



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:24 PM UTC

PDB ID : 9DYQ / pdb_00009dyq
Title : Crystal structure of human dysferlin C2G domain
Authors : Dominguez, M.J.; Sutton, R.B.
Deposited on : 2024-10-14
Resolution : 2.05 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

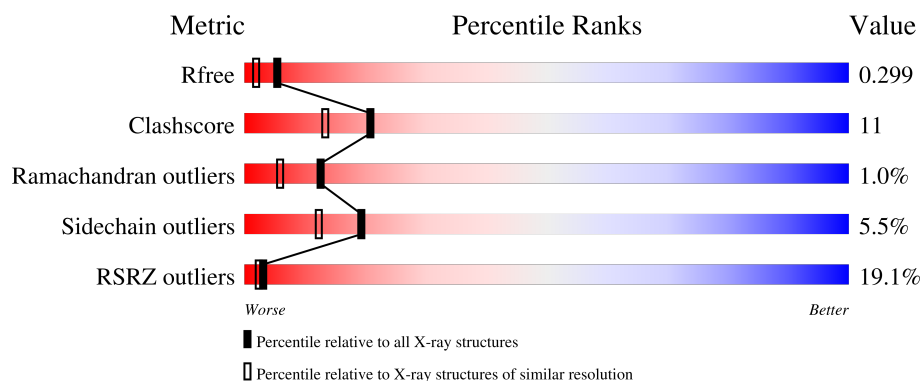
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	200	<div> <div>21%</div> <div>72%</div> <div>22%</div> <div>• •</div> </div>
1	B	200	<div> <div>16%</div> <div>76%</div> <div>19%</div> <div>• •</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6626 atoms, of which 3247 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 Dysferlin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	194	Total	C	H	N	O	S	0	9	0
			3261	1067	1611	274	300	9			
1	B	194	Total	C	H	N	O	S	0	10	0
			3286	1077	1622	277	301	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1802	GLY	-	expression tag	UNP O75923
A	1803	ASP	-	expression tag	UNP O75923
A	1804	ILE	-	expression tag	UNP O75923
A	1805	THR	-	expression tag	UNP O75923
A	1806	HIS	-	expression tag	UNP O75923
A	1807	MET	-	expression tag	UNP O75923
B	1802	GLY	-	expression tag	UNP O75923
B	1803	ASP	-	expression tag	UNP O75923
B	1804	ILE	-	expression tag	UNP O75923
B	1805	THR	-	expression tag	UNP O75923
B	1806	HIS	-	expression tag	UNP O75923
B	1807	MET	-	expression tag	UNP O75923

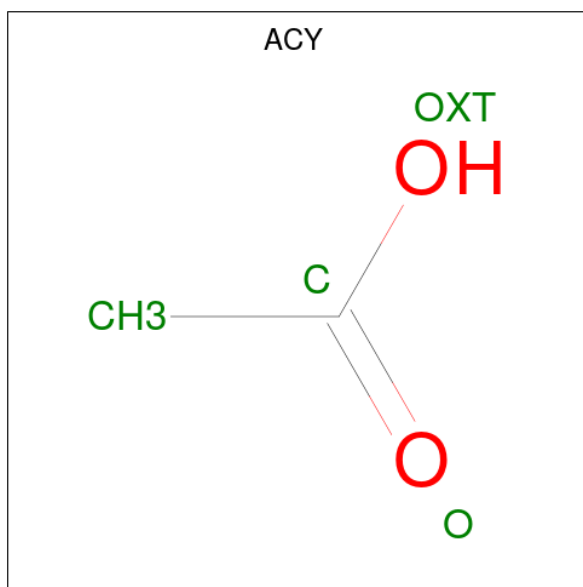
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Ca	0	0
			3	3		
2	B	3	Total	Ca	0	0
			3	3		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	2	Total	Cl	0	0
			2	2		

- Molecule 4 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			7	2	3	2		
4	B	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			14	3	8	3		

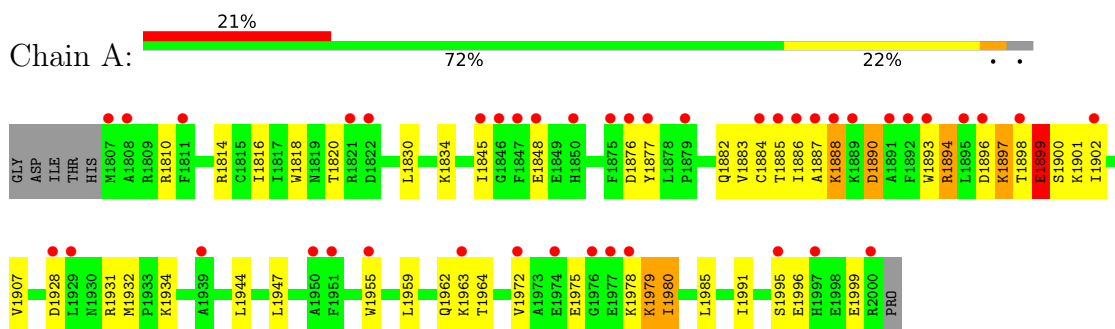
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	21	Total	O	0	0
			21	21		
6	B	21	Total	O	0	0
			21	21		

