



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:53 AM UTC

PDB ID : 6LXK / pdb_00006lxk
Title : Crystal structure of Z2B3 D102R Fab in complex with influenza virus neuraminidase from A/Serbia/NS-601/2014 (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 : 3.61 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

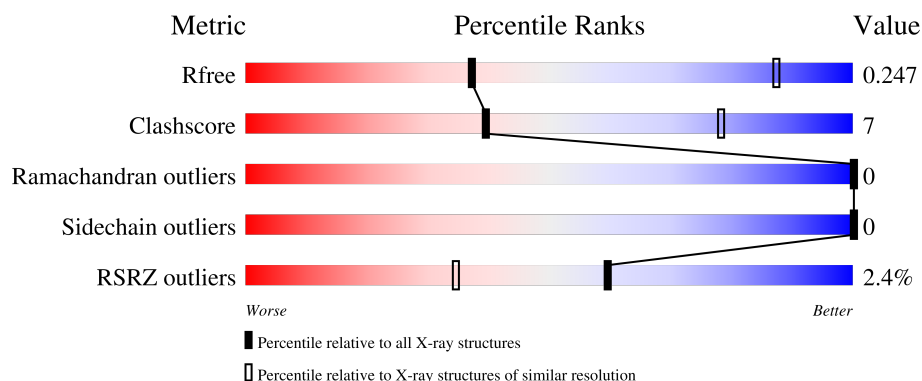
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.61 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.



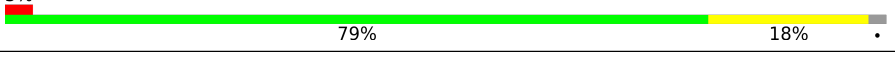
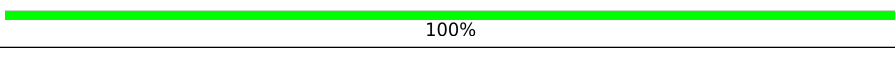
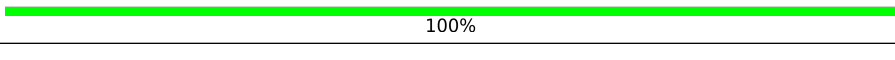
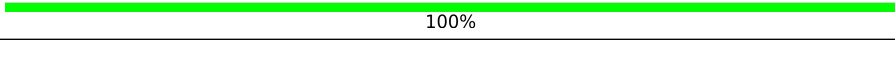
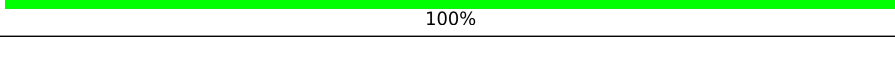
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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 $\leq 5\%$. 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	469	
1	B	469	
1	C	469	
1	D	469	
2	E	237	

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Mol	Chain	Length	Quality of chain
2	H	237	
2	J	237	
3	F	216	
3	K	216	
3	L	216	
4	G	3	
4	I	3	
4	M	3	
4	N	3	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21987 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
			2986	1876	512	577	21			
1	B	387	Total	C	N	O	S	0	0	0
			2986	1876	512	577	21			
1	C	387	Total	C	N	O	S	0	0	0
			2986	1876	512	577	21			
1	D	387	Total	C	N	O	S	0	0	0
			2986	1876	512	577	21			

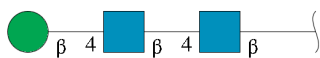
- Molecule 2 is a protein called Heavy chain of Z2B3-D102R Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	232	Total	C	N	O	S	0	0	0
			1730	1093	284	346	7			
2	E	232	Total	C	N	O	S	0	0	0
			1730	1093	284	346	7			
2	J	232	Total	C	N	O	S	0	0	0
			1730	1093	284	346	7			

- Molecule 3 is a protein called Light chain of Z2B3-D102R 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	F	211	Total	C	N	O	S	0	0	0
			1563	973	260	325	5			
3	K	211	Total	C	N	O	S	0	0	0
			1563	973	260	325	5			

- Molecule 4 is an oligosaccharide called 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
4	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	M	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	N	3	Total	C	N	O	0	0	0
			39	22	2	15			

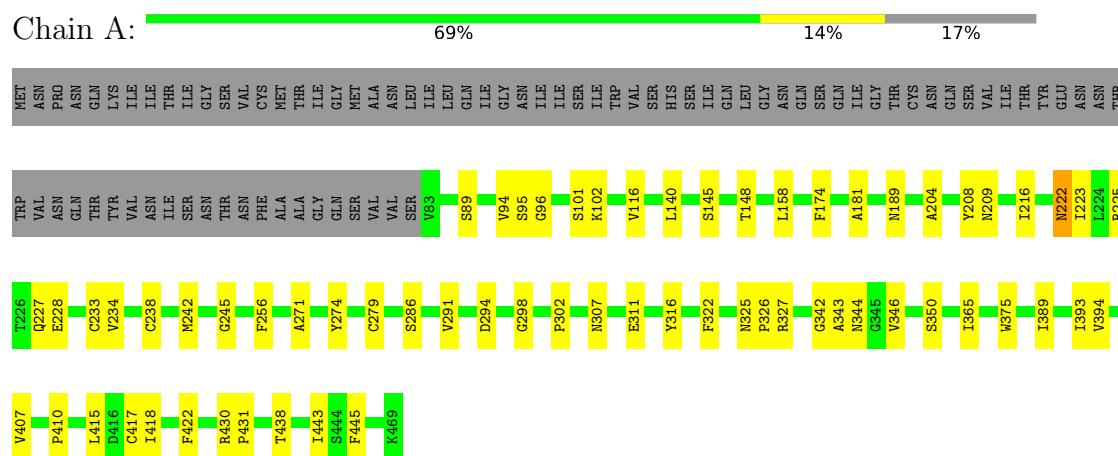
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

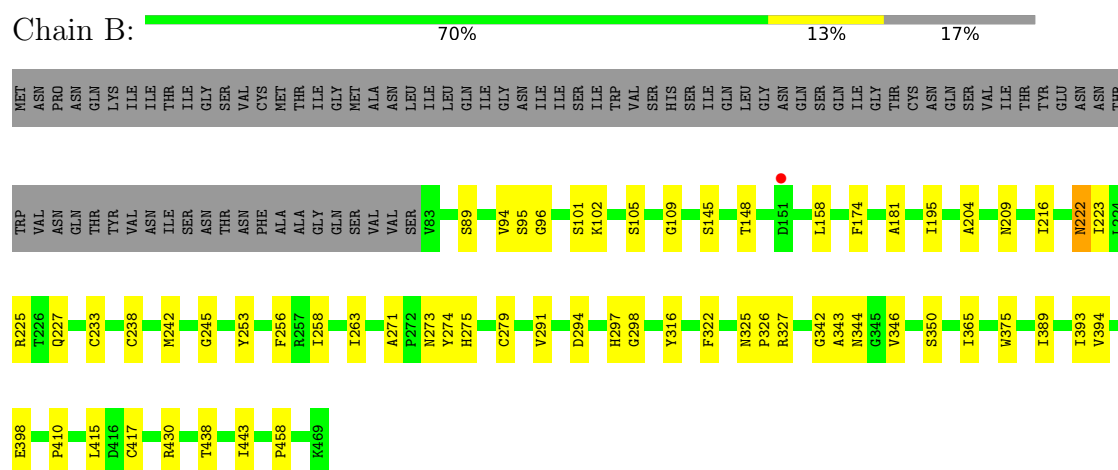
3 Residue-property plots

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.

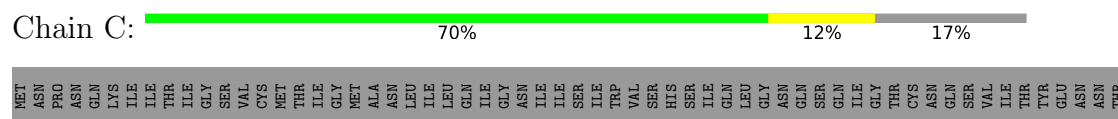
• Molecule 1: Neuraminidase

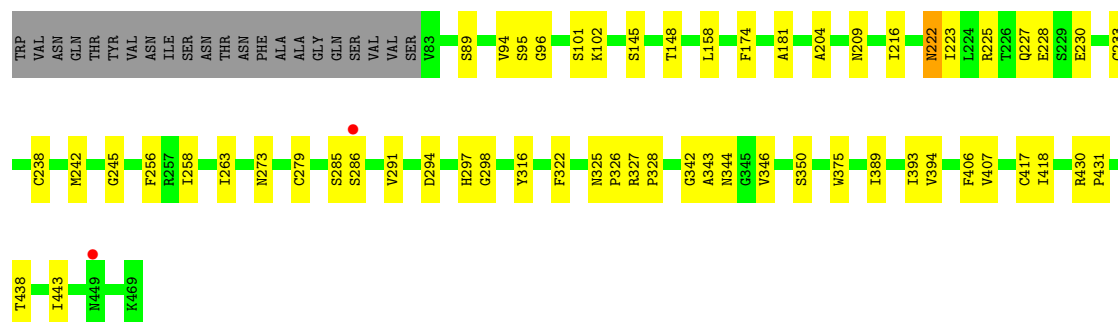


• Molecule 1: Neuraminidase



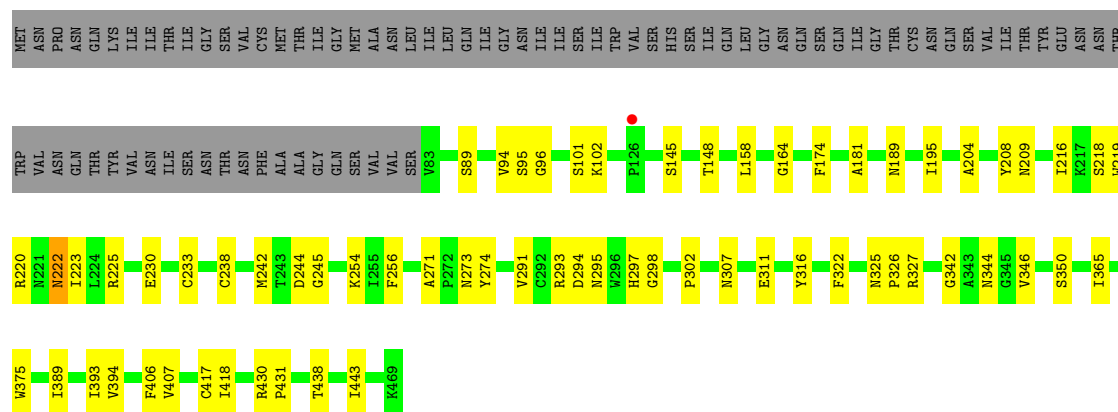
• Molecule 1: Neuraminidase





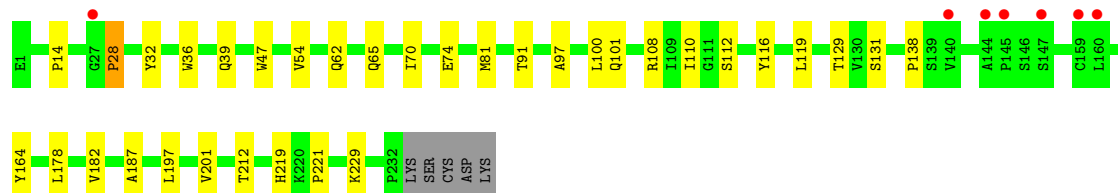
• Molecule 1: Neuraminidase

Chain D: 68% 14% 17%



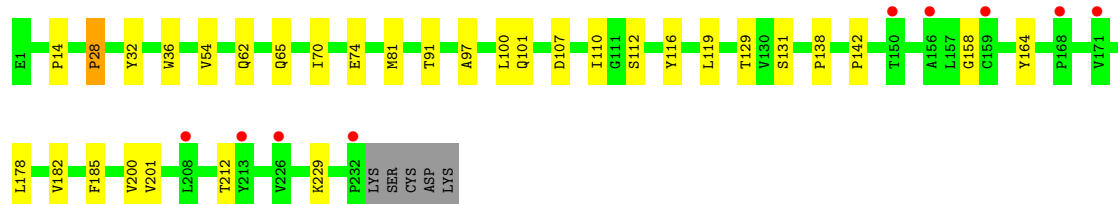
• Molecule 2: Heavy chain of Z2B3-D102R Fab

