



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2021 – 04:09 PM JST

PDB ID : 7CYM
Title : Crystal structure of LI-Cadherin EC1-4
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Deposited on : 2020-09-03
Resolution : 2.70 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 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 : 2.23.1
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) : 2.23.1

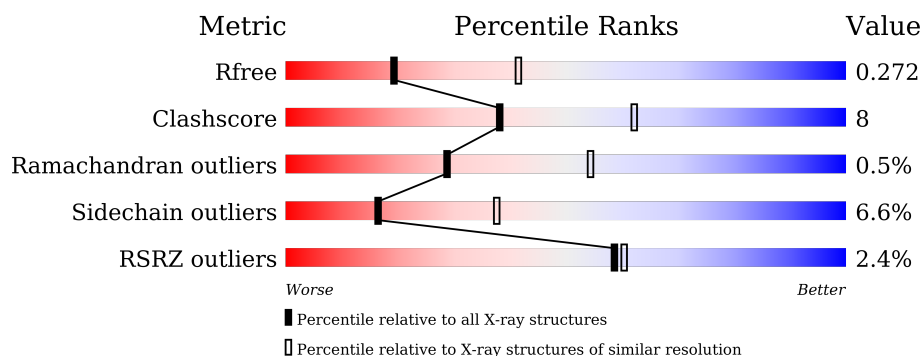
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	440	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>19%</div> <div>• 5%</div> </div> </div>
1	B	440	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>19%</div> <div>• 5%</div> </div> </div>
2	C	4	<div> <div>50%</div> <div>50%</div> </div>
2	E	4	<div> <div>50%</div> <div>50%</div> </div>
3	D	2	<div> <div>50%</div> <div>50%</div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6879 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 Cadherin-17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3324	2111	549	655	9			
1	B	418	Total	C	N	O	S	0	1	0
			3340	2121	553	657	9			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	442	GLU	-	expression tag	UNP Q12864
A	443	GLN	-	expression tag	UNP Q12864
A	444	LYS	-	expression tag	UNP Q12864
A	445	LEU	-	expression tag	UNP Q12864
A	446	ILE	-	expression tag	UNP Q12864
A	447	SER	-	expression tag	UNP Q12864
A	448	GLU	-	expression tag	UNP Q12864
A	449	GLU	-	expression tag	UNP Q12864
A	450	ASP	-	expression tag	UNP Q12864
A	451	LEU	-	expression tag	UNP Q12864
A	452	ASN	-	expression tag	UNP Q12864
A	453	SER	-	expression tag	UNP Q12864
A	454	ALA	-	expression tag	UNP Q12864
A	455	VAL	-	expression tag	UNP Q12864
A	456	ASP	-	expression tag	UNP Q12864
A	457	HIS	-	expression tag	UNP Q12864
A	458	HIS	-	expression tag	UNP Q12864
A	459	HIS	-	expression tag	UNP Q12864
A	460	HIS	-	expression tag	UNP Q12864
A	461	HIS	-	expression tag	UNP Q12864
A	462	HIS	-	expression tag	UNP Q12864
B	442	GLU	-	expression tag	UNP Q12864
B	443	GLN	-	expression tag	UNP Q12864
B	444	LYS	-	expression tag	UNP Q12864
B	445	LEU	-	expression tag	UNP Q12864

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Chain	Residue	Modelled	Actual	Comment	Reference
B	446	ILE	-	expression tag	UNP Q12864
B	447	SER	-	expression tag	UNP Q12864
B	448	GLU	-	expression tag	UNP Q12864
B	449	GLU	-	expression tag	UNP Q12864
B	450	ASP	-	expression tag	UNP Q12864
B	451	LEU	-	expression tag	UNP Q12864
B	452	ASN	-	expression tag	UNP Q12864
B	453	SER	-	expression tag	UNP Q12864
B	454	ALA	-	expression tag	UNP Q12864
B	455	VAL	-	expression tag	UNP Q12864
B	456	ASP	-	expression tag	UNP Q12864
B	457	HIS	-	expression tag	UNP Q12864
B	458	HIS	-	expression tag	UNP Q12864
B	459	HIS	-	expression tag	UNP Q12864
B	460	HIS	-	expression tag	UNP Q12864
B	461	HIS	-	expression tag	UNP Q12864
B	462	HIS	-	expression tag	UNP Q12864

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- 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	6	Total	Ca	0	0
			6	6		
5	B	6	Total	Ca	0	0
			6	6		

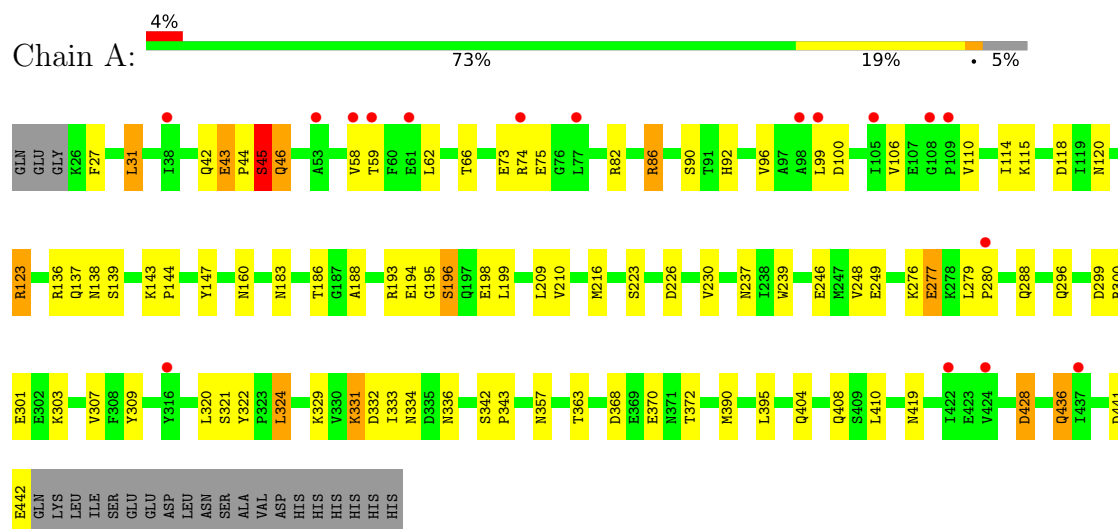
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	12	Total	O	0	0
			12	12		
6	B	21	Total	O	0	0
			21	21		

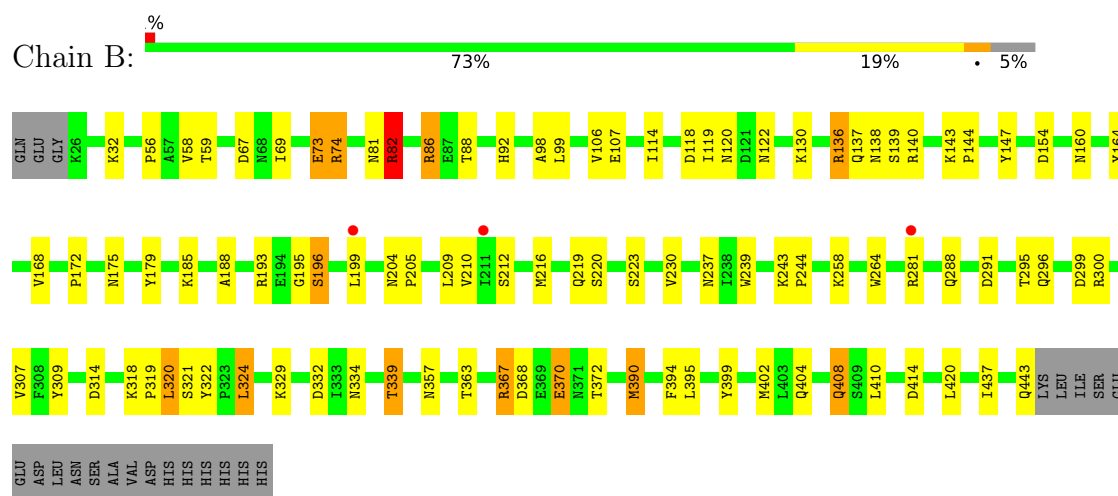
3 Residue-property plots

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: Cadherin-17



• Molecule 1: Cadherin-17



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





- Molecule 2: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.36Å 70.84Å 134.22Å 90.00° 98.69° 90.00°	Depositor
Resolution (Å)	55.25 – 2.70 55.19 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (55.25-2.70) 99.9 (55.19-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.222 , 0.274 0.225 , 0.272	Depositor DCC
R_{free} test set	2040 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	56.4	Xtriage
Anisotropy	0.784	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6879	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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

5.1 Standard geometry

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

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	0.68	4/3399 (0.1%)	0.90	1/4628 (0.0%)
1	B	0.69	0/3419	0.90	4/4655 (0.1%)
All	All	0.68	4/6818 (0.1%)	0.90	5/9283 (0.1%)

