



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2023 – 06:03 PM EDT

PDB ID : 8TYS
Title : Adaptive mechanism of collagen IV scaffold assembly in Drosophila: crystal structure of tissue-extracted NC1 hexamer
Authors : Boudko, S.P.
Deposited on : 2023-08-25
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
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

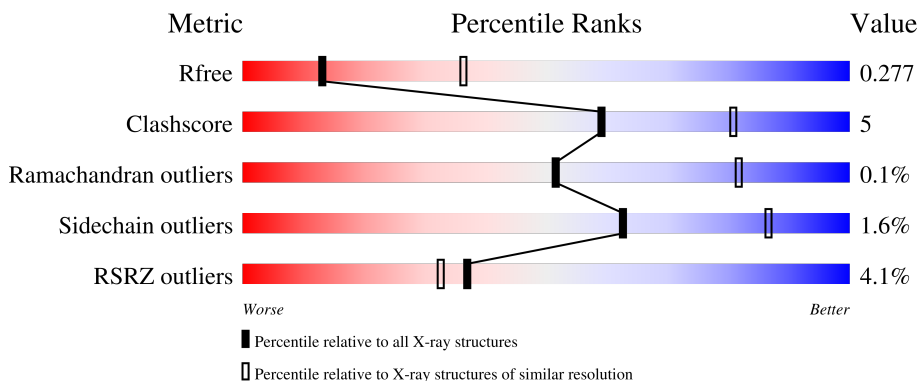
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	230	
1	C	230	
1	D	230	
1	F	230	
2	B	230	

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Mol	Chain	Length	Quality of chain
2	E	230	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a small red segment on the left labeled '2%', a large green segment in the middle labeled '86%', and a small yellow segment on the right labeled '12%'. A small grey dot is visible at the far right end of the bar.</p>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10472 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 Collagen alpha-1(IV) chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	223	Total 1719	C 1071	N 300	O 330	S 18	0	0	0
1	C	226	Total 1739	C 1087	N 301	O 333	S 18	0	0	0
1	D	226	Total 1740	C 1084	N 303	O 335	S 18	0	0	0
1	F	226	Total 1746	C 1090	N 303	O 335	S 18	0	0	0

- Molecule 2 is a protein called Collagen IV, chain Viking.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	226	Total 1763	C 1096	N 311	O 333	S 23	0	0	0
2	E	225	Total 1759	C 1094	N 310	O 332	S 23	0	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	1	Total 1 Cl 1	0	0
3	C	1	Total 1 Cl 1	0	0
3	D	1	Total 1 Cl 1	0	0
3	F	1	Total 1 Cl 1	0	0

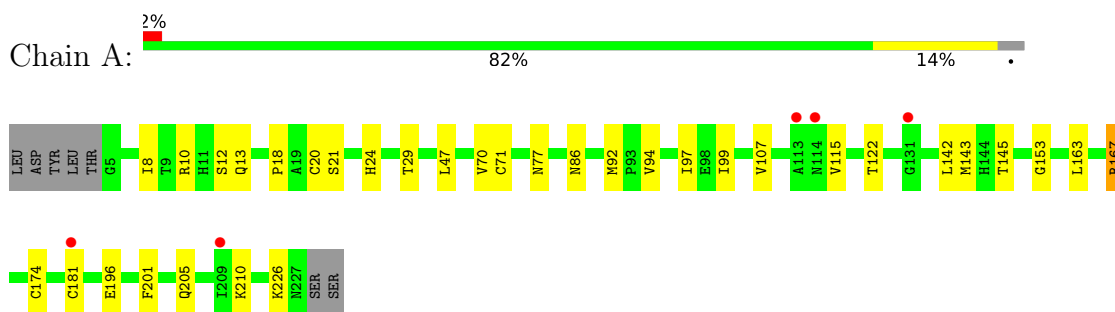
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total 1	Ca 1	0	0
4	F	1	Total 1	Ca 1	0	0

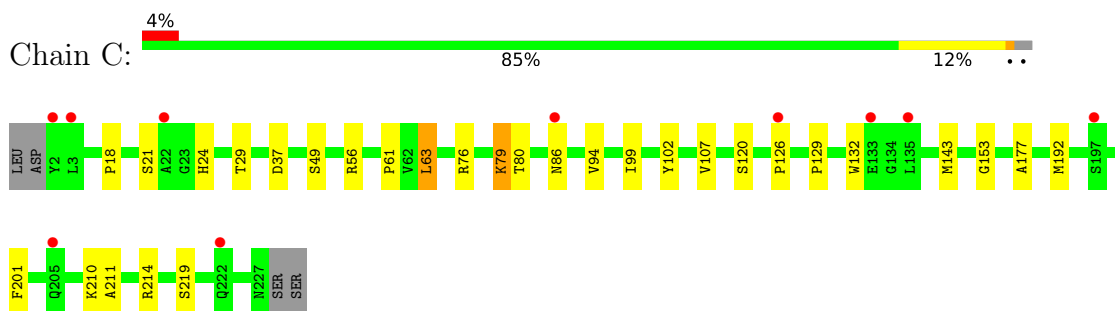
3 Residue-property plots [i](#)

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.