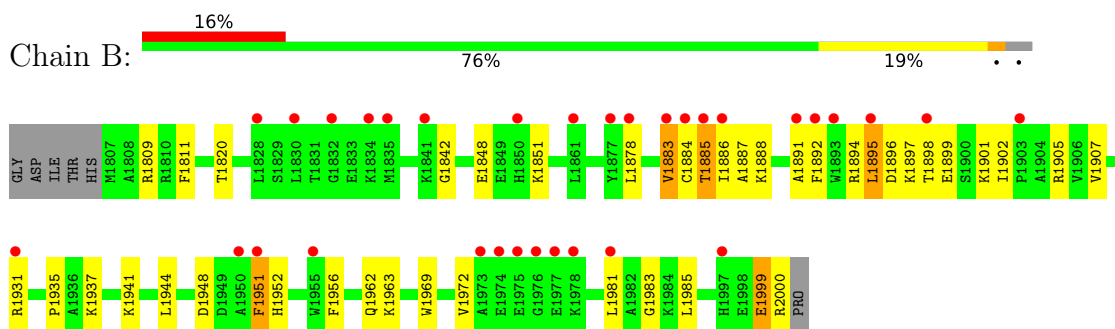
3 Residue-property plots [i](#)

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: Dysferlin



• Molecule 1: Dysferlin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	83.94Å 109.76Å 59.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.04 – 2.05 52.04 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.4 (52.04-2.05) 97.5 (52.04-2.05)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.245 , 0.273 (Not available) , 0.299	Depositor DCC
R_{free} test set	1680 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 61.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6626	wwPDB-VP
Average B, all atoms (Å ²)	89.0	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 45.68 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2771e-04. 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: ACY, CL, CA, GOL

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	0.52	3/1736 (0.2%)	0.78	3/2341 (0.1%)
1	B	0.37	0/1751	0.65	1/2361 (0.0%)
All	All	0.45	3/3487 (0.1%)	0.72	4/4702 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1980[A]	ILE	N-CA	6.03	1.53	1.46
1	A	1980[B]	ILE	N-CA	6.03	1.53	1.46
1	A	1996	GLU	C-O	-5.45	1.18	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1951	PHE	N-CA-CB	-6.81	100.73	110.81
1	A	1975	GLU	N-CA-C	-5.28	101.69	109.62
1	A	1830	LEU	N-CA-C	-5.23	105.58	111.28
1	A	1899	GLU	CB-CG-CD	-5.10	103.93	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1650	1611	1557	41	0
1	B	1664	1622	1569	32	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
4	A	4	3	3	0	0
4	B	4	3	3	0	0
5	A	6	8	8	0	0
6	A	21	0	0	0	0
6	B	21	0	0	1	0
All	All	3379	3247	3140	73	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 11.