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	7
1	B	0	9
All	All	0	16

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	301	GLU	CG-CD	8.15	1.64	1.51
1	A	73	GLU	CD-OE1	7.21	1.33	1.25
1	A	442	GLU	CD-OE1	5.95	1.32	1.25
1	A	226	ASP	CB-CG	5.40	1.63	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	414	ASP	CB-CA-C	7.13	124.66	110.40
1	A	296	GLN	CB-CA-C	-5.89	98.62	110.40
1	B	296	GLN	CB-CA-C	-5.51	99.38	110.40
1	B	339	THR	CA-CB-OG1	-5.45	97.56	109.00
1	B	408	GLN	CB-CA-C	-5.36	99.68	110.40

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	ARG	Sidechain
1	A	136	ARG	Sidechain
1	A	45	SER	Peptide
1	A	74	ARG	Sidechain
1	A	75	GLU	Peptide
1	A	82	ARG	Sidechain
1	A	86	ARG	Sidechain
1	B	136	ARG	Sidechain
1	B	140	ARG	Sidechain
1	B	193	ARG	Sidechain
1	B	205	PRO	Peptide
1	B	281	ARG	Sidechain
1	B	367	ARG	Sidechain
1	B	74	ARG	Sidechain
1	B	82	ARG	Sidechain
1	B	86	ARG	Sidechain

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	3324	0	3263	48	0
1	B	3340	0	3280	55	0
2	C	50	0	43	3	0
2	E	50	0	43	2	0
3	D	28	0	25	0	0
4	A	28	0	26	0	0
4	B	14	0	13	1	0
5	A	6	0	0	0	0
5	B	6	0	0	0	0
6	A	12	0	0	0	0
6	B	21	0	0	1	0
All	All	6879	0	6693	103	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 8.

All (103) 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:419:ASN:OD1	1:A:436:GLN:NE2	2.16	0.78
1:B:137:GLN:HE21	1:B:237:ASN:H	1.34	0.76
1:A:137:GLN:HE21	1:A:237:ASN:H	1.32	0.74
1:A:300:ARG:HD3	1:A:332:ASP:HB2	1.73	0.70
1:B:300:ARG:HD3	1:B:332:ASP:HB2	1.74	0.69
1:B:179:TYR:CD2	1:B:199:LEU:HD13	2.28	0.69
1:B:86:ARG:HD3	1:B:118:ASP:HB2	1.78	0.64
1:A:239:TRP:CE2	1:A:324:LEU:HD22	2.34	0.63
1:B:239:TRP:CE2	1:B:324:LEU:HD22	2.34	0.63
1:A:139:SER:O	1:A:196:SER:OG	2.18	0.62
1:B:395:LEU:C	1:B:395:LEU:HD12	2.22	0.60
1:A:336:ASN:HD22	2:C:2:NAG:H5	1.65	0.60
1:A:58:VAL:HG23	1:A:59:THR:HG23	1.83	0.59
1:B:139:SER:O	1:B:196:SER:OG	2.20	0.59
1:A:147:TYR:CE1	1:A:188:ALA:HB2	2.38	0.59
1:A:277:GLU:HB2	1:A:279:LEU:HD21	1.85	0.59
1:B:147:TYR:CE1	1:B:188:ALA:HB2	2.38	0.58
1:A:279:LEU:HB3	1:A:280:PRO:HD2	1.85	0.58
1:A:336:ASN:ND2	2:C:2:NAG:H5	2.19	0.58
1:A:395:LEU:HD12	1:A:395:LEU:C	2.24	0.57
1:B:420:LEU:HD11	1:B:437:ILE:CD1	2.35	0.56
1:B:73:GLU:OE2	1:B:73:GLU:HA	2.06	0.55
1:A:299:ASP:HB2	2:C:1:NAG:H81	1.87	0.55
1:B:420:LEU:HD11	1:B:437:ILE:HD12	1.88	0.55
2:E:1:NAG:H61	2:E:2:NAG:C7	2.36	0.55
1:A:147:TYR:HE1	1:A:186:THR:HG22	1.70	0.55
1:A:86:ARG:HD3	1:A:118:ASP:HB2	1.89	0.55
1:B:59:THR:HG21	1:B:74:ARG:HH21	1.71	0.55
1:B:136:ARG:HG3	1:B:136:ARG:HH11	1.73	0.54
1:B:367:ARG:HH11	1:B:367:ARG:CG	2.21	0.53
1:B:264:TRP:CD1	1:B:320:LEU:HD23	2.44	0.53
1:A:31:LEU:HD12	1:A:110:VAL:CG2	2.39	0.53
1:B:390:MET:SD	1:B:408:GLN:NE2	2.83	0.52
1:B:395:LEU:HD11	1:B:404:GLN:HB2	1.90	0.52
1:B:122:ASN:HB2	1:B:154:ASP:OD1	2.09	0.52
1:B:395:LEU:HD12	1:B:395:LEU:O	2.10	0.52
1:A:246:GLU:HB3	1:A:331:LYS:CE	2.41	0.51
1:B:367:ARG:HH11	1:B:367:ARG:HG2	1.76	0.51
1:B:81:ASN:O	1:B:82:ARG:HB3	2.11	0.51
1:B:58:VAL:HG23	1:B:59:THR:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ASN:O	1:A:404:GLN:HA	2.11	0.50
1:B:56:PRO:HG2	1:B:106:VAL:HG11	1.94	0.50
1:A:334:ASN:ND2	1:A:428:ASP:OD1	2.45	0.50
1:A:248:VAL:HG12	1:A:249:GLU:O	2.12	0.49
1:A:216:MET:HB2	1:A:223:SER:HB3	1.95	0.49
1:A:137:GLN:HG2	1:A:237:ASN:HB2	1.95	0.49
1:A:31:LEU:HD21	1:A:96:VAL:HG12	1.96	0.48
1:A:210:VAL:HG11	1:B:399:TYR:CE2	2.49	0.48
1:B:216:MET:HB2	1:B:223:SER:HB3	1.95	0.48
1:B:318:LYS:O	1:B:320:LEU:N	2.46	0.48
1:B:138:ASN:HA	1:B:196:SER:O	2.14	0.48
1:B:321:SER:OG	1:B:322:TYR:N	2.46	0.48
1:B:119:ILE:HA	6:B:615:HOH:O	2.13	0.48
1:B:120:ASN:HA	1:B:154:ASP:OD2	2.14	0.48
1:B:92:HIS:HB2	1:B:114:ILE:HB	1.96	0.47
1:A:195:GLY:O	1:A:199:LEU:HB2	2.14	0.47
1:A:370:GLU:O	1:A:372:THR:HG23	2.14	0.47
1:B:179:TYR:CD2	1:B:199:LEU:CD1	2.95	0.47
1:B:164:TYR:CE1	4:B:501:NAG:H82	2.49	0.47
1:A:309:TYR:HA	1:A:324:LEU:O	2.15	0.47
1:A:43:GLU:O	1:A:45:SER:N	2.49	0.46
1:A:62:LEU:CD1	1:A:66:THR:HG22	2.44	0.46
1:B:209:LEU:HB2	1:B:230:VAL:HB	1.97	0.46
1:B:137:GLN:HG2	1:B:237:ASN:HB2	1.97	0.46
1:A:137:GLN:HG2	1:A:237:ASN:CB	2.46	0.46
1:A:183:ASN:ND2	1:A:186:THR:HB	2.31	0.46
1:B:172:PRO:HG3	1:B:204:ASN:HD21	1.81	0.46
1:A:209:LEU:HB2	1:A:230:VAL:HB	1.98	0.45
1:A:321:SER:OG	1:A:322:TYR:N	2.49	0.45
1:B:239:TRP:CZ2	1:B:324:LEU:HD22	2.51	0.45
1:A:45:SER:O	1:A:46:GLN:HB2	2.16	0.45
1:B:195:GLY:O	1:B:199:LEU:HB2	2.16	0.45
1:B:258:LYS:HE2	1:B:291:ASP:CG	2.36	0.45
1:A:92:HIS:HB2	1:A:114:ILE:HB	1.98	0.45
1:A:248:VAL:HG13	1:A:333:ILE:HG12	1.97	0.45
1:A:239:TRP:CZ2	1:A:324:LEU:HD22	2.51	0.45
1:A:138:ASN:HA	1:A:196:SER:O	2.17	0.45
1:A:395:LEU:HD12	1:A:395:LEU:O	2.17	0.44
1:B:370:GLU:O	1:B:372:THR:HG23	2.17	0.44
1:B:309:TYR:HA	1:B:324:LEU:O	2.16	0.44
1:B:394:PHE:CD2	1:B:420:LEU:HD21	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ASN:HB2	1:A:160:ASN:OD1	2.17	0.44
1:B:120:ASN:HB2	1:B:160:ASN:OD1	2.17	0.44
1:B:334:ASN:HA	1:B:368:ASP:OD2	2.18	0.43
1:A:31:LEU:HD12	1:A:110:VAL:HG22	2.00	0.43
1:A:334:ASN:HA	1:A:368:ASP:OD2	2.19	0.43
1:A:31:LEU:CD1	1:A:110:VAL:HG22	2.48	0.43
1:B:98:ALA:HB3	1:B:107:GLU:HB2	2.00	0.43
1:B:168:VAL:HB	1:B:210:VAL:HG12	2.00	0.43
1:B:299:ASP:HB2	2:E:1:NAG:H81	2.00	0.43
1:B:314:ASP:N	1:B:320:LEU:HD13	2.33	0.43
1:A:100:ASP:HB3	1:A:106:VAL:HG11	2.01	0.42
1:B:243:LYS:HD3	1:B:244:PRO:HD2	2.02	0.42
1:A:194:GLU:O	1:A:198:GLU:HG2	2.21	0.41
1:B:307:VAL:O	1:B:307:VAL:HG23	2.21	0.41
1:A:143:LYS:HA	1:A:144:PRO:HD2	1.87	0.41
1:A:246:GLU:HB3	1:A:331:LYS:HE2	2.03	0.41
1:B:67:ASP:O	1:B:69:ILE:HG13	2.20	0.41
1:B:86:ARG:CD	1:B:118:ASP:HB2	2.49	0.40
1:B:143:LYS:HA	1:B:144:PRO:HD3	1.99	0.40
1:B:394:PHE:CE1	1:B:437:ILE:HD13	2.57	0.40
1:B:175:ASN:HD22	1:B:175:ASN:HA	1.72	0.40
1:A:342:SER:HB2	1:A:343:PRO:HD2	2.03	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	415/440 (94%)	390 (94%)	23 (6%)	2 (0%)	29	54
1	B	417/440 (95%)	393 (94%)	22 (5%)	2 (0%)	29	54
All	All	832/880 (94%)	783 (94%)	45 (5%)	4 (0%)	29	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	PRO
1	A	46	GLN
1	B	319	PRO
1	B	370	GLU