Chain H: 3% 84% 14%

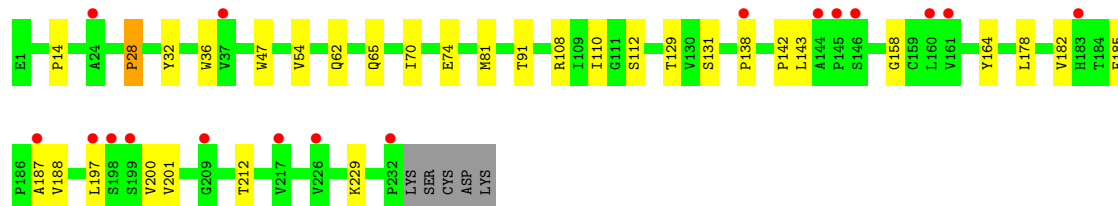
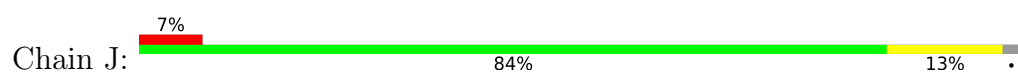


• Molecule 2: Heavy chain of Z2B3-D102R Fab

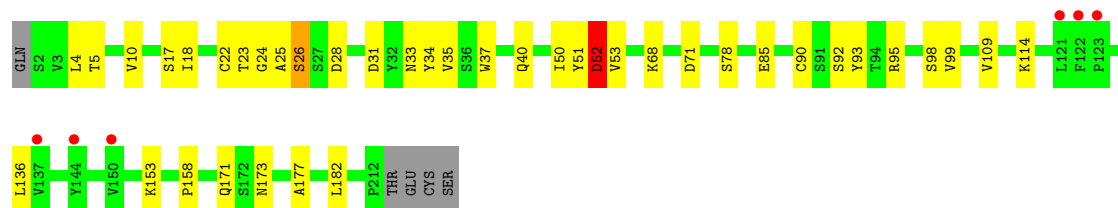
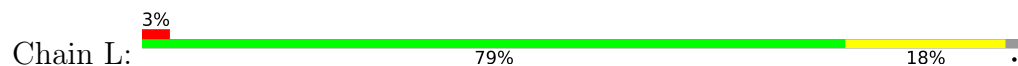
Chain E: 4% 84% 13%



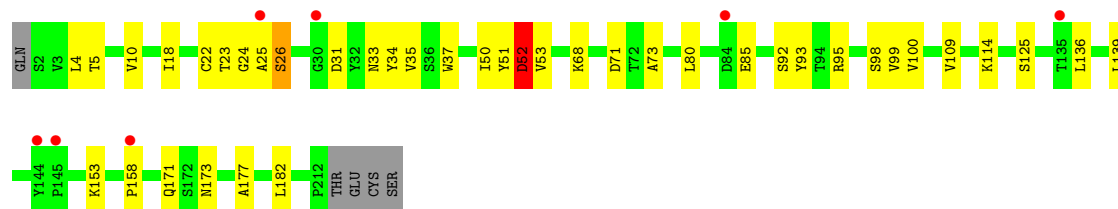
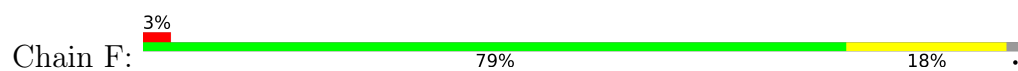
• Molecule 2: Heavy chain of Z2B3-D102R Fab



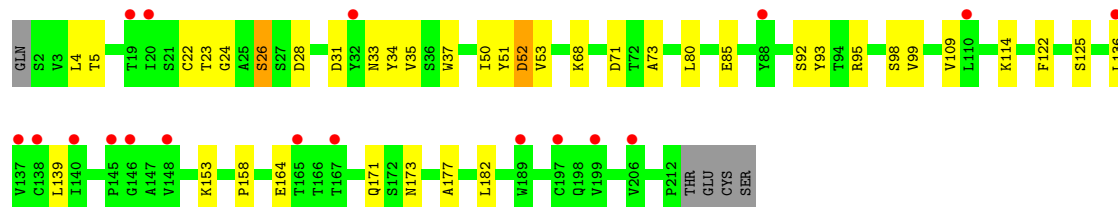
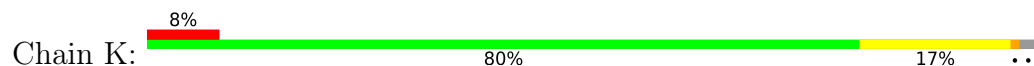
- Molecule 3: Light chain of Z2B3-D102R Fab



- Molecule 3: Light chain of Z2B3-D102R Fab



- Molecule 3: Light chain of Z2B3-D102R Fab



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



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

Chain I:  100%

HA01
HA02
BM03

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

Chain M:  100%

HA01
HA02
BM03

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

Chain N:  100%

HA01
HA02
BM03

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	214.44Å 214.44Å 168.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.46 – 3.61 25.46 – 3.61	Depositor EDS
% Data completeness (in resolution range)	99.5 (25.46-3.61) 99.1 (25.46-3.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 3.64Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.215 , 0.249 0.214 , 0.247	Depositor DCC
R_{free} test set	2522 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	65.5	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	21987	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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: NAG, BMA, CA

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	0.12	0/3068	0.36	0/4169
1	B	0.13	0/3068	0.38	0/4169
1	C	0.12	0/3068	0.36	0/4169
1	D	0.12	0/3068	0.37	0/4169
2	E	0.10	0/1772	0.30	0/2416
2	H	0.10	0/1772	0.29	0/2416
2	J	0.10	0/1772	0.30	0/2416
3	F	0.14	0/1600	0.50	4/2183 (0.2%)
3	K	0.15	0/1600	0.51	4/2183 (0.2%)
3	L	0.15	0/1600	0.49	6/2183 (0.3%)
All	All	0.12	0/22388	0.39	14/30473 (0.0%)

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	2
1	B	0	2
1	C	0	2
1	D	0	1
2	E	0	1
2	H	0	1
2	J	0	1
3	F	0	1
3	K	0	1
3	L	0	1
All	All	0	13

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	26	SER	CA-C-N	6.57	132.72	121.29
3	F	26	SER	C-N-CA	6.57	132.72	121.29
3	K	26	SER	CA-C-N	6.37	133.71	121.54
3	K	26	SER	C-N-CA	6.37	133.71	121.54
3	L	26	SER	CA-C-N	6.27	133.52	121.54
3	L	26	SER	C-N-CA	6.27	133.52	121.54
3	K	28	ASP	CA-C-N	5.37	131.63	121.97
3	K	28	ASP	C-N-CA	5.37	131.63	121.97
3	F	52	ASP	CA-C-N	5.14	131.23	121.97
3	F	52	ASP	C-N-CA	5.14	131.23	121.97
3	L	28	ASP	CA-C-N	5.12	131.18	121.97
3	L	28	ASP	C-N-CA	5.12	131.18	121.97
3	L	52	ASP	CA-C-N	5.11	131.17	121.97
3	L	52	ASP	C-N-CA	5.11	131.17	121.97

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	222	ASN	Peptide
1	A	343	ALA	Peptide
1	B	222	ASN	Peptide
1	B	343	ALA	Peptide
1	C	222	ASN	Peptide
1	C	343	ALA	Peptide
1	D	222	ASN	Peptide
2	E	28	PRO	Peptide
3	F	52	ASP	Peptide
2	H	28	PRO	Peptide
2	J	28	PRO	Peptide
3	K	52	ASP	Peptide
3	L	52	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2986	0	2809	38	0
1	B	2986	0	2809	34	0
1	C	2986	0	2809	35	0
1	D	2986	0	2809	41	0
2	E	1730	0	1695	20	0
2	H	1730	0	1695	23	0
2	J	1730	0	1695	22	0
3	F	1563	0	1505	34	0
3	K	1563	0	1505	33	0
3	L	1563	0	1505	33	0
4	G	39	0	34	0	0
4	I	39	0	34	0	0
4	M	39	0	34	0	0
4	N	39	0	34	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
All	All	21987	0	20972	286	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 7.

