W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Aug 22, 2023 – 07:22 pm BST

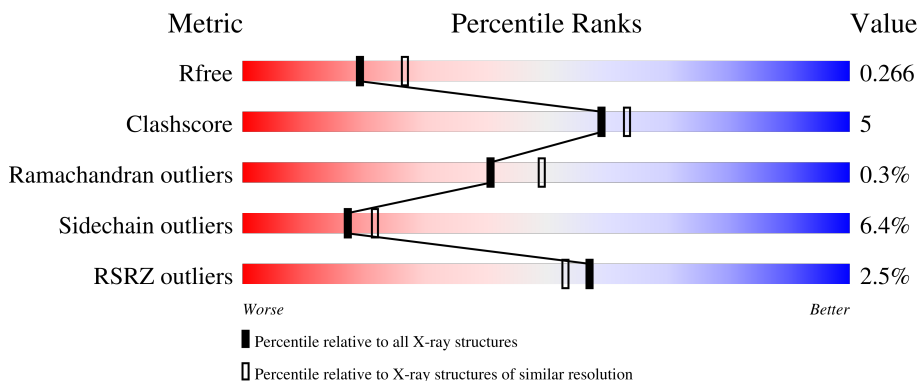|		
PDB ID	:	8CQ6
Title	:	Bifunctional cyclohexadienyl dehydratase/chorismate mutase from Duganella sacchari
Authors	:	Khatanbaatar, T.; Cordara, G.; Krengel, U.
Deposited on	:	2023-03-03
Resolution	:	2.44 Å(reported)

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 2.44 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	Percentile Ranks	Value
Rfree		0.266
Clashscore		5
Ramachandran outliers		0.3%
Sidechain outliers		6.4%
RSRZ outliers		2.5%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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

Mol	Chain	Length	Quality of chain
1	A	416	2% / 74% 16% · 9%
1	B	416	2% / 74% 16% · 8%
1	C	416	4% / 73% 17% · 6%
1	D	416	2% / 75% 17% · 6%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 12234 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 chorismate mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	0	0
			2954	1865	530	552	7			
1	B	384	Total	C	N	O	S	0	6	0
			3034	1916	546	565	7			
1	C	389	Total	C	N	O	S	0	7	0
			3098	1957	563	571	7			
1	D	389	Total	C	N	O	S	0	3	0
			3067	1938	558	564	7			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	409	LEU	-	expression tag	UNP A0A1M7QNQ8
A	410	GLU	-	expression tag	UNP A0A1M7QNQ8
A	411	HIS	-	expression tag	UNP A0A1M7QNQ8
A	412	HIS	-	expression tag	UNP A0A1M7QNQ8
A	413	HIS	-	expression tag	UNP A0A1M7QNQ8
A	414	HIS	-	expression tag	UNP A0A1M7QNQ8
A	415	HIS	-	expression tag	UNP A0A1M7QNQ8
A	416	HIS	-	expression tag	UNP A0A1M7QNQ8
B	409	LEU	-	expression tag	UNP A0A1M7QNQ8
B	410	GLU	-	expression tag	UNP A0A1M7QNQ8
B	411	HIS	-	expression tag	UNP A0A1M7QNQ8
B	412	HIS	-	expression tag	UNP A0A1M7QNQ8
B	413	HIS	-	expression tag	UNP A0A1M7QNQ8
B	414	HIS	-	expression tag	UNP A0A1M7QNQ8
B	415	HIS	-	expression tag	UNP A0A1M7QNQ8
B	416	HIS	-	expression tag	UNP A0A1M7QNQ8
C	409	LEU	-	expression tag	UNP A0A1M7QNQ8
C	410	GLU	-	expression tag	UNP A0A1M7QNQ8
C	411	HIS	-	expression tag	UNP A0A1M7QNQ8
C	412	HIS	-	expression tag	UNP A0A1M7QNQ8
C	413	HIS	-	expression tag	UNP A0A1M7QNQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	414	HIS	-	expression tag	UNP A0A1M7QNQ8
C	415	HIS	-	expression tag	UNP A0A1M7QNQ8
C	416	HIS	-	expression tag	UNP A0A1M7QNQ8
D	409	LEU	-	expression tag	UNP A0A1M7QNQ8
D	410	GLU	-	expression tag	UNP A0A1M7QNQ8
D	411	HIS	-	expression tag	UNP A0A1M7QNQ8
D	412	HIS	-	expression tag	UNP A0A1M7QNQ8
D	413	HIS	-	expression tag	UNP A0A1M7QNQ8
D	414	HIS	-	expression tag	UNP A0A1M7QNQ8
D	415	HIS	-	expression tag	UNP A0A1M7QNQ8
D	416	HIS	-	expression tag	UNP A0A1M7QNQ8

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Na 2　2	0	0
2	B	2	Total Na 2　2	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Cl 3　3	0	0
3	B	1	Total Cl 1　1	0	0
3	C	1	Total Cl 1　1	0	0
3	D	1	Total Cl 1　1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	17	Total O 17　17	0	0
4	B	18	Total O 18　18	0	0

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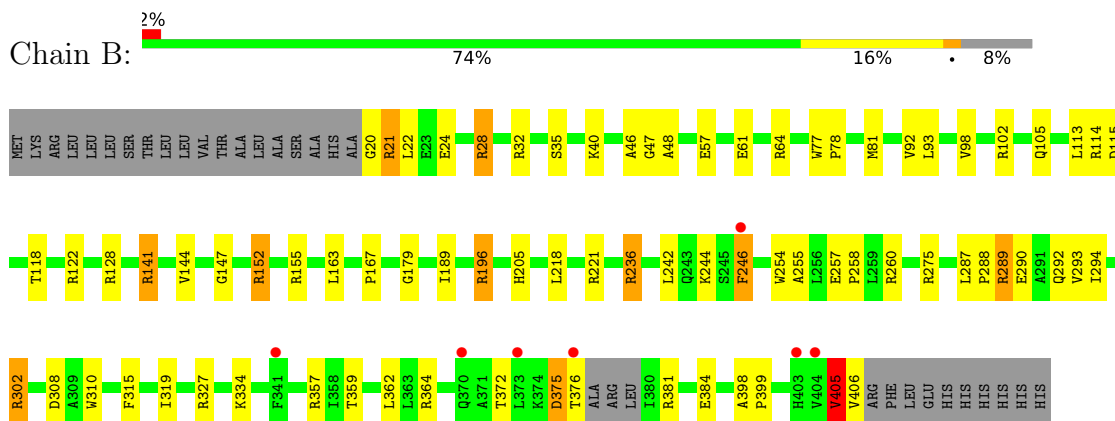| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	15	Total 15	O 15	0	0
4	D	21	Total 21	O 21	0	0