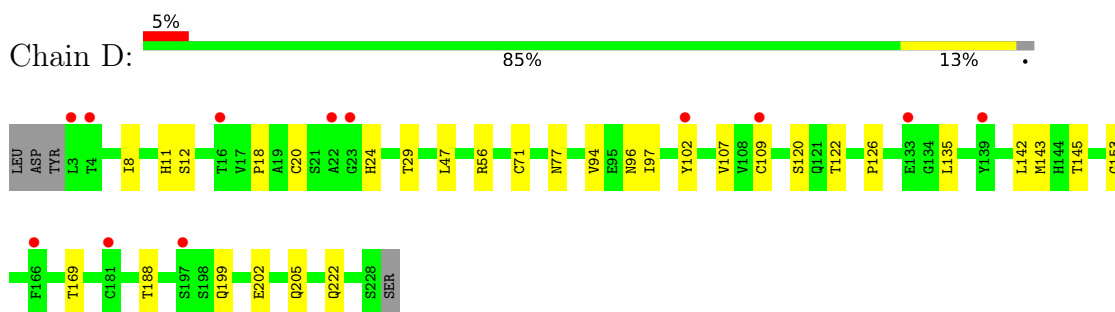
- Molecule 1: Collagen alpha-1(IV) chain



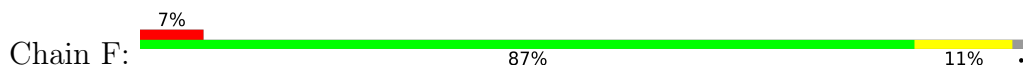
- Molecule 1: Collagen alpha-1(IV) chain

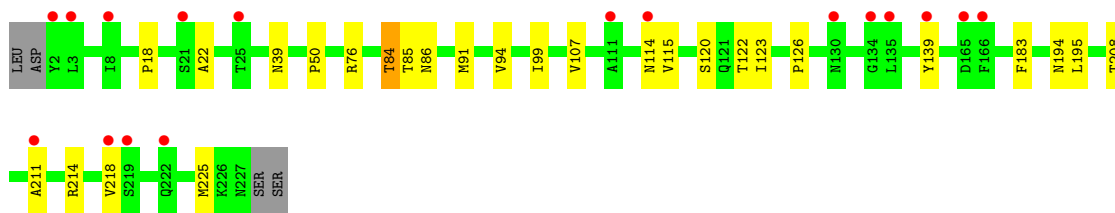


- Molecule 1: Collagen alpha-1(IV) chain

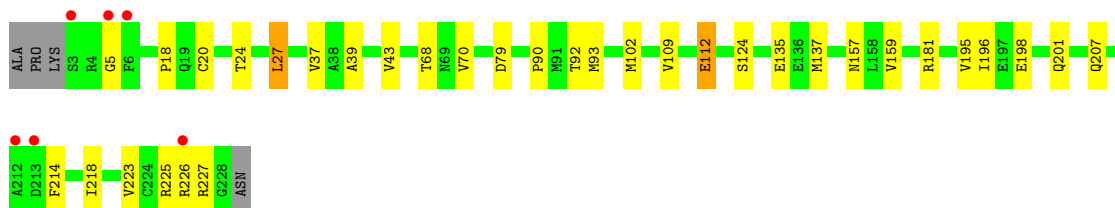
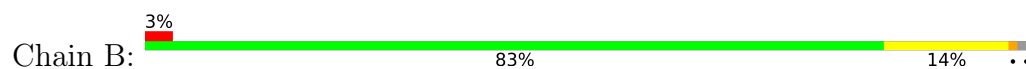


- Molecule 1: Collagen alpha-1(IV) chain

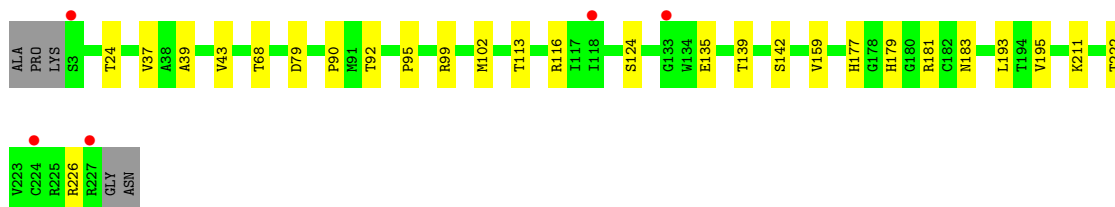
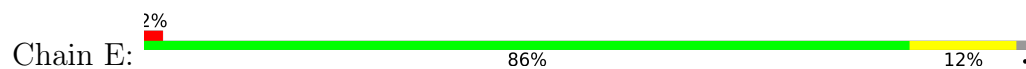




- Molecule 2: Collagen IV, chain Viking



- Molecule 2: Collagen IV, chain Viking



4 Data and refinement statistics i

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	145.21Å 145.21Å 106.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.63 – 2.90 40.63 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.63-2.90) 100.0 (40.63-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.54 (at 2.90Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.241 , 0.277 0.240 , 0.277	Depositor DCC
R_{free} test set	1335 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	76.6	Xtrriage
Anisotropy	0.085	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.045 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10472	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.24	0/1764	0.50	0/2402
1	C	0.24	0/1785	0.48	0/2432
1	D	0.24	0/1785	0.50	0/2431
1	F	0.24	0/1792	0.48	0/2441
2	B	0.24	0/1805	0.51	0/2448
2	E	0.24	0/1801	0.52	0/2443
All	All	0.24	0/10732	0.50	0/14597

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	A	1719	0	1611	28	0
1	C	1739	0	1628	18	0
1	D	1740	0	1634	21	0
1	F	1746	0	1638	18	0
2	B	1763	0	1675	21	0
2	E	1759	0	1672	15	0
3	A	1	0	0	0	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	1	0	0	0	0
3	F	1	0	0	0	0
4	C	1	0	0	0	0
4	F	1	0	0	0	0
All	All	10472	0	9858	96	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.