All (286) 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:430:ARG:NH1	2:H:74:GLU:OE2	2.05	0.90
1:C:430:ARG:NH1	2:J:74:GLU:OE2	2.09	0.84
3:K:35:VAL:HB	3:K:53:VAL:HG22	1.60	0.81
3:L:35:VAL:HB	3:L:53:VAL:HG22	1.65	0.79
3:K:171:GLN:HE21	3:K:177:ALA:HB2	1.50	0.77
3:L:171:GLN:HE21	3:L:177:ALA:HB2	1.49	0.77
2:H:138:PRO:HB3	2:H:164:TYR:HB3	1.66	0.77
2:E:138:PRO:HB3	2:E:164:TYR:HB3	1.65	0.76
3:F:35:VAL:HB	3:F:53:VAL:HG22	1.67	0.76
2:J:138:PRO:HB3	2:J:164:TYR:HB3	1.68	0.76
2:J:158:GLY:HA3	2:J:200:VAL:HG12	1.70	0.74
3:F:171:GLN:HE21	3:F:177:ALA:HB2	1.52	0.74
3:F:4:LEU:HG	3:F:100:VAL:HG23	1.70	0.73
1:D:430:ARG:NH1	2:E:74:GLU:OE2	2.15	0.71
3:L:51:TYR:CD2	3:L:52:ASP:HB2	2.25	0.70
3:K:51:TYR:CD2	3:K:52:ASP:HB2	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:33:ASN:OD1	3:K:68:LYS:NZ	2.27	0.68
3:L:33:ASN:OD1	3:L:68:LYS:NZ	2.25	0.68
1:D:375:TRP:HB3	1:D:389:ILE:HB	1.75	0.67
3:F:51:TYR:CD2	3:F:52:ASP:HB2	2.30	0.66
3:F:98:SER:O	3:F:99:VAL:HG13	1.97	0.65
1:A:294:ASP:OD2	1:A:316:TYR:OH	2.14	0.65
1:C:375:TRP:HB3	1:C:389:ILE:HB	1.78	0.64
3:F:33:ASN:OD1	3:F:68:LYS:NZ	2.31	0.64
1:A:228:GLU:OE2	2:H:108:ARG:NH2	2.32	0.63
2:J:110:ILE:HG22	2:J:112:SER:H	1.64	0.62
1:A:431:PRO:HB3	2:H:54:VAL:HG21	1.82	0.61
1:D:431:PRO:HB3	2:E:54:VAL:HG21	1.81	0.61
2:H:110:ILE:HG22	2:H:112:SER:H	1.66	0.61
1:A:223:ILE:O	1:A:225:ARG:NH1	2.33	0.60
2:E:110:ILE:HG22	2:E:112:SER:H	1.66	0.60
3:K:98:SER:O	3:K:99:VAL:HG13	2.01	0.60
1:A:375:TRP:HB3	1:A:389:ILE:HB	1.82	0.60
1:B:375:TRP:HB3	1:B:389:ILE:HB	1.83	0.60
1:D:219:TRP:CE2	1:D:254:LYS:HE3	2.38	0.59
1:B:209:ASN:O	1:B:209:ASN:ND2	2.36	0.59
3:L:5:THR:HB	3:L:23:THR:HG23	1.84	0.59
3:F:4:LEU:HG	3:F:100:VAL:CG2	2.32	0.58
1:C:209:ASN:O	1:C:209:ASN:ND2	2.36	0.58
1:B:223:ILE:O	1:B:225:ARG:NH1	2.36	0.58
1:D:209:ASN:O	1:D:209:ASN:ND2	2.36	0.58
3:L:98:SER:O	3:L:99:VAL:HG13	2.05	0.57
3:K:34:TYR:HB2	3:K:93:TYR:HB3	1.87	0.57
3:F:4:LEU:CG	3:F:100:VAL:HG23	2.35	0.57
3:K:136:LEU:HD12	3:K:182:LEU:HD23	1.86	0.57
1:A:209:ASN:ND2	1:A:209:ASN:O	2.36	0.56
3:K:5:THR:HB	3:K:23:THR:HG23	1.87	0.56
3:L:93:TYR:HD1	3:L:98:SER:O	1.88	0.56
1:D:293:ARG:NH1	2:E:107:ASP:OD2	2.36	0.56
3:F:114:LYS:H	3:F:114:LYS:CD	2.19	0.56
1:D:89:SER:HB2	1:D:417:CYS:HA	1.88	0.56
2:J:142:PRO:O	3:K:125:SER:HB3	2.05	0.56
2:J:178:LEU:HD21	2:J:201:VAL:HG11	1.88	0.56
1:C:431:PRO:HB3	2:J:54:VAL:HG21	1.87	0.56
1:C:223:ILE:O	1:C:225:ARG:NH1	2.38	0.55
2:J:182:VAL:HG22	2:J:201:VAL:HG22	1.87	0.55
3:K:114:LYS:H	3:K:114:LYS:CD	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:114:LYS:CD	3:L:114:LYS:H	2.19	0.55
3:F:100:VAL:HG23	3:F:100:VAL:O	2.06	0.55
1:B:95:SER:O	1:B:95:SER:OG	2.21	0.55
3:F:5:THR:HB	3:F:23:THR:HG23	1.87	0.55
3:K:4:LEU:HD22	3:K:24:GLY:HA3	1.88	0.55
3:F:136:LEU:HD12	3:F:182:LEU:HD23	1.89	0.55
1:D:291:VAL:HG21	1:D:350:SER:HB2	1.89	0.54
1:D:242:MET:HB2	1:D:256:PHE:HE2	1.73	0.54
3:F:93:TYR:HD1	3:F:98:SER:O	1.90	0.54
3:L:136:LEU:HD12	3:L:182:LEU:HD23	1.90	0.54
1:C:94:VAL:HG12	1:C:96:GLY:H	1.73	0.54
2:E:158:GLY:HA3	2:E:200:VAL:HG12	1.89	0.53
3:K:93:TYR:HD1	3:K:98:SER:O	1.91	0.53
1:A:94:VAL:HG12	1:A:96:GLY:H	1.72	0.53
3:L:85:GLU:HB2	3:L:109:VAL:HG23	1.91	0.53
1:B:158:LEU:HD22	1:B:181:ALA:HB1	1.91	0.53
1:A:89:SER:HB2	1:A:417:CYS:HA	1.90	0.53
1:D:220:ARG:HB3	1:D:244:ASP:OD1	2.09	0.53
1:A:102:LYS:HG3	1:A:443:ILE:HG22	1.91	0.53
3:F:34:TYR:HB2	3:F:93:TYR:HB3	1.91	0.53
2:H:39:GLN:OE1	3:L:40:GLN:NE2	2.38	0.53
3:L:34:TYR:HB2	3:L:93:TYR:HB3	1.90	0.53
2:H:47:TRP:CG	3:L:99:VAL:HG21	2.44	0.52
1:C:228:GLU:OE2	2:J:108:ARG:NH2	2.42	0.52
2:J:91:THR:HG23	2:J:129:THR:HA	1.92	0.52
1:B:298:GLY:N	1:B:342:GLY:O	2.43	0.52
1:B:322:PHE:HB2	1:B:327:ARG:HD2	1.92	0.52
2:H:212:THR:HG23	2:H:229:LYS:HE3	1.92	0.52
1:C:322:PHE:HB2	1:C:327:ARG:HD2	1.90	0.51
1:B:326:PRO:HD2	1:B:344:ASN:O	2.09	0.51
1:D:223:ILE:O	1:D:225:ARG:NH1	2.41	0.51
2:E:36:TRP:CE2	2:E:81:MET:HB2	2.46	0.51
2:E:182:VAL:HG22	2:E:201:VAL:HG22	1.92	0.51
1:A:393:ILE:HG22	1:A:394:VAL:HG23	1.92	0.51
3:L:17:SER:HB3	3:L:78:SER:HA	1.92	0.51
3:L:31:ASP:OD2	3:L:95:ARG:HD3	2.10	0.51
1:C:242:MET:HB2	1:C:256:PHE:HE2	1.76	0.51
1:D:94:VAL:HG12	1:D:96:GLY:H	1.76	0.51
2:H:36:TRP:CE2	2:H:81:MET:HB2	2.46	0.51
2:H:178:LEU:HD21	2:H:201:VAL:HG11	1.93	0.51
1:B:89:SER:HB2	1:B:417:CYS:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:MET:HB2	1:B:256:PHE:HE2	1.77	0.50
2:J:185:PHE:CZ	3:K:139:LEU:HB3	2.46	0.50
1:B:148:THR:HG23	1:B:438:THR:H	1.76	0.50
1:B:393:ILE:HG22	1:B:394:VAL:HG23	1.93	0.50
1:D:148:THR:HG23	1:D:438:THR:H	1.77	0.50
2:E:28:PRO:HB3	2:E:32:TYR:CD1	2.47	0.50
1:A:326:PRO:HD2	1:A:344:ASN:O	2.12	0.50
1:B:94:VAL:HG12	1:B:96:GLY:H	1.77	0.50
1:C:393:ILE:HG22	1:C:394:VAL:HG23	1.94	0.50
2:J:36:TRP:HD1	2:J:70:ILE:HD13	1.77	0.50
3:K:171:GLN:OE1	3:K:173:ASN:ND2	2.44	0.50
1:D:95:SER:O	1:D:95:SER:OG	2.22	0.49
2:J:188:VAL:HG21	3:K:164:GLU:HB3	1.93	0.49
2:E:178:LEU:HD21	2:E:201:VAL:HG11	1.93	0.49
1:A:95:SER:O	1:A:95:SER:OG	2.22	0.49
1:A:222:ASN:HB3	1:A:245:GLY:HA2	1.94	0.49
1:C:158:LEU:HD22	1:C:181:ALA:HB1	1.94	0.49
3:K:85:GLU:HB2	3:K:109:VAL:HG23	1.94	0.49
2:E:142:PRO:O	3:F:125:SER:HB3	2.13	0.49
1:A:158:LEU:HD22	1:A:181:ALA:HB1	1.94	0.49
1:A:322:PHE:HB2	1:A:327:ARG:HD2	1.95	0.49
1:C:326:PRO:HD2	1:C:344:ASN:O	2.13	0.48
1:C:148:THR:HG23	1:C:438:THR:H	1.78	0.48
1:D:273:ASN:O	1:D:297:HIS:NE2	2.38	0.48
1:D:102:LYS:HG3	1:D:443:ILE:HG22	1.94	0.48
1:D:393:ILE:HG22	1:D:394:VAL:HG23	1.95	0.48
1:D:326:PRO:HD2	1:D:344:ASN:O	2.12	0.48
1:D:322:PHE:HB2	1:D:327:ARG:HD2	1.94	0.48
2:J:36:TRP:CE2	2:J:81:MET:HB2	2.48	0.48
2:H:182:VAL:HG22	2:H:201:VAL:HG22	1.95	0.48
1:A:242:MET:HB2	1:A:256:PHE:HE2	1.79	0.48
1:B:204:ALA:HB3	1:B:216:ILE:HG23	1.96	0.48
1:B:291:VAL:HG21	1:B:350:SER:HB2	1.95	0.47
2:E:116:TYR:O	3:F:34:TYR:HD1	1.97	0.47
2:H:36:TRP:HD1	2:H:70:ILE:HD13	1.79	0.47
1:C:258:ILE:HD12	1:C:263:ILE:HG12	1.96	0.47
1:B:294:ASP:OD2	1:B:316:TYR:OH	2.24	0.47
2:J:212:THR:HG23	2:J:229:LYS:HE3	1.95	0.47
1:B:222:ASN:HB3	1:B:245:GLY:HA2	1.95	0.47
3:L:171:GLN:NE2	3:L:177:ALA:HB2	2.25	0.47
1:C:204:ALA:HB3	1:C:216:ILE:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:VAL:HG21	1:C:418:ILE:HD11	1.97	0.47
2:E:212:THR:HG23	2:E:229:LYS:HE3	1.96	0.47
2:H:28:PRO:HB3	2:H:32:TYR:CD1	2.50	0.47
3:F:22:CYS:O	3:F:73:ALA:N	2.47	0.46
3:L:22:CYS:CB	3:L:90:CYS:SG	3.02	0.46
3:F:114:LYS:H	3:F:114:LYS:HD2	1.80	0.46
1:B:258:ILE:HD12	1:B:263:ILE:HG12	1.96	0.46
3:L:114:LYS:H	3:L:114:LYS:HD2	1.81	0.46
3:K:114:LYS:H	3:K:114:LYS:HD2	1.81	0.46
3:L:37:TRP:HB2	3:L:50:ILE:HB	1.98	0.46
1:A:204:ALA:HB3	1:A:216:ILE:HG23	1.98	0.46
1:C:102:LYS:HG3	1:C:443:ILE:HG22	1.97	0.46
1:C:230:GLU:OE2	1:C:406:PHE:HA	2.15	0.46
2:J:187:ALA:HB2	2:J:197:LEU:HD23	1.97	0.46
1:A:325:ASN:O	1:A:346:VAL:HG23	2.15	0.46
3:F:171:GLN:OE1	3:F:173:ASN:ND2	2.46	0.46
1:C:325:ASN:O	1:C:346:VAL:HG23	2.16	0.46
3:F:10:VAL:HB	3:F:18:ILE:HD11	1.97	0.46
1:B:227:GLN:HB3	1:B:279:CYS:O	2.17	0.45
1:D:158:LEU:HD22	1:D:181:ALA:HB1	1.97	0.45
1:D:298:GLY:N	1:D:342:GLY:O	2.49	0.45
2:J:62:GLN:HA	2:J:65:GLN:HG3	1.99	0.45
2:H:91:THR:HG23	2:H:129:THR:HA	1.97	0.45
3:L:26:SER:HB2	3:L:71:ASP:HA	1.98	0.45
3:L:171:GLN:OE1	3:L:173:ASN:ND2	2.48	0.45
1:C:89:SER:HB2	1:C:417:CYS:HA	1.97	0.45
1:D:325:ASN:O	1:D:346:VAL:HG23	2.17	0.45
1:A:298:GLY:N	1:A:342:GLY:O	2.50	0.45
2:E:91:THR:HG23	2:E:129:THR:HA	1.98	0.45
3:K:93:TYR:CD1	3:K:98:SER:O	2.70	0.45
3:F:4:LEU:HD22	3:F:25:ALA:H	1.80	0.45
3:K:31:ASP:OD2	3:K:95:ARG:HD3	2.15	0.45
3:L:31:ASP:OD1	3:L:31:ASP:N	2.49	0.45
1:C:95:SER:O	1:C:95:SER:OG	2.22	0.45
3:F:4:LEU:HD22	3:F:24:GLY:HA3	1.98	0.45
3:F:153:LYS:HG2	3:F:158:PRO:HA	1.99	0.45
3:L:153:LYS:HG2	3:L:158:PRO:HA	1.98	0.45
1:D:204:ALA:HB3	1:D:216:ILE:HG23	1.99	0.45
1:D:233:CYS:HA	1:D:238:CYS:HA	1.99	0.45
2:E:36:TRP:HD1	2:E:70:ILE:HD13	1.81	0.45
1:B:102:LYS:HG3	1:B:443:ILE:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:26:SER:HB2	3:F:71:ASP:HA	1.99	0.45
3:F:85:GLU:HB2	3:F:109:VAL:HG23	1.98	0.45
1:A:174:PHE:CZ	1:C:101:SER:HA	2.52	0.44
3:L:26:SER:CB	3:L:71:ASP:HA	2.47	0.44
1:C:298:GLY:N	1:C:342:GLY:O	2.51	0.44
2:E:185:PHE:CZ	3:F:139:LEU:HB3	2.52	0.44
1:A:291:VAL:HG21	1:A:350:SER:HB2	1.99	0.44
1:C:222:ASN:HB3	1:C:245:GLY:HA2	2.00	0.44
1:D:145:SER:O	1:D:148:THR:HG22	2.17	0.44
1:A:145:SER:O	1:A:148:THR:HG22	2.17	0.44
3:K:68:LYS:HE2	3:K:68:LYS:HB3	1.81	0.44
1:A:233:CYS:HA	1:A:238:CYS:HA	1.98	0.44
3:F:31:ASP:OD2	3:F:95:ARG:HD3	2.18	0.44
2:J:28:PRO:HB3	2:J:32:TYR:CD1	2.52	0.44
1:D:222:ASN:HB3	1:D:245:GLY:HA2	1.99	0.44
3:F:26:SER:CB	3:F:71:ASP:HA	2.48	0.44
1:A:148:THR:HG23	1:A:438:THR:H	1.83	0.43
2:H:116:TYR:O	3:L:34:TYR:HD1	2.00	0.43
1:B:273:ASN:O	1:B:297:HIS:NE2	2.47	0.43
1:C:145:SER:O	1:C:148:THR:HG22	2.18	0.43
2:H:187:ALA:HB2	2:H:197:LEU:HD23	1.99	0.43
1:C:174:PHE:CG	1:D:164:GLY:HA3	2.53	0.43
1:C:273:ASN:O	1:C:297:HIS:NE2	2.45	0.43
1:A:189:ASN:HB2	1:A:208:TYR:CZ	2.53	0.43
2:J:185:PHE:CD1	3:K:139:LEU:HD22	2.53	0.43
3:L:92:SER:O	3:L:99:VAL:HA	2.18	0.43
1:D:195:ILE:HG12	1:D:204:ALA:HB2	2.00	0.43
3:K:26:SER:CB	3:K:71:ASP:HA	2.49	0.43
3:K:37:TRP:HB2	3:K:50:ILE:HB	2.01	0.43
3:L:4:LEU:HD13	3:L:22:CYS:SG	2.59	0.43
1:B:327:ARG:O	1:B:365:ILE:HG22	2.18	0.43
1:D:189:ASN:HB2	1:D:208:TYR:CZ	2.54	0.43
2:E:100:LEU:HG	2:E:101:GLN:HG3	2.01	0.43
1:C:291:VAL:HG21	1:C:350:SER:HB2	2.01	0.43
1:D:218:SER:OG	1:D:244:ASP:OD2	2.35	0.43
1:B:105:SER:O	1:B:109:GLY:N	2.51	0.43
1:C:174:PHE:CZ	1:D:101:SER:HA	2.53	0.43
1:A:234:VAL:HG11	1:A:286:SER:HA	2.00	0.43
2:H:108:ARG:HA	2:H:108:ARG:HD3	1.79	0.43
3:L:26:SER:OG	3:L:71:ASP:HA	2.19	0.43
3:K:92:SER:O	3:K:99:VAL:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ASN:O	1:B:346:VAL:HG23	2.19	0.42
2:E:62:GLN:HA	2:E:65:GLN:HG3	2.00	0.42
3:F:26:SER:OG	3:F:71:ASP:HA	2.19	0.42
3:K:26:SER:HB2	3:K:71:ASP:HA	2.01	0.42
1:B:145:SER:O	1:B:148:THR:HG22	2.19	0.42
1:C:285:SER:O	1:C:286:SER:OG	2.36	0.42
1:A:101:SER:HA	1:B:174:PHE:CZ	2.54	0.42
3:F:92:SER:O	3:F:99:VAL:HA	2.19	0.42
1:A:116:VAL:HG22	1:A:140:LEU:HD23	2.00	0.42
2:E:14:PRO:HD3	2:E:131:SER:O	2.19	0.42
3:K:153:LYS:HG2	3:K:158:PRO:HA	2.01	0.42
2:H:14:PRO:HD3	2:H:131:SER:O	2.19	0.42
1:D:327:ARG:O	1:D:365:ILE:HG22	2.19	0.42
1:A:407:VAL:HG21	1:A:418:ILE:HD11	2.02	0.42
2:H:62:GLN:HA	2:H:65:GLN:HG3	2.00	0.42
1:D:294:ASP:OD2	1:D:316:TYR:OH	2.18	0.42
1:D:307:ASN:ND2	1:D:311:GLU:OE1	2.48	0.42
3:K:26:SER:OG	3:K:71:ASP:HA	2.19	0.42
1:A:302:PRO:HB3	1:A:316:TYR:CZ	2.54	0.42
1:B:430:ARG:HB2	1:B:438:THR:OG1	2.20	0.42
3:K:80:LEU:HD23	3:K:80:LEU:HA	1.84	0.42
1:A:227:GLN:HB3	1:A:279:CYS:O	2.19	0.42
3:L:4:LEU:HD22	3:L:24:GLY:HA3	2.02	0.42
1:B:101:SER:HA	1:D:174:PHE:CZ	2.55	0.42
1:C:430:ARG:HB2	1:C:438:THR:OG1	2.20	0.42
3:F:93:TYR:CD1	3:F:98:SER:O	2.72	0.42
2:J:143:LEU:HB3	3:K:122:PHE:CD1	2.54	0.42
3:K:136:LEU:HB2	3:K:182:LEU:HB3	2.02	0.42
3:K:98:SER:O	3:K:99:VAL:CG1	2.68	0.41
3:L:10:VAL:HB	3:L:18:ILE:HD11	2.01	0.41
2:H:97:ALA:HB3	2:H:119:LEU:HD13	2.02	0.41
3:L:4:LEU:HD22	3:L:25:ALA:H	1.85	0.41
3:L:93:TYR:CD1	3:L:98:SER:O	2.70	0.41
2:H:219:HIS:CD2	2:H:221:PRO:HD2	2.56	0.41
1:C:227:GLN:HB3	1:C:279:CYS:O	2.19	0.41
1:A:271:ALA:HB1	1:A:274:TYR:HB2	2.01	0.41
1:A:327:ARG:O	1:A:365:ILE:HG22	2.20	0.41
1:A:410:PRO:HB3	1:A:415:LEU:O	2.20	0.41
2:J:47:TRP:CG	3:K:99:VAL:CG2	3.03	0.41
1:D:294:ASP:HB2	1:D:302:PRO:HD3	2.03	0.41
1:D:407:VAL:HG21	1:D:418:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:CYS:HA	1:B:238:CYS:HA	2.03	0.41
1:C:233:CYS:HA	1:C:238:CYS:HA	2.01	0.41
1:C:322:PHE:CE2	1:C:328:PRO:HG2	2.55	0.41
3:F:37:TRP:HB2	3:F:50:ILE:HB	2.02	0.41
1:A:307:ASN:ND2	1:A:311:GLU:OE1	2.48	0.41
2:H:47:TRP:CG	3:L:99:VAL:CG2	3.04	0.41
1:B:195:ILE:HG12	1:B:204:ALA:HB2	2.03	0.41
1:B:398:GLU:OE1	1:B:458:PRO:HG3	2.21	0.41
1:B:410:PRO:HB3	1:B:415:LEU:O	2.21	0.41
1:C:294:ASP:OD2	1:C:316:TYR:OH	2.29	0.41
3:F:114:LYS:CD	3:F:114:LYS:N	2.84	0.41
1:A:422:PHE:CE1	1:A:445:PHE:HB2	2.56	0.41
1:D:293:ARG:NH2	1:D:295:ASN:OD1	2.42	0.41
2:H:100:LEU:HG	2:H:101:GLN:HG3	2.02	0.40
3:F:80:LEU:HD23	3:F:80:LEU:HA	1.84	0.40
1:D:271:ALA:HB1	1:D:274:TYR:HB2	2.03	0.40
2:E:97:ALA:HB3	2:E:119:LEU:HD13	2.03	0.40
2:J:14:PRO:HD3	2:J:131:SER:O	2.21	0.40
1:B:253:TYR:OH	1:B:275:HIS:HA	2.22	0.40
1:B:271:ALA:HB1	1:B:274:TYR:HB2	2.03	0.40
1:D:230:GLU:OE2	1:D:406:PHE:HA	2.21	0.40
1:A:430:ARG:HB2	1:A:438:THR:OG1	2.22	0.40
1:D:430:ARG:HB2	1:D:438:THR:OG1	2.22	0.40
3:K:22:CYS:O	3:K:73:ALA:N	2.52	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	385/469 (82%)	384 (100%)	1 (0%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	385/469 (82%)	383 (100%)	2 (0%)	0	100	100
1	C	385/469 (82%)	383 (100%)	2 (0%)	0	100	100
1	D	385/469 (82%)	384 (100%)	1 (0%)	0	100	100
2	E	230/237 (97%)	230 (100%)	0	0	100	100
2	H	230/237 (97%)	230 (100%)	0	0	100	100
2	J	230/237 (97%)	230 (100%)	0	0	100	100
3	F	209/216 (97%)	204 (98%)	5 (2%)	0	100	100
3	K	209/216 (97%)	204 (98%)	5 (2%)	0	100	100
3	L	209/216 (97%)	204 (98%)	5 (2%)	0	100	100
All	All	2857/3235 (88%)	2836 (99%)	21 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	332/407 (82%)	332 (100%)	0	100	100
1	B	332/407 (82%)	332 (100%)	0	100	100
1	C	332/407 (82%)	332 (100%)	0	100	100
1	D	332/407 (82%)	332 (100%)	0	100	100
2	E	195/200 (98%)	195 (100%)	0	100	100
2	H	195/200 (98%)	195 (100%)	0	100	100
2	J	195/200 (98%)	195 (100%)	0	100	100
3	F	178/183 (97%)	178 (100%)	0	100	100
3	K	178/183 (97%)	178 (100%)	0	100	100
3	L	178/183 (97%)	178 (100%)	0	100	100
All	All	2447/2777 (88%)	2447 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	409	HIS
2	H	117	ASN
3	L	171	GLN
3	L	173	ASN
2	E	117	ASN
3	F	132	ASN
3	F	171	GLN
3	F	173	ASN
3	F	201	HIS
2	J	39	GLN
2	J	117	ASN
3	K	40	GLN
3	K	171	GLN
3	K	173	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 ⓘ

