Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2023 – 04:22 PM JST

PDB ID	:	6LXI
Title	:	Crystal structure of Z2B3 Fab in complex with influenza virus neuraminidase from A/Brevig Mission/1/1918 (H1N1)
Authors	:	Jiang, H.; Peng, W.; Qi, J.; Chai, Y.; Song, H.; Shi, Y.; Gao, G.F.; Wu, Y.
Deposited on	:	2020-02-11
Resolution	:	2.50 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:

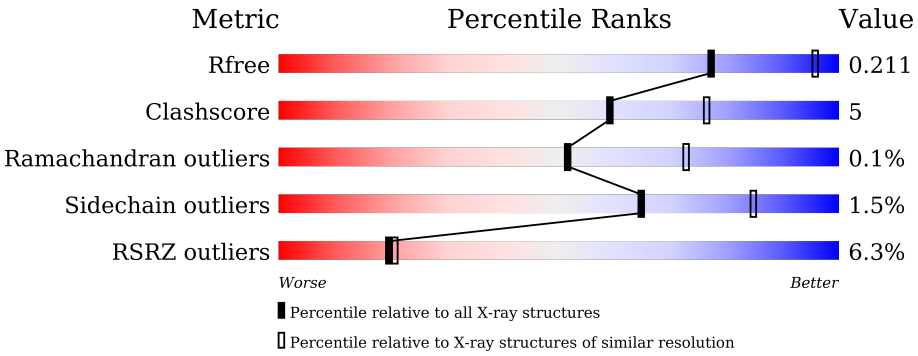
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	469	79% · 17%
1	B	469	76% 6% 17%
2	C	237	12% 78% 12% 10%
2	H	237	% 92% 6% ·
3	D	216	25% 70% 19% · 9%
3	L	216	8% 79% 17% ··

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Mol	Chain	Length	Quality of chain
4	E	5	20% 60% 20%
4	F	5	60% 40%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12997 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 Neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			2980	1866	512	579	23			
1	B	387	Total	C	N	O	S	0	0	0
			2980	1866	512	579	23			

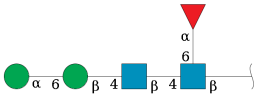
- Molecule 2 is a protein called Heavy chain of Z2B3 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	232	Total	C	N	O	S	0	0	0
			1727	1091	281	348	7			
2	C	214	Total	C	N	O	S	0	0	0
			1611	1023	261	320	7			

- Molecule 3 is a protein called Light chain of Z2B3 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	211	Total	C	N	O	S	0	0	0
			1563	973	260	325	5			
3	D	196	Total	C	N	O	S	0	0	0
			1447	902	237	303	5			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	5	Total	C	N	O	0	0	0
			60	34	2	24			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	F	5	Total C N O 60 34 2 24	0	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 6 is water.

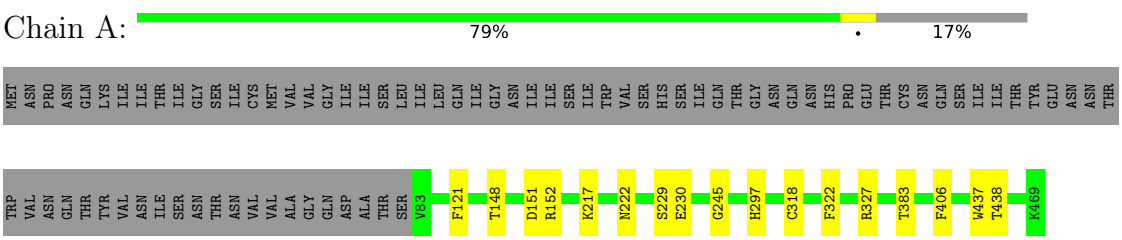
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	221	Total O 221 221	0	0
6	H	69	Total O 69 69	0	0
6	L	46	Total O 46 46	0	0
6	B	165	Total O 165 165	0	0
6	C	46	Total O 46 46	0	0
6	D	18	Total O 18 18	0	0

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.

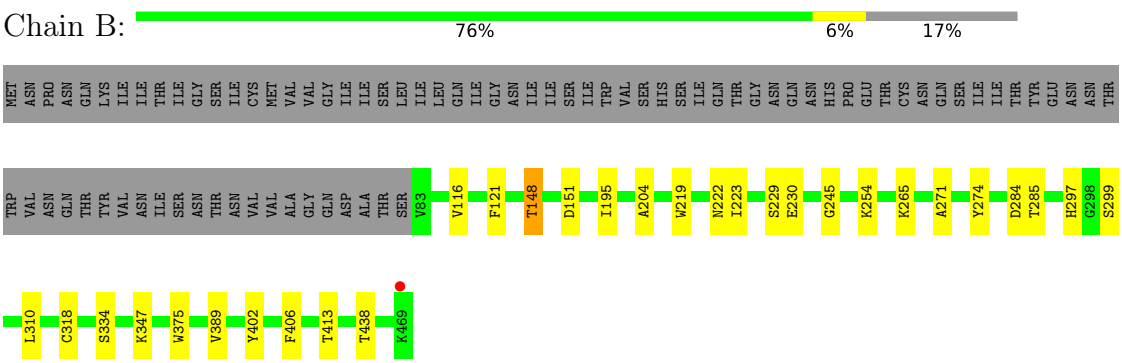
• Molecule 1: Neuraminidase

Chain A:



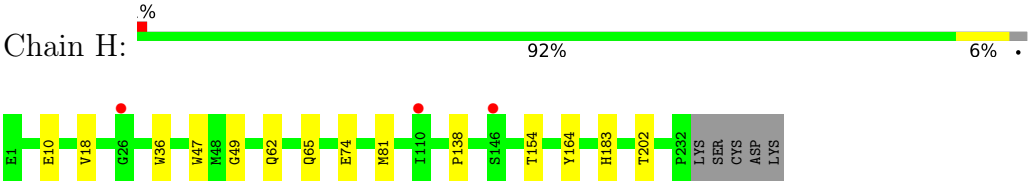
• Molecule 1: Neuraminidase

Chain B:



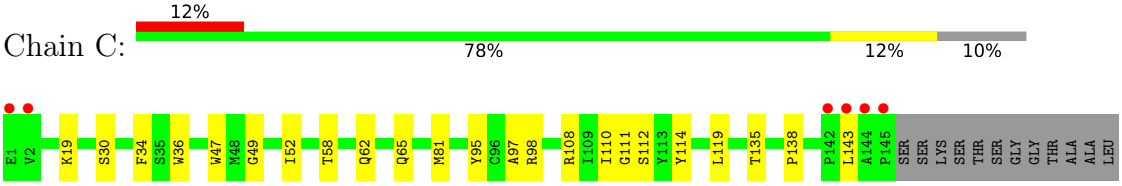
• Molecule 2: Heavy chain of Z2B3 Fab

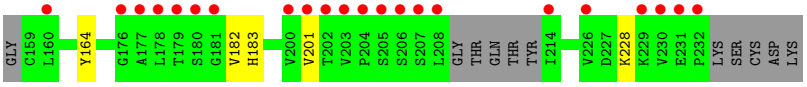
Chain H:



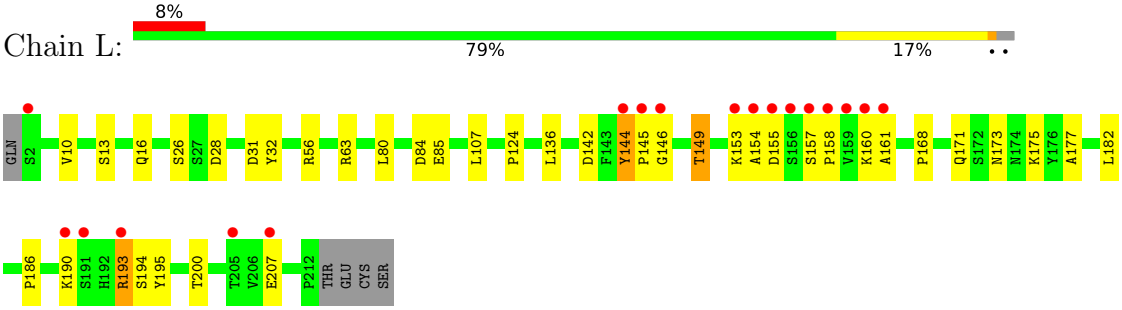
• Molecule 2: Heavy chain of Z2B3 Fab

Chain C:

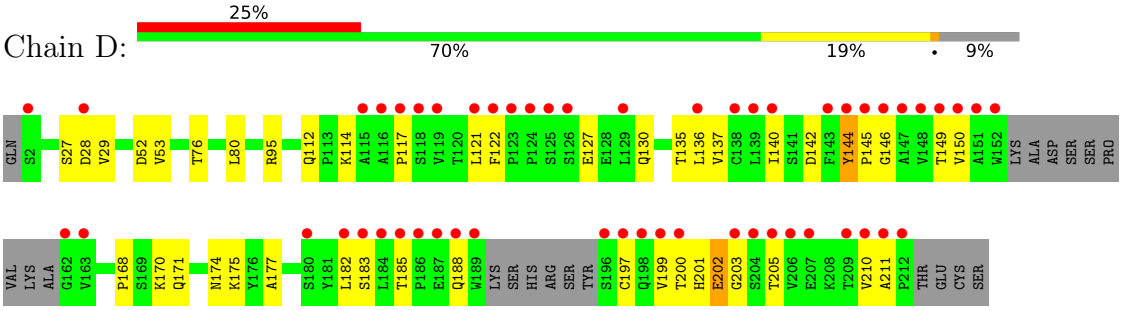




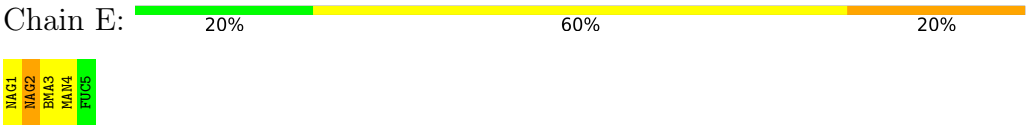
• Molecule 3: Light chain of Z2B3 Fab



• Molecule 3: Light chain of Z2B3 Fab



• Molecule 4: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 4: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	163.13Å 163.13Å 190.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.93 – 2.50 47.93 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.93-2.50) 99.0 (47.93-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.06 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.18.2-3874_1692	Depositor
R, R_{free}	0.183 , 0.212 0.183 , 0.211	Depositor DCC
R_{free} test set	4442 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	38.1	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12997	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: FUC, MAN, NAG, CA, BMA

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	0.67	0/3061	0.63	0/4160
1	B	0.64	0/3061	0.62	0/4160
2	C	0.55	0/1650	0.57	0/2249
2	H	0.56	0/1769	0.56	0/2413
3	D	0.53	0/1479	0.64	0/2018
3	L	0.54	0/1600	0.61	0/2183
All	All	0.60	0/12620	0.61	0/17183

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

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	2980	0	2802	10	0
1	B	2980	0	2802	18	0
2	C	1611	0	1573	18	0
2	H	1727	0	1686	7	0
3	D	1447	0	1385	34	0
3	L	1563	0	1505	24	0
4	E	60	0	52	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	60	0	52	3	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	221	0	0	1	1
6	B	165	0	0	2	1
6	C	46	0	0	1	0
6	D	18	0	0	0	1
6	H	69	0	0	0	0
6	L	46	0	0	2	0
All	All	12997	0	11857	114	2