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.
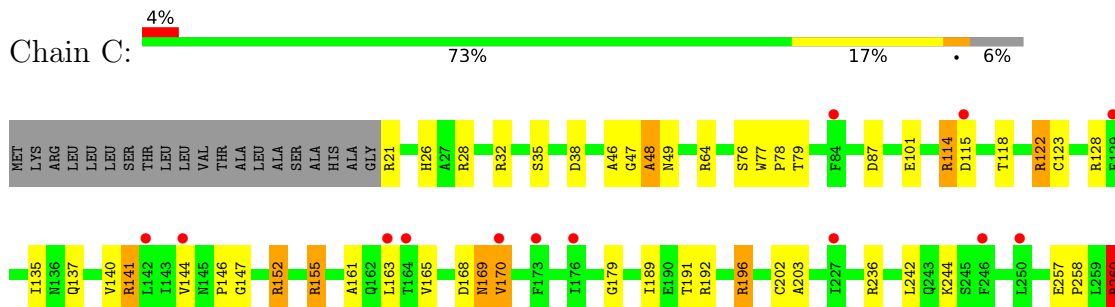
- Molecule 1: chorismate mutase
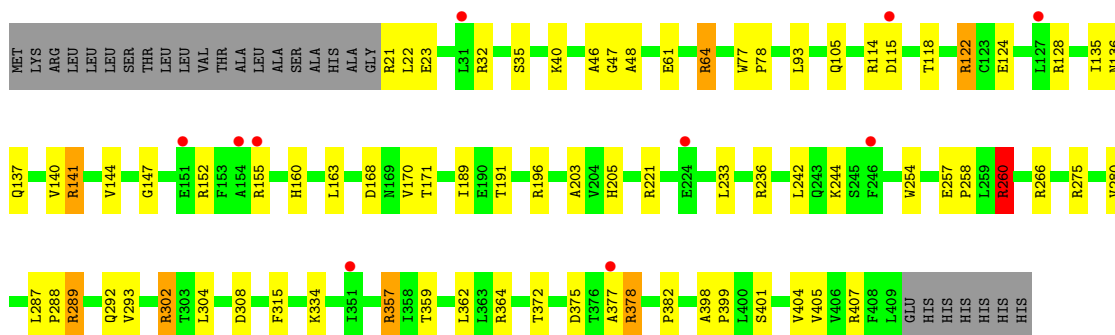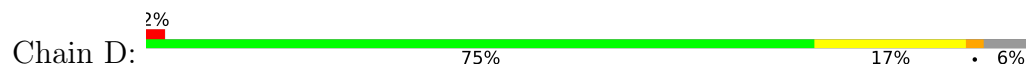
Chain A:

- Molecule 1: chorismate mutase

Chain B:

- Molecule 1: chorismate mutase

Chain C:

Q261 E265 R266 R275 A276 V280 Q281 L287 P288 R289 Q292 V293 L304 G305 L306 P307 D308 F315 R327 R357 I358 T359 L362 L363 R364 A367 T372 D375 T376 A377 R378 L379 P382 A398 P399 L400 S401 V404 V405 V406 R407 F408 L409 GLU

HIS HIS HIS HIS HIS

• Molecule 1: chorismate mutase

Chain D:

2%

75%   17%   6%

MET LYS ARG LEU LEU LEU SER THR LEU LEU VAL THR ALA LEU ALA SER ALA HIS ALA GLY R21 L22 E23 L31 R32 S35 K40 A46 G47 A48 E61 R64 W77 P78 L93 Q105 R114 D115 T118 R122 C123 E124 L127 R128 I135 N136

Q137 V140 R141 V144 G147 E151 R152 F153 A154 R155 H160 L163 D168 N169 V170 T171 I189 E190 T191 R196 A203 V204 H205 R221 E224 L233 R236 L242 Q243 K244 S245 F246 W254 E257 P258 L259 R260 R266 R275 V280

L287 P288 R289 Q292 V293 R302 T303 L304 D308 F315 K334 I351 R357 I358 T359 L362 L363 R364 T372 D375 T376 A377 R378 P382 A398 P399 L400 S401 V404 V405 V406 R407 F408 L409 GLU HIS HIS HIS HIS HIS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	92.11Å 111.93Å 221.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.90 – 2.44 99.89 – 2.44	Depositor EDS
% Data completeness (in resolution range)	60.3 (99.90-2.44) 60.3 (99.89-2.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.8.0350	Depositor
R, R_{free}	0.225 , 0.265 0.226 , 0.266	Depositor DCC
R_{free} test set	2573 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	52.4	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 38.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12234	wwPDB-VP
Average B, all atoms (Å^2)	59.0	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 48.01 % 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 9.1447e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.29	0/3013	0.51	0/4101
1	B	0.29	0/3094	0.52	0/4212
1	C	0.28	0/3161	0.53	0/4302
1	D	0.29	0/3130	0.50	0/4260
All	All	0.29	0/12398	0.52	0/16875

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	24
1	B	0	24
1	C	0	29
1	D	0	25
All	All	0	102

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 102 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	20	GLY	Peptide
1	A	21	ARG	Sidechain
1	A	32	ARG	Sidechain
1	A	46	ALA	Peptide
1	A	47	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	2954	0	2954	23	0
1	B	3034	0	3037	36	0
1	C	3098	0	3110	35	0
1	D	3067	0	3078	27	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	17	0	0	0	0
4	B	18	0	0	1	0
4	C	15	0	0	1	0
4	D	21	0	0	0	0
All	All	12234	0	12179	115	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 5.