12 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	G	1	4,1	14,14,15	0.23	0	17,19,21	0.38	0
4	NAG	G	2	4	14,14,15	0.19	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BMA	G	3	4	11,11,12	0.62	0	15,15,17	0.71	0
4	NAG	I	1	4,1	14,14,15	0.24	0	17,19,21	0.38	0
4	NAG	I	2	4	14,14,15	0.20	0	17,19,21	0.42	0
4	BMA	I	3	4	11,11,12	0.59	0	15,15,17	0.71	0
4	NAG	M	1	4,1	14,14,15	0.22	0	17,19,21	0.40	0
4	NAG	M	2	4	14,14,15	0.20	0	17,19,21	0.44	0
4	BMA	M	3	4	11,11,12	0.61	0	15,15,17	0.72	0
4	NAG	N	1	4,1	14,14,15	0.21	0	17,19,21	0.40	0
4	NAG	N	2	4	14,14,15	0.19	0	17,19,21	0.43	0
4	BMA	N	3	4	11,11,12	0.63	0	15,15,17	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
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	NAG	I	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	BMA	I	3	4	-	0/2/19/22	0/1/1/1
4	NAG	M	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
4	BMA	M	3	4	-	0/2/19/22	0/1/1/1
4	NAG	N	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	0/6/23/26	0/1/1/1
4	BMA	N	3	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

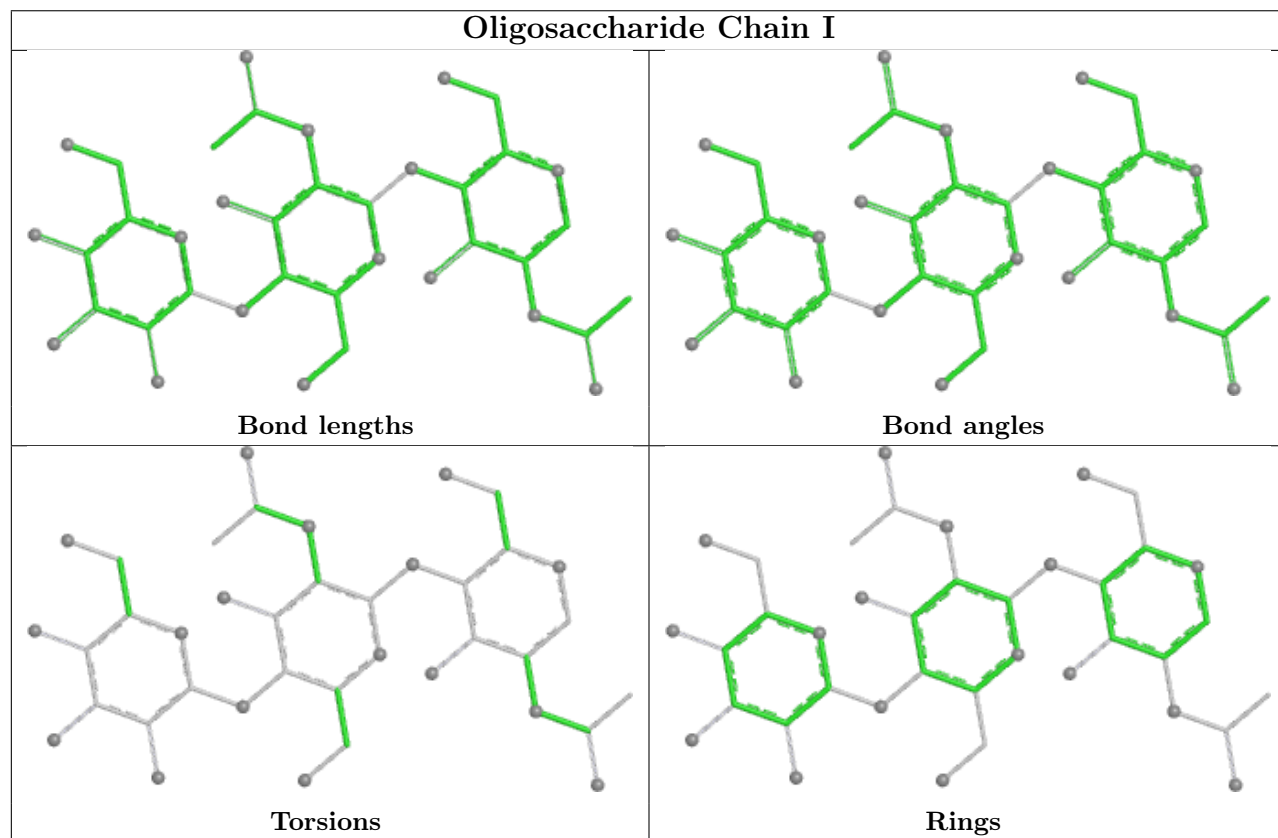
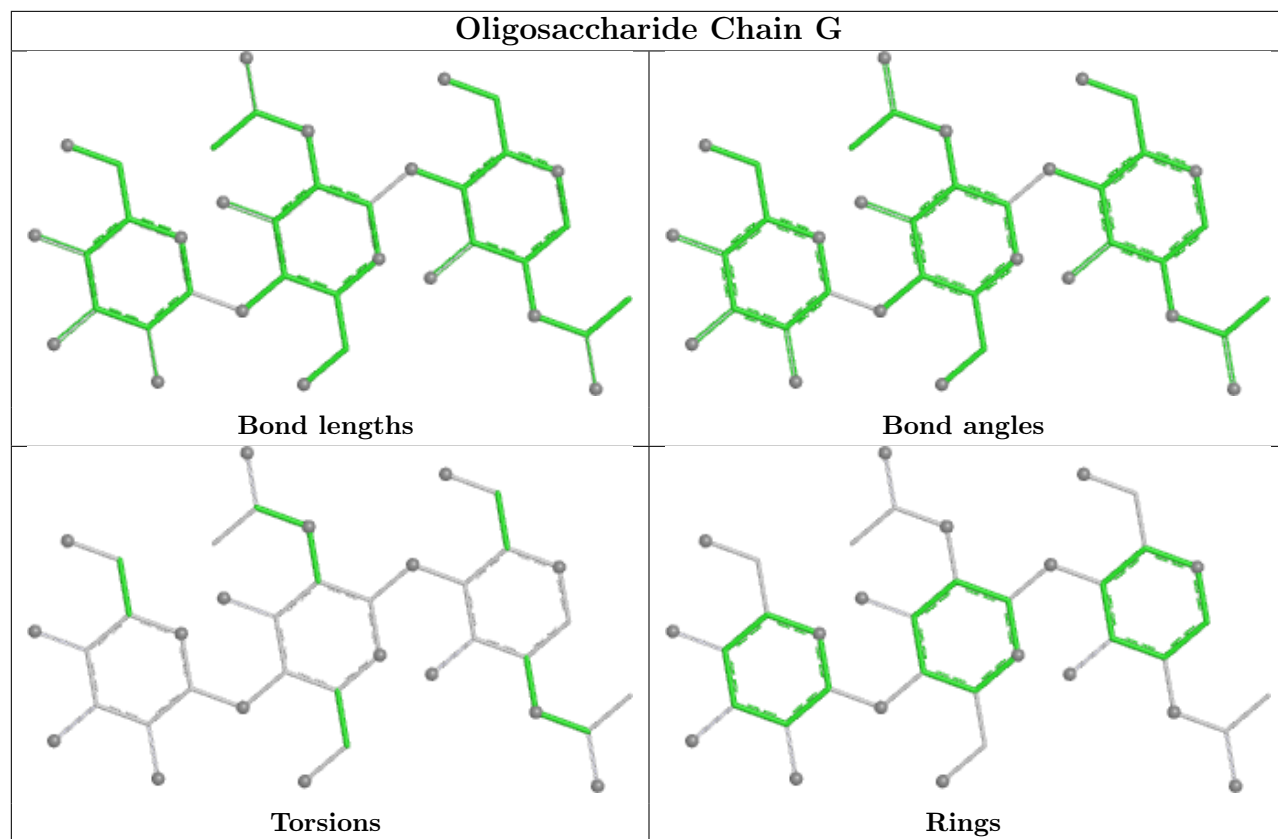
There are no chirality outliers.