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 (114) 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)
4:F:3:BMA:H62	4:F:4:MAN:H5	1.55	0.85
3:D:135:THR:HG22	3:D:183:SER:HA	1.69	0.75
4:E:3:BMA:H62	4:E:4:MAN:H5	1.68	0.74
3:L:171:GLN:OE1	3:L:173:ASN:ND2	2.21	0.73
1:B:413:THR:O	6:B:601:HOH:O	2.05	0.73
3:L:171:GLN:HE21	3:L:177:ALA:HB2	1.53	0.72
3:D:127:GLU:HG2	3:D:130:GLN:NE2	2.07	0.70
1:B:230:GLU:OE1	6:B:602:HOH:O	2.11	0.69
3:D:127:GLU:O	3:D:130:GLN:NE2	2.24	0.68
3:D:130:GLN:N	3:D:130:GLN:OE1	2.26	0.68
4:E:3:BMA:C6	4:E:4:MAN:H5	2.23	0.68
3:L:173:ASN:OD1	3:L:175:LYS:HG3	1.93	0.68
3:D:136:LEU:HD12	3:D:182:LEU:HD23	1.77	0.67
2:C:182:VAL:HG12	2:C:201:VAL:HG22	1.78	0.66
3:L:171:GLN:HB2	3:L:173:ASN:ND2	2.12	0.64
3:L:136:LEU:HD12	3:L:182:LEU:HD23	1.79	0.64
2:C:110:ILE:HG22	2:C:111:GLY:H	1.65	0.62
3:D:200:THR:HB	3:D:205:THR:HG23	1.81	0.61
1:B:148:THR:CG2	1:B:438:THR:H	2.13	0.61
3:D:170:LYS:HD2	3:D:174:ASN:OD1	1.99	0.61
3:D:185:THR:N	3:D:188:GLN:OE1	2.33	0.60
2:C:143:LEU:HD13	3:D:137:VAL:HG21	1.81	0.60
3:D:144:TYR:CD1	3:D:145:PRO:HA	2.37	0.59
1:A:148:THR:CG2	1:A:438:THR:H	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:149:THR:HB	3:D:200:THR:CG2	2.33	0.58
1:A:217:LYS:O	6:A:603:HOH:O	2.17	0.58
2:C:36:TRP:CE2	2:C:81:MET:HB2	2.39	0.58
2:C:138:PRO:HB3	2:C:164:TYR:HB3	1.85	0.58
3:L:144:TYR:HD1	3:L:145:PRO:CA	2.17	0.57
3:L:160:LYS:HG3	3:L:161:ALA:N	2.18	0.57
3:L:153:LYS:HG2	3:L:158:PRO:HA	1.85	0.57
3:L:155:ASP:OD1	3:L:193:ARG:HB3	2.04	0.57
1:B:223:ILE:O	1:B:223:ILE:HG22	2.05	0.57
1:B:284:ASP:OD1	1:B:285:THR:HG23	2.04	0.56
1:B:148:THR:HG22	1:B:438:THR:H	1.71	0.55
1:B:222:ASN:HB3	1:B:245:GLY:HA2	1.88	0.55
1:A:230:GLU:OE2	1:A:406:PHE:HA	2.07	0.55
3:L:26:SER:O	3:L:31:ASP:HB2	2.06	0.55
2:H:36:TRP:CE2	2:H:81:MET:HB2	2.41	0.55
2:C:58:THR:O	2:C:112:SER:HA	2.06	0.55
2:C:62:GLN:HA	2:C:65:GLN:HG3	1.89	0.55
2:C:110:ILE:HG22	2:C:111:GLY:N	2.24	0.53
1:B:195:ILE:HG12	1:B:204:ALA:HB2	1.89	0.53
1:A:148:THR:HG22	1:A:437:TRP:HA	1.90	0.53
2:H:10:GLU:HG2	2:H:18:VAL:HG23	1.91	0.53
1:B:265:LYS:HG2	1:B:310:LEU:HD12	1.92	0.52
2:H:62:GLN:HA	2:H:65:GLN:HG3	1.92	0.52
3:D:117:PRO:HD3	3:D:201:HIS:ND1	2.24	0.51
3:L:63:ARG:NH2	3:L:84:ASP:OD2	2.44	0.51
3:L:154:ALA:HB2	3:L:195:TYR:CE2	2.46	0.51
3:D:146:GLY:O	3:D:168:PRO:HG2	2.11	0.51
3:L:31:ASP:OD2	6:L:302:HOH:O	2.19	0.51
2:C:19:LYS:NZ	4:F:4:MAN:O5	2.44	0.50
3:D:140:ILE:HD11	3:D:150:VAL:HG21	1.93	0.50
3:D:201:HIS:O	3:D:203:GLY:O	2.29	0.49
2:C:228:LYS:HE2	2:C:228:LYS:HA	1.94	0.49
4:E:1:NAG:H62	4:E:2:NAG:C7	2.43	0.49
3:D:112:GLN:NE2	3:D:144:TYR:CD2	2.81	0.49
1:A:151:ASP:OD2	1:A:152:ARG:HG3	2.13	0.48
3:L:144:TYR:HD1	3:L:145:PRO:HA	1.78	0.48
3:D:112:GLN:NE2	3:D:144:TYR:HD2	2.11	0.48
1:B:121:PHE:CG	1:B:229:SER:HA	2.49	0.48
2:C:95:TYR:OH	6:C:301:HOH:O	2.20	0.48
3:D:122:PHE:HB2	3:D:137:VAL:HG22	1.95	0.48
3:D:28:ASP:OD1	3:D:29:VAL:N	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:3:BMA:H61	4:F:4:MAN:H2	1.35	0.47
2:C:47:TRP:CH2	2:C:49:GLY:HA2	2.50	0.47
4:E:3:BMA:H61	4:E:4:MAN:H2	1.42	0.47
3:D:199:VAL:O	3:D:205:THR:HA	2.14	0.47
1:B:116:VAL:HG11	1:B:148:THR:HG21	1.96	0.46
1:B:271:ALA:HB1	1:B:274:TYR:HB2	1.96	0.46
3:L:10:VAL:HG23	3:L:107:LEU:HD13	1.98	0.46
2:H:138:PRO:HB3	2:H:164:TYR:HB3	1.98	0.45
3:D:149:THR:HB	3:D:200:THR:HG23	1.99	0.45
2:C:97:ALA:HB1	2:C:119:LEU:HB3	1.99	0.45
2:H:36:TRP:CD2	2:H:81:MET:HB2	2.52	0.45
3:L:149:THR:HG23	3:L:200:THR:OG1	2.17	0.45
3:D:144:TYR:CD1	3:D:145:PRO:CA	2.99	0.45
3:D:200:THR:HA	3:D:205:THR:HA	1.98	0.45
1:B:347:LYS:HB3	1:B:402:TYR:CG	2.52	0.45
3:L:146:GLY:O	3:L:168:PRO:HG2	2.17	0.44
1:B:219:TRP:CE2	1:B:254:LYS:HE3	2.53	0.44
1:B:151:ASP:OD2	2:C:108:ARG:HD3	2.18	0.44
2:C:183:HIS:CE1	3:D:177:ALA:HB3	2.52	0.44
3:L:31:ASP:OD2	3:L:32:TYR:CE1	2.70	0.44
3:L:124:PRO:HD3	3:L:136:LEU:HD23	1.99	0.43
2:C:52:ILE:HD11	2:C:114:TYR:HA	1.99	0.43
3:L:16:GLN:HB3	6:L:329:HOH:O	2.17	0.43
2:C:36:TRP:CD2	2:C:81:MET:HB2	2.52	0.43
3:D:127:GLU:HG2	3:D:130:GLN:HE22	1.83	0.43
3:D:142:ASP:H	3:D:171:GLN:HE22	1.66	0.43
3:D:142:ASP:H	3:D:171:GLN:NE2	2.16	0.43
1:A:148:THR:HG23	1:A:438:THR:H	1.83	0.43
3:D:121:LEU:HD22	3:D:197:CYS:HB2	1.99	0.43
3:D:142:ASP:CA	3:D:175:LYS:HD3	2.49	0.43
1:A:322:PHE:HB2	1:A:327:ARG:HD2	2.00	0.42
3:L:186:PRO:O	3:L:190:LYS:HG2	2.19	0.42
2:C:34:PHE:CZ	2:C:98:ARG:HD2	2.54	0.42
3:D:112:GLN:HG2	3:D:144:TYR:CE2	2.54	0.42
2:H:47:TRP:CH2	2:H:49:GLY:HA2	2.54	0.42
1:A:121:PHE:CG	1:A:229:SER:HA	2.54	0.42
3:D:27:SER:HB2	3:D:95:ARG:HG3	2.01	0.42
2:H:154:THR:OG1	2:H:202:THR:HG22	2.20	0.42
1:B:318:CYS:HA	1:B:334:SER:O	2.20	0.42
1:A:222:ASN:HB3	1:A:245:GLY:HA2	2.01	0.42
3:D:52:ASP:O	3:D:53:VAL:HB	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:142:ASP:H	3:L:171:GLN:HE22	1.67	0.42
3:D:210:VAL:HG12	3:D:211:ALA:H	1.85	0.41
3:L:85:GLU:HG3	3:L:107:LEU:O	2.21	0.41
1:B:375:TRP:HB3	1:B:389:VAL:HB	2.02	0.41
3:D:202:GLU:HB3	3:D:203:GLY:H	1.75	0.41
1:A:318:CYS:O	1:A:383:THR:HA	2.21	0.40
3:L:207:GLU:OE1	3:L:207:GLU:N	2.54	0.40
1:B:230:GLU:OE2	1:B:406:PHE:HA	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:709:HOH:O	6:D:318:HOH:O[7_555]	2.06	0.14
6:A:719:HOH:O	6:A:739:HOH:O[3_455]	2.13	0.07