The worst 5 of 115 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:B:24[B]:GLU:HA	1:B:24[B]:GLU:OE1	1.38	1.19
1:B:375:ASP:HB3	1:B:376:THR:HG23	1.64	0.79
1:A:113:LEU:HD13	1:A:246:PHE:CZ	2.19	0.78
1:B:113:LEU:HD13	1:B:246:PHE:CZ	2.19	0.78
1:A:214:GLU:OE2	1:D:114:ARG:HD3	1.89	0.72

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	376/416 (90%)	364 (97%)	12 (3%)	0	100	100
1	B	386/416 (93%)	373 (97%)	12 (3%)	1 (0%)	41	49
1	C	394/416 (95%)	378 (96%)	13 (3%)	3 (1%)	19	22
1	D	390/416 (94%)	374 (96%)	15 (4%)	1 (0%)	41	49
All	All	1546/1664 (93%)	1489 (96%)	52 (3%)	5 (0%)	41	49

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	405	VAL
1	C	169	ASN
1	D	48	ALA
1	C	48	ALA
1	C	170	VAL

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	304/335 (91%)	285 (94%)	19 (6%)	18	23
1	B	313/335 (93%)	294 (94%)	19 (6%)	18	24
1	C	319/335 (95%)	298 (93%)	21 (7%)	16	20
1	D	316/335 (94%)	293 (93%)	23 (7%)	14	17
All	All	1252/1340 (93%)	1170 (94%)	82 (6%)	17	21

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	379	LEU
1	D	242	LEU
1	D	22	LEU
1	D	122	ARG
1	D	302	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	162	GLN
1	D	136	ASN
1	C	157	HIS
1	D	103	GLN
1	C	145	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å²)	Q<0.9
1	A	380/416 (91%)	0.31	7 (1%)	68	64	33, 53, 82, 117	0
1	B	384/416 (92%)	0.36	7 (1%)	68	64	31, 54, 87, 146	0
1	C	389/416 (93%)	0.49	15 (3%)	39	36	32, 64, 94, 121	0
1	D	389/416 (93%)	0.37	10 (2%)	56	52	31, 57, 82, 124	0
All	All	1542/1664 (92%)	0.38	39 (2%)	57	53	31, 57, 89, 146	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	373	LEU	7.7
1	B	403	HIS	4.9
1	C	250	LEU	4.2
1	C	246	PHE	4.2
1	D	377	ALA	3.5