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	378/399 (95%)	351 (93%)	27 (7%)	14	34
1	B	380/399 (95%)	357 (94%)	23 (6%)	18	41
All	All	758/798 (95%)	708 (93%)	50 (7%)	16	38

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	PHE
1	A	31	LEU
1	A	42	GLN
1	A	43	GLU
1	A	45	SER
1	A	90	SER
1	A	99	LEU
1	A	115	LYS
1	A	123	ARG
1	A	193	ARG
1	A	196	SER
1	A	276	LYS
1	A	277	GLU
1	A	288	GLN
1	A	303	LYS
1	A	307	VAL
1	A	320	LEU
1	A	324	LEU
1	A	329	LYS

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Mol	Chain	Res	Type
1	A	331	LYS
1	A	363	THR
1	A	390	MET
1	A	408	GLN
1	A	410	LEU
1	A	428	ASP
1	A	436	GLN
1	A	441	ASP
1	B	32	LYS
1	B	73	GLU
1	B	82	ARG
1	B	88	THR
1	B	99	LEU
1	B	130	LYS
1	B	185	LYS
1	B	196	SER
1	B	212	SER
1	B	219	GLN
1	B	220	SER
1	B	288	GLN
1	B	295	THR
1	B	320	LEU
1	B	324	LEU
1	B	329	LYS
1	B	339	THR
1	B	357	ASN
1	B	363	THR
1	B	390	MET
1	B	402	MET
1	B	410	LEU
1	B	443	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	336	ASN
1	A	417	GLN
1	B	137	GLN
1	B	175	ASN
1	B	197	GLN
1	B	204	ASN

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Mol	Chain	Res	Type
1	B	219	GLN
1	B	350	GLN

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 ⓘ

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	$\# Z > 2$
2	NAG	C	1	1,2,5	14,14,15	0.83	0	17,19,21	1.57	4 (23%)
2	NAG	C	2	2	14,14,15	0.60	0	17,19,21	1.48	1 (5%)
2	BMA	C	3	2	11,11,12	0.68	0	15,15,17	1.78	3 (20%)
2	MAN	C	4	2	11,11,12	0.94	0	15,15,17	3.65	7 (46%)
3	NAG	D	1	1,3	14,14,15	0.71	1 (7%)	17,19,21	1.46	4 (23%)
3	NAG	D	2	3	14,14,15	0.35	0	17,19,21	0.69	0
2	NAG	E	1	1,2,5	14,14,15	0.63	0	17,19,21	1.67	5 (29%)
2	NAG	E	2	2	14,14,15	0.88	0	17,19,21	2.50	8 (47%)
2	BMA	E	3	2	11,11,12	1.53	3 (27%)	15,15,17	2.42	5 (33%)
2	MAN	E	4	2	11,11,12	1.65	3 (27%)	15,15,17	1.79	4 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2,5	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	3/6/23/26	0/1/1/1
2	NAG	E	1	1,2,5	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	MAN	E	4	2	-	0/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	4	MAN	C1-C2	3.06	1.59	1.52
2	E	3	BMA	C4-C3	2.89	1.59	1.52
2	E	4	MAN	C2-C3	2.65	1.56	1.52
2	E	4	MAN	O2-C2	2.60	1.48	1.43
2	E	3	BMA	C4-C5	2.33	1.57	1.53
2	E	3	BMA	O3-C3	2.32	1.48	1.43
3	D	1	NAG	C1-C2	2.00	1.55	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	MAN	C1-C2-C3	9.25	121.03	109.67
2	C	4	MAN	C1-O5-C5	7.80	122.76	112.19
2	E	2	NAG	O5-C5-C6	6.36	117.18	107.20
2	C	2	NAG	O5-C1-C2	-5.22	103.05	111.29
2	E	3	BMA	O2-C2-C1	-5.19	98.52	109.15
2	E	3	BMA	O3-C3-C4	4.99	121.89	110.35
2	C	3	BMA	O5-C1-C2	-4.42	103.95	110.77
2	E	4	MAN	C1-C2-C3	4.19	114.82	109.67
2	E	2	NAG	C3-C4-C5	4.07	117.50	110.24
2	C	1	NAG	C8-C7-N2	-3.98	109.35	116.10
2	E	1	NAG	C4-C3-C2	-3.71	105.58	111.02
3	D	1	NAG	C1-O5-C5	3.47	116.89	112.19
2	C	3	BMA	C1-C2-C3	3.38	113.81	109.67
2	E	3	BMA	C6-C5-C4	3.32	120.78	113.00
2	E	2	NAG	C6-C5-C4	-3.31	105.25	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	MAN	O5-C1-C2	3.18	115.67	110.77
2	C	4	MAN	O5-C5-C4	3.12	118.42	110.83
2	E	4	MAN	O2-C2-C1	2.95	115.18	109.15
2	E	2	NAG	C1-C2-N2	2.93	115.49	110.49
2	E	4	MAN	O5-C5-C6	2.92	111.78	107.20
2	E	2	NAG	O4-C4-C3	-2.92	103.61	110.35
2	C	4	MAN	C3-C4-C5	2.89	115.40	110.24
2	C	1	NAG	O7-C7-N2	2.82	127.13	121.95
2	C	4	MAN	C2-C3-C4	2.65	115.49	110.89
2	C	1	NAG	O4-C4-C5	2.60	115.74	109.30
2	E	3	BMA	O2-C2-C3	2.52	115.20	110.14
2	E	1	NAG	O5-C5-C6	2.47	111.08	107.20
2	C	3	BMA	O5-C5-C4	-2.43	104.91	110.83
2	E	2	NAG	C4-C3-C2	2.43	114.58	111.02
2	E	4	MAN	O4-C4-C3	2.21	115.45	110.35
2	C	1	NAG	C1-O5-C5	2.17	115.14	112.19
3	D	1	NAG	O3-C3-C4	-2.14	105.41	110.35
2	E	2	NAG	O3-C3-C4	-2.13	105.43	110.35
2	E	1	NAG	C3-C4-C5	-2.12	106.46	110.24
2	E	1	NAG	C8-C7-N2	-2.10	112.54	116.10
2	E	2	NAG	C8-C7-N2	-2.09	112.56	116.10
2	C	4	MAN	C6-C5-C4	-2.08	108.14	113.00
2	E	3	BMA	C3-C4-C5	2.05	113.89	110.24
2	E	1	NAG	O3-C3-C4	2.04	115.06	110.35
3	D	1	NAG	O5-C5-C6	2.03	110.38	107.20
3	D	1	NAG	O4-C4-C3	-2.00	105.72	110.35

There are no chirality outliers.