All (73) 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:A:1886:ILE:HG13	1:A:1900:SER:HB3	1.59	0.85
1:A:1820:THR:HG22	1:A:1985:LEU:HD12	1.60	0.81
1:B:1948:ASP:OD1	1:B:1951:PHE:HB2	1.84	0.77
1:A:1886:ILE:CG1	1:A:1900:SER:HB3	2.16	0.75
1:B:1820:THR:HG22	1:B:1985:LEU:HD13	1.69	0.73
1:B:1894:ARG:O	1:B:1896:ASP:N	2.20	0.73
1:B:1848[B]:GLU:O	1:B:1851:LYS:HG3	1.95	0.65
1:B:1885:THR:HG22	1:B:1899:GLU:HG3	1.79	0.65
1:B:1820:THR:HG22	1:B:1985:LEU:CD1	2.26	0.64
1:B:1848[A]:GLU:O	1:B:1851:LYS:HG3	1.99	0.63
1:A:1887:ALA:HA	1:A:1896:ASP:HB2	1.80	0.62
1:B:1885:THR:HG22	1:B:1899:GLU:CG	2.30	0.61
1:A:1931:ARG:O	1:A:1931:ARG:HG3	2.00	0.61
1:A:1944:LEU:HD21	1:A:1972:VAL:HG22	1.85	0.59
1:A:1886:ILE:CD1	1:A:1896:ASP:HB3	2.34	0.57
1:A:1814:ARG:CZ	1:A:1816:ILE:HD11	2.34	0.57
1:A:1877[A]:TYR:OH	1:A:1882:GLN:HA	2.04	0.57
1:A:1885:THR:HG23	1:A:1899:GLU:HA	1.87	0.57
1:A:1888:LYS:HB2	1:A:1894:ARG:HG3	1.86	0.56
1:B:1931[A]:ARG:HG3	1:B:1956[A]:PHE:HB3	1.89	0.55
1:A:1845:ILE:HD11	1:A:1907:VAL:CG2	2.37	0.55
1:A:1820:THR:HG22	1:A:1985:LEU:CD1	2.33	0.54
1:A:1887:ALA:HB1	1:A:1894:ARG:HE	1.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1809:ARG:HB3	1:B:1811:PHE:HE1	1.71	0.54
1:A:1928[A]:ASP:O	1:A:1932:MET:HB3	2.09	0.52
1:A:1883:VAL:HG21	1:A:1901:LYS:HB3	1.93	0.51
1:B:1883:VAL:CG2	1:B:1901:LYS:HZ3	2.23	0.51
1:B:1894:ARG:HG2	1:B:1897:LYS:CG	2.41	0.50
1:B:1809:ARG:HB3	1:B:1811:PHE:CE1	2.46	0.50
1:A:1886:ILE:HD12	1:A:1896:ASP:HB3	1.95	0.49
1:A:1810:ARG:NH1	1:A:1876:ASP:OD1	2.47	0.48
1:A:1886:ILE:HD13	1:A:1896:ASP:HB3	1.96	0.48
1:B:1897:LYS:HA	1:B:1897:LYS:HE2	1.96	0.48
1:B:1948:ASP:CG	1:B:1951:PHE:HB2	2.40	0.47
1:A:1887:ALA:HB2	1:A:1896:ASP:O	2.14	0.47
1:A:1816:ILE:HG21	1:A:1818:TRP:CZ2	2.50	0.47
1:A:1877[A]:TYR:CZ	1:A:1882:GLN:HA	2.48	0.47
1:B:1999:GLU:O	1:B:2000:ARG:C	2.58	0.47
1:A:1887:ALA:HB1	1:A:1897:LYS:O	2.16	0.46
1:B:1894:ARG:O	1:B:1895:LEU:C	2.58	0.46
1:B:1951:PHE:C	1:B:1952:HIS:HD2	2.23	0.46
1:B:1842:GLY:HA2	1:B:1907:VAL:O	2.15	0.46
1:A:1899:GLU:OE2	1:A:1901:LYS:HE3	2.16	0.45
1:A:1848[A]:GLU:H	1:A:1848[A]:GLU:CD	2.23	0.45
1:A:1972:VAL:HG13	1:A:1979:LYS:HG3	1.98	0.45
1:B:1944:LEU:HD21	1:B:1972:VAL:HG12	1.98	0.45
1:B:1883:VAL:HG21	1:B:1901:LYS:HZ3	1.82	0.45
1:B:1894:ARG:HG2	1:B:1897:LYS:HG2	1.98	0.44
1:A:1947:LEU:HD23	1:A:1947:LEU:N	2.33	0.44
1:B:1891:ALA:O	1:B:1892:PHE:CB	2.65	0.44
1:B:1887:ALA:HA	1:B:1899:GLU:HA	2.00	0.43
1:B:1935:PRO:HB3	1:B:1969:TRP:CZ2	2.53	0.43
1:B:1884:CYS:N	1:B:1902:ILE:O	2.49	0.43
1:A:1962:GLN:O	1:A:1963[A]:LYS:HB2	2.18	0.43
1:B:1981:LEU:HD13	1:B:1983:GLY:H	1.83	0.43
1:A:1887:ALA:HB1	1:A:1894:ARG:NE	2.32	0.42
1:A:1944:LEU:CD2	1:A:1972:VAL:HG22	2.49	0.42
1:A:1890:ASP:O	1:A:1894:ARG:NH1	2.50	0.42
1:A:1928[A]:ASP:HB3	1:A:1931:ARG:O	2.18	0.42
1:B:1895:LEU:O	1:B:1898:THR:HB	2.20	0.42
1:B:1962:GLN:O	1:B:1963:LYS:HB2	2.20	0.42
1:A:1810:ARG:HH22	1:A:1888:LYS:HD3	1.85	0.42
1:B:1905:ARG:HD2	6:B:2205:HOH:O	2.20	0.42
1:B:1894:ARG:O	1:B:1894:ARG:HG3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1959:LEU:HG	1:A:1991:ILE:HD12	2.02	0.41
1:A:1899:GLU:HB3	1:A:1900:SER:H	1.62	0.41
1:A:1883:VAL:HG11	1:A:1901:LYS:HD3	2.01	0.41
1:A:1897:LYS:HB2	1:A:1898:THR:H	1.48	0.41
1:A:1886:ILE:CG2	1:A:1902:ILE:HD13	2.51	0.41
1:A:1934:LYS:HG3	1:A:1955:TRP:O	2.21	0.41
1:A:1816:ILE:HG21	1:A:1818:TRP:CE2	2.57	0.41
1:B:1894:ARG:HB3	1:B:1897:LYS:HB2	2.02	0.41

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	201/200 (100%)	191 (95%)	7 (4%)	3 (2%)	8	2
1	B	202/200 (101%)	192 (95%)	9 (4%)	1 (0%)	24	16
All	All	403/400 (101%)	383 (95%)	16 (4%)	4 (1%)	12	6

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1888	LYS
1	B	1895	LEU
1	A	1890	ASP
1	A	1897	LYS

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	182/178 (102%)	170 (93%)	12 (7%)	15	9
1	B	183/178 (103%)	174 (95%)	9 (5%)	22	15
All	All	365/356 (102%)	344 (94%)	21 (6%)	19	11

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1834	LYS
1	A	1884	CYS
1	A	1893	TRP
1	A	1894	ARG
1	A	1899	GLU
1	A	1964	THR
1	A	1978	LYS
1	A	1979	LYS
1	A	1980[A]	ILE
1	A	1980[B]	ILE
1	A	1995	SER
1	A	1999	GLU
1	B	1878[A]	LEU
1	B	1878[B]	LEU
1	B	1883	VAL
1	B	1885	THR
1	B	1886	ILE
1	B	1888	LYS
1	B	1937	LYS
1	B	1941	LYS
1	B	1999	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1926	GLN
1	A	1930	ASN
1	B	1926	GLN
1	B	1930	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 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	$\# Z > 2$
5	GOL	A	2106	-	5,5,5	0.54	0	5,5,5	0.31	0
4	ACY	B	2106	-	3,3,3	1.03	0	3,3,3	0.90	0
4	ACY	A	2105	-	3,3,3	1.07	0	3,3,3	0.70	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
5	GOL	A	2106	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2106	GOL	O1-C1-C2-O2
5	A	2106	GOL	O1-C1-C2-C3