All (96) 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:D:199:GLN:HB2	1:D:202:GLU:HG3	1.65	0.77
1:F:94:VAL:HG23	1:F:99:ILE:HG22	1.72	0.72
2:B:93:MET:SD	2:E:211:LYS:NZ	2.67	0.67
2:B:198:GLU:OE1	2:B:201:GLN:NE2	2.29	0.65
2:E:24:THR:HG22	2:E:113:THR:HB	1.79	0.65
2:B:124:SER:HA	2:B:195:VAL:HG13	1.83	0.61
2:B:20:CYS:HB3	2:B:24:THR:HG23	1.83	0.61
1:A:13:GLN:O	1:A:167:ARG:NH2	2.35	0.59
2:E:37:VAL:HB	2:E:79:ASP:HB2	1.84	0.59
2:B:27:LEU:HD11	2:B:112:GLU:HB3	1.85	0.58
1:D:56:ARG:NH2	1:F:195:LEU:O	2.35	0.58
1:C:143:MET:HA	1:C:153:GLY:HA2	1.87	0.57
1:A:122:THR:HG23	1:A:196:GLU:HB3	1.86	0.57
1:D:29:THR:HG22	1:D:107:VAL:HG23	1.88	0.56
2:B:137:MET:HB2	2:B:223:VAL:HG23	1.88	0.56
1:D:120:SER:OG	1:D:122:THR:OG1	2.24	0.56
1:A:18:PRO:HG2	1:A:107:VAL:HG12	1.88	0.55
1:A:70:VAL:HG22	1:C:210:LYS:HG2	1.89	0.54
2:B:181:ARG:NH2	1:F:76:ARG:O	2.35	0.54
2:B:135:GLU:OE2	2:B:227:ARG:NH2	2.41	0.53
1:A:77:ASN:HB2	1:D:77:ASN:HB2	1.91	0.53
1:F:115:VAL:HG22	1:F:225:MET:HB2	1.91	0.52
2:E:90:PRO:HB2	2:E:92:THR:HG22	1.91	0.52
2:B:137:MET:HE2	2:B:225:ARG:HD2	1.92	0.52
1:A:20:CYS:HB3	1:A:24:HIS:HB2	1.90	0.52
1:A:12:SER:HB3	1:A:18:PRO:HD3	1.93	0.51
1:A:8:ILE:HG12	1:A:115:VAL:HG11	1.93	0.51
1:D:20:CYS:HB3	1:D:24:HIS:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:THR:HG22	1:A:107:VAL:HG23	1.92	0.50
2:E:124:SER:HA	2:E:195:VAL:HG13	1.94	0.49
1:F:120:SER:HB3	1:F:126:PRO:HB3	1.94	0.49
1:A:97:ILE:HD13	1:C:201:PHE:HB2	1.94	0.49
2:B:37:VAL:HB	2:B:79:ASP:HB2	1.93	0.49
1:D:12:SER:HB3	1:D:18:PRO:HD3	1.96	0.48
2:B:18:PRO:HG2	2:B:109:VAL:HG22	1.96	0.48
1:C:21:SER:HB3	1:C:24:HIS:CE1	2.49	0.48
1:A:210:LYS:NZ	1:F:91:MET:HB3	2.29	0.47
1:C:94:VAL:HG23	1:C:99:ILE:HG12	1.96	0.47
1:A:153:GLY:HA3	2:B:43:VAL:HG11	1.96	0.47
1:C:120:SER:HB3	1:C:126:PRO:HB3	1.96	0.47
1:D:126:PRO:O	1:D:222:GLN:NE2	2.46	0.46
1:A:174:CYS:HA	1:A:181:CYS:HA	1.98	0.46
1:D:199:GLN:HB3	2:E:99:ARG:HH22	1.81	0.46
1:A:86:ASN:HB3	1:A:167:ARG:NH1	2.30	0.46
1:A:71:CYS:SG	1:C:214:ARG:HD2	2.55	0.46
1:F:211:ALA:HA	1:F:214:ARG:NH1	2.30	0.46
1:F:39:ASN:OD1	1:F:76:ARG:NH1	2.46	0.46
1:A:94:VAL:HG22	1:A:99:ILE:HG22	1.98	0.45
1:D:96:ASN:HB3	1:D:97:ILE:HD12	1.98	0.45
1:A:13:GLN:HB3	1:A:167:ARG:HH21	1.81	0.45
1:A:226:LYS:NZ	2:B:112:GLU:OE2	2.42	0.45
1:A:210:LYS:HG2	2:B:70:VAL:HG12	1.98	0.45
1:C:129:PRO:HB2	1:C:132:TRP:CD1	2.52	0.45
2:E:139:THR:HG22	2:E:222:THR:HG23	1.98	0.45
1:A:10:ARG:HH22	1:A:21:SER:HG	1.62	0.45
1:A:13:GLN:HB3	1:A:167:ARG:NH2	2.32	0.44
1:F:84:THR:HG22	1:F:85:THR:H	1.82	0.44
2:E:159:VAL:HG21	1:F:50:PRO:HG2	2.00	0.44
1:C:61:PRO:HD2	1:C:80:THR:HG21	2.00	0.44
1:D:142:LEU:HG	1:D:143:MET:HG3	1.99	0.44
2:E:116:ARG:NH2	1:F:114:ASN:OD1	2.51	0.44
1:F:122:THR:HA	1:F:194:ASN:OD1	2.17	0.44
1:D:153:GLY:HA3	2:E:43:VAL:HG11	2.00	0.43
1:A:47:LEU:HD23	1:A:163:LEU:HD21	1.99	0.43
2:B:90:PRO:HB2	2:B:92:THR:HG22	1.99	0.43
1:D:205:GLN:O	1:D:205:GLN:HG2	2.18	0.43
1:D:145:THR:OG1	1:D:188:THR:OG1	2.36	0.43
2:B:196:ILE:O	1:C:56:ARG:HD3	2.19	0.43
1:D:135:LEU:HD23	1:D:135:LEU:HA	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:ILE:HG23	1:D:109:CYS:HB2	2.00	0.42
2:E:142:SER:HB2	2:E:193:LEU:HB2	2.01	0.42
1:D:18:PRO:HG2	1:D:107:VAL:HG12	2.01	0.42
1:F:84:THR:HG21	1:F:183:PHE:HZ	1.84	0.42
1:D:11:HIS:NE2	1:D:47:LEU:O	2.51	0.42
1:A:145:THR:HG21	2:B:39:ALA:HB3	2.02	0.42
2:B:218:ILE:HD13	1:C:63:LEU:HD21	2.01	0.42
1:C:76:ARG:HA	2:E:177:HIS:CE1	2.55	0.42
1:F:139:TYR:HB3	1:F:218:VAL:HG11	2.01	0.42
1:C:192:MET:HB2	1:C:219:SER:HB3	2.02	0.42
1:D:145:THR:HG21	2:E:39:ALA:HB3	2.02	0.42
2:B:157:ASN:OD1	2:B:159:VAL:HG12	2.19	0.41
1:C:177:ALA:HB3	2:E:179:HIS:CE1	2.55	0.41
1:C:37:ASP:HB3	1:C:79:LYS:HG2	2.01	0.41
1:A:205:GLN:OE1	1:A:205:GLN:N	2.38	0.41
1:A:142:LEU:HG	1:A:143:MET:HG3	2.02	0.41
1:F:123:ILE:HG23	1:F:194:ASN:ND2	2.35	0.41
1:A:92:MET:HG2	1:F:208:THR:OG1	2.21	0.41
1:C:29:THR:HG22	1:C:107:VAL:HG23	2.03	0.41
1:D:71:CYS:SG	1:F:214:ARG:HD2	2.61	0.41
1:A:226:LYS:HD2	2:B:5:GLY:HA3	2.02	0.41
1:F:18:PRO:HG2	1:F:107:VAL:HG12	2.02	0.40
1:D:94:VAL:HG11	1:D:102:TYR:HE2	1.87	0.40
1:C:18:PRO:HG2	1:C:107:VAL:HG12	2.03	0.40
2:E:95:PRO:HA	2:E:183:ASN:HB2	2.02	0.40
1:A:201:PHE:CE2	2:B:102:MET:HG2	2.57	0.40
1:C:94:VAL:HG11	1:C:102:TYR:CE2	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	A	221/230 (96%)	209 (95%)	12 (5%)	0	100	100
1	C	224/230 (97%)	212 (95%)	11 (5%)	1 (0%)	34	66
1	D	224/230 (97%)	210 (94%)	14 (6%)	0	100	100
1	F	224/230 (97%)	212 (95%)	11 (5%)	1 (0%)	34	66
2	B	224/230 (97%)	218 (97%)	6 (3%)	0	100	100
2	E	223/230 (97%)	219 (98%)	4 (2%)	0	100	100
All	All	1340/1380 (97%)	1280 (96%)	58 (4%)	2 (0%)	51	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	211	ALA
1	F	22	ALA