All (11) torsion outliers are listed below:

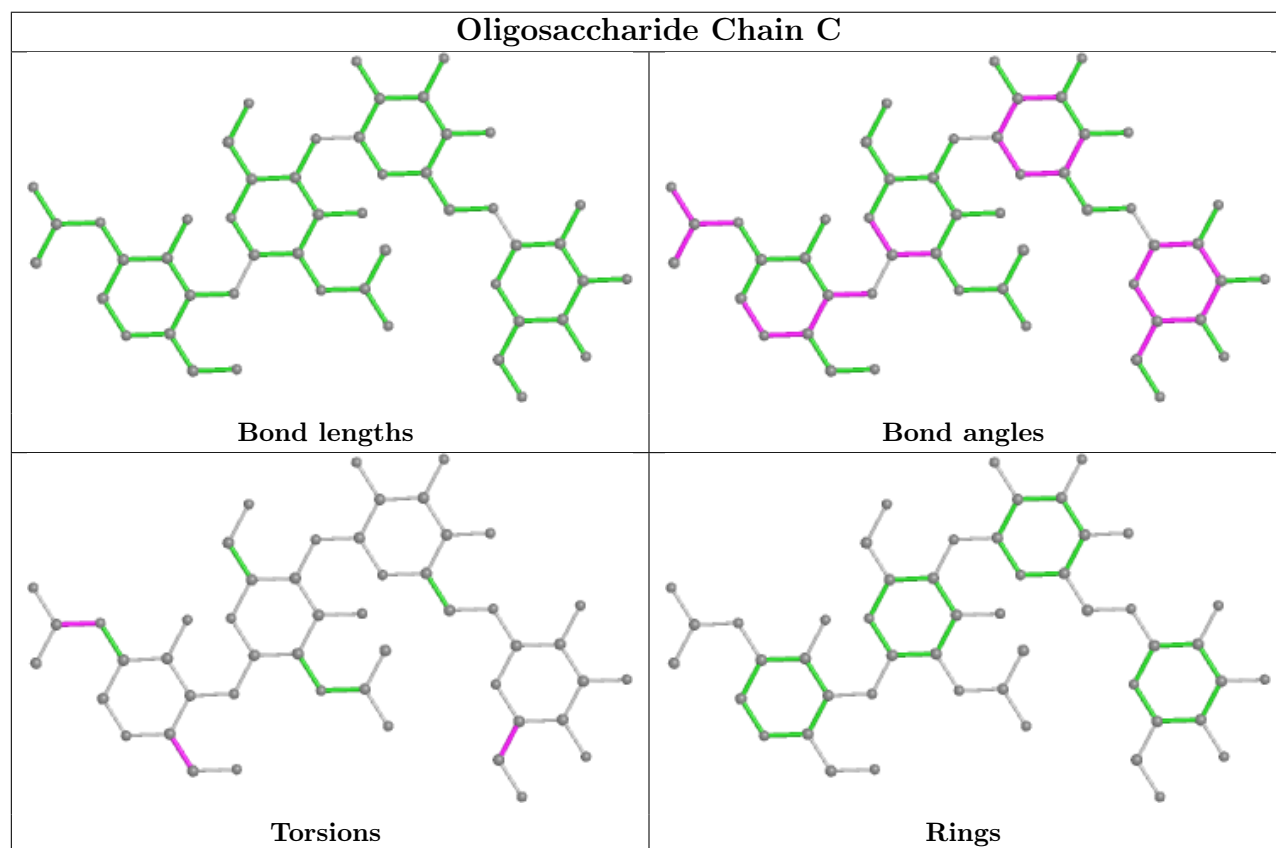
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	O5-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
3	D	2	NAG	C8-C7-N2-C2
2	E	1	NAG	O5-C5-C6-O6
3	D	2	NAG	O7-C7-N2-C2
2	C	4	MAN	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	C4-C5-C6-O6

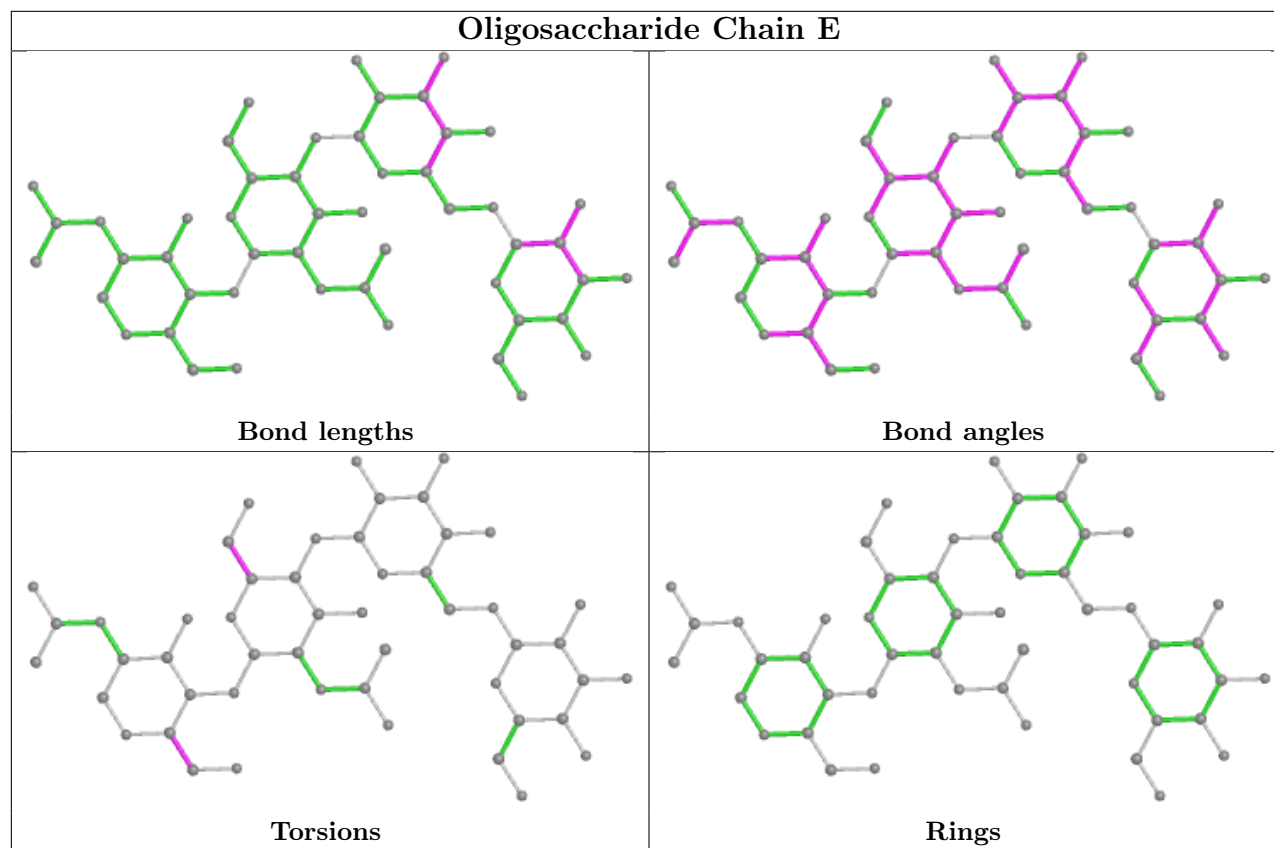
There are no ring outliers.