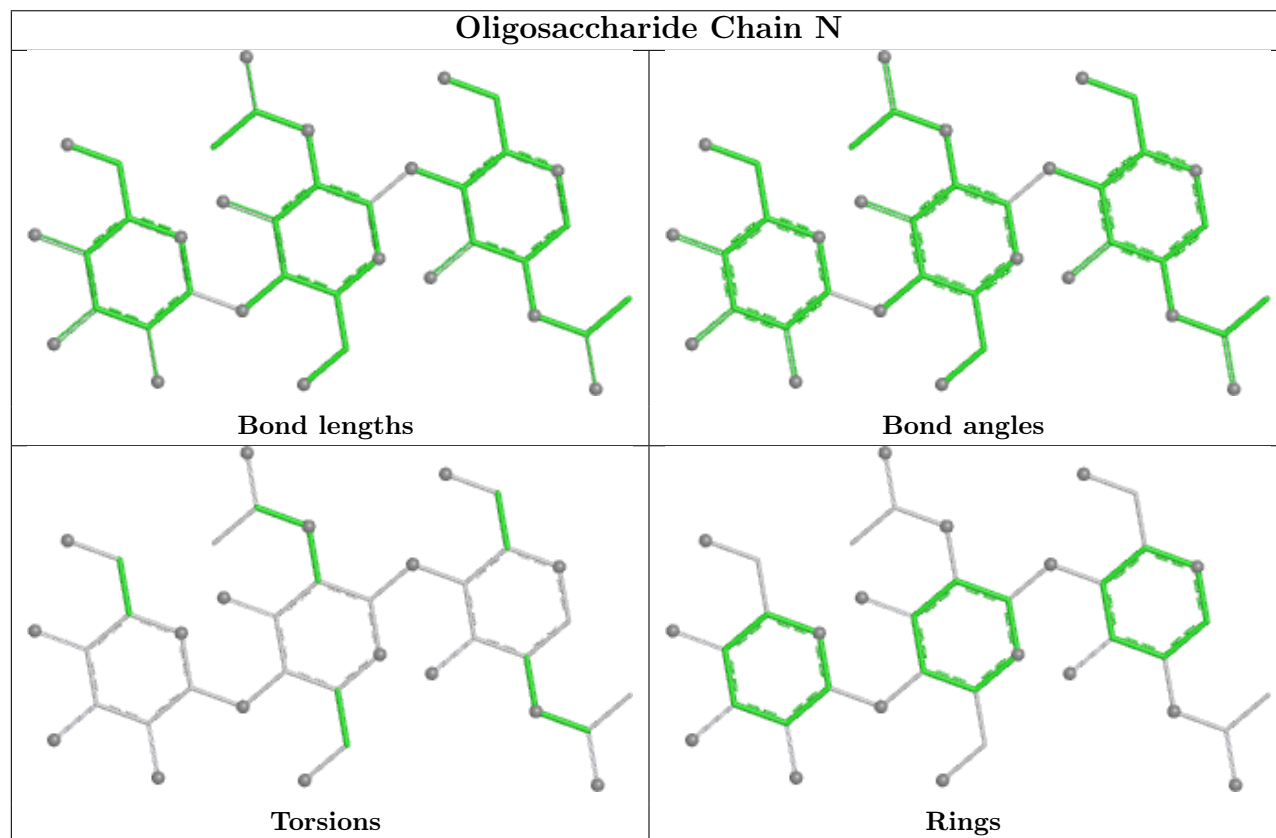
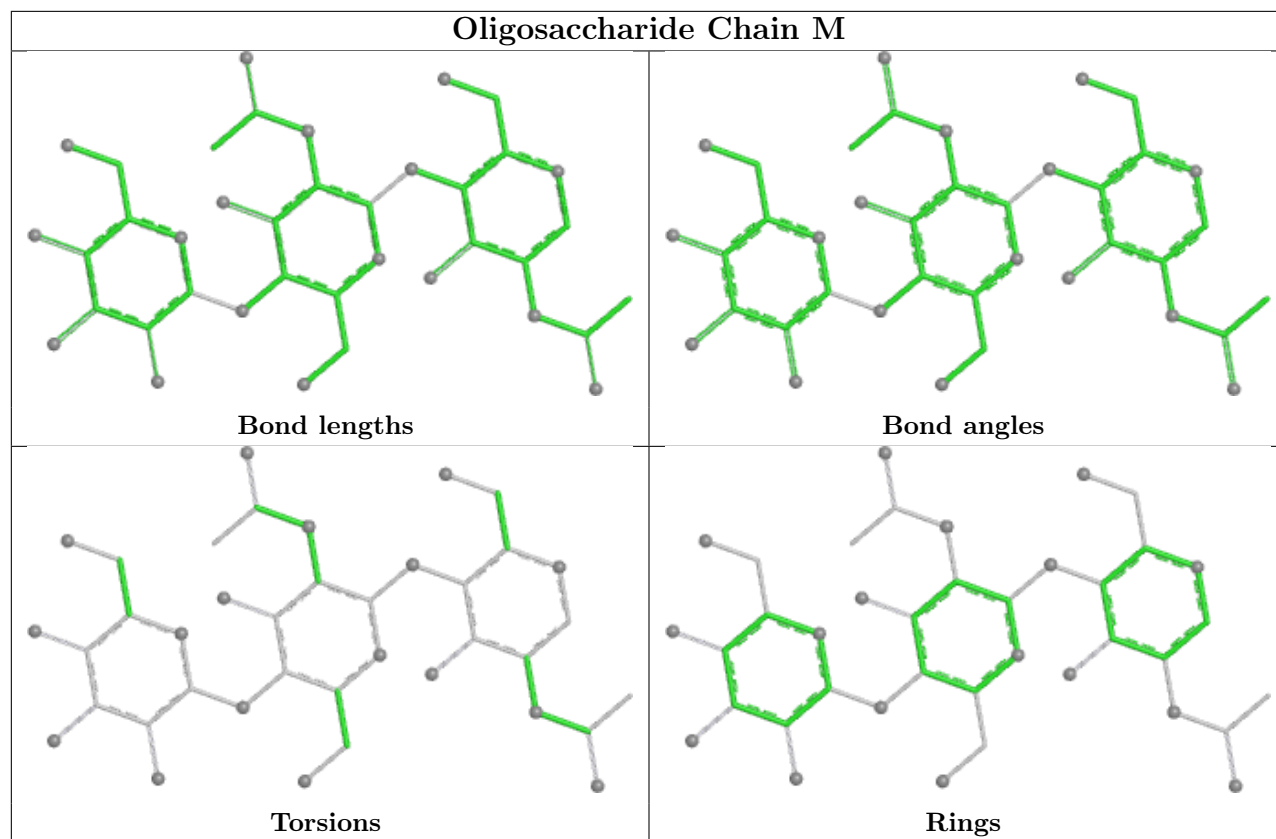
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	387/469 (82%)	-0.19	0 100 100	21, 49, 77, 106	0
1	B	387/469 (82%)	-0.20	1 (0%) 90 75	22, 48, 77, 144	0
1	C	387/469 (82%)	-0.13	2 (0%) 87 66	32, 53, 84, 101	0
1	D	387/469 (82%)	-0.14	1 (0%) 90 75	24, 52, 81, 145	0
2	E	232/237 (97%)	0.42	9 (3%) 43 24	43, 104, 224, 361	0
2	H	232/237 (97%)	0.29	7 (3%) 52 30	41, 101, 234, 393	0
2	J	232/237 (97%)	0.77	17 (7%) 21 14	50, 156, 399, 524	0
3	F	211/216 (97%)	0.51	7 (3%) 49 28	64, 124, 178, 224	0
3	K	211/216 (97%)	0.99	18 (8%) 16 12	101, 210, 388, 547	0
3	L	211/216 (97%)	0.35	6 (2%) 55 31	44, 101, 199, 264	0
All	All	2877/3235 (88%)	0.17	68 (2%) 59 34	21, 66, 260, 547	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	148	VAL	4.2
3	K	137	VAL	4.1
2	J	197	LEU	3.9
2	J	161	VAL	3.9
2	J	198	SER	3.7
2	E	208	LEU	3.5
2	H	160	LEU	3.4
2	E	156	ALA	3.2
3	K	197	CYS	3.2
3	L	123	PRO	3.2
2	E	150	THR	3.2
3	K	138	CYS	3.1
2	H	159	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
3	K	88	TYR	3.0
2	H	140	VAL	2.8
2	J	217	VAL	2.8
3	F	144	TYR	2.8
2	J	232	PRO	2.7
2	J	145	PRO	2.7
3	L	150	VAL	2.7
3	L	121	LEU	2.7
1	C	449	ASN	2.6
3	K	167	THR	2.6
3	F	30	GLY	2.6
2	H	145	PRO	2.6
2	J	37	VAL	2.5
2	J	160	LEU	2.5
2	H	144	ALA	2.4
2	J	187	ALA	2.4
2	J	226	VAL	2.4
2	E	159	CYS	2.4
1	C	286	SER	2.4
3	K	20	ILE	2.4
1	B	151	ASP	2.4
2	J	209	GLY	2.4
3	K	19	THR	2.4
2	E	213	TYR	2.4
3	L	122	PHE	2.3
3	F	158	PRO	2.3
3	K	206	VAL	2.3
3	K	146	GLY	2.3
3	F	135	THR	2.3
2	J	138	PRO	2.3
3	F	84	ASP	2.3
2	J	146	SER	2.2
2	E	232	PRO	2.2
2	J	24	ALA	2.2
2	E	168	PRO	2.2
3	K	165	THR	2.2
2	E	226	VAL	2.2
3	L	137	VAL	2.2
1	D	126	PRO	2.2
2	J	144	ALA	2.1
2	J	199	SER	2.1
2	J	183	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	147	SER	2.1
3	K	199	VAL	2.1
3	F	145	PRO	2.1
3	K	140	ILE	2.1
3	L	144	TYR	2.1
3	F	25	ALA	2.1
3	K	110	LEU	2.1
3	K	136	LEU	2.1
3	K	145	PRO	2.0
3	K	189	TRP	2.0
2	H	27	GLY	2.0
3	K	32	TYR	2.0
2	E	171	VAL	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](#)