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	385/469 (82%)	369 (96%)	16 (4%)	0	100	100
1	B	385/469 (82%)	368 (96%)	17 (4%)	0	100	100
2	C	208/237 (88%)	203 (98%)	5 (2%)	0	100	100
2	H	230/237 (97%)	225 (98%)	5 (2%)	0	100	100
3	D	190/216 (88%)	184 (97%)	5 (3%)	1 (0%)	29	48
3	L	209/216 (97%)	204 (98%)	5 (2%)	0	100	100
All	All	1607/1844 (87%)	1553 (97%)	53 (3%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	202	GLU

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	332/407 (82%)	331 (100%)	1 (0%)	92 97
1	B	332/407 (82%)	329 (99%)	3 (1%)	78 92
2	C	183/200 (92%)	181 (99%)	2 (1%)	73 89
2	H	195/200 (98%)	193 (99%)	2 (1%)	76 90
3	D	165/183 (90%)	161 (98%)	4 (2%)	49 74
3	L	178/183 (97%)	169 (95%)	9 (5%)	24 45
All	All	1385/1580 (88%)	1364 (98%)	21 (2%)	65 85

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

Mol	Chain	Res	Type
1	A	297	HIS
2	H	74	GLU
2	H	183	HIS
3	L	13	SER
3	L	28	ASP
3	L	56	ARG
3	L	80	LEU
3	L	144	TYR
3	L	149	THR
3	L	157	SER
3	L	193	ARG
3	L	194	SER
1	B	148	THR
1	B	297	HIS
1	B	299	SER
2	C	30	SER
2	C	135	THR
3	D	76	THR

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Mol	Chain	Res	Type
3	D	80	LEU
3	D	114	LYS
3	D	144	TYR

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)

10 monosaccharides are modelled in this entry.

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	$\#\|Z\| > 2$
4	NAG	E	1	1,4	14,14,15	0.31	0	17,19,21	0.63	0
4	NAG	E	2	4	14,14,15	0.31	0	17,19,21	0.89	1 (5%)
4	BMA	E	3	4	11,11,12	0.26	0	15,15,17	0.64	0
4	MAN	E	4	4	11,11,12	0.26	0	15,15,17	0.66	0
4	FUC	E	5	4	10,10,11	0.30	0	14,14,16	0.64	0
4	NAG	F	1	1,4	14,14,15	0.32	0	17,19,21	0.57	0
4	NAG	F	2	4	14,14,15	0.30	0	17,19,21	0.65	0
4	BMA	F	3	4	11,11,12	0.27	0	15,15,17	0.59	0
4	MAN	F	4	4	11,11,12	0.26	0	15,15,17	0.68	0
4	FUC	F	5	4	10,10,11	0.30	0	14,14,16	0.63	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
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	1/2/19/22	0/1/1/1
4	FUC	E	5	4	-	-	0/1/1/1
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	2/2/19/22	0/1/1/1
4	MAN	F	4	4	-	2/2/19/22	0/1/1/1
4	FUC	F	5	4	-	-	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	2	NAG	O5-C1-C2	-2.39	107.52	111.29

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	3	BMA	C4-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6
4	F	4	MAN	C4-C5-C6-O6
4	F	4	MAN	O5-C5-C6-O6
4	E	4	MAN	O5-C5-C6-O6

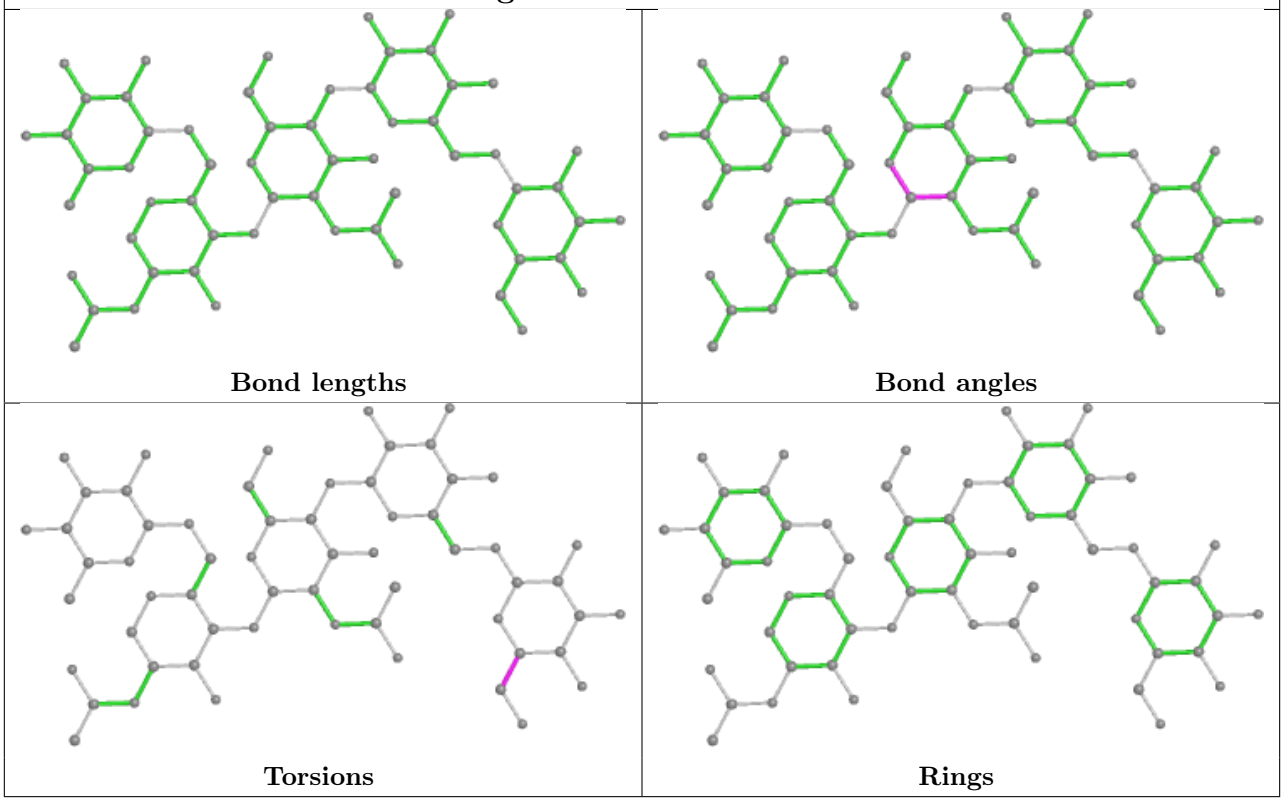
There are no ring outliers.

