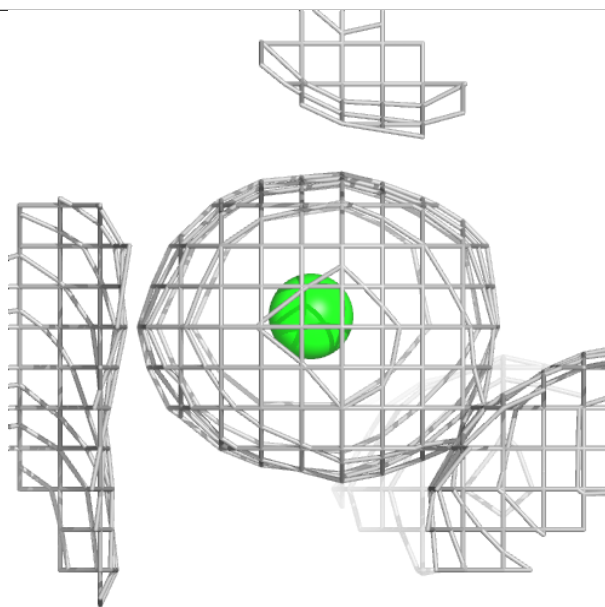
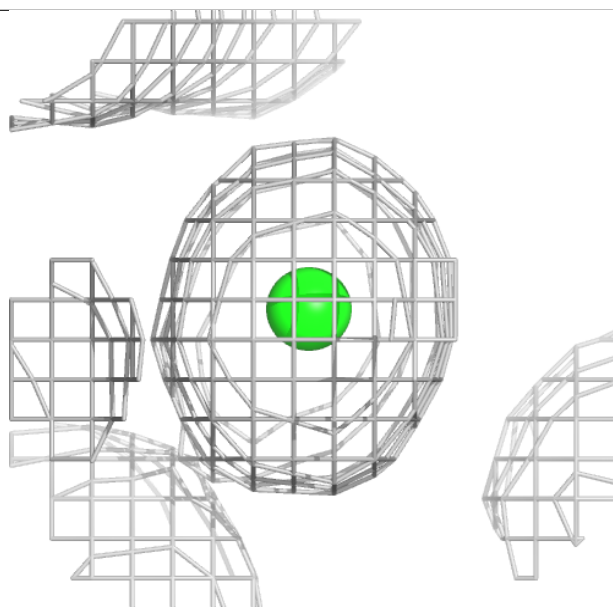
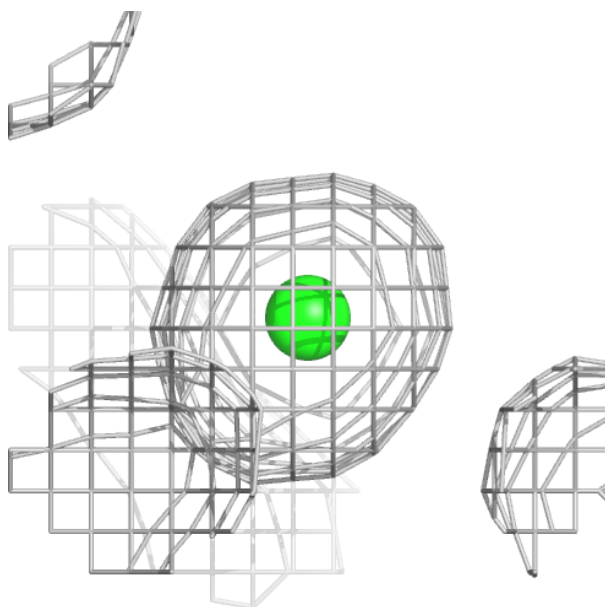
Electron density around CL B 202:

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



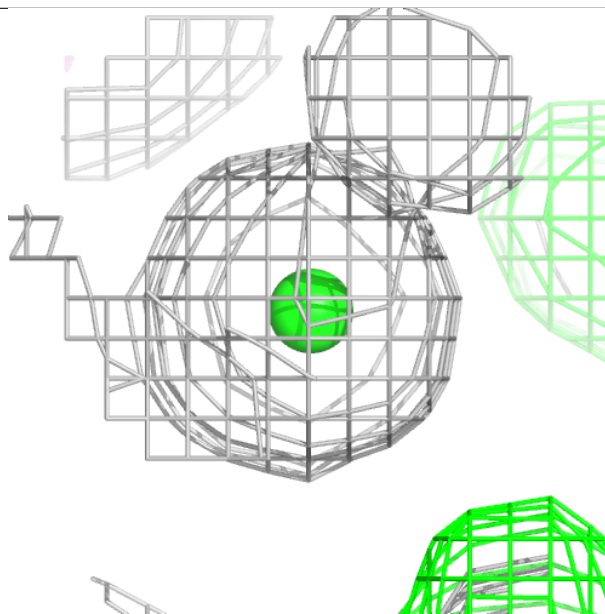
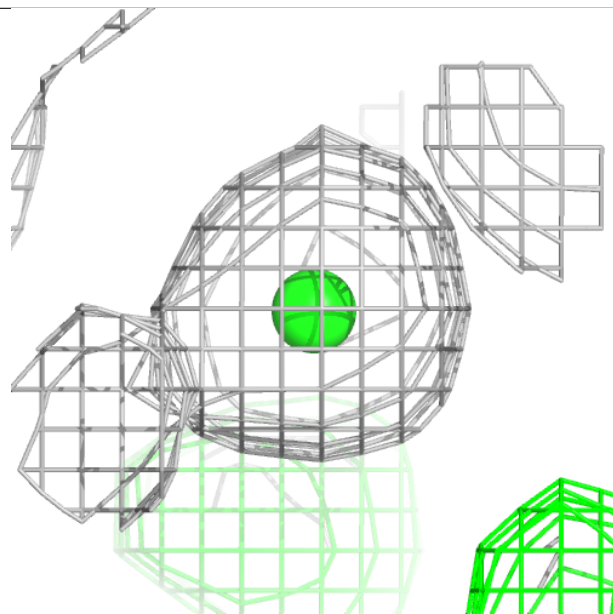
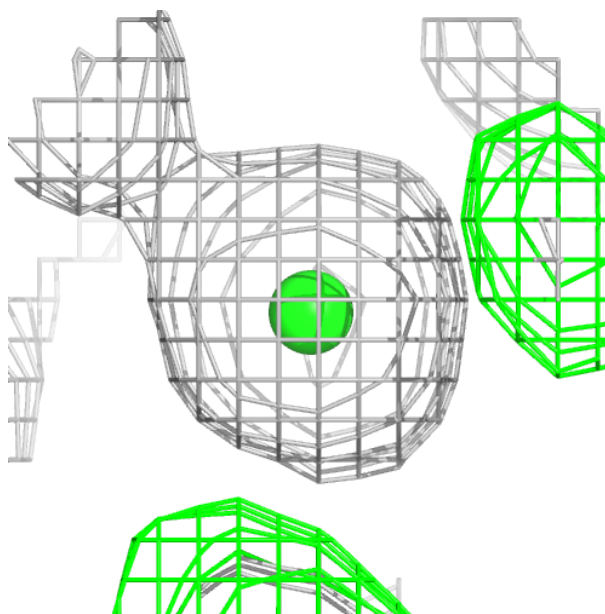
Electron density around CL G 202:

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



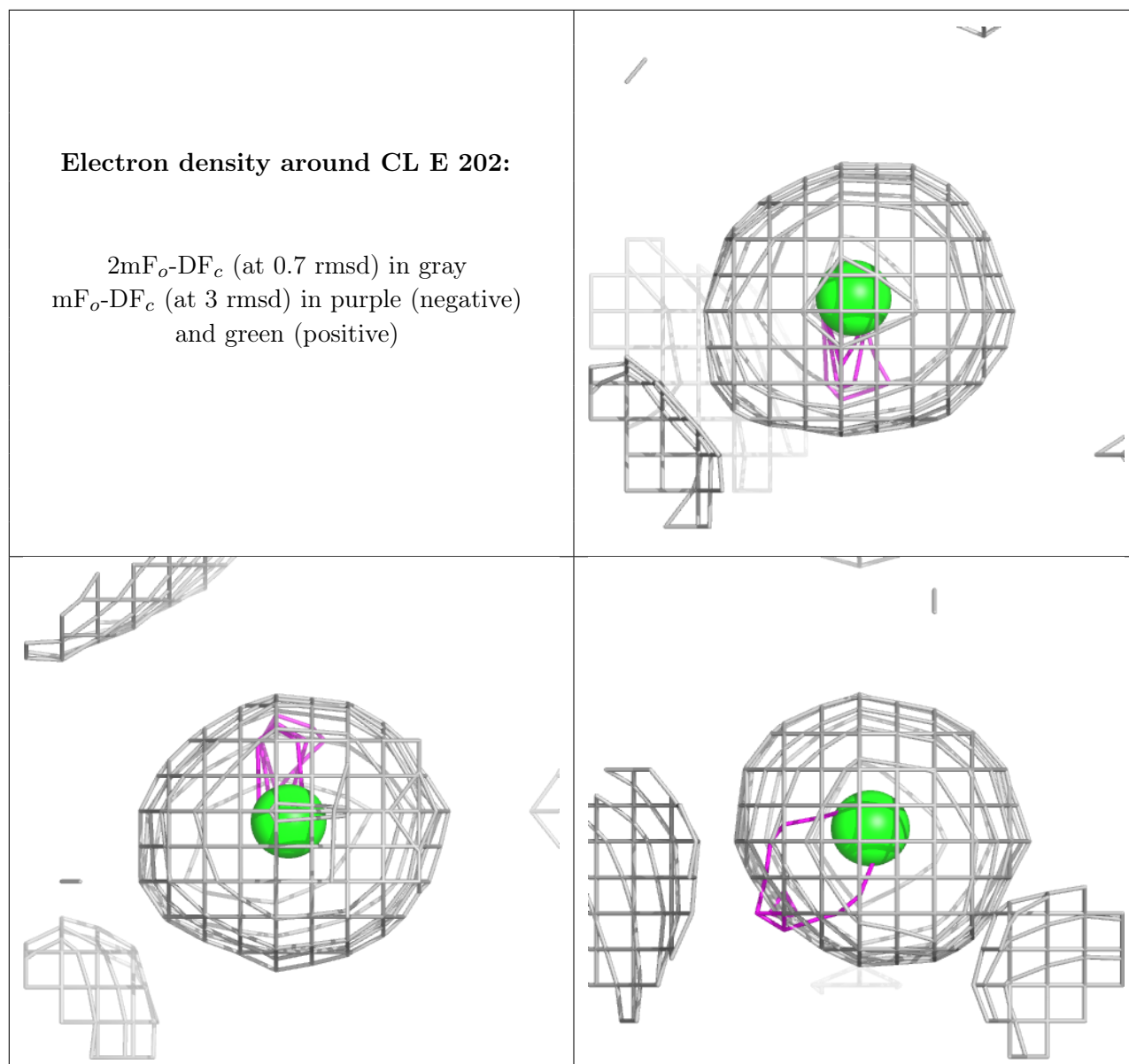
Electron density around CL E 201:

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



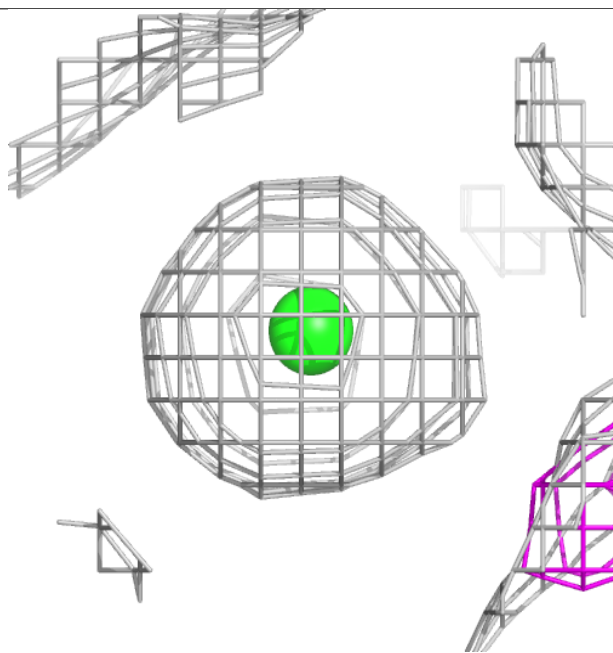
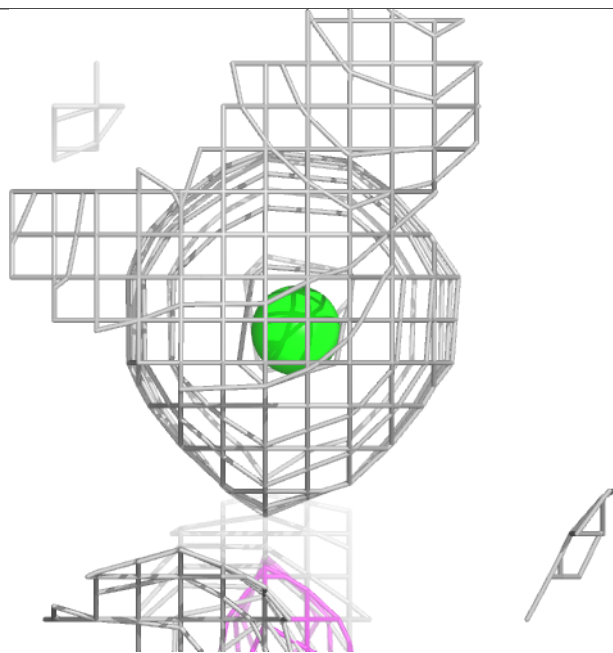
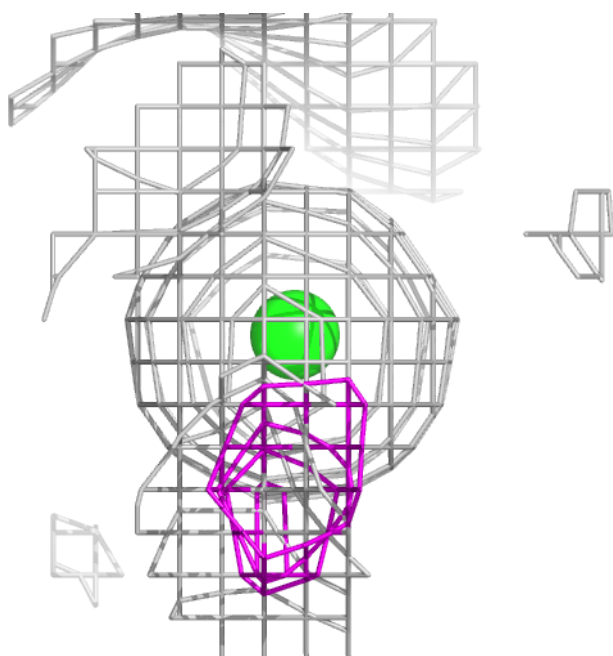
Electron density around CL E 202:

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



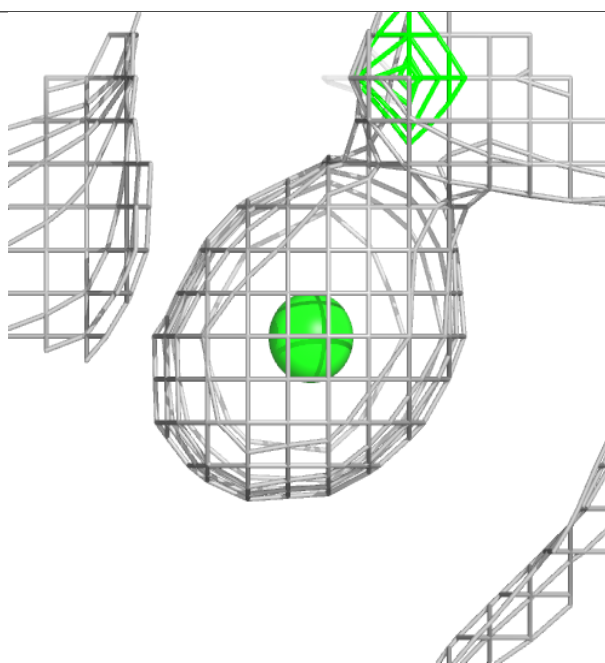
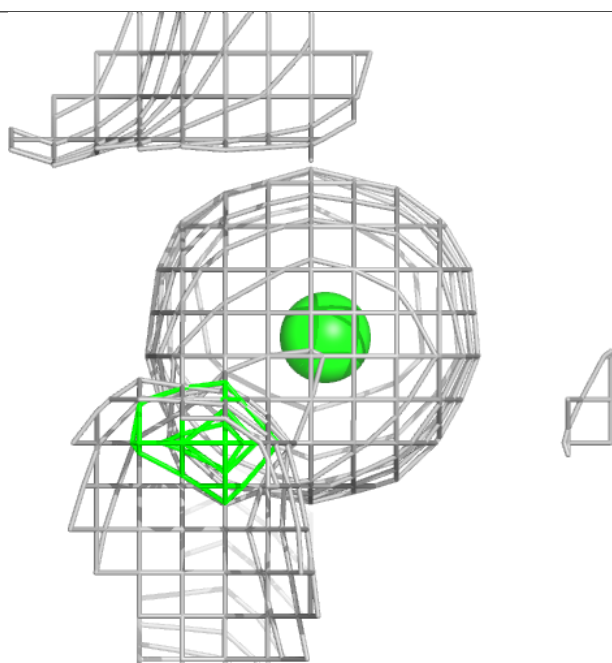
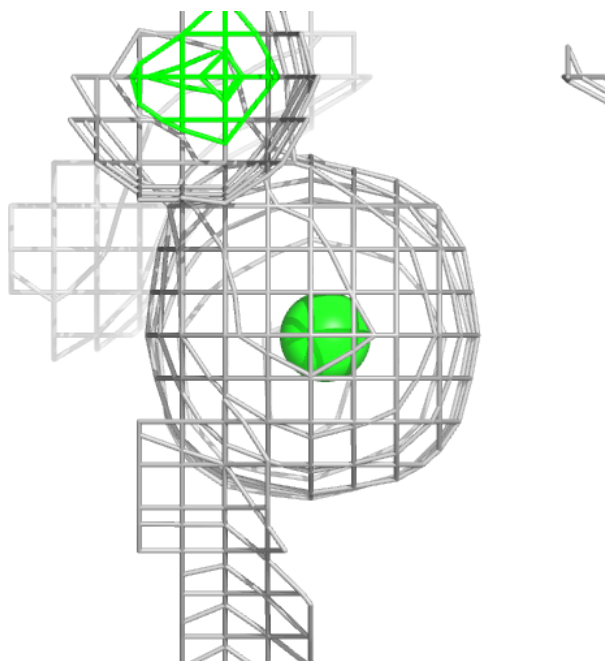
Electron density around CL B 204:

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



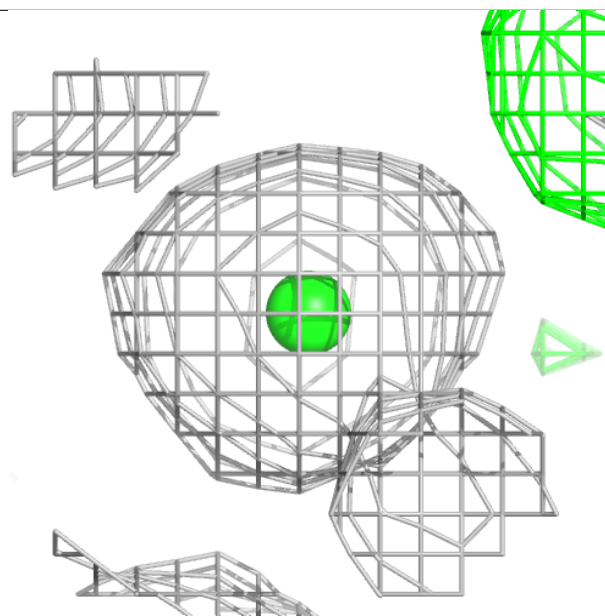
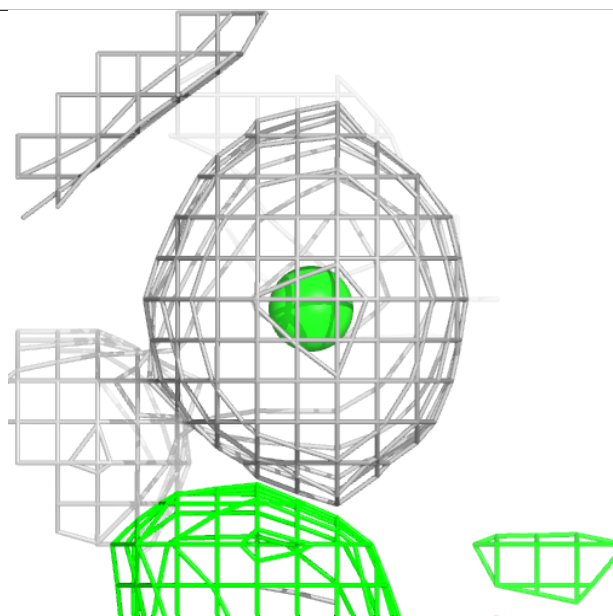
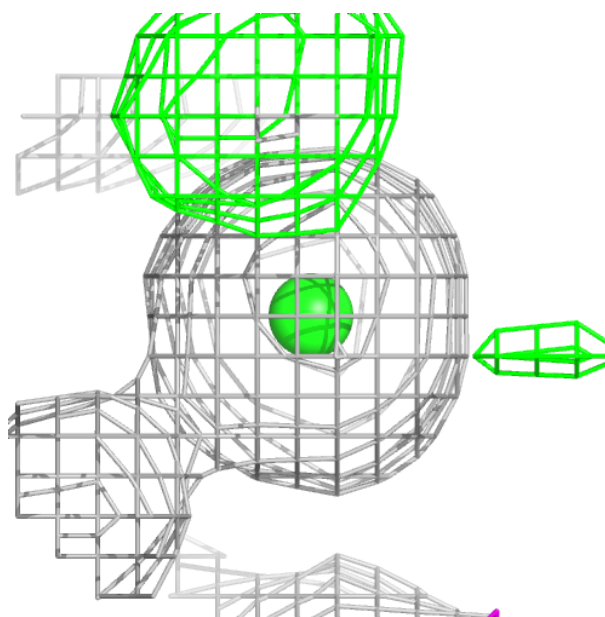
Electron density around CL A 203:

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



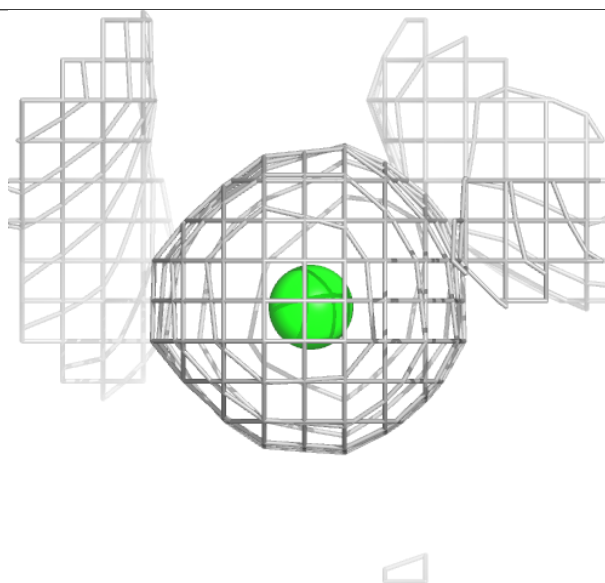
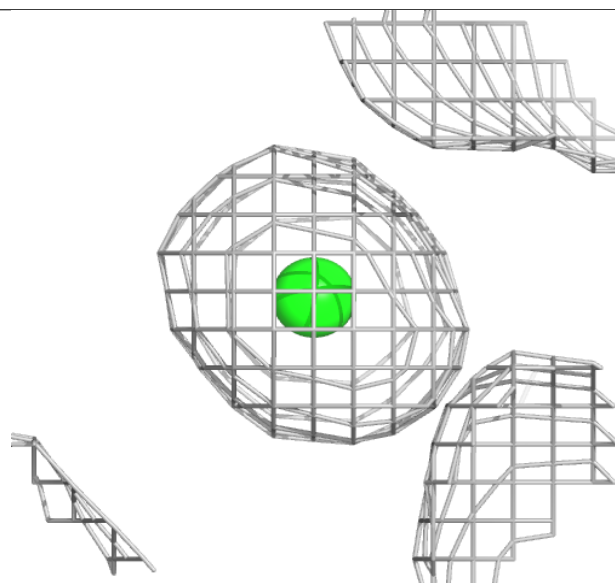
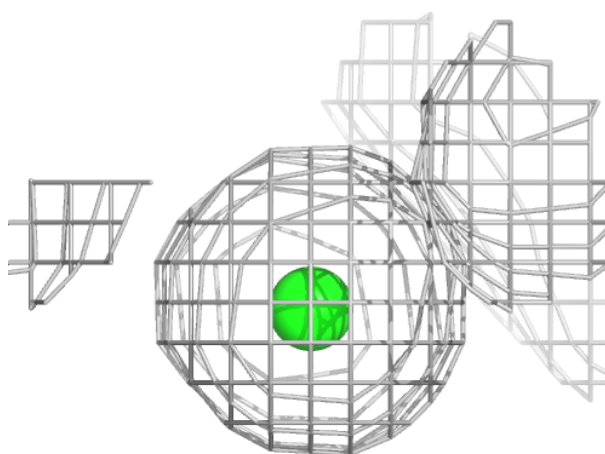
Electron density around CL A 202:

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



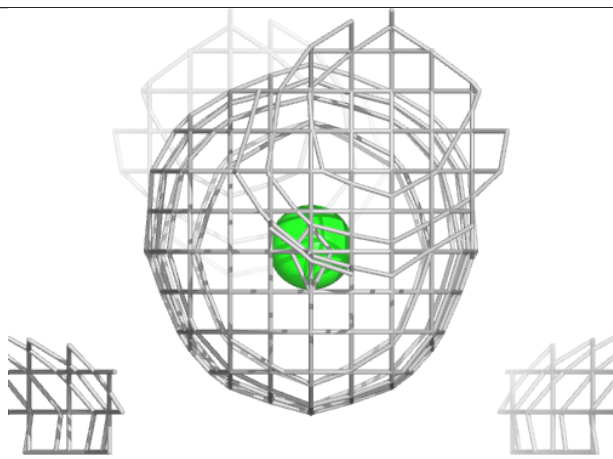
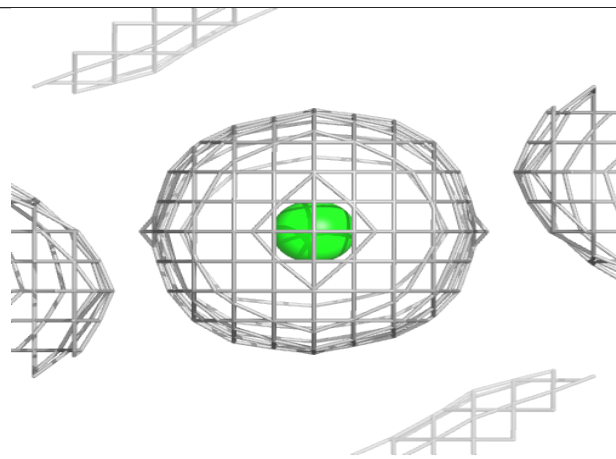
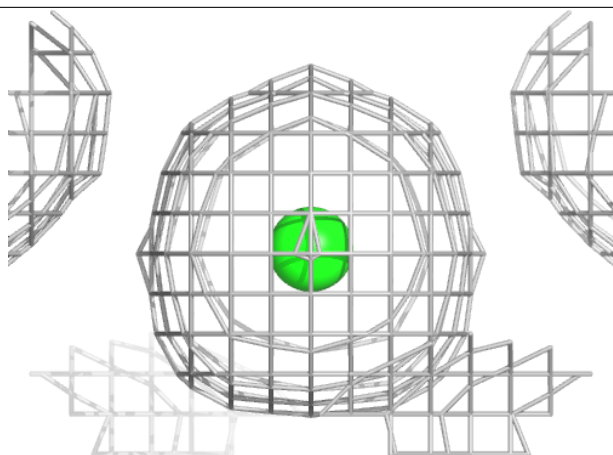
Electron density around CL H 202:

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



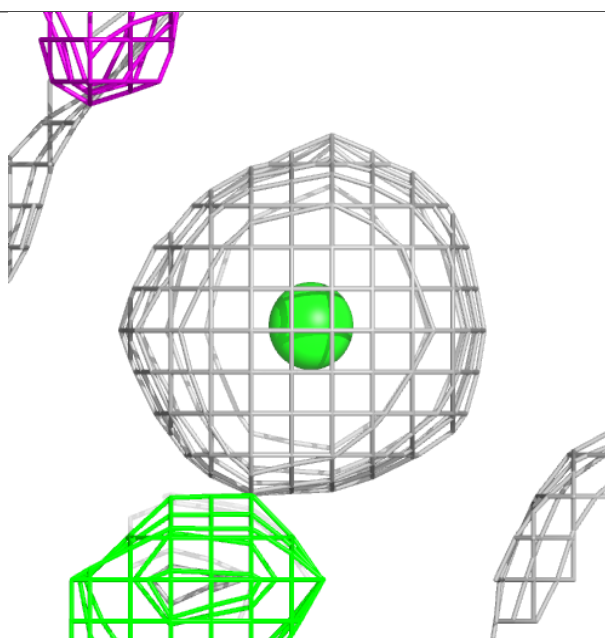
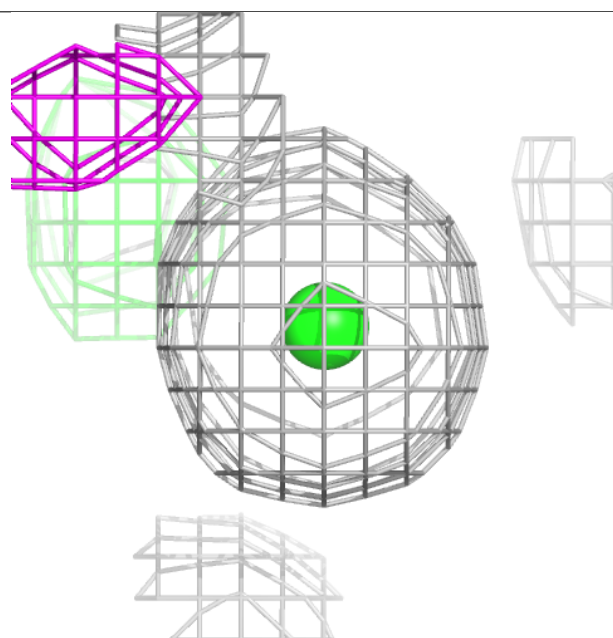
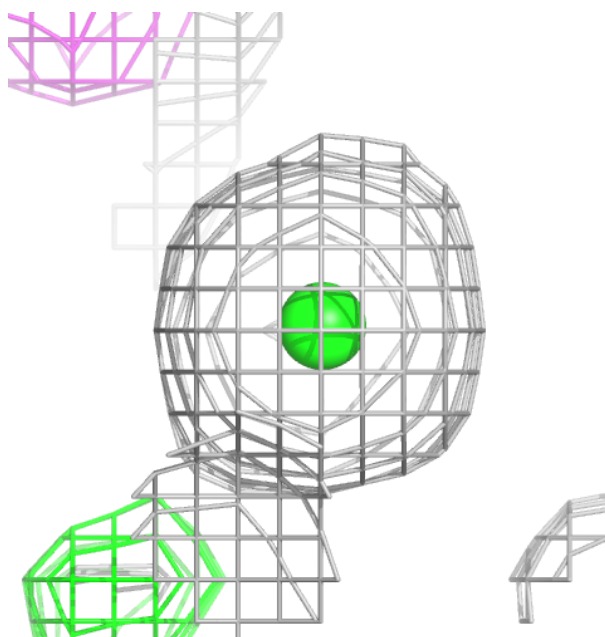
Electron density around CL F 202:

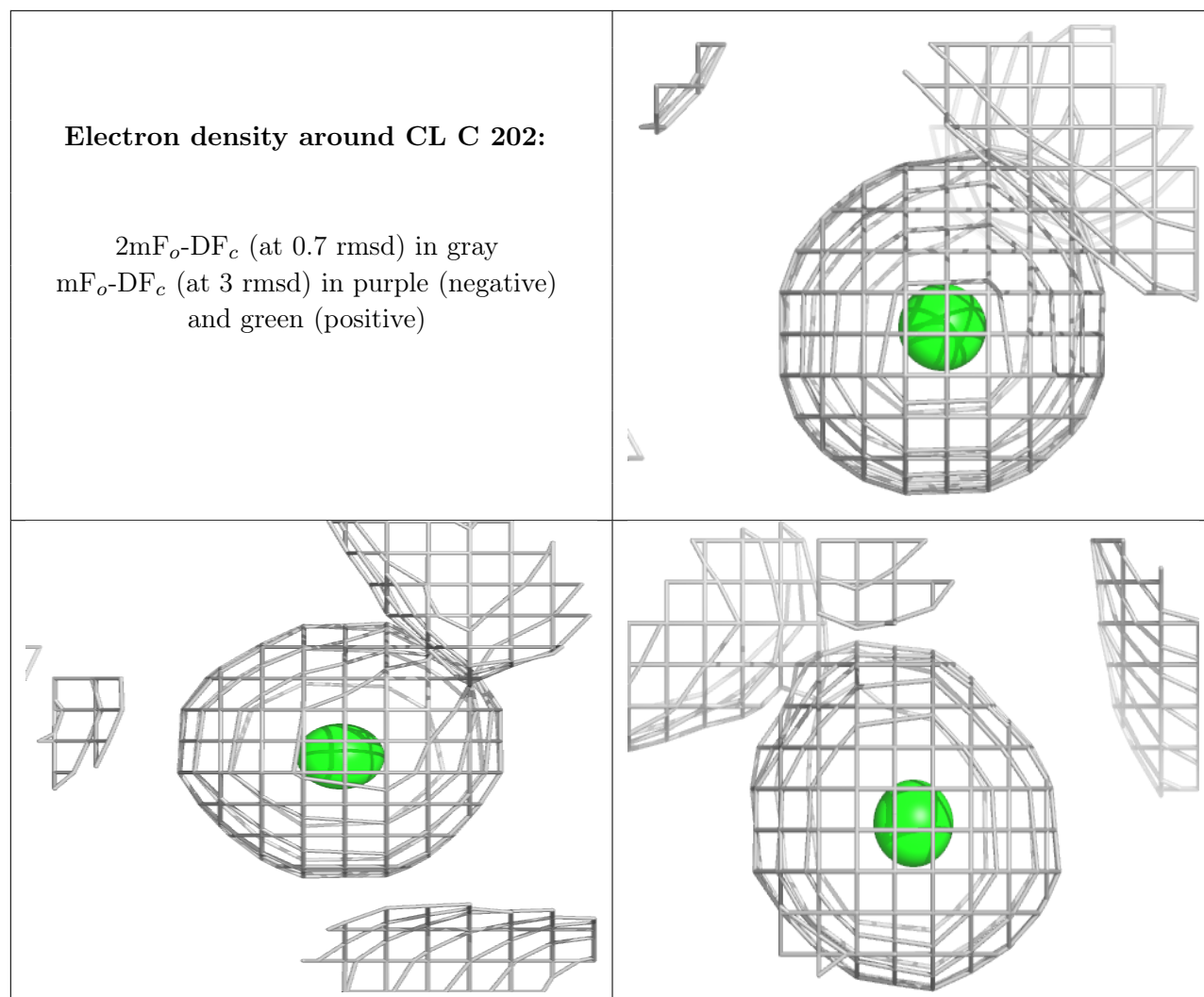
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CL 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.