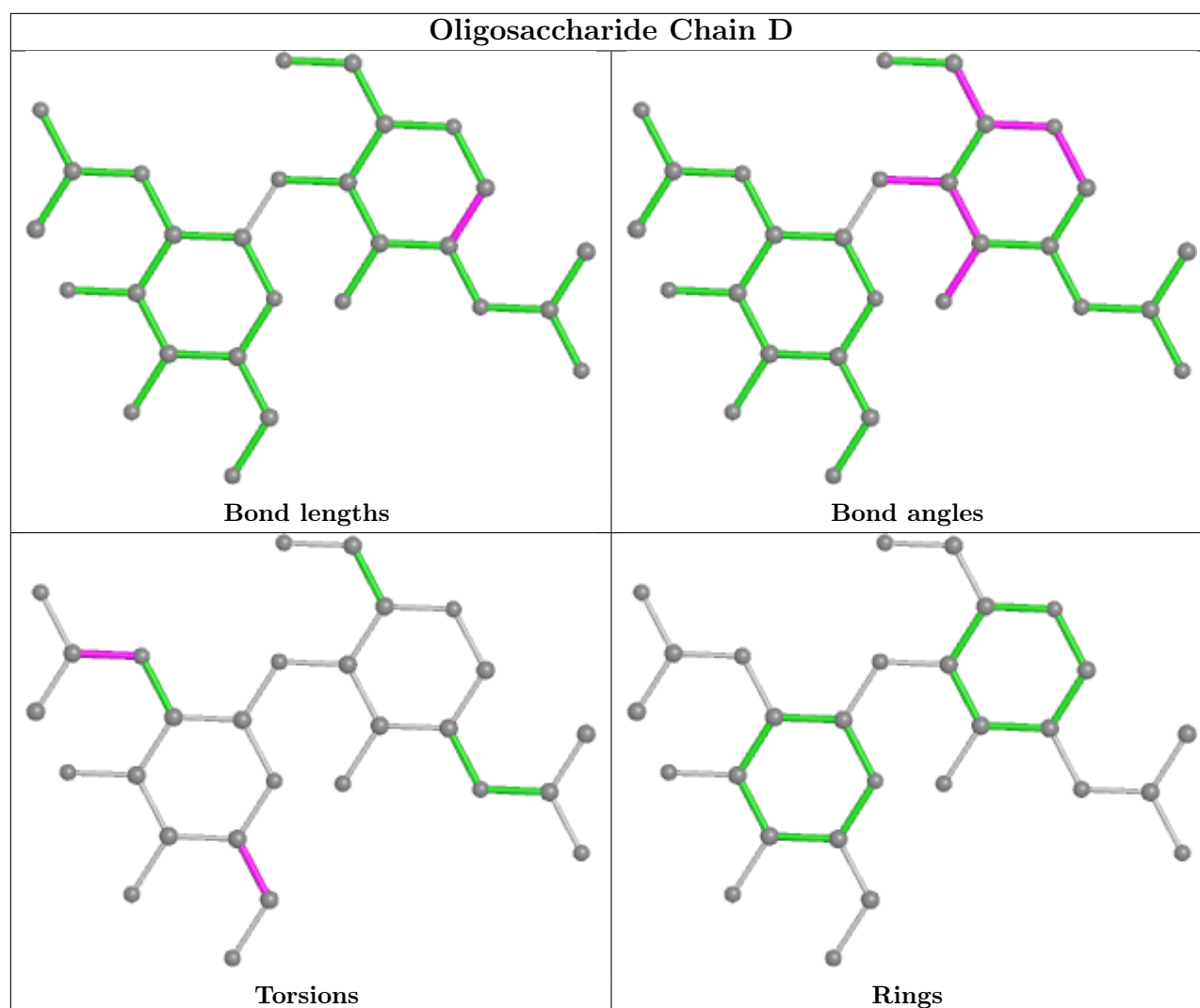
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	1	0
2	E	1	NAG	2	0
2	C	1	NAG	1	0
2	C	2	NAG	2	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.







5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 12 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	$\# Z > 2$
4	NAG	A	501	1	14,14,15	1.99	5 (35%)	17,19,21	3.48	11 (64%)
4	NAG	B	501	1	14,14,15	0.72	0	17,19,21	1.08	1 (5%)
4	NAG	A	502	1	14,14,15	0.94	0	17,19,21	1.67	2 (11%)

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	A	501	1	-	0/6/23/26	0/1/1/1
4	NAG	B	501	1	-	0/6/23/26	0/1/1/1
4	NAG	A	502	1	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	NAG	C2-N2	3.59	1.52	1.46
4	A	501	NAG	O5-C1	3.29	1.49	1.43
4	A	501	NAG	C1-C2	2.69	1.56	1.52
4	A	501	NAG	C3-C2	2.54	1.57	1.52
4	A	501	NAG	O5-C5	2.47	1.48	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	NAG	C2-N2-C7	7.12	133.04	122.90
4	A	501	NAG	C1-O5-C5	6.87	121.50	112.19
4	A	501	NAG	O5-C5-C6	6.51	117.41	107.20
4	A	502	NAG	C1-O5-C5	5.02	119.00	112.19
4	A	501	NAG	O5-C1-C2	3.66	117.07	111.29
4	A	501	NAG	O7-C7-C8	-3.12	116.26	122.06
4	A	502	NAG	C6-C5-C4	-3.09	105.77	113.00
4	A	501	NAG	O7-C7-N2	2.94	127.35	121.95
4	A	501	NAG	C4-C3-C2	2.71	114.99	111.02
4	A	501	NAG	O3-C3-C2	2.67	115.00	109.47
4	B	501	NAG	C2-N2-C7	-2.25	119.69	122.90
4	A	501	NAG	O3-C3-C4	-2.12	105.45	110.35
4	A	501	NAG	C6-C5-C4	-2.10	108.09	113.00
4	A	501	NAG	C3-C4-C5	2.05	113.89	110.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	417/440 (94%)	0.29	17 (4%) 37 36	57, 80, 115, 139	0
1	B	418/440 (95%)	0.19	3 (0%) 87 89	54, 69, 91, 128	0
All	All	835/880 (94%)	0.24	20 (2%) 59 60	54, 74, 108, 139	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	59	THR	4.1
1	A	108	GLY	4.1
1	A	99	LEU	3.9
1	A	98	ALA	3.8
1	A	74	ARG	3.4
1	A	58	VAL	3.4
1	A	77	LEU	2.9
1	A	280	PRO	2.9
1	B	199	LEU	2.8
1	A	105	ILE	2.7
1	B	211	ILE	2.7
1	A	53	ALA	2.5
1	A	38	ILE	2.4
1	A	61	GLU	2.3
1	A	422	ILE	2.3
1	A	109	PRO	2.2
1	A	424	VAL	2.1
1	A	437	ILE	2.1
1	B	281	ARG	2.0
1	A	316	TYR	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](#)

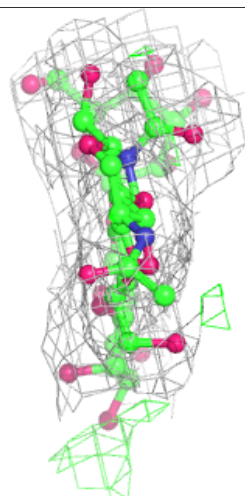
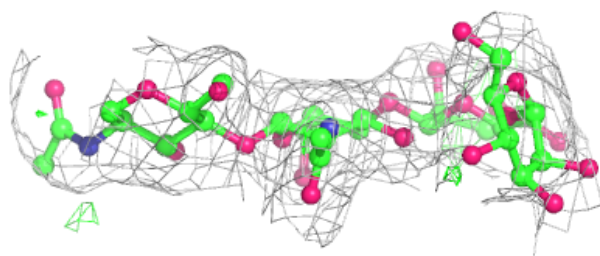
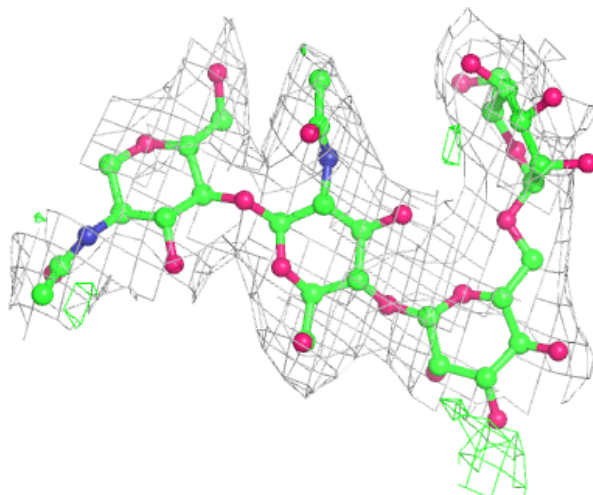
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MAN	E	4	11/12	0.79	0.16	94,103,108,110	0
3	NAG	D	2	14/15	0.82	0.12	131,137,142,146	0
2	BMA	C	3	11/12	0.84	0.13	107,113,118,119	0
2	BMA	E	3	11/12	0.87	0.12	94,99,101,102	0
2	MAN	C	4	11/12	0.88	0.16	113,118,127,129	0
3	NAG	D	1	14/15	0.89	0.10	116,120,127,130	0
2	NAG	C	2	14/15	0.90	0.11	100,110,118,120	0
2	NAG	C	1	14/15	0.93	0.13	91,96,102,107	0
2	NAG	E	2	14/15	0.93	0.14	75,90,95,98	0
2	NAG	E	1	14/15	0.95	0.16	62,69,75,80	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.