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	A	190/197 (96%)	189 (100%)	1 (0%)	88	96
1	C	191/197 (97%)	187 (98%)	4 (2%)	53	81
1	D	193/197 (98%)	192 (100%)	1 (0%)	88	96
1	F	193/197 (98%)	191 (99%)	2 (1%)	76	92
2	B	197/200 (98%)	191 (97%)	6 (3%)	41	75
2	E	197/200 (98%)	192 (98%)	5 (2%)	47	78
All	All	1161/1188 (98%)	1142 (98%)	19 (2%)	62	86

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	ARG
2	B	27	LEU
2	B	68	THR

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Mol	Chain	Res	Type
2	B	112	GLU
2	B	207	GLN
2	B	214	PHE
2	B	226	ARG
1	C	49	SER
1	C	63	LEU
1	C	79	LYS
1	C	86	ASN
1	D	169	THR
2	E	68	THR
2	E	102	MET
2	E	135	GLU
2	E	181	ARG
2	E	226	ARG
1	F	84	THR
1	F	86	ASN

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 6 ligands modelled in this entry, 6 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 [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

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(Å ²)	Q<0.9
1	A	223/230 (96%)	0.32	5 (2%) 62 59	51, 80, 102, 120	0
1	C	226/230 (98%)	0.27	10 (4%) 34 30	45, 81, 104, 118	0
1	D	226/230 (98%)	0.47	12 (5%) 26 22	54, 89, 114, 124	0
1	F	226/230 (98%)	0.48	17 (7%) 14 11	43, 82, 119, 137	0
2	B	226/230 (98%)	0.07	6 (2%) 54 50	41, 63, 95, 111	0
2	E	225/230 (97%)	0.11	5 (2%) 62 59	47, 70, 102, 116	0
All	All	1352/1380 (97%)	0.29	55 (4%) 37 32	41, 77, 110, 137	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	130	ASN	4.6
1	F	211	ALA	4.1
1	F	25	THR	3.9
2	B	213	ASP	3.9
1	D	181	CYS	3.5
1	F	218	VAL	3.5
1	D	139	TYR	3.5
1	A	113	ALA	3.3
1	C	197	SER	3.2
2	E	224	CYS	3.2
1	D	23	GLY	3.2
2	B	212	ALA	3.2
1	C	126	PRO	3.1
1	C	135	LEU	3.1
2	B	3	SER	3.0
1	D	133	GLU	3.0
1	C	86	ASN	3.0
2	B	226	ARG	3.0
1	F	8	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	2	TYR	2.9
1	D	102	TYR	2.9
1	D	166	PHE	2.8
1	F	3	LEU	2.8
1	D	197	SER	2.8
1	F	114	ASN	2.7
1	F	166	PHE	2.7
1	F	222	GLN	2.7
1	D	16	THR	2.7
1	C	22	ALA	2.7
1	D	3	LEU	2.6
1	F	135	LEU	2.6
2	B	6	PHE	2.6
1	C	222	GLN	2.6
1	F	111	ALA	2.6
1	C	205	GLN	2.5
2	E	227	ARG	2.5
1	F	21	SER	2.5
1	A	209	ILE	2.5
1	F	165	ASP	2.4
1	C	2	TYR	2.4
2	E	133	GLY	2.4
1	C	3	LEU	2.4
1	D	22	ALA	2.4
1	F	134	GLY	2.3
1	F	219	SER	2.3
1	C	133	GLU	2.3
2	E	118	ILE	2.3
1	A	181	CYS	2.2
1	D	109	CYS	2.2
1	A	131	GLY	2.2
2	E	3	SER	2.1
1	D	4	THR	2.0
1	F	139	TYR	2.0
1	A	114	ASN	2.0
2	B	5	GLY	2.0