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	194/200 (97%)	1.20	42 (21%)	2 1	40, 71, 236, 362	4 (2%)
1	B	194/200 (97%)	1.11	32 (16%)	4 4	34, 70, 179, 218	5 (2%)
All	All	388/400 (97%)	1.16	74 (19%)	3 2	34, 70, 198, 362	9 (2%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1893	TRP	6.0
1	B	1892	PHE	5.4
1	B	1976	GLY	4.9
1	A	1895	LEU	4.5
1	B	1832	GLY	4.5
1	A	1886	ILE	4.4
1	A	1977	GLU	4.2
1	A	1892	PHE	4.1
1	A	1888	LYS	4.1
1	A	1877[A]	TYR	3.9
1	B	1931[A]	ARG	3.8
1	B	1877[A]	TYR	3.6
1	B	1951	PHE	3.4
1	A	1885	THR	3.4
1	A	1893	TRP	3.3
1	A	1884	CYS	3.3
1	A	1891	ALA	3.3
1	A	1951	PHE	3.3
1	A	1898	THR	3.2
1	B	1878[A]	LEU	3.2
1	B	1886	ILE	3.1
1	B	1883	VAL	3.1
1	B	1977	GLU	3.1
1	A	1845	ILE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1876	ASP	3.0
1	A	1847	PHE	3.0
1	B	1828	LEU	3.0
1	A	1807	MET	3.0
1	B	1884	CYS	2.9
1	A	1846	GLY	2.9
1	A	1811	PHE	2.9
1	A	1887	ALA	2.9
1	B	1891	ALA	2.9
1	B	1950	ALA	2.9
1	B	1895	LEU	2.9
1	A	1902	ILE	2.8
1	A	1875	PHE	2.8
1	A	1976	GLY	2.8
1	A	1955	TRP	2.8
1	A	1822	ASP	2.8
1	A	1963[A]	LYS	2.8
1	B	1830	LEU	2.7
1	A	2000	ARG	2.7
1	A	1879	PRO	2.7
1	A	1808	ALA	2.7
1	B	1841	LYS	2.6
1	A	1972	VAL	2.5
1	B	1978	LYS	2.5
1	A	1821	ARG	2.5
1	A	1928[A]	ASP	2.4
1	B	1975	GLU	2.4
1	A	1896	ASP	2.4
1	B	1850	HIS	2.4
1	B	1885	THR	2.3
1	A	1848[A]	GLU	2.3
1	A	1939	ALA	2.3
1	B	1973	ALA	2.3
1	B	1861	LEU	2.3
1	B	1898	THR	2.2
1	A	1997	HIS	2.2
1	A	1889	LYS	2.2
1	A	1950	ALA	2.2
1	A	1929[A]	LEU	2.2
1	B	1834[A]	LYS	2.2
1	B	1835	MET	2.2
1	A	1974	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1981	LEU	2.2
1	A	1995	SER	2.2
1	B	1903	PRO	2.1
1	B	1997	HIS	2.1
1	A	1850	HIS	2.1
1	A	1978	LYS	2.1
1	B	1974	GLU	2.1
1	B	1955	TRP	2.1

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 oligosaccharides in this entry.