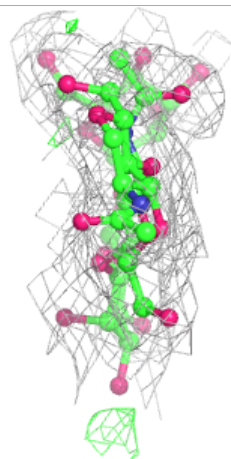
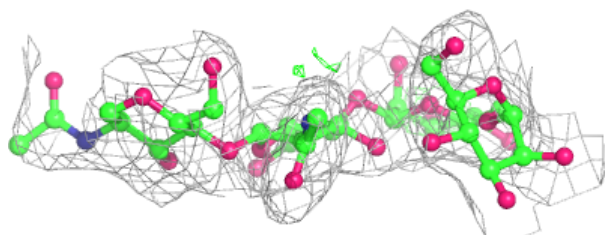
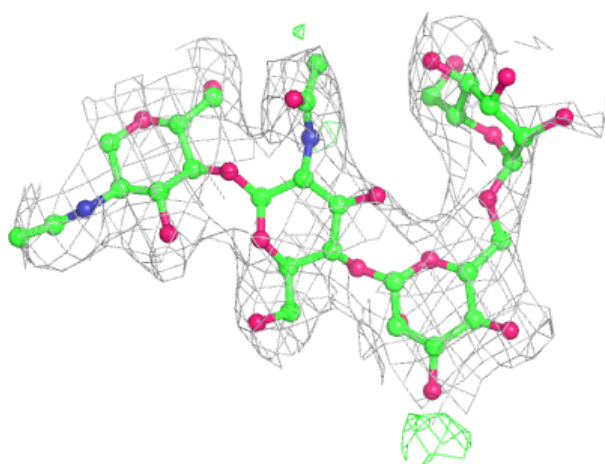
Electron density around Chain C:

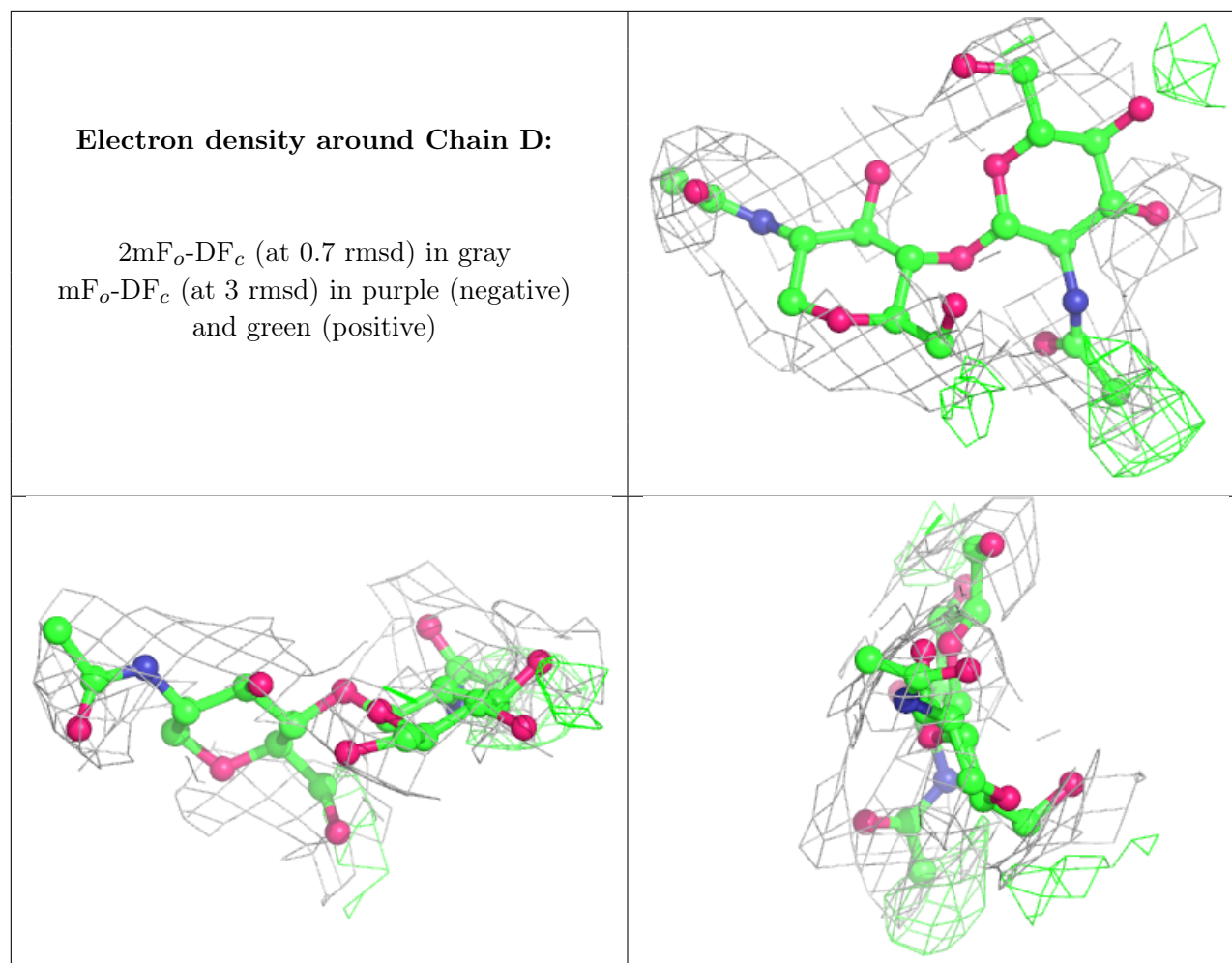
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain E:

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





6.4 Ligands ⓘ

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.

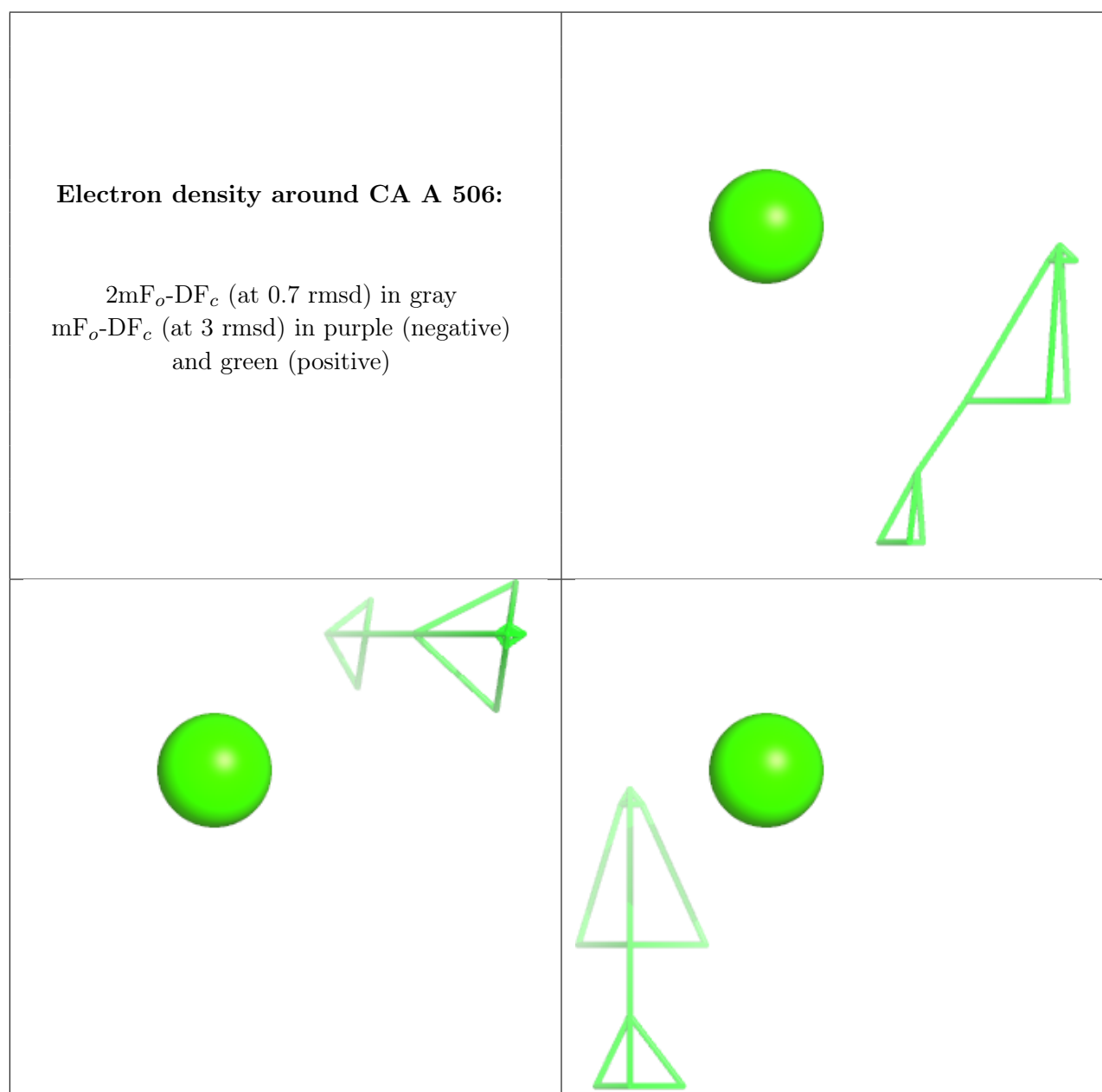
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	501	14/15	0.79	0.14	96,112,116,117	0
4	NAG	A	502	14/15	0.89	0.12	90,95,111,114	0
4	NAG	B	501	14/15	0.93	0.07	94,99,103,106	0
5	CA	A	506	1/1	0.96	0.21	84,84,84,84	0
5	CA	A	505	1/1	0.97	0.16	70,70,70,70	0
5	CA	B	502	1/1	0.97	0.19	66,66,66,66	0
5	CA	A	507	1/1	0.98	0.17	72,72,72,72	0
5	CA	B	503	1/1	0.98	0.13	72,72,72,72	0
5	CA	B	506	1/1	0.98	0.19	68,68,68,68	0
5	CA	A	508	1/1	0.99	0.17	75,75,75,75	0

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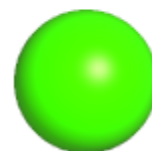
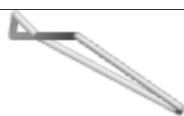
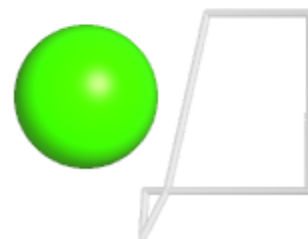
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	CA	B	504	1/1	0.99	0.13	69,69,69,69	0
5	CA	B	505	1/1	0.99	0.21	59,59,59,59	0
5	CA	A	503	1/1	0.99	0.18	66,66,66,66	0
5	CA	B	507	1/1	0.99	0.20	57,57,57,57	0
5	CA	A	504	1/1	1.00	0.20	67,67,67,67	0

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.