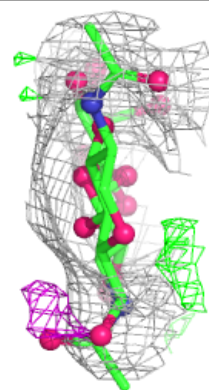
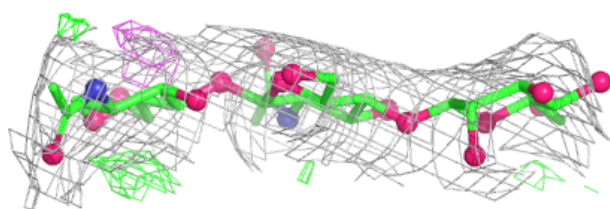
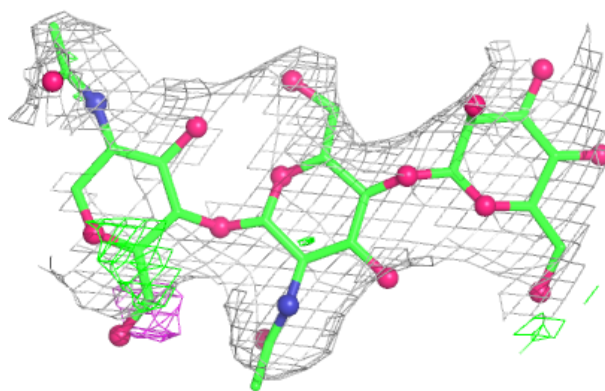
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	G	1	14/15	-	-	71,90,107,122	0
4	NAG	G	2	14/15	-	-	94,102,114,120	0
4	BMA	G	3	11/12	-	-	138,154,164,167	0
4	NAG	I	1	14/15	-	-	89,119,162,183	0
4	NAG	I	2	14/15	-	-	188,208,226,230	0
4	BMA	I	3	11/12	-	-	183,185,194,206	0
4	BMA	N	3	11/12	0.58	0.13	121,143,160,164	0
4	BMA	M	3	11/12	0.60	0.10	120,139,150,153	0
4	NAG	N	2	14/15	0.80	0.12	94,109,124,129	0
4	NAG	N	1	14/15	0.80	0.14	73,83,103,115	0
4	NAG	M	2	14/15	0.83	0.12	124,139,150,159	0
4	NAG	M	1	14/15	0.84	0.12	72,89,113,120	0

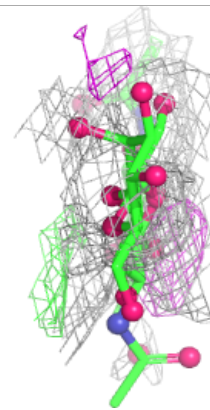
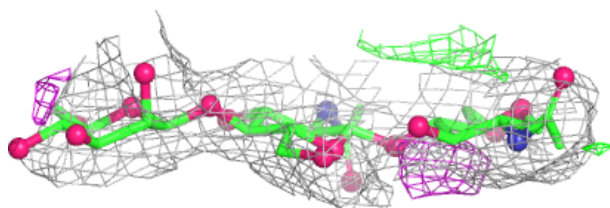
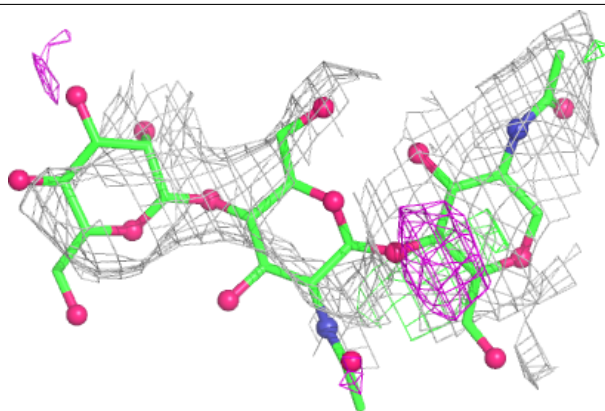
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

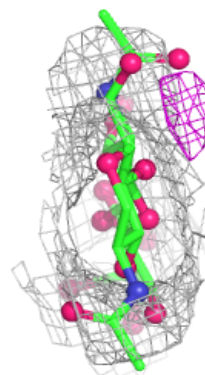
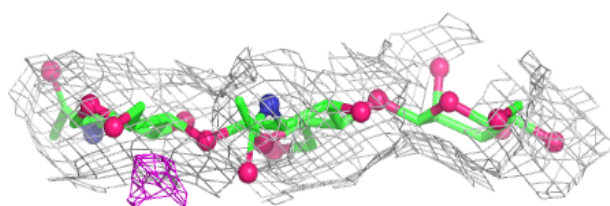
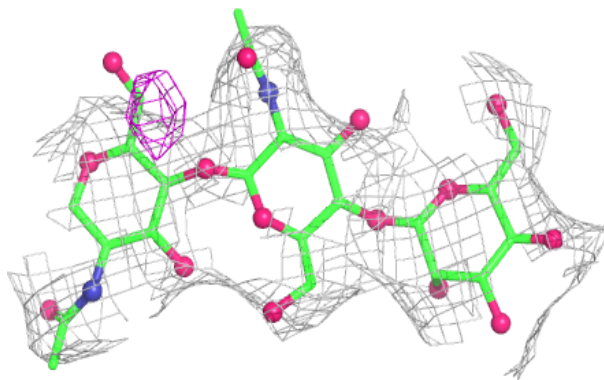
**Electron density around Chain I:**

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

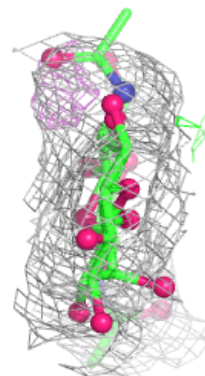
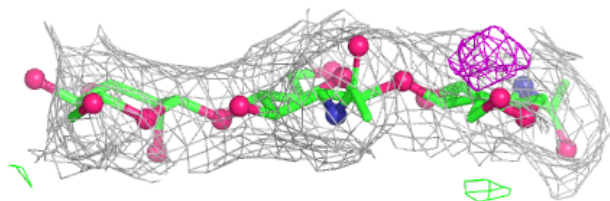
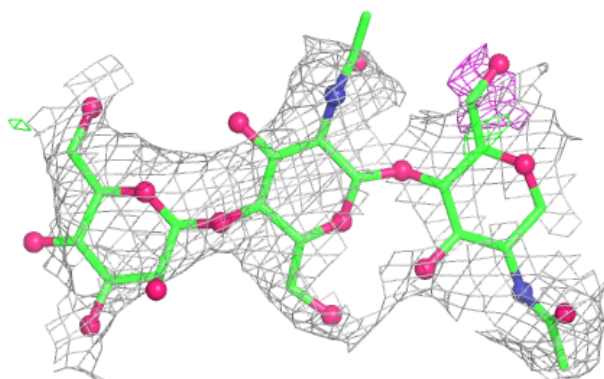


Electron density around Chain M:

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

**Electron density around Chain N:**

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



6.4 Ligands

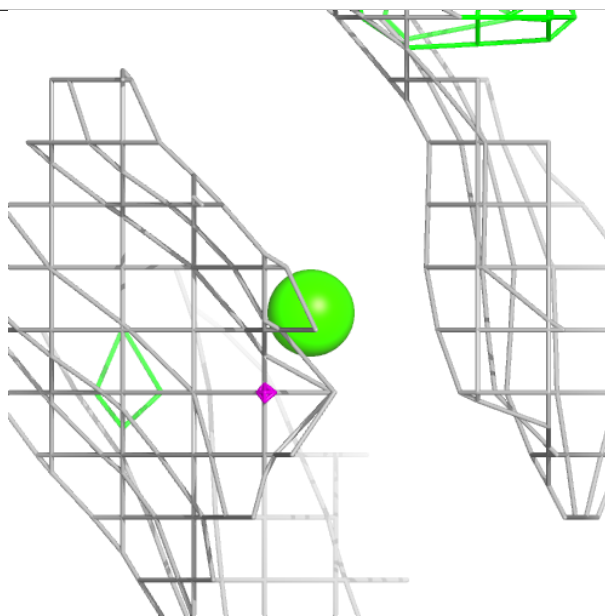
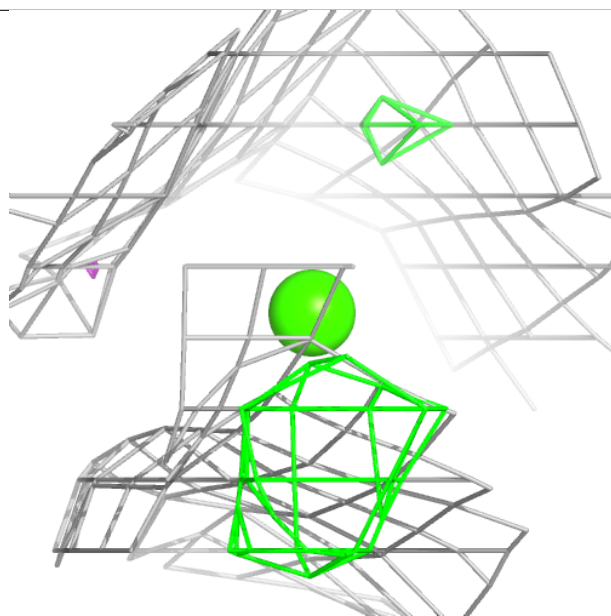
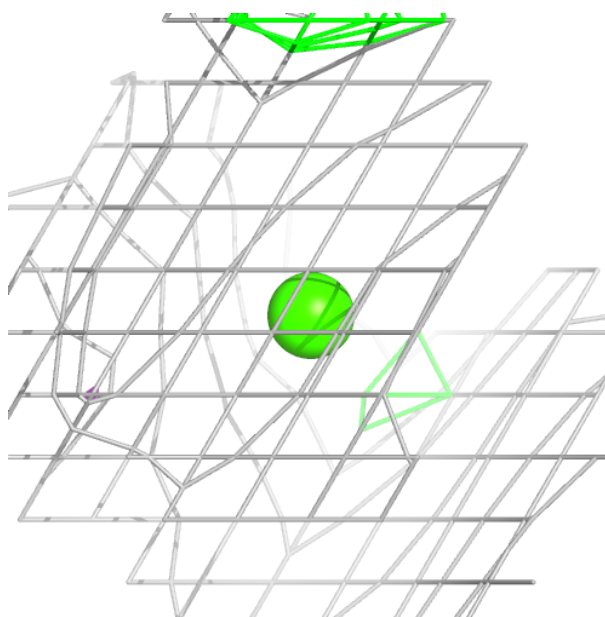
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	CA	D	502	1/1	0.90	0.09	81,81,81,81	0
5	CA	B	502	1/1	0.92	0.07	96,96,96,96	0
5	CA	C	502	1/1	0.93	0.08	70,70,70,70	0
5	CA	A	502	1/1	0.94	0.05	72,72,72,72	0
5	CA	B	501	1/1	0.96	0.05	54,54,54,54	0
5	CA	D	501	1/1	0.97	0.07	45,45,45,45	0
5	CA	A	501	1/1	0.97	0.07	36,36,36,36	0
5	CA	C	501	1/1	0.98	0.06	52,52,52,52	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.