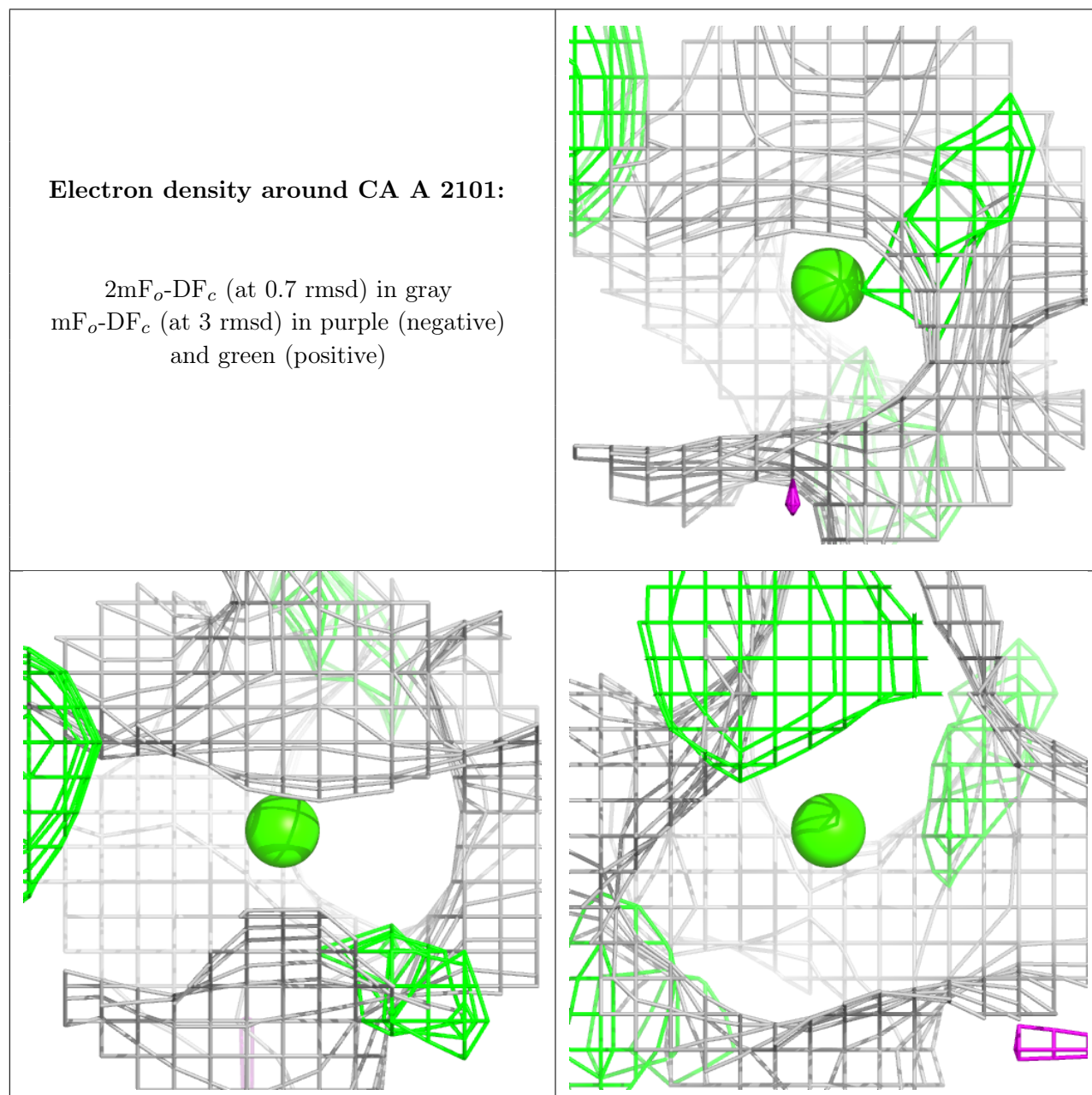
6.4 Ligands ⓘ

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
4	ACY	A	2105	4/4	0.81	0.19	77,86,93,93	0
5	GOL	A	2106	6/6	0.86	0.12	66,89,108,108	0
4	ACY	B	2106	4/4	0.87	0.18	70,84,101,101	0
3	CL	B	2105	1/1	0.87	0.16	63,63,63,63	0
3	CL	B	2104	1/1	0.92	0.15	62,62,62,62	0
2	CA	A	2101	1/1	0.97	0.04	43,43,43,43	0
2	CA	B	2101	1/1	0.97	0.04	55,55,55,55	0
2	CA	B	2102	1/1	0.97	0.05	53,53,53,53	0
2	CA	B	2103	1/1	0.97	0.08	55,55,55,55	0
3	CL	A	2104	1/1	0.97	0.08	55,55,55,55	0
2	CA	A	2102	1/1	0.98	0.04	38,38,38,38	0
2	CA	A	2103	1/1	0.99	0.02	37,37,37,37	0

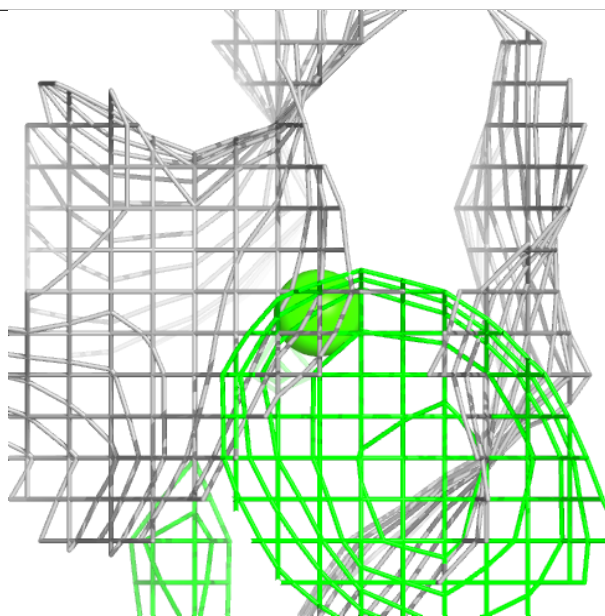
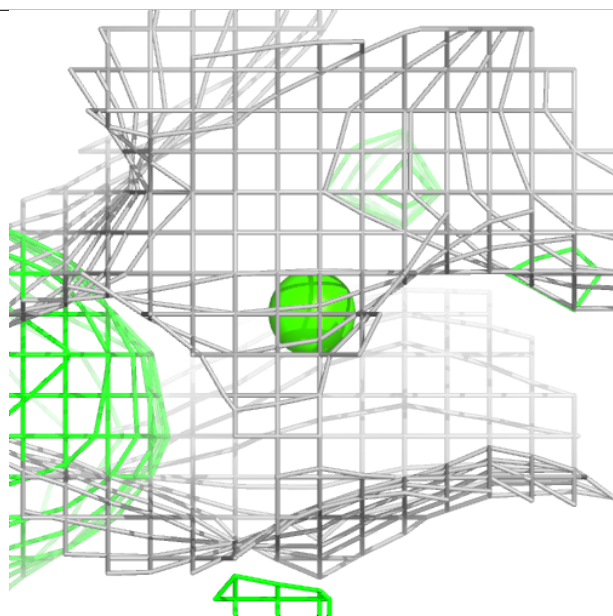
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