6 monomers are involved in 7 short contacts:

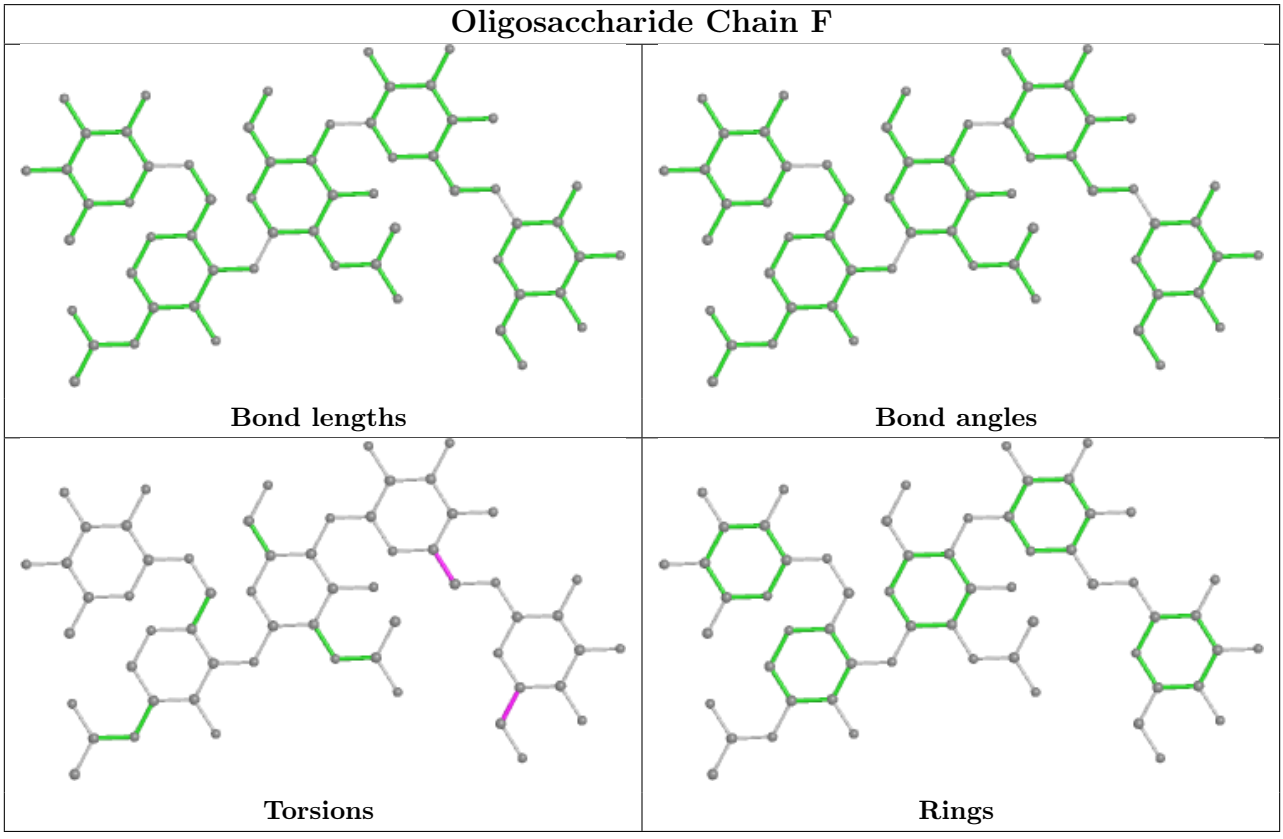
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	4	MAN	3	0
4	E	1	NAG	1	0
4	E	3	BMA	3	0
4	E	4	MAN	3	0
4	F	3	BMA	2	0
4	E	2	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain E



Oligosaccharide Chain F



5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 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, 95^{th} 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	387/469 (82%)	-0.30	0 100 100	17, 26, 35, 60	0
1	B	387/469 (82%)	-0.35	1 (0%) 94 94	18, 29, 42, 72	0
2	C	214/237 (90%)	0.18	28 (13%) 3 3	26, 44, 102, 130	0
2	H	232/237 (97%)	-0.38	3 (1%) 77 79	24, 37, 58, 89	0
3	D	196/216 (90%)	1.01	53 (27%) 0 0	30, 68, 119, 145	0
3	L	211/216 (97%)	0.23	18 (8%) 10 10	22, 49, 93, 114	0
All	All	1627/1844 (88%)	-0.03	103 (6%) 20 21	17, 33, 92, 145	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	204	SER	6.6
3	D	189	TRP	5.6
2	C	208	LEU	5.5
2	C	203	VAL	5.2
2	C	177	ALA	5.2
3	D	2	SER	4.8
3	D	205	THR	4.8
3	D	147	ALA	4.7
3	D	184	LEU	4.6
3	D	126	SER	4.6
3	D	200	THR	4.6
3	D	152	TRP	4.6
3	D	196	SER	4.4
2	C	144	ALA	4.4
3	D	121	LEU	4.4
2	C	201	VAL	4.4
3	D	118	SER	4.3
3	L	159	VAL	4.3
2	C	202	THR	4.3

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Mol	Chain	Res	Type	RSRZ
3	D	211	ALA	4.3
3	D	187	GLU	4.2
3	D	209	THR	4.2
3	D	136	LEU	4.2
3	D	119	VAL	4.2
2	C	206	SER	4.1
3	L	160	LYS	4.1
3	L	2	SER	4.0
3	D	182	LEU	3.9
2	C	207	SER	3.9
3	D	207	GLU	3.8
3	L	158	PRO	3.8
3	L	146	GLY	3.8
3	D	146	GLY	3.8
2	C	145	PRO	3.7
3	D	210	VAL	3.7
3	D	150	VAL	3.7
3	D	140	ILE	3.6
2	C	230	VAL	3.5
3	D	199	VAL	3.5
3	D	197	CYS	3.5
2	C	232	PRO	3.5
3	D	123	PRO	3.5
3	D	198	GLN	3.4
3	D	117	PRO	3.3
3	D	145	PRO	3.3
2	C	204	PRO	3.2
3	L	190	LYS	3.2
3	D	115	ALA	3.2
3	D	185	THR	3.2
3	L	153	LYS	3.2
2	C	200	VAL	3.1
3	D	151	ALA	3.1
3	D	186	PRO	3.1
2	C	143	LEU	3.1
3	L	157	SER	3.1
3	L	207	GLU	3.1
3	D	138	CYS	3.0
3	D	122	PHE	3.0
3	L	144	TYR	3.0
3	D	206	VAL	2.9
2	C	178	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
3	L	145	PRO	2.8
3	D	124	PRO	2.8
2	C	214	ILE	2.8
3	D	163	VAL	2.7
3	D	148	VAL	2.7
3	D	162	GLY	2.7
3	D	143	PHE	2.7
3	D	203	GLY	2.6
3	D	212	PRO	2.6
3	L	156	SER	2.6
3	L	161	ALA	2.6
2	C	142	PRO	2.6
2	C	160	LEU	2.6
3	D	129	LEU	2.6
2	C	181	GLY	2.5
3	D	149	THR	2.5
3	D	188	GLN	2.5
3	L	193	ARG	2.5
2	C	229	LYS	2.5
2	H	146	SER	2.4
3	D	116	ALA	2.4
3	L	191	SER	2.4
3	D	125	SER	2.4
2	C	231	GLU	2.3
2	C	179	THR	2.3
3	D	183	SER	2.3
2	C	205	SER	2.3
2	C	226	VAL	2.2
2	C	180	SER	2.2
3	D	28	ASP	2.1
3	L	154	ALA	2.1
3	D	139	LEU	2.1
3	L	155	ASP	2.1
2	C	176	GLY	2.1
2	C	1	GLU	2.1
3	D	144	TYR	2.1
3	D	180	SER	2.0
1	B	469	LYS	2.0
3	L	205	THR	2.0
2	C	2	VAL	2.0
2	H	26	GLY	2.0
2	H	110	ILE	2.0