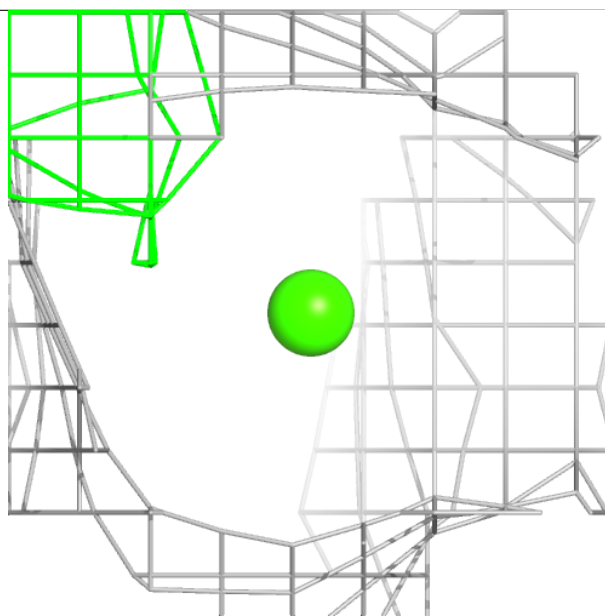
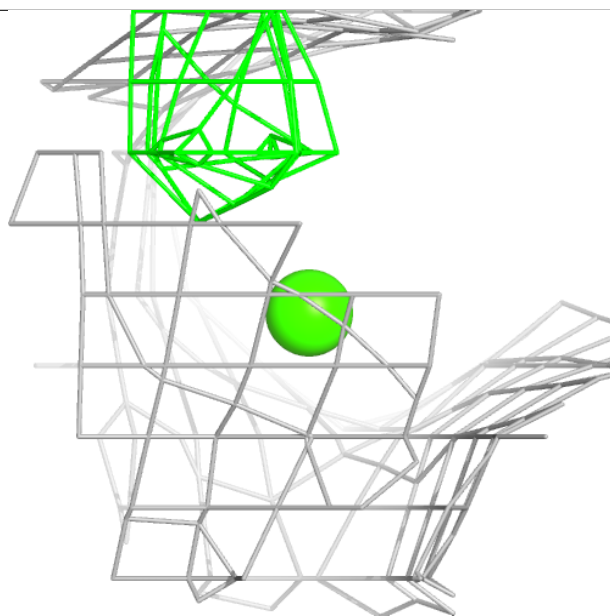
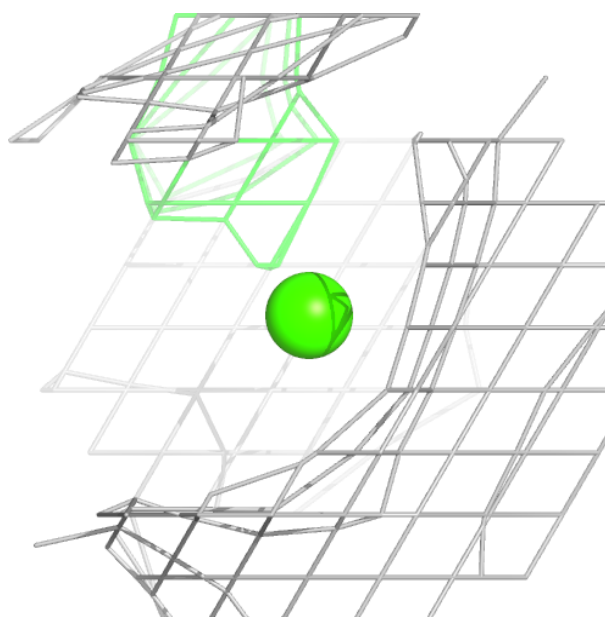
Electron density around CA D 502:

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



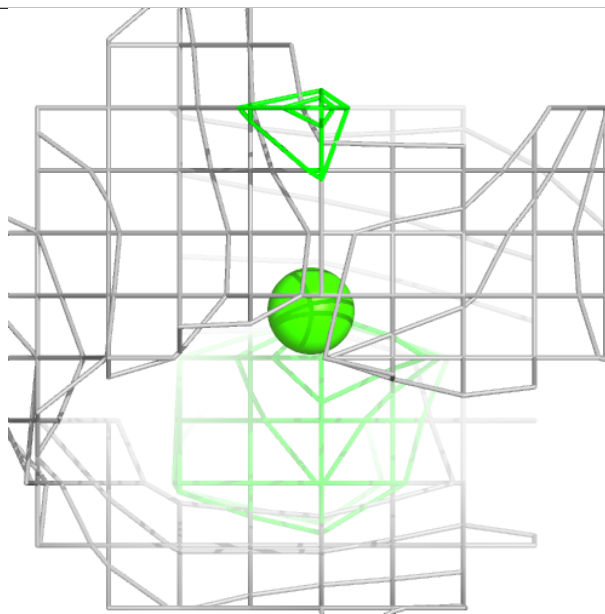
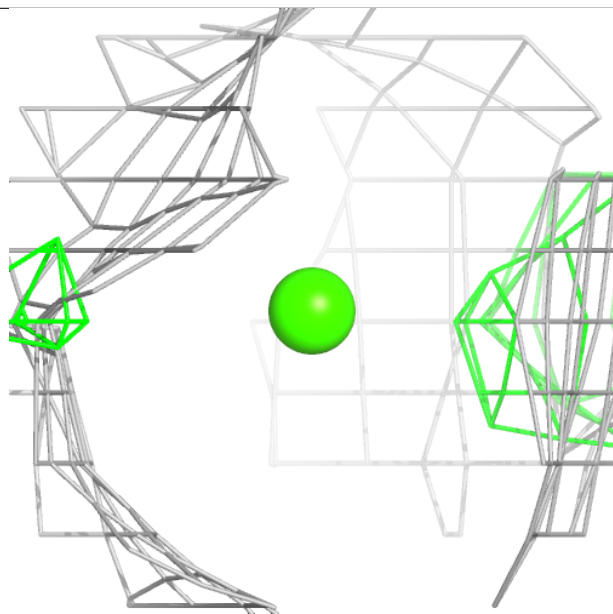
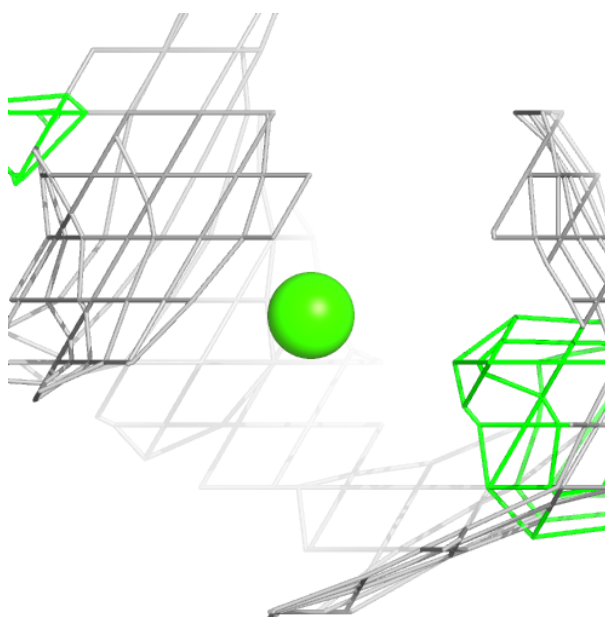
Electron density around CA B 502:

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



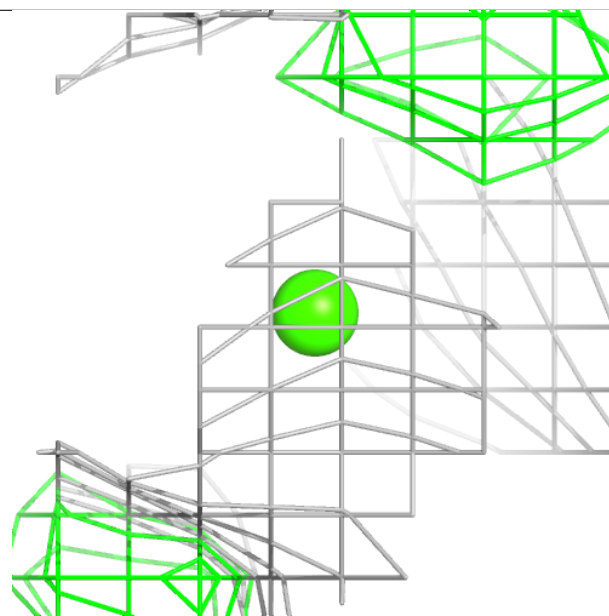
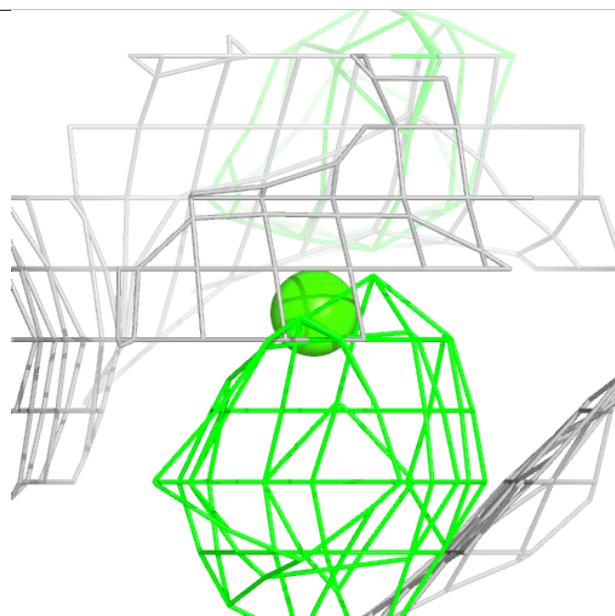
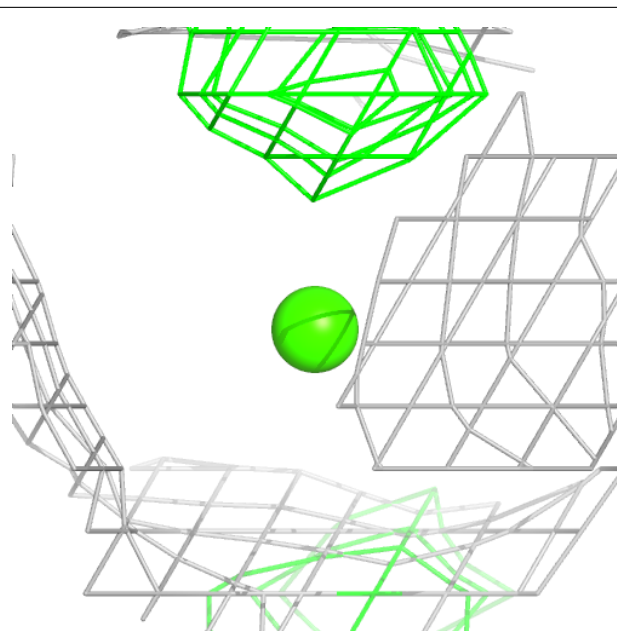
Electron density around CA C 502:

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



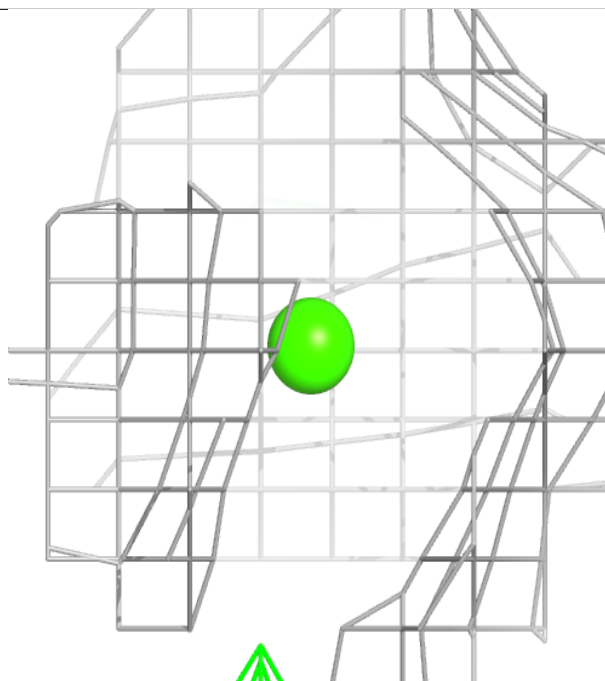
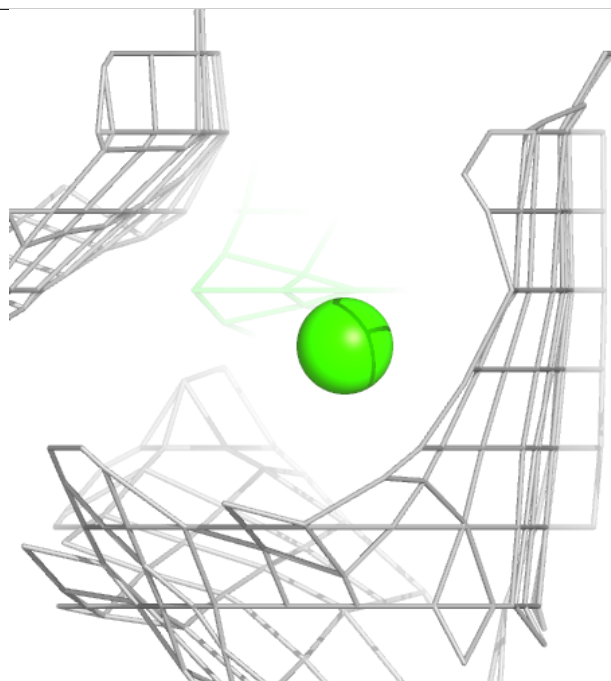
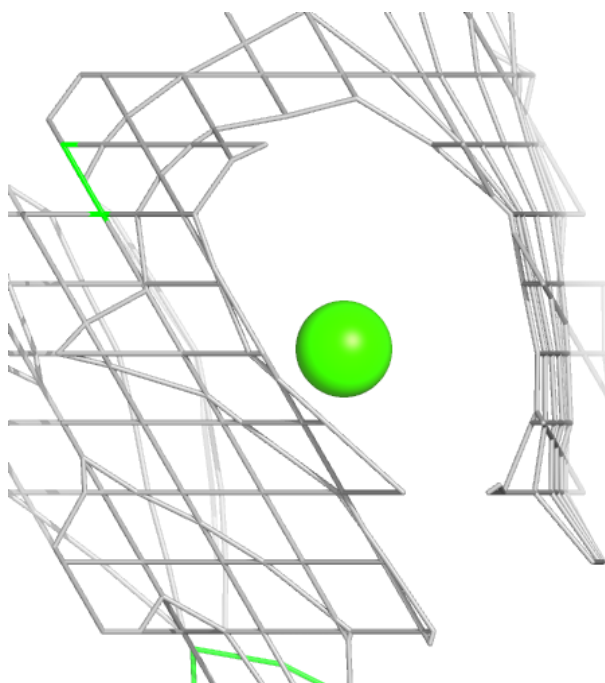
Electron density around CA A 502:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