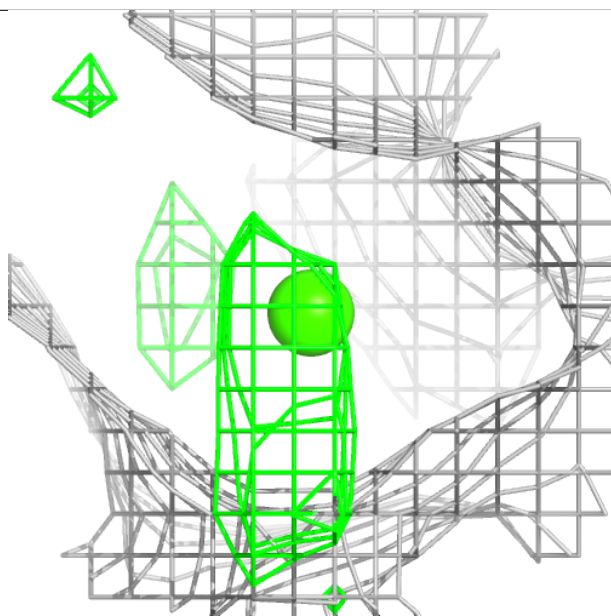
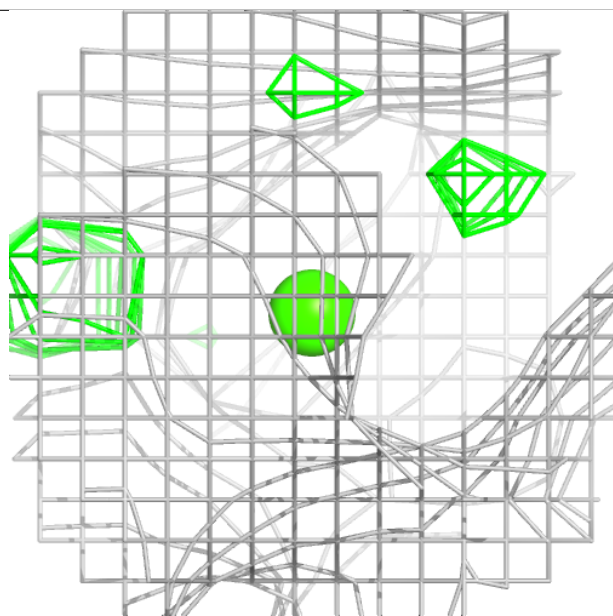
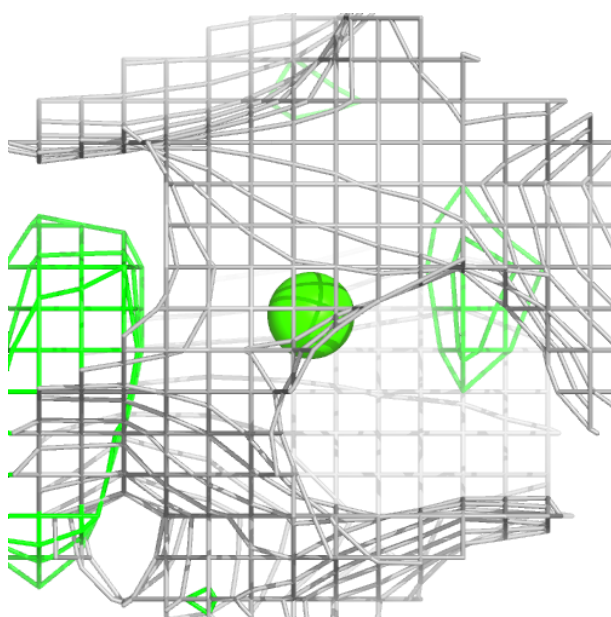
Electron density around CA B 2101:

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



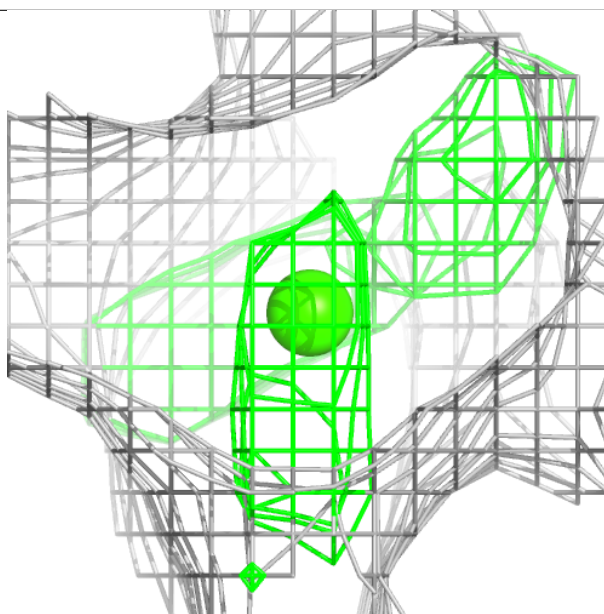
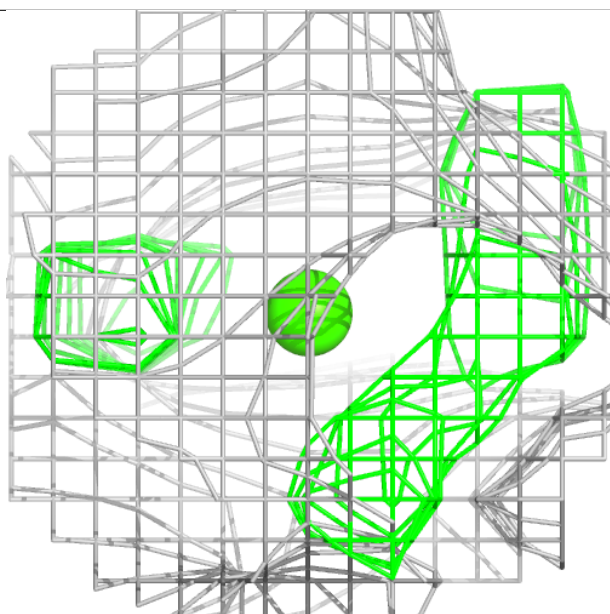
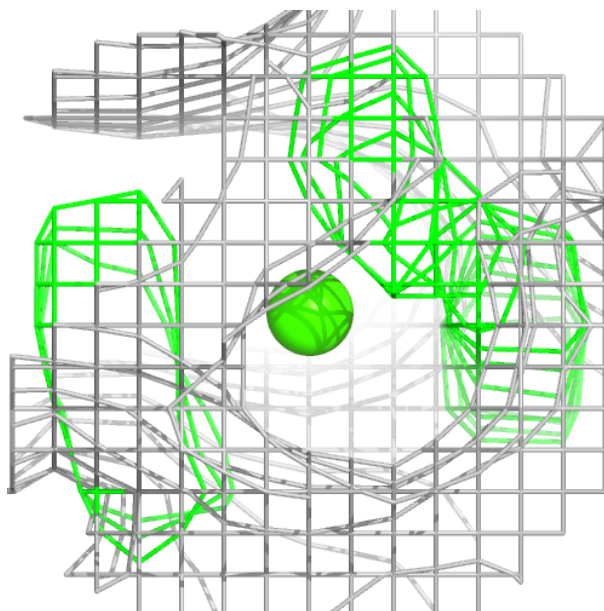
Electron density around CA B 2102:

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



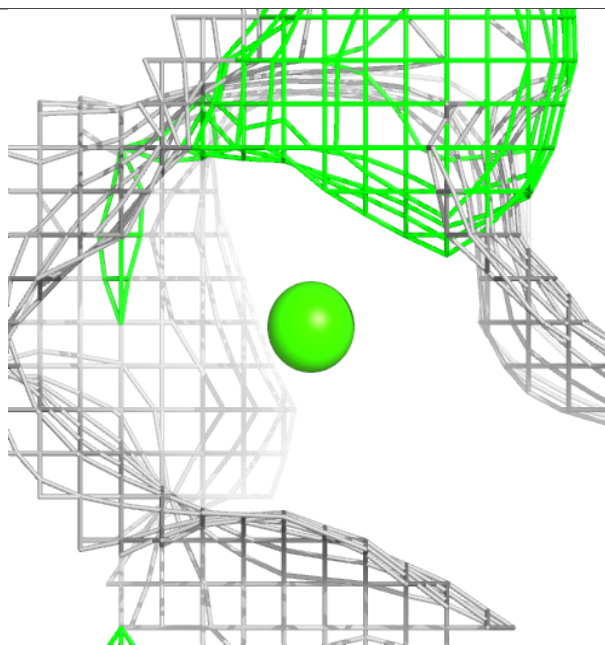
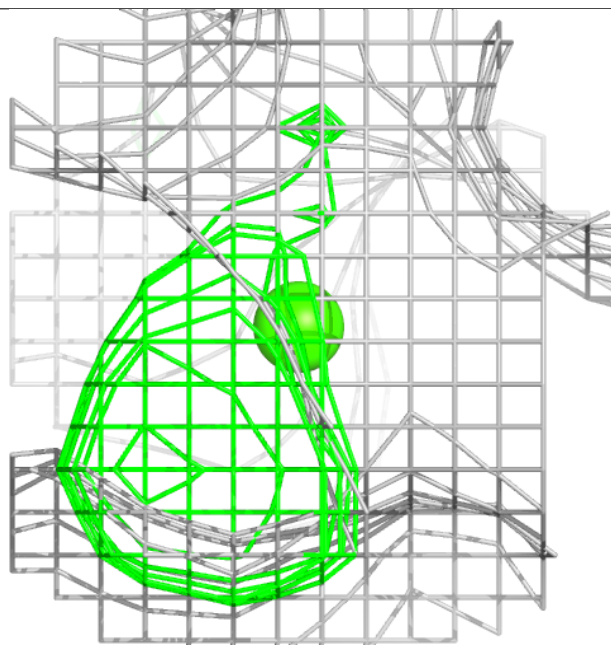
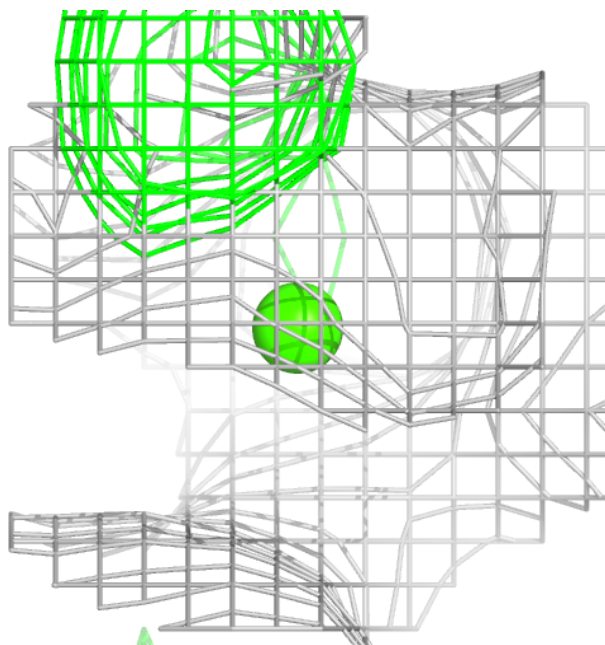
Electron density around CA B 2103:

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



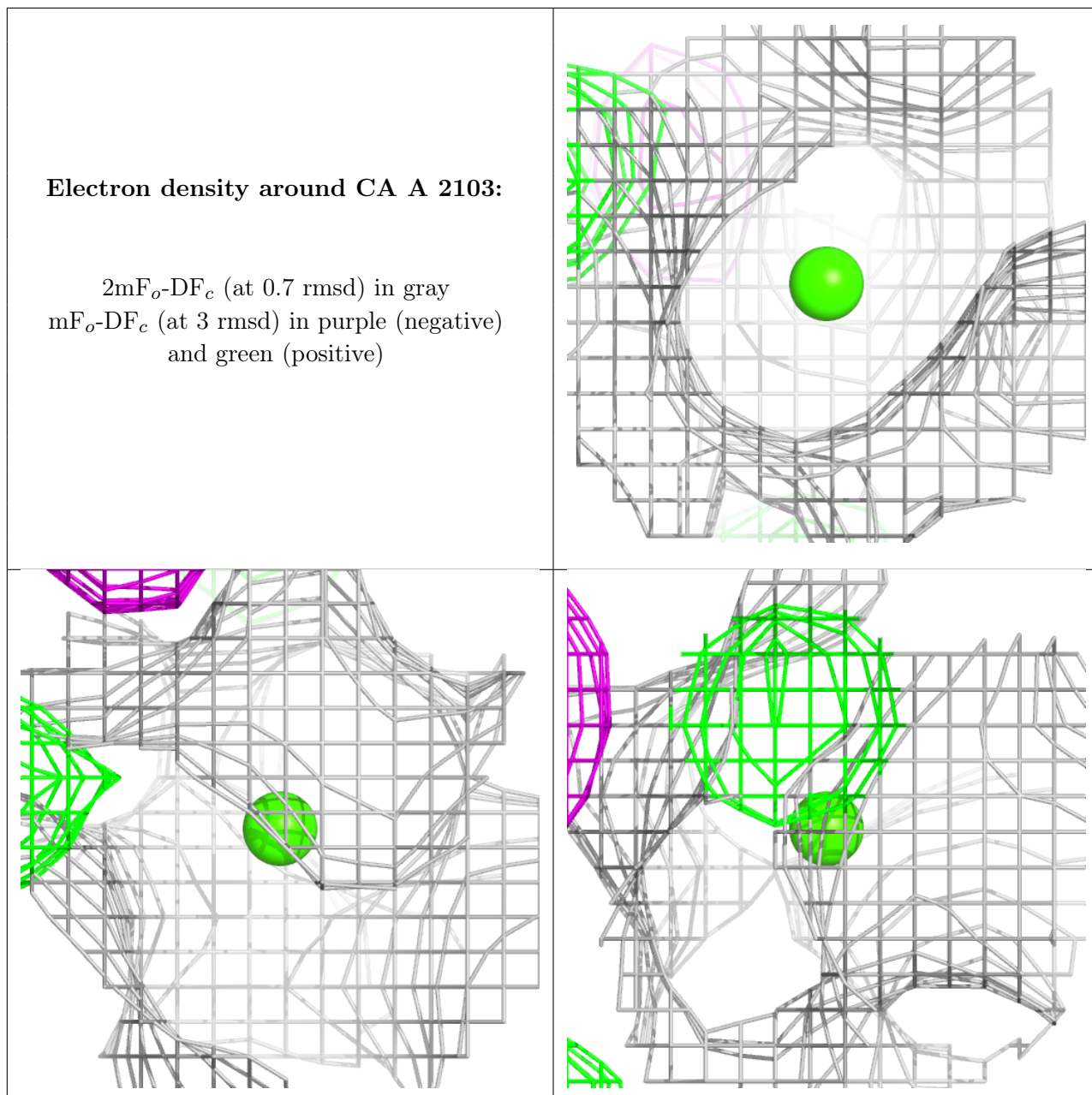
Electron density around CA A 2102:

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



Electron density around CA A 2103:

$2mF_o-DF_c$ (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.