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)

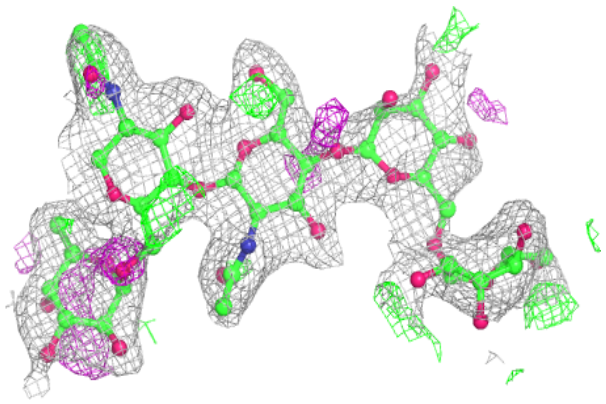
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

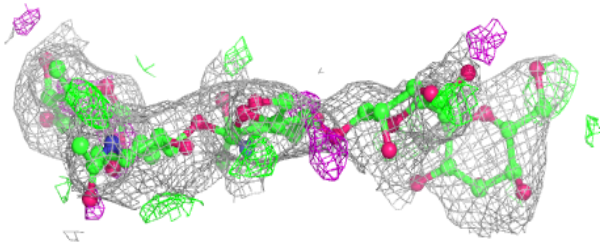
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BMA	E	3	11/12	0.70	0.39	96,106,112,113	0
4	FUC	E	5	10/11	0.72	0.26	44,58,62,68	0
4	BMA	F	3	11/12	0.72	0.30	87,96,108,116	0
4	MAN	F	4	11/12	0.75	0.27	87,94,100,101	0
4	MAN	E	4	11/12	0.79	0.30	78,87,90,91	0
4	NAG	E	2	14/15	0.86	0.24	46,57,70,79	0
4	NAG	E	1	14/15	0.87	0.20	52,64,69,76	0
4	NAG	F	1	14/15	0.87	0.20	42,49,60,60	0
4	FUC	F	5	10/11	0.90	0.18	44,51,55,57	0
4	NAG	F	2	14/15	0.92	0.21	38,48,53,61	0

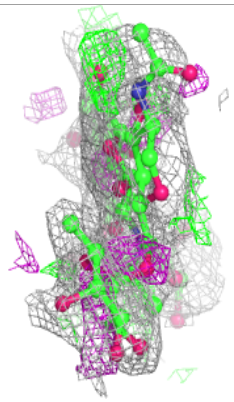
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

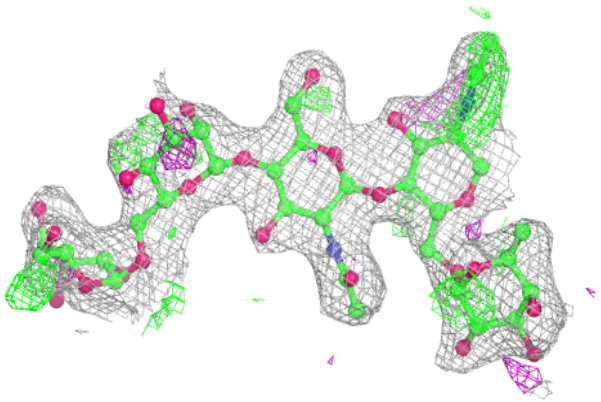


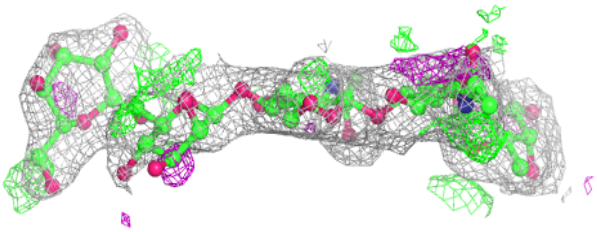


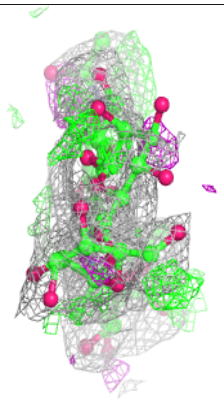


Electron density around Chain F:

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







6.4 Ligands (i)

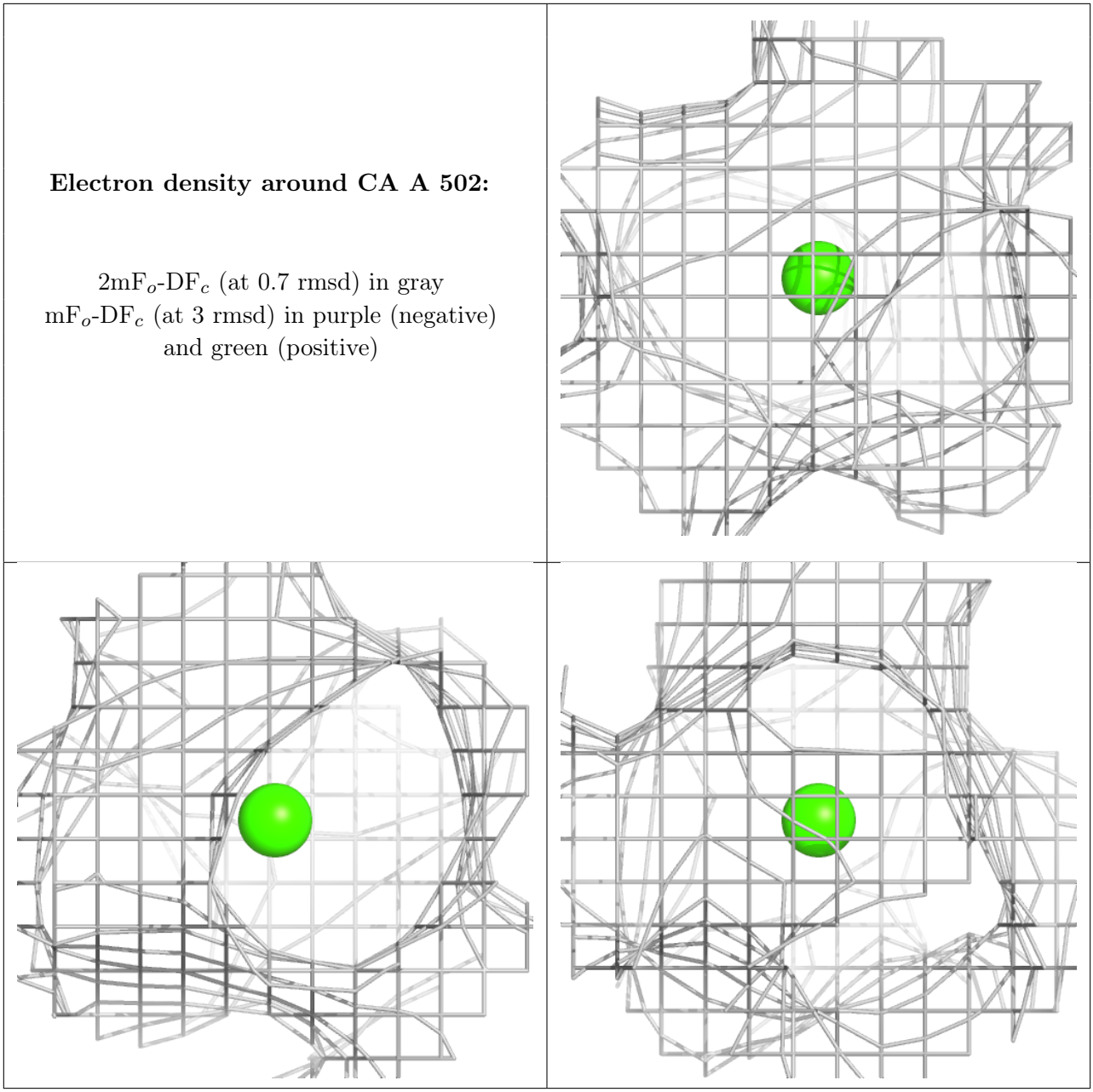
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	CA	A	502	1/1	0.98	0.03	33,33,33,33	0
5	CA	A	501	1/1	0.99	0.12	27,27,27,27	0
5	CA	B	501	1/1	0.99	0.14	32,32,32,32	0
5	CA	B	502	1/1	0.99	0.04	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.

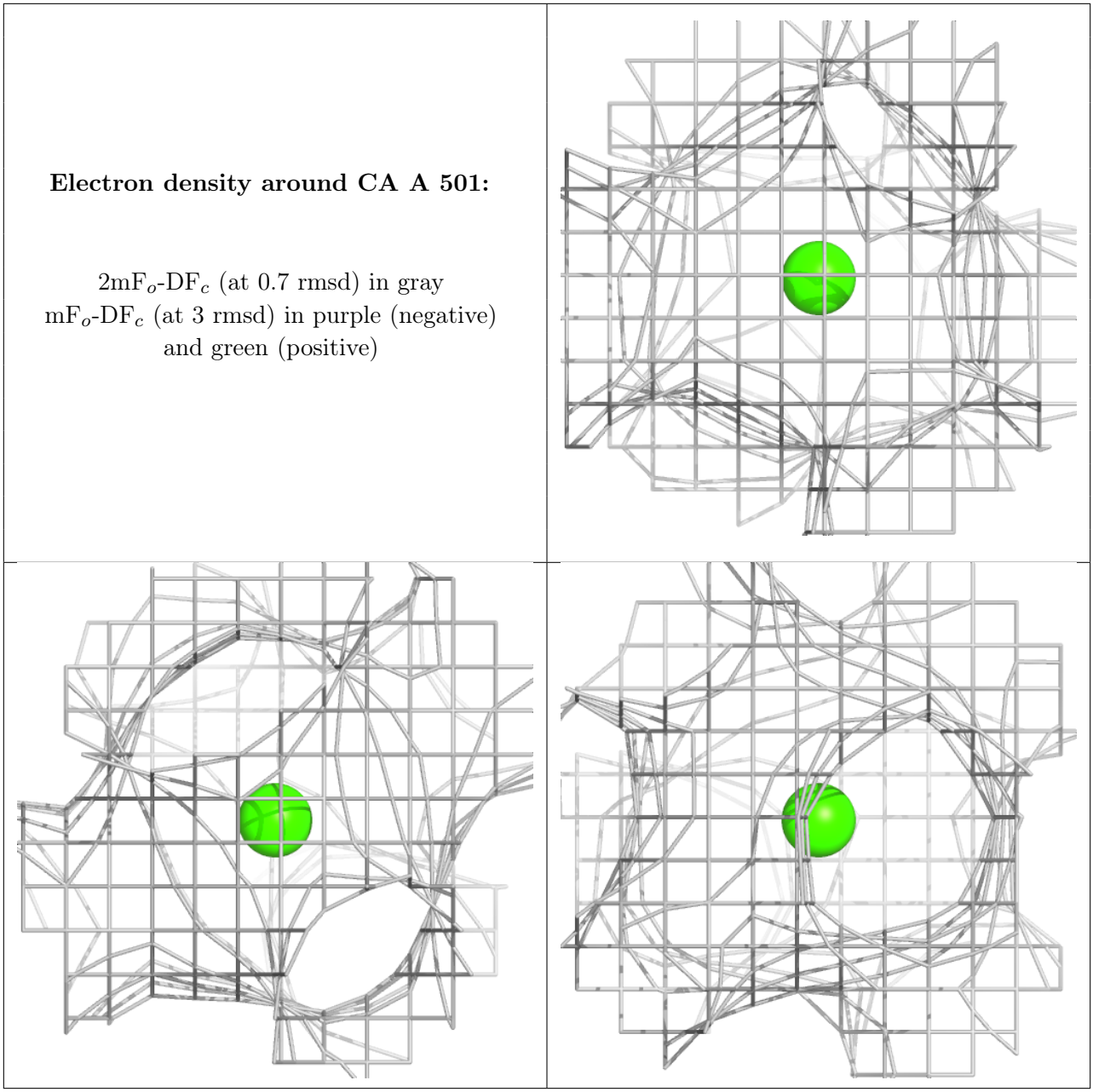
Electron density around CA A 502:

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



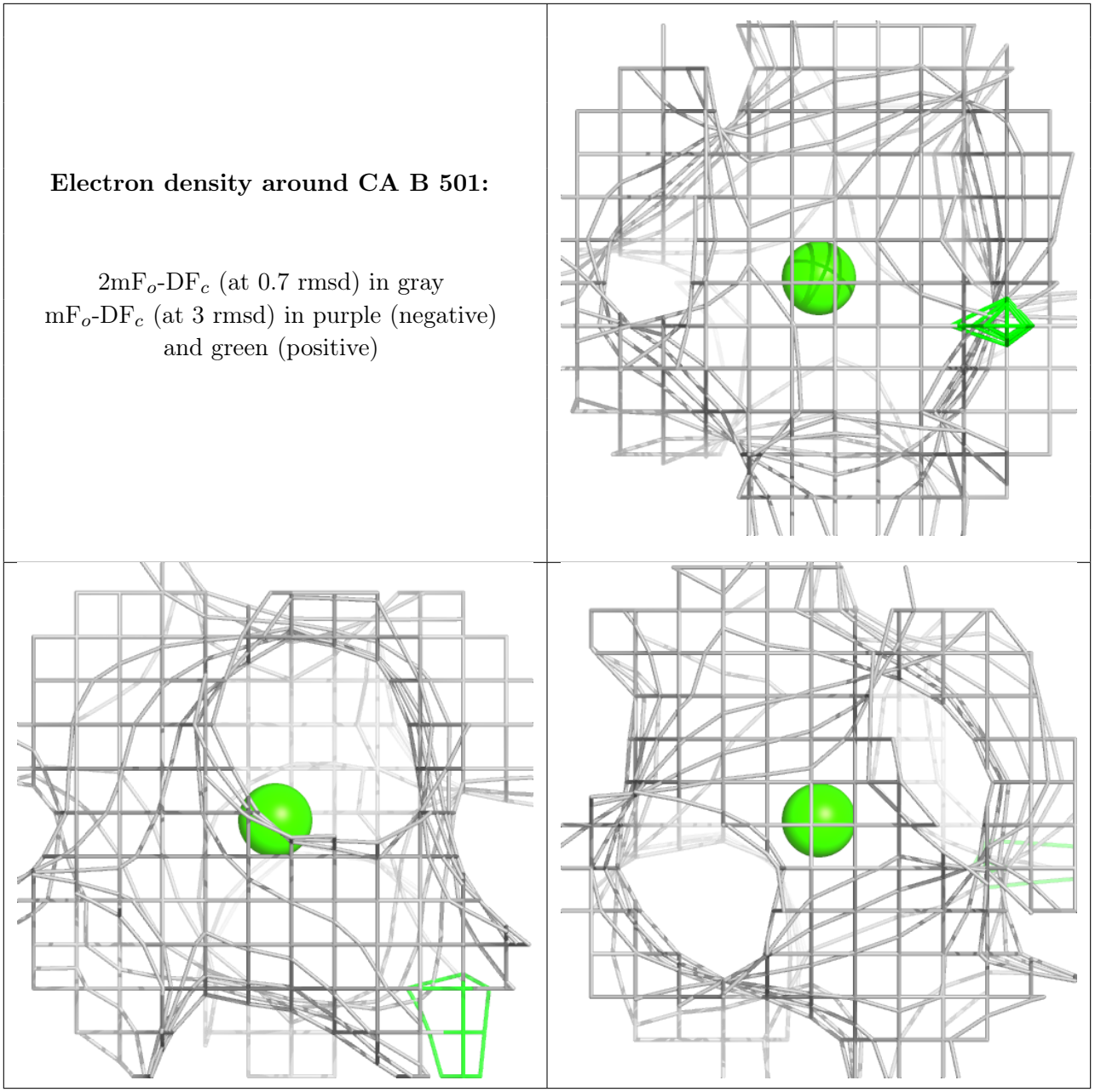
Electron density around CA A 501:

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



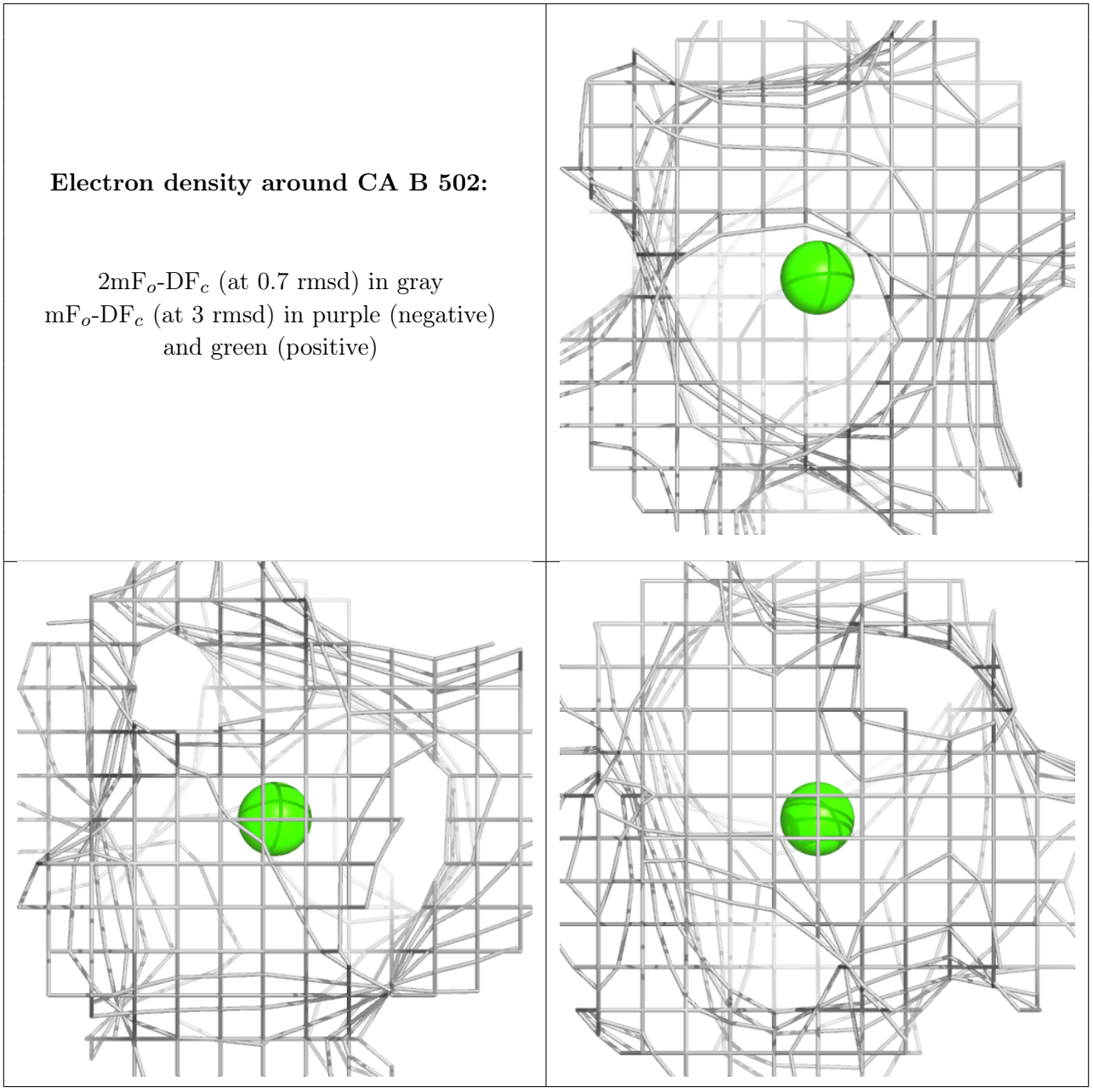
Electron density around CA B 501:

$2mF_o$-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 502:

$2mF_o$-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.