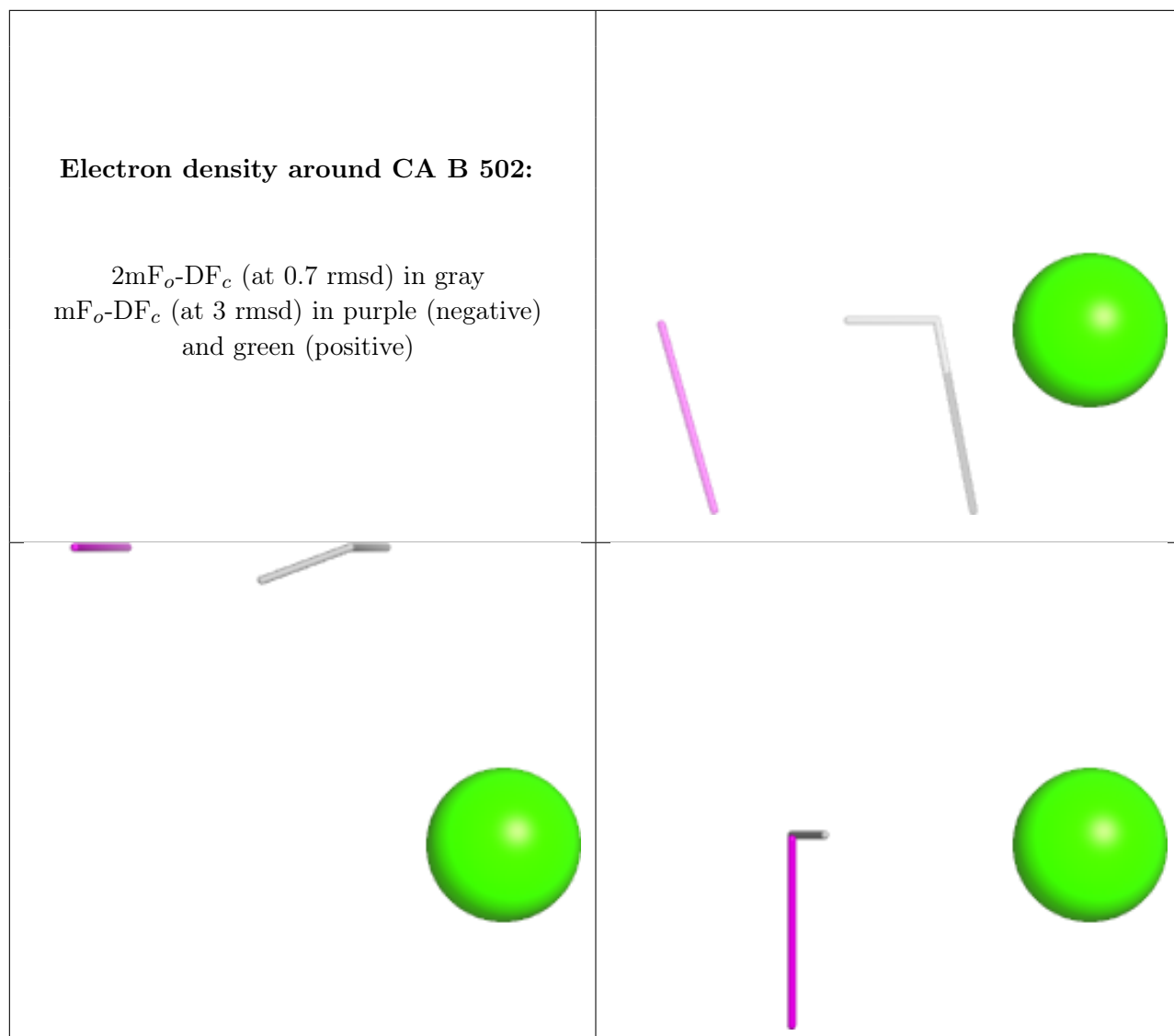
Electron density around CA A 505:

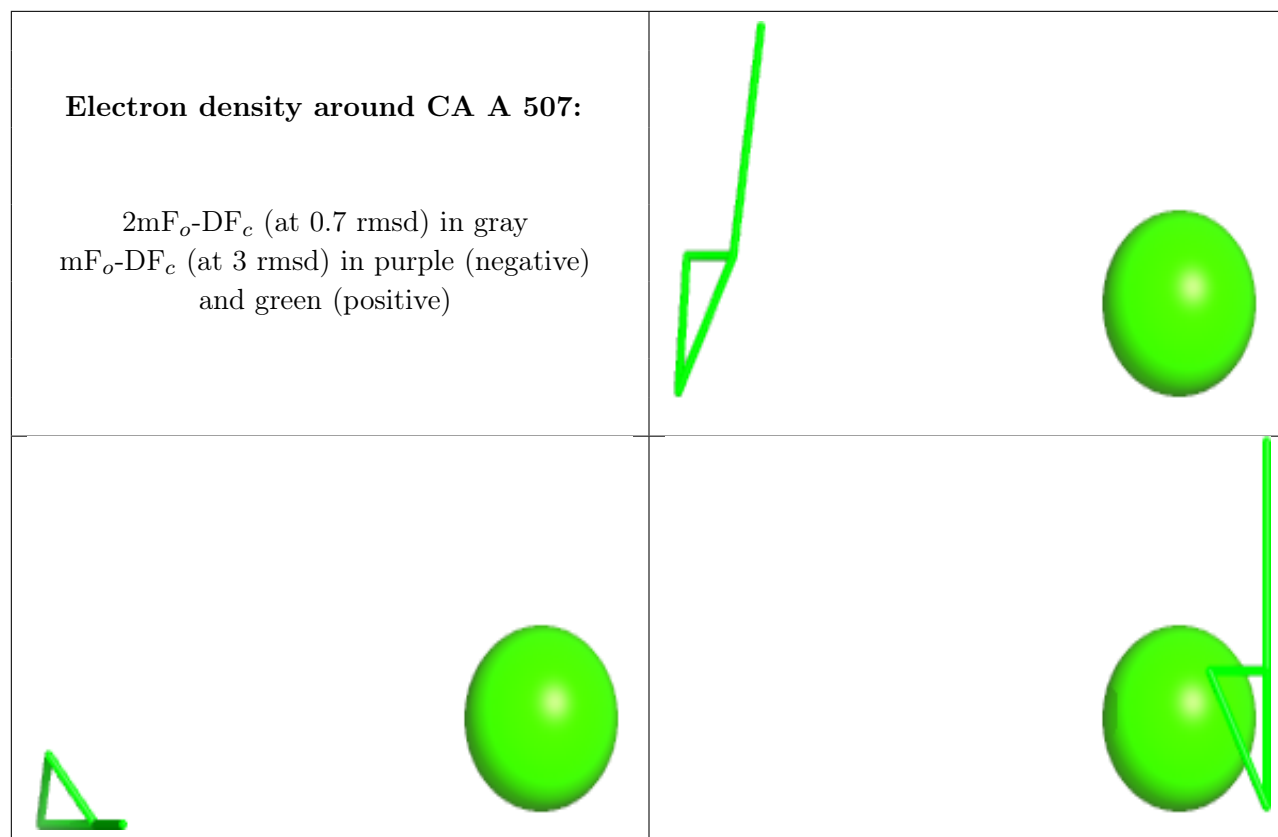
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA B 502:

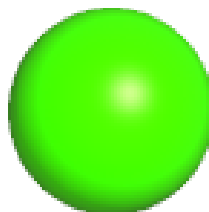
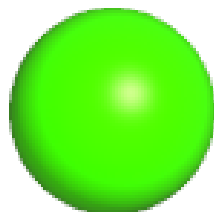
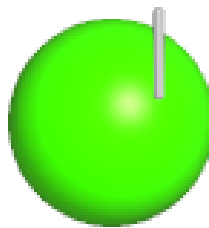
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