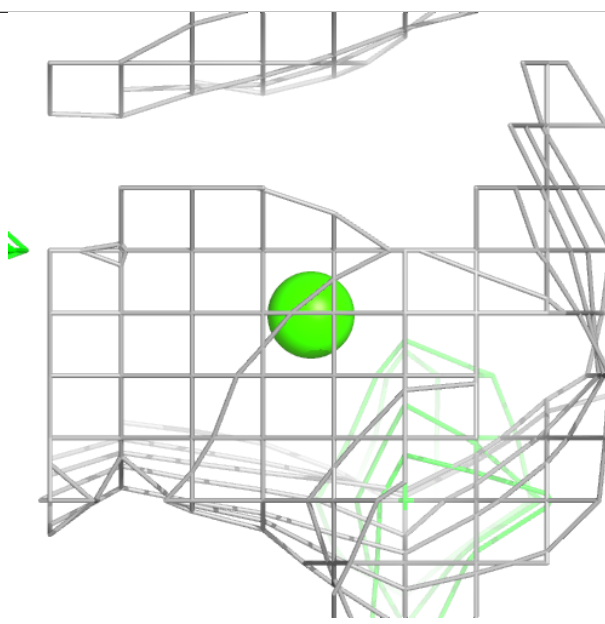
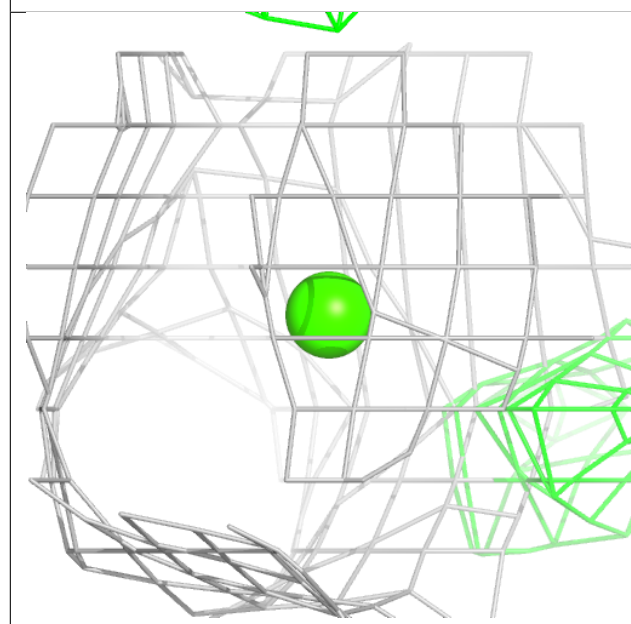
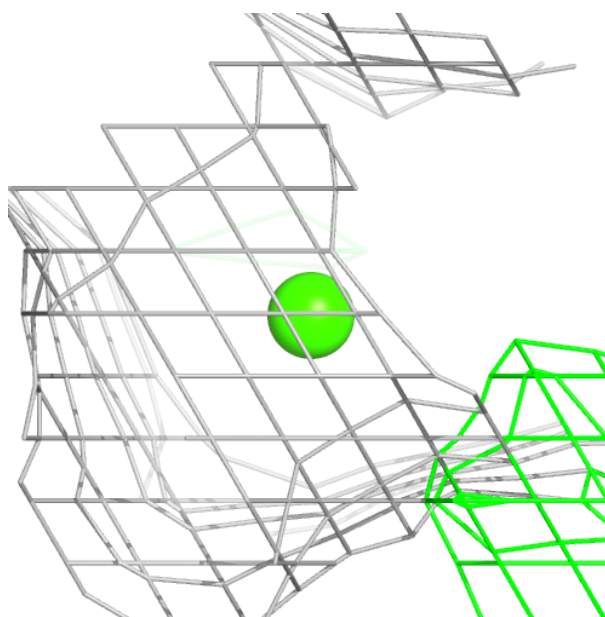
Electron density around CA B 501:

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



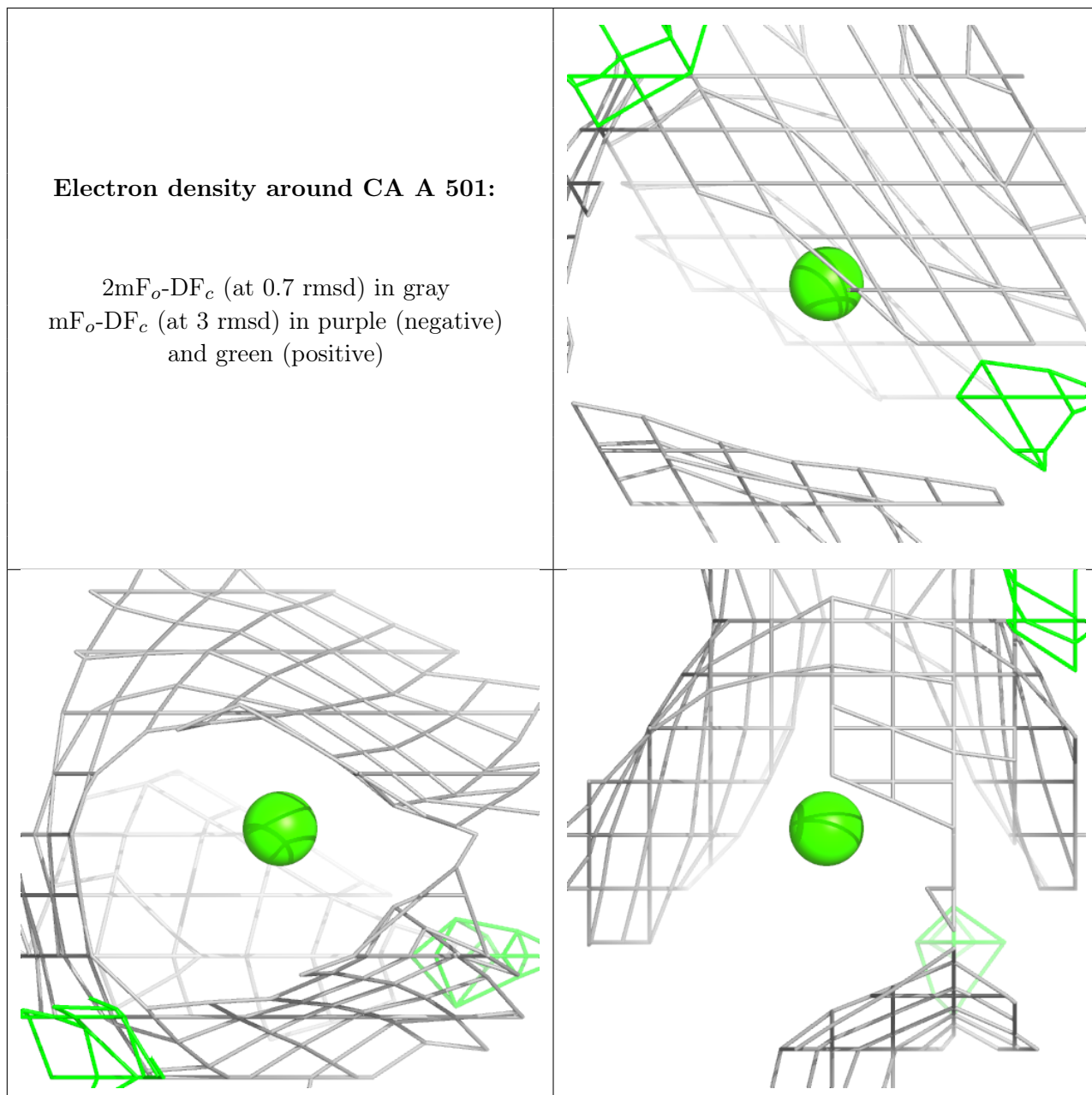
Electron density around CA D 501:

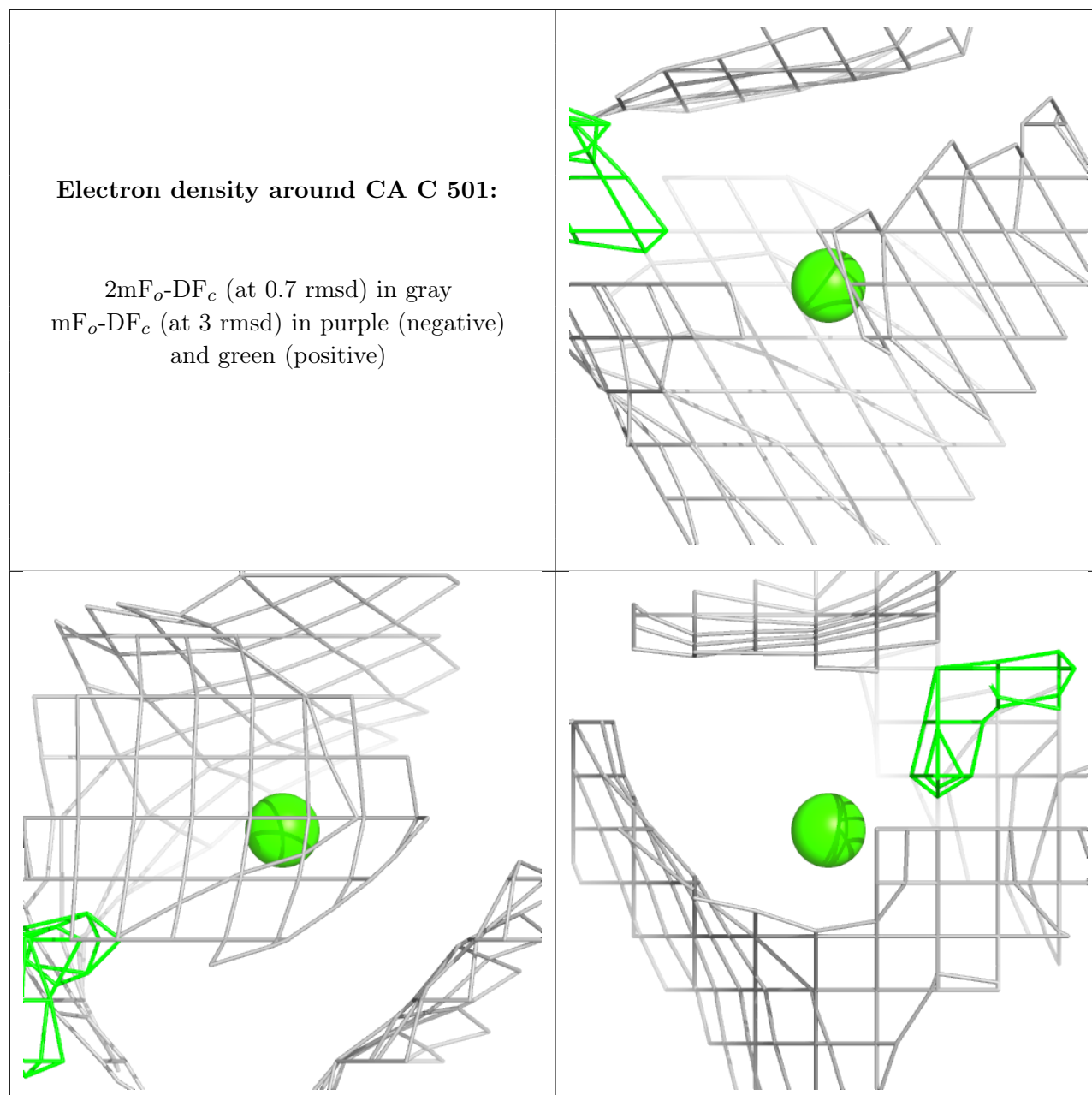
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.