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 [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

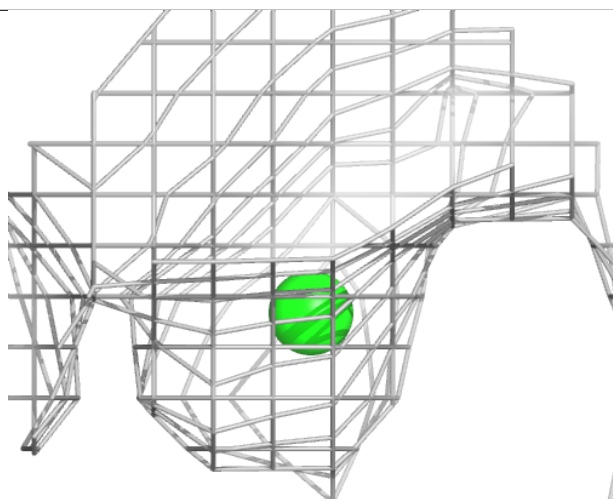
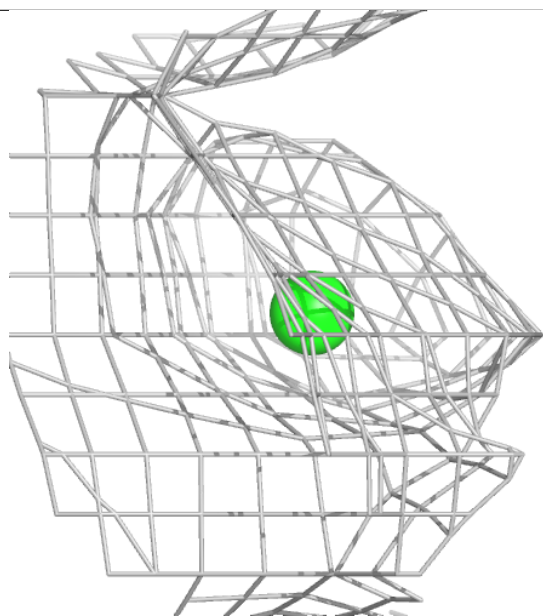
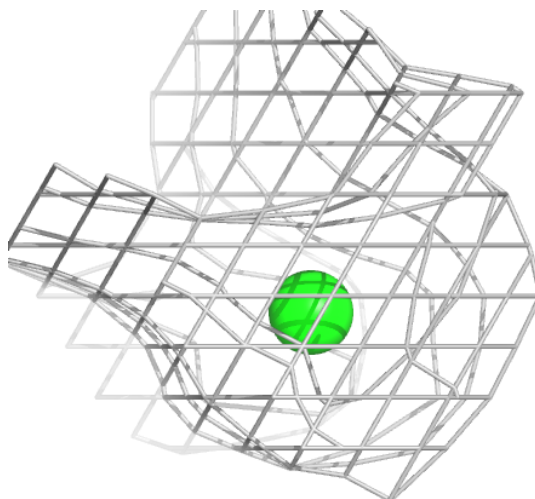
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CL	D	301	1/1	0.77	0.18	85,85,85,85	0
3	CL	A	301	1/1	0.88	0.23	69,69,69,69	0
3	CL	F	301	1/1	0.92	0.15	54,54,54,54	0
3	CL	C	301	1/1	0.94	0.13	57,57,57,57	0
4	CA	F	302	1/1	0.97	0.42	74,74,74,74	0
4	CA	C	302	1/1	0.98	0.24	62,62,62,62	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.