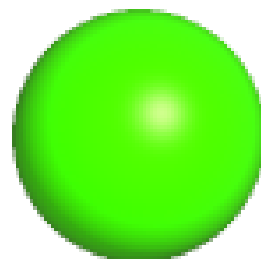
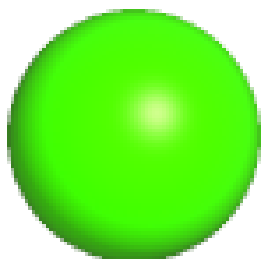
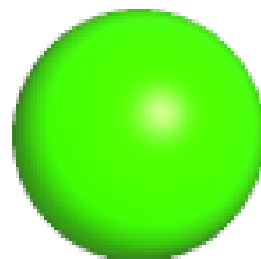
Electron density around CA B 503:

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



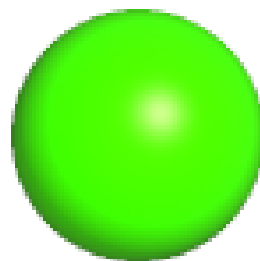
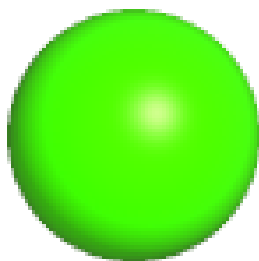
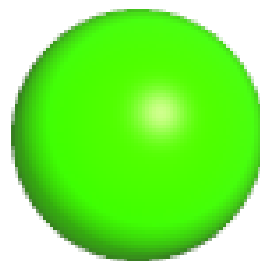
Electron density around CA B 506:

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



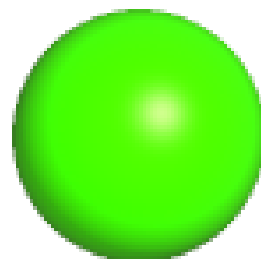
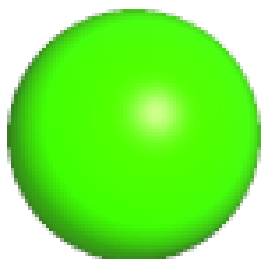
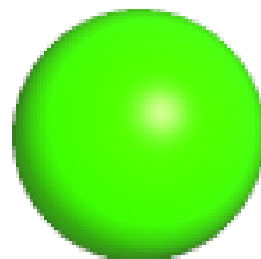
Electron density around CA A 508:

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



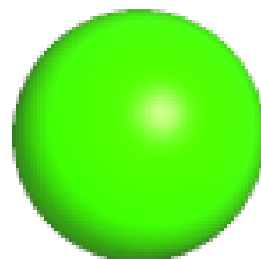
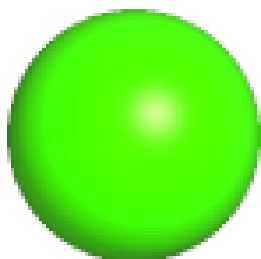
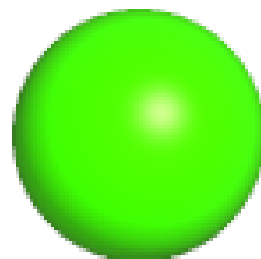
Electron density around CA B 504:

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



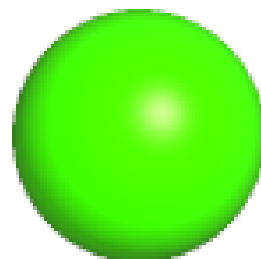
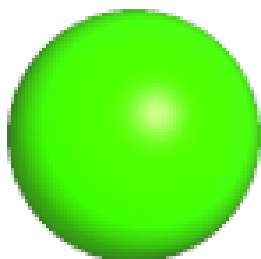
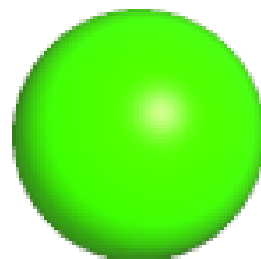
Electron density around CA B 505:

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



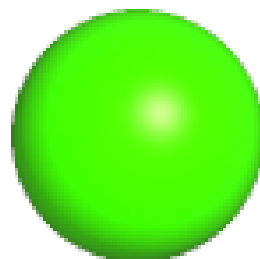
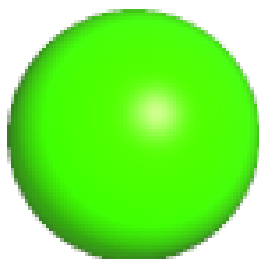
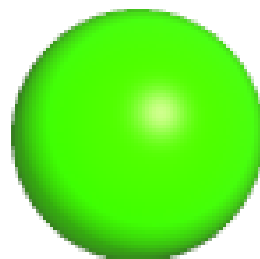
Electron density around CA A 503:

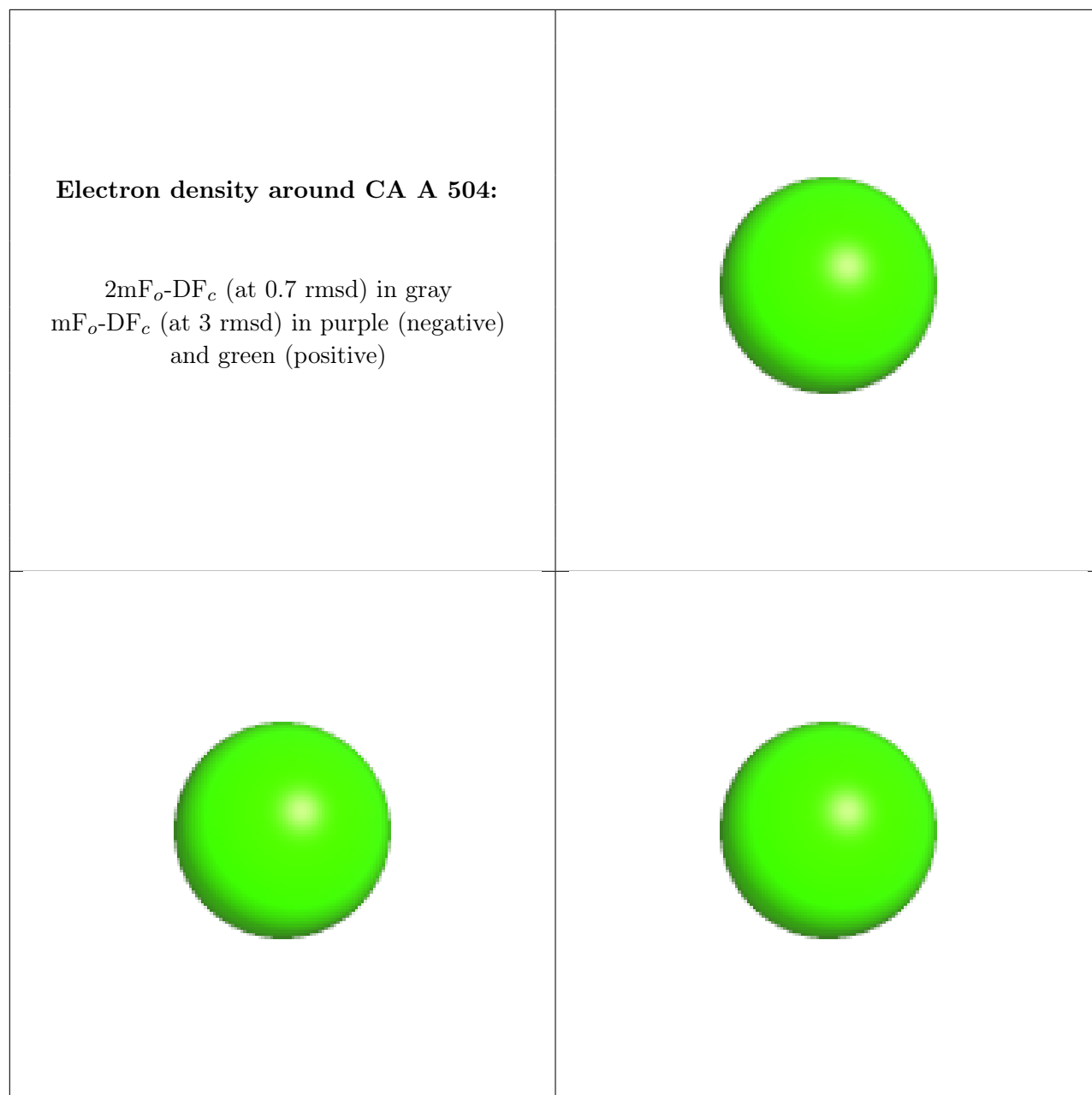
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA B 507:

$2mF_o-DF_c$ (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.