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides 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	NA	A	502	1/1	0.92	0.11	64,64,64,64	0
2	NA	B	501	1/1	0.92	0.07	46,46,46,46	0
2	NA	A	501	1/1	0.96	0.11	51,51,51,51	0
3	CL	A	503	1/1	0.97	0.07	51,51,51,51	0
3	CL	A	504	1/1	0.97	0.07	62,62,62,62	0
3	CL	A	505	1/1	0.97	0.06	48,48,48,48	0
3	CL	B	503	1/1	0.97	0.08	51,51,51,51	0
2	NA	B	502	1/1	0.98	0.10	51,51,51,51	0
3	CL	C	501	1/1	0.98	0.10	51,51,51,51	0
3	CL	D	501	1/1	0.98	0.07	44,44,44,44	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.
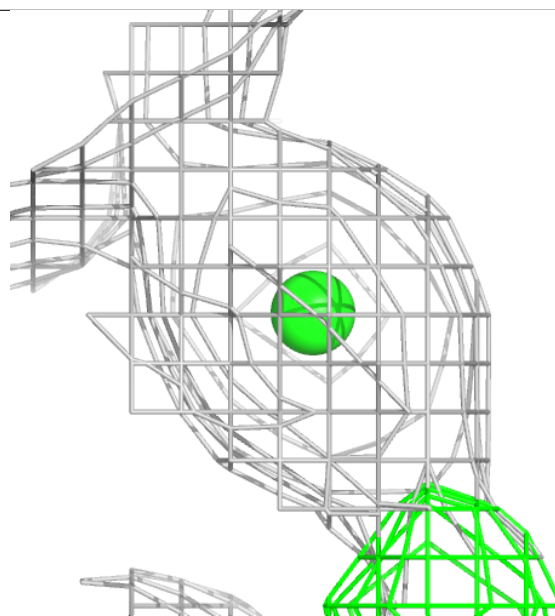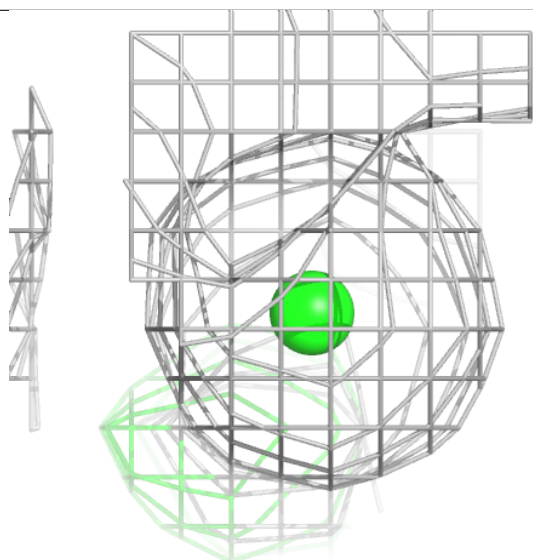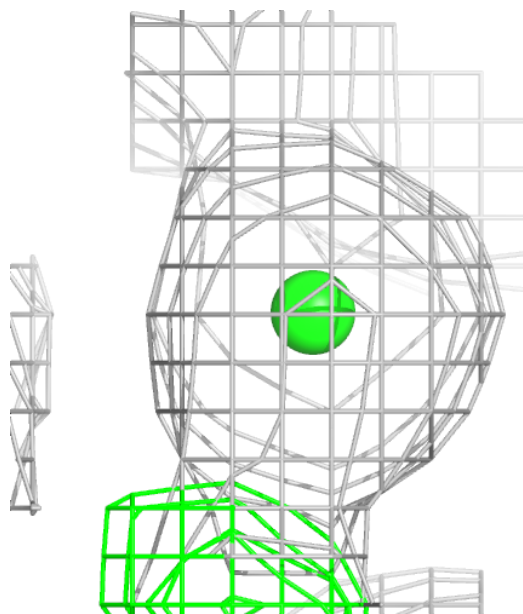
Electron density around NA A 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
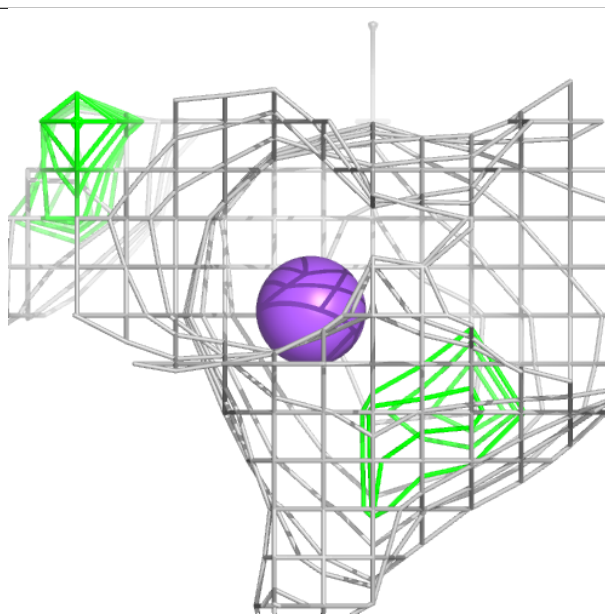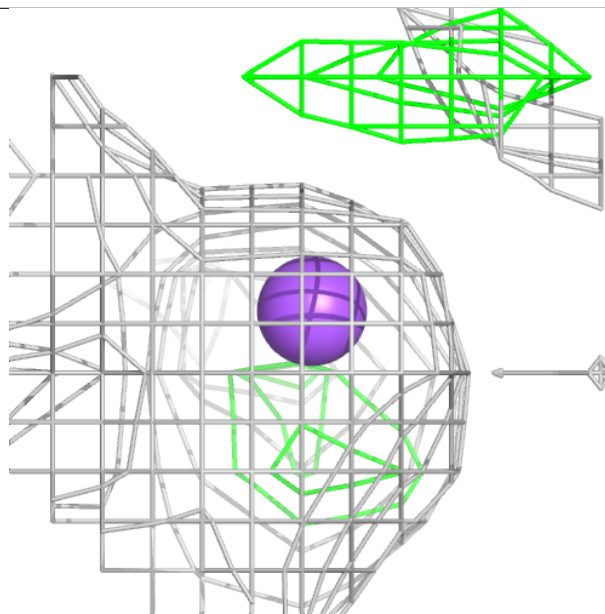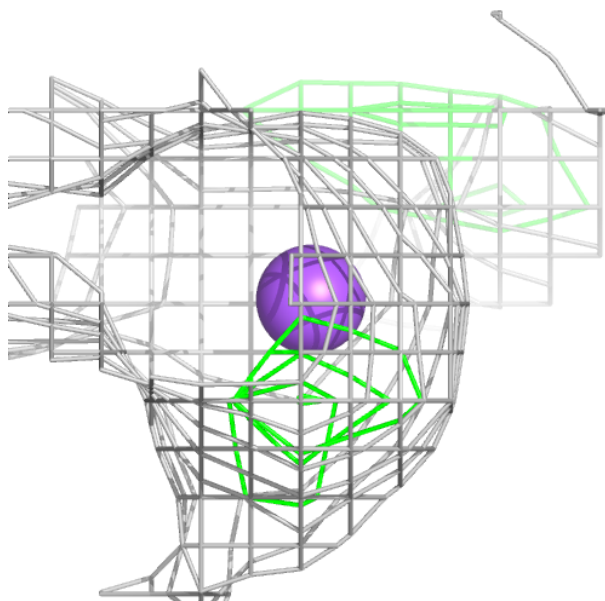
Electron density around NA B 501:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