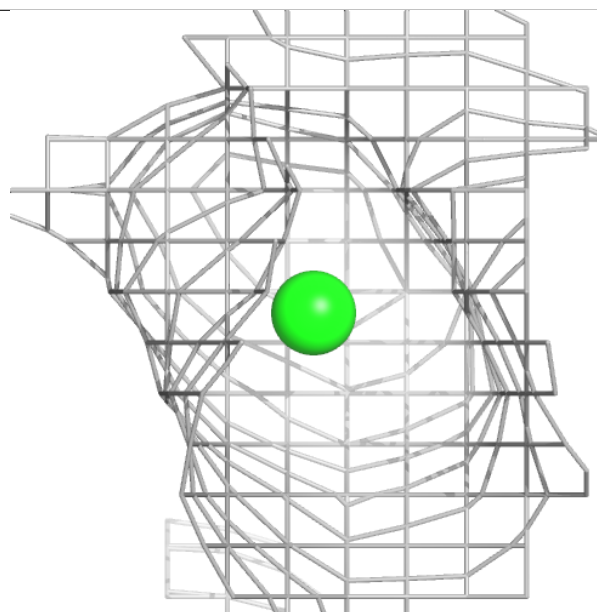
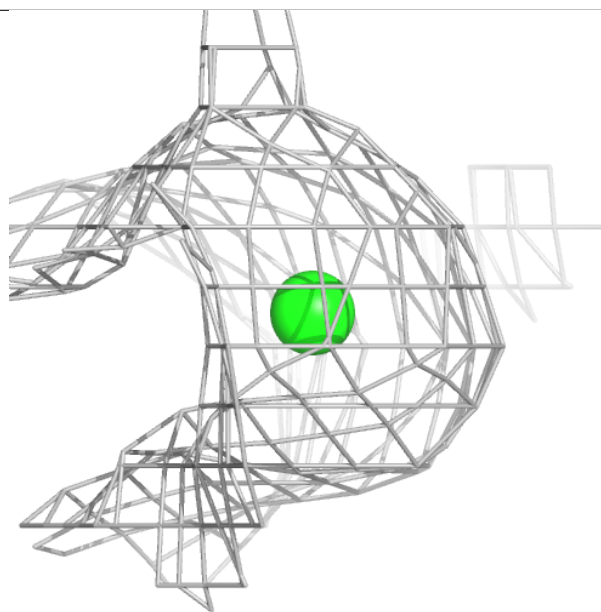
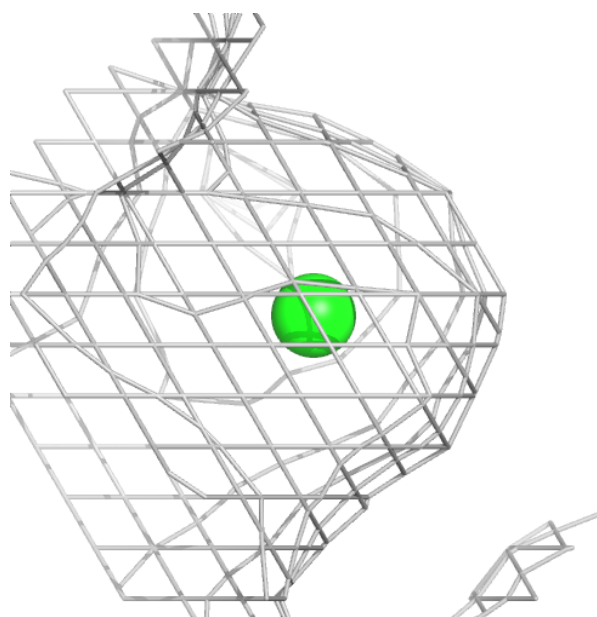
Electron density around CL D 301:

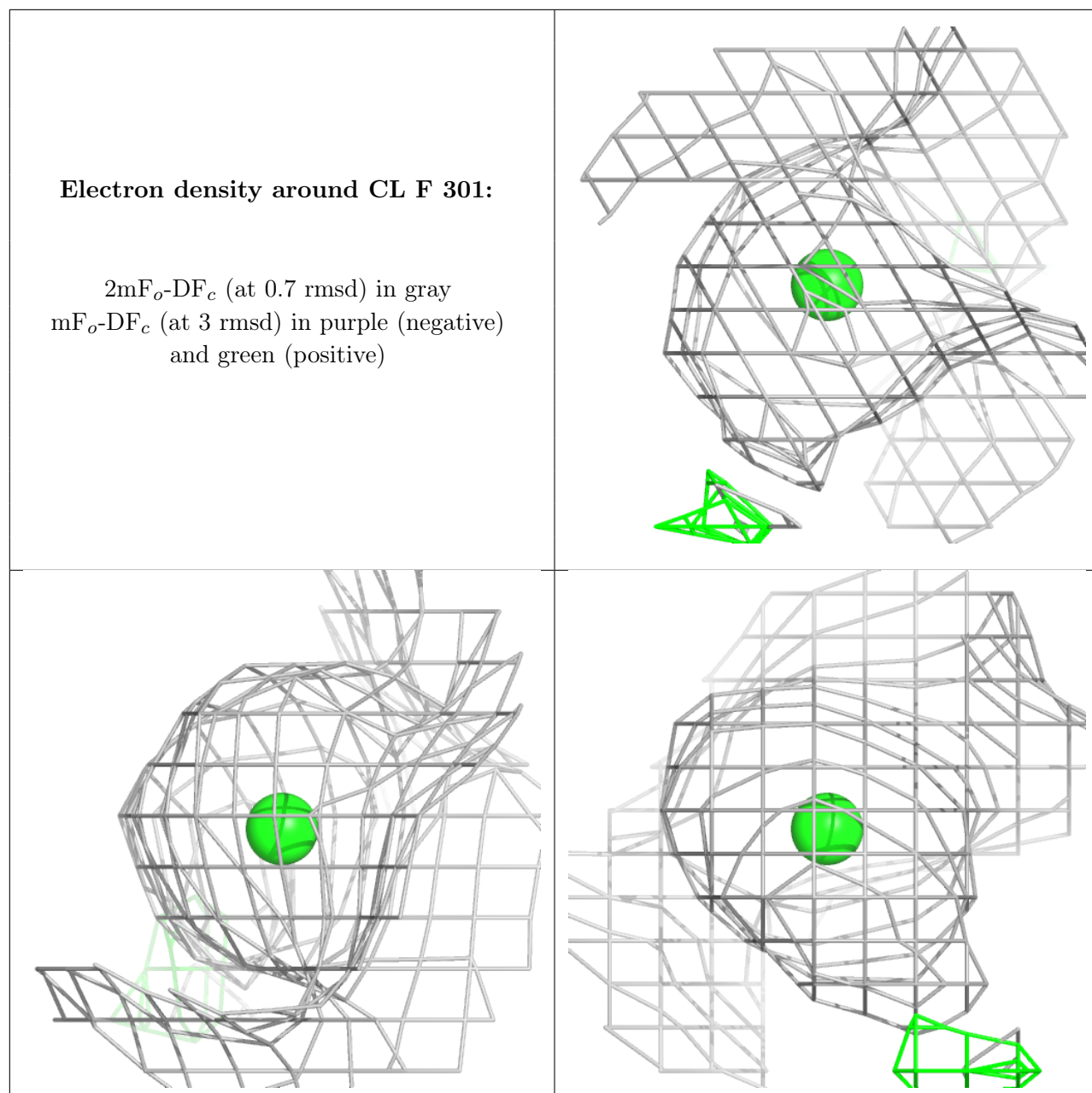
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CL A 301:

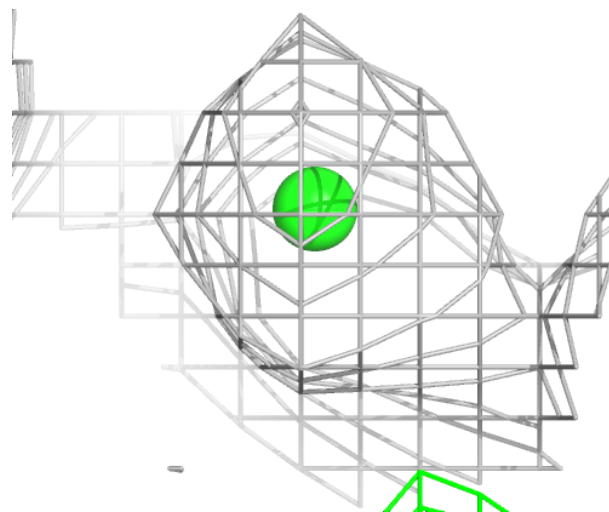
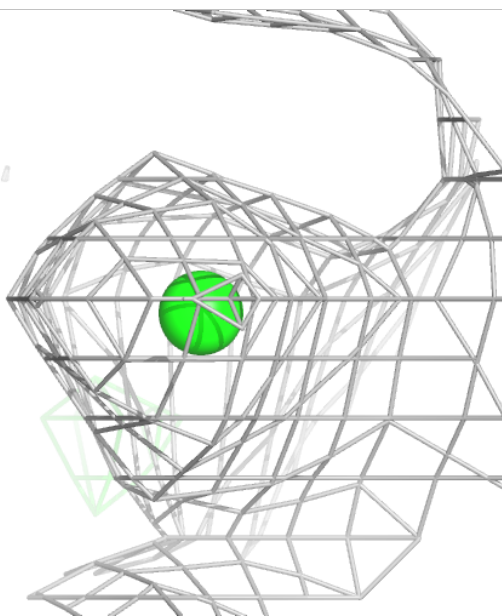
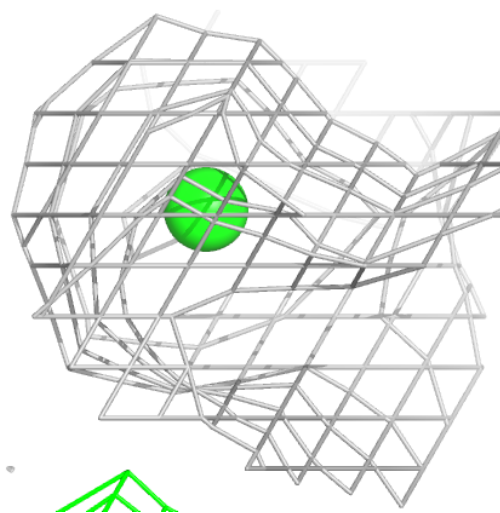
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





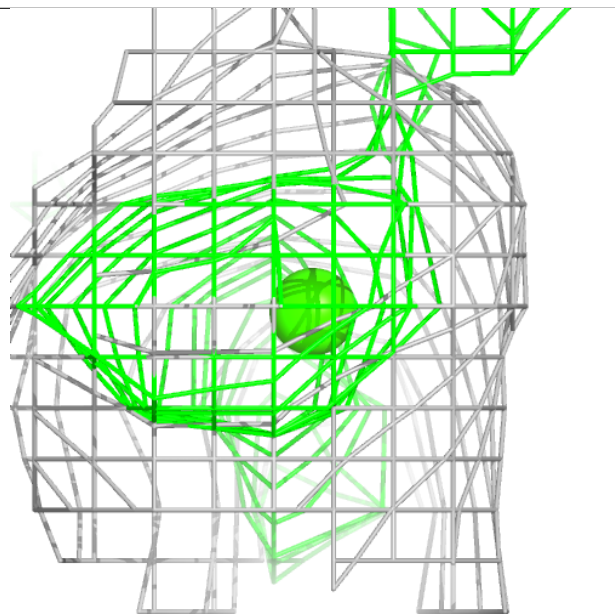
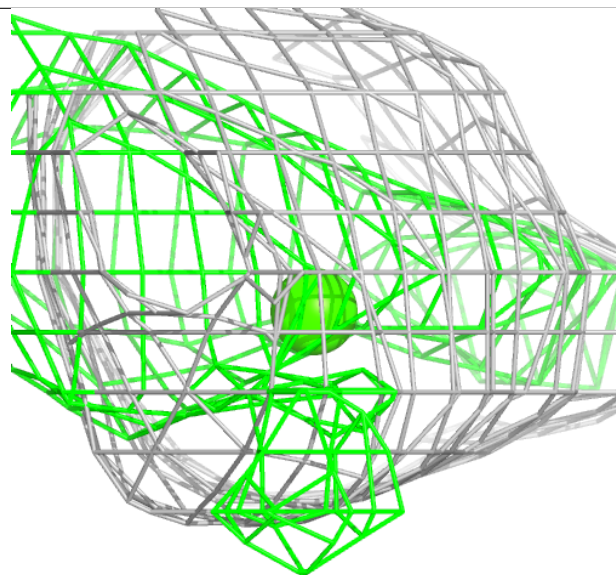
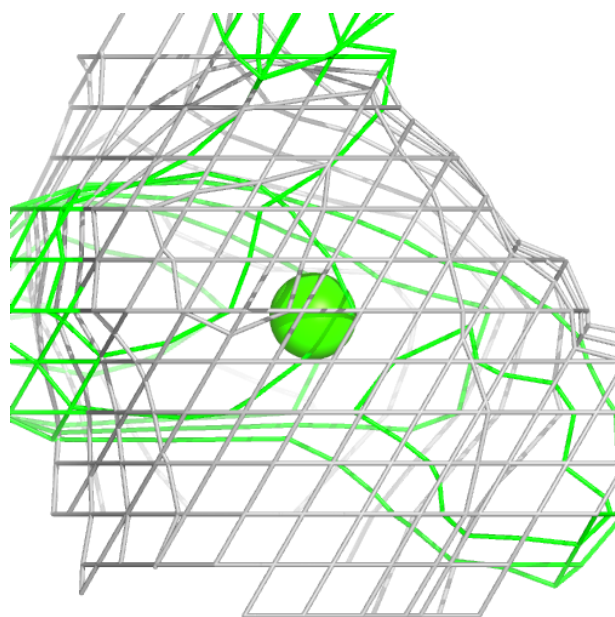
Electron density around CL C 301:

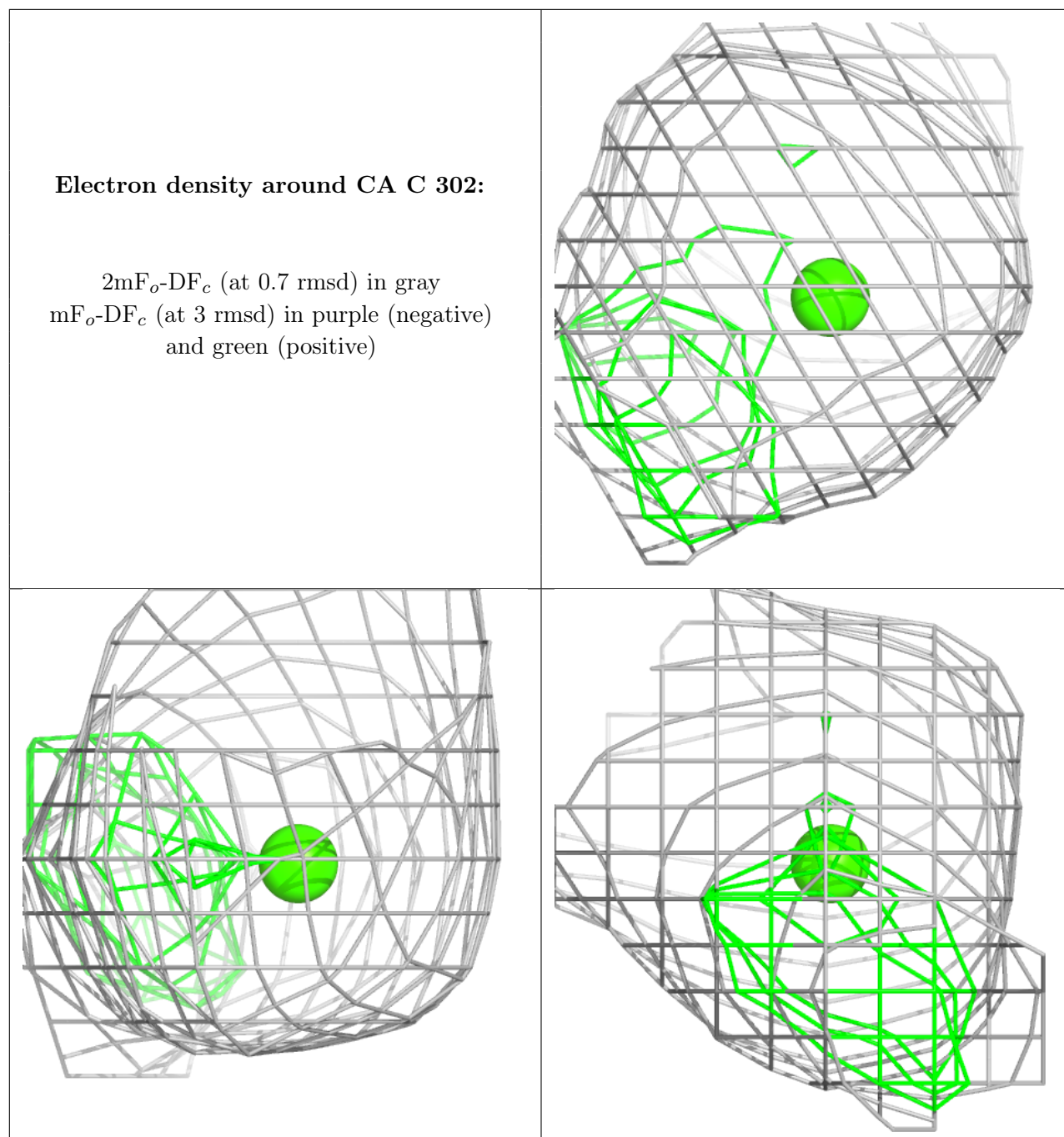
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA F 302:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.