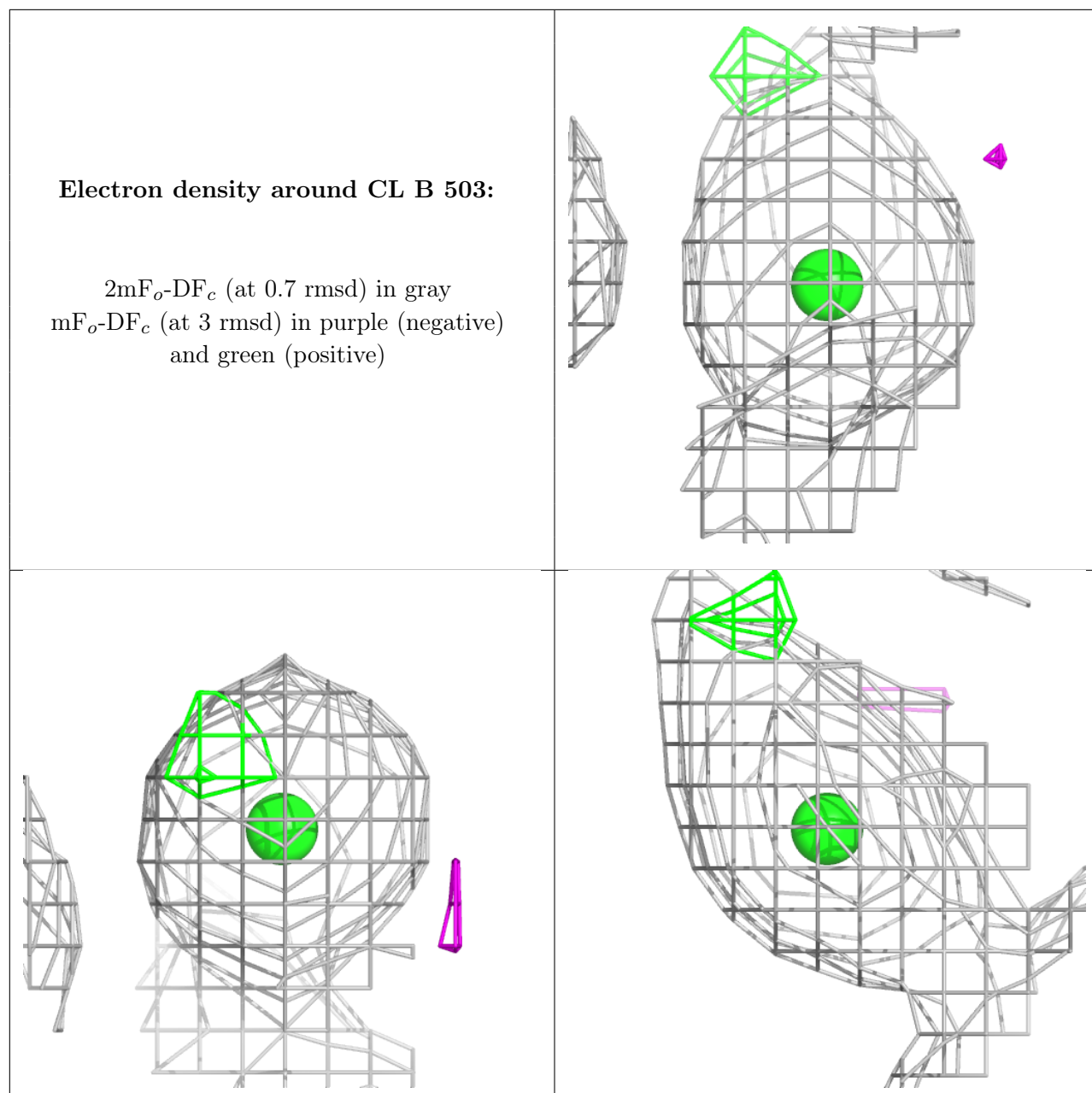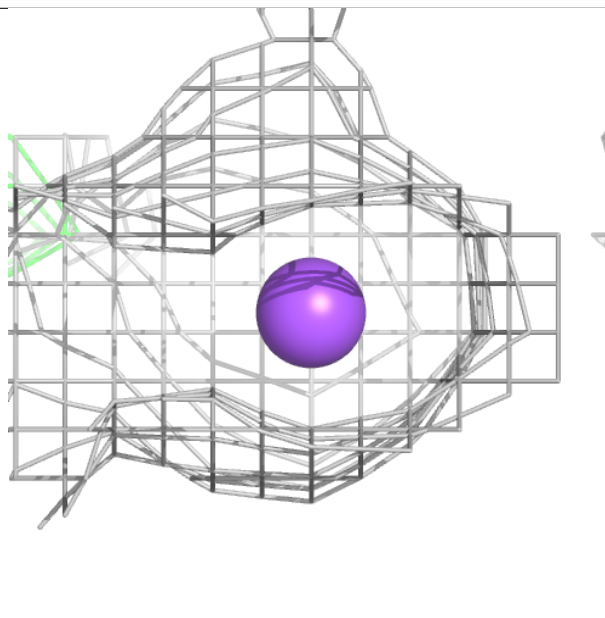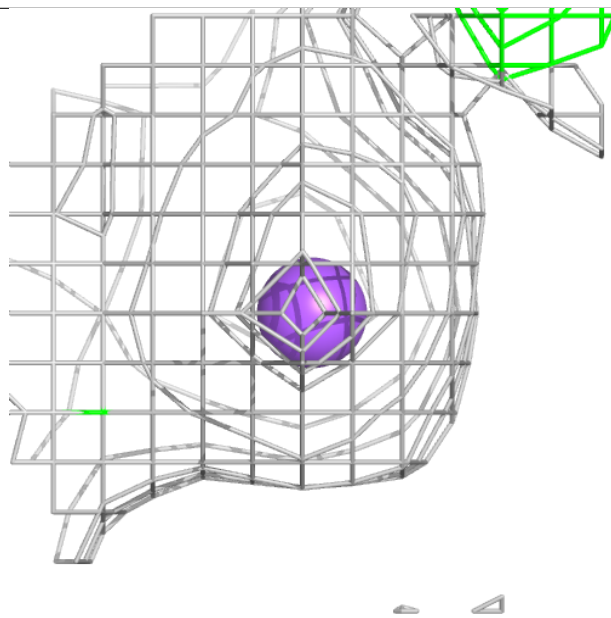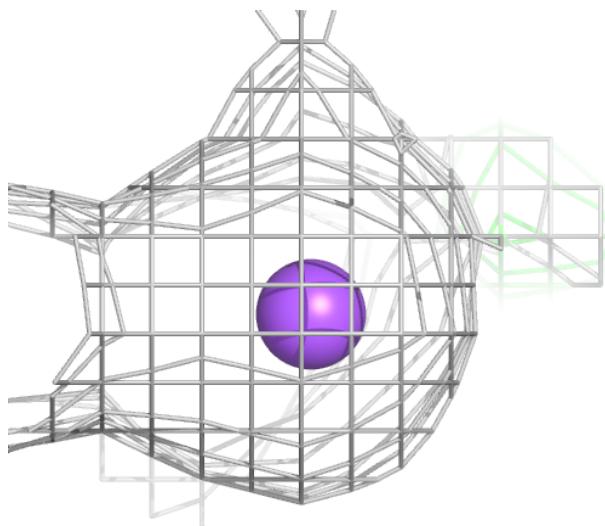and green (positive)
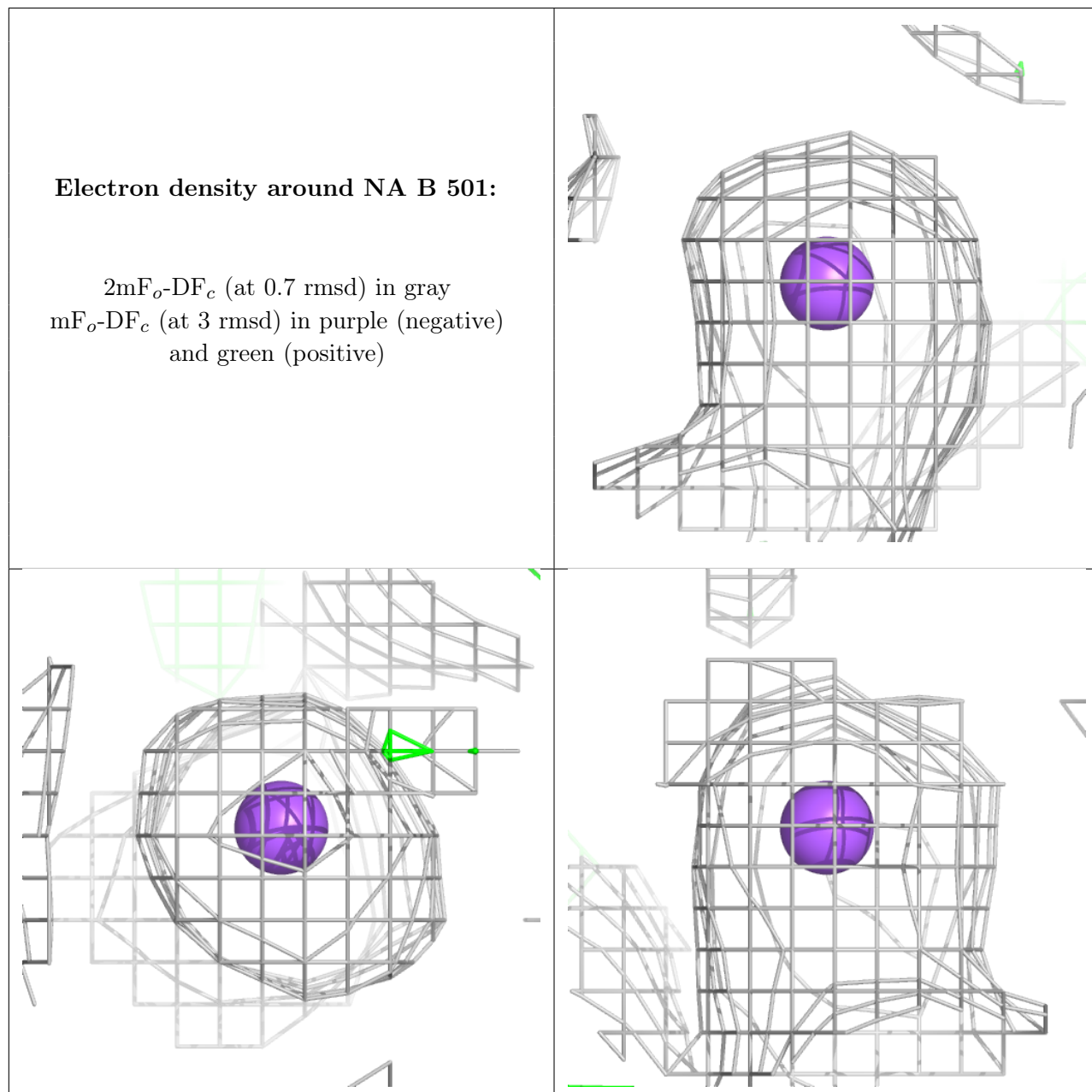
Electron density around NA A 501:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
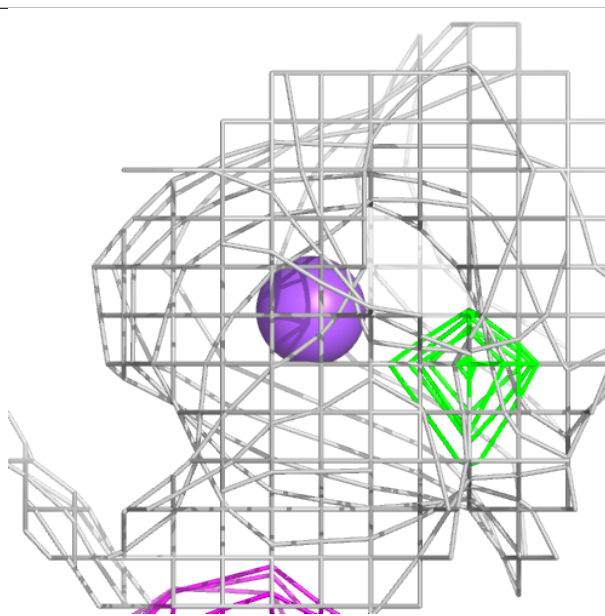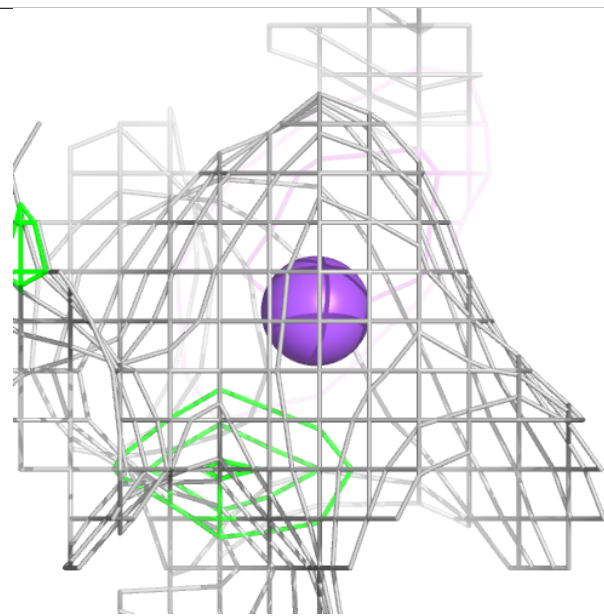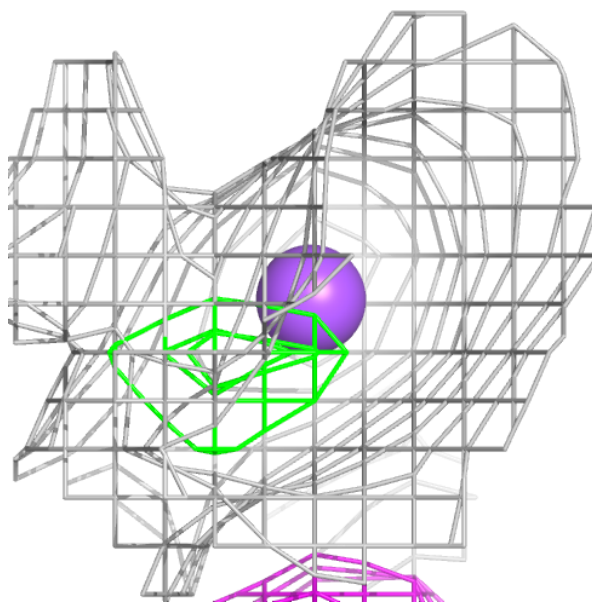
Electron density around CL A 503:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
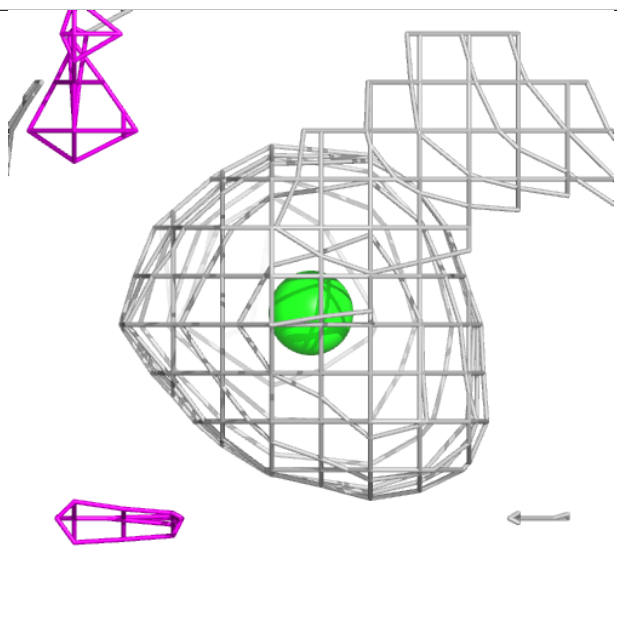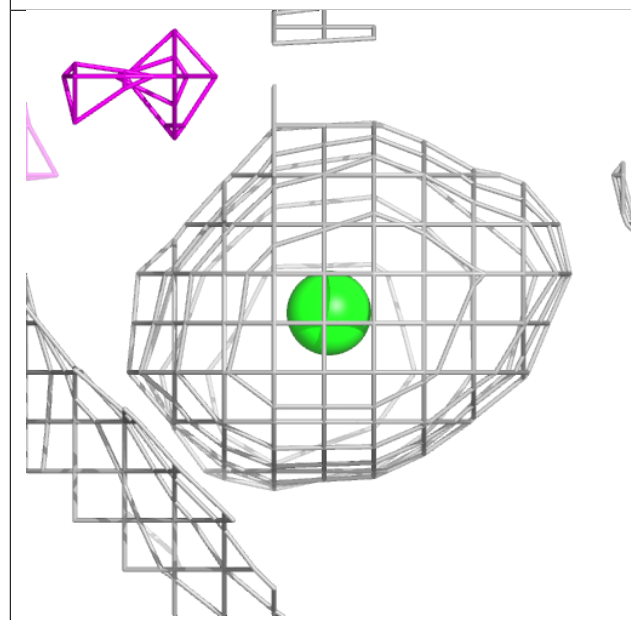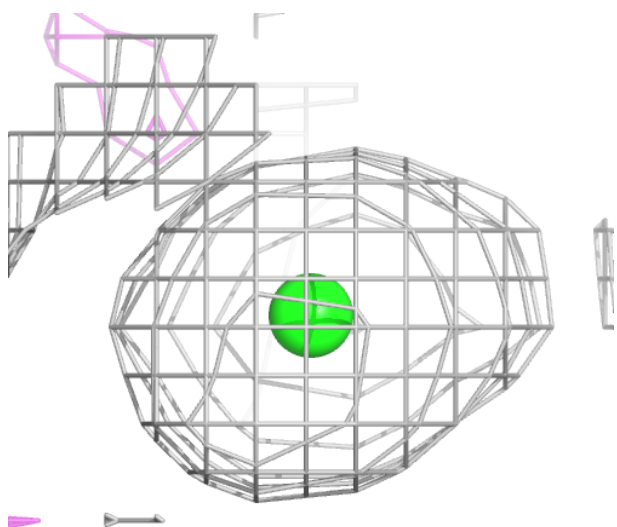
Electron density around CL A 504:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
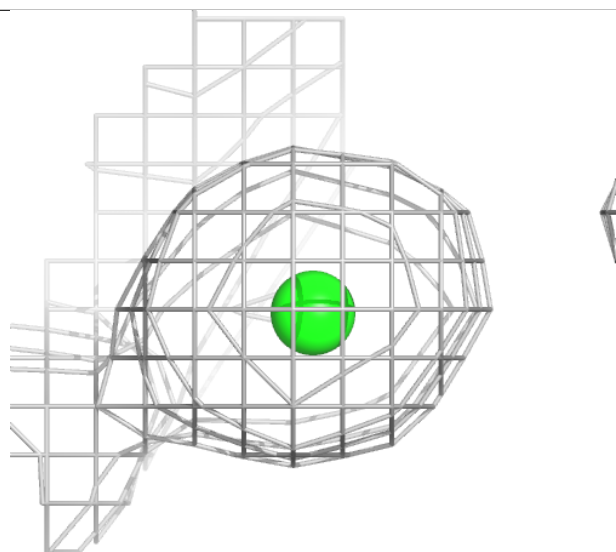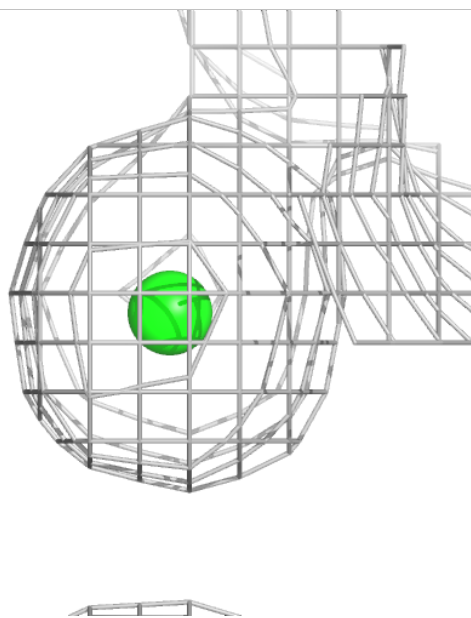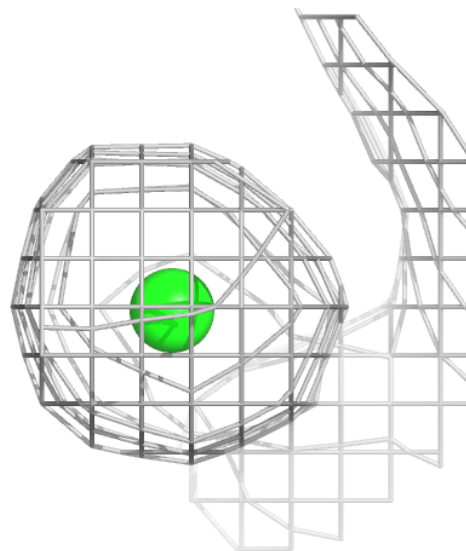
Electron density around CL A 505:

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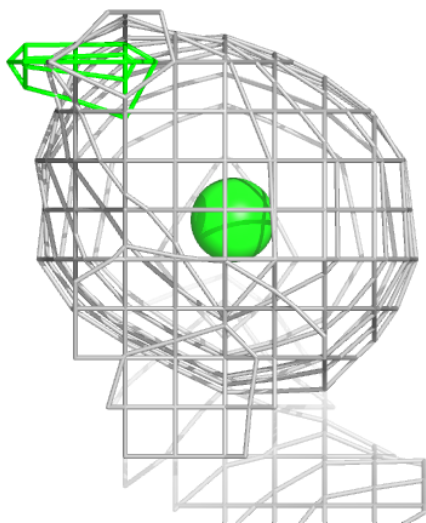$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around CL B 503:

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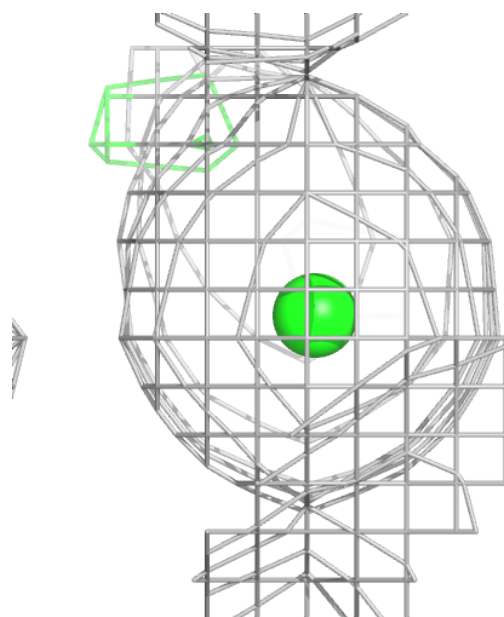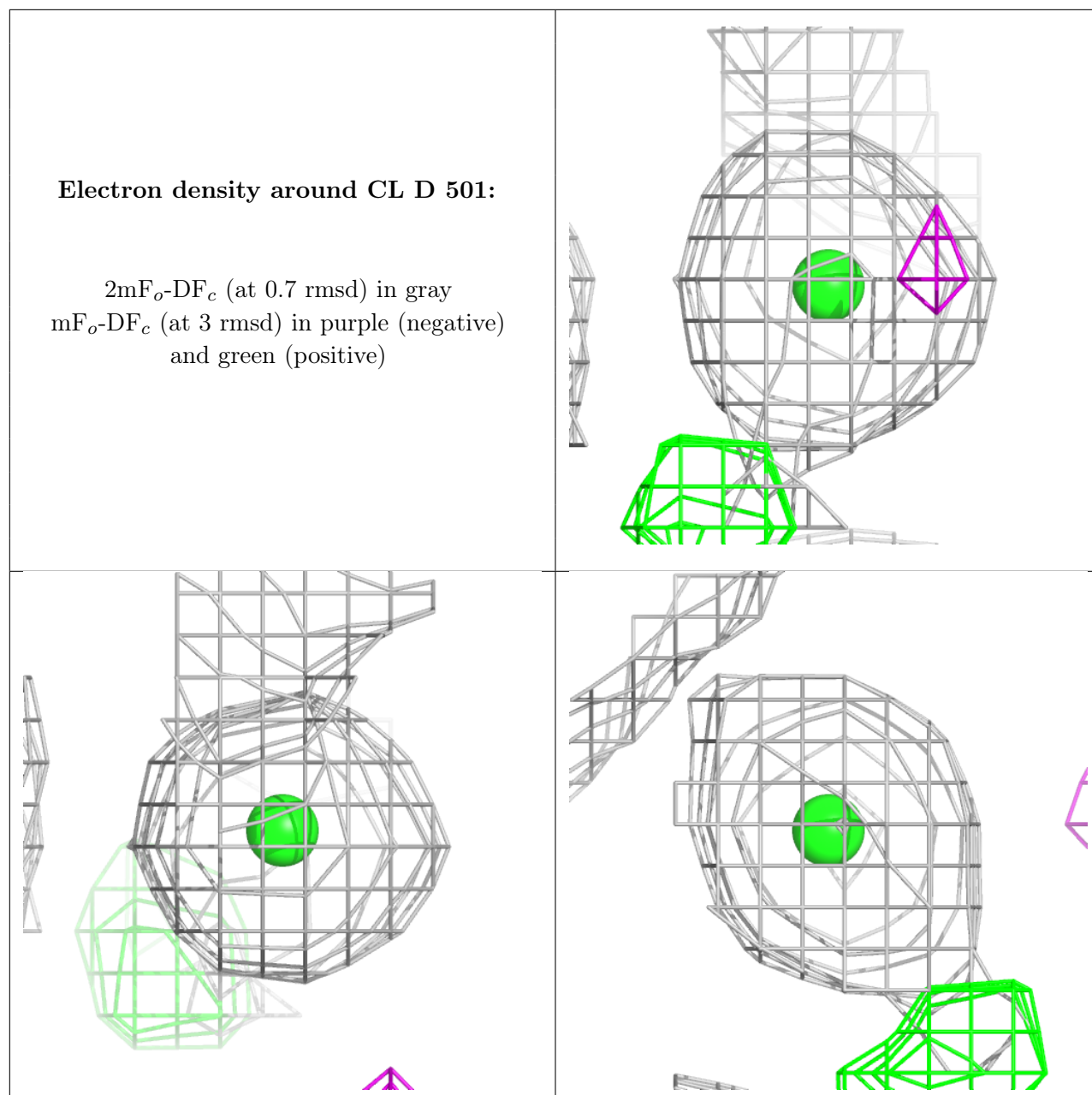and green (positive)

Electron density around NA B 502:

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

Electron density around CL C 501:

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

Electron density around CL D 501:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.