



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2020 – 02:13 PM JST

PDB ID : 6LXK  
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](mailto: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.

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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 : 2.14.6  
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) : 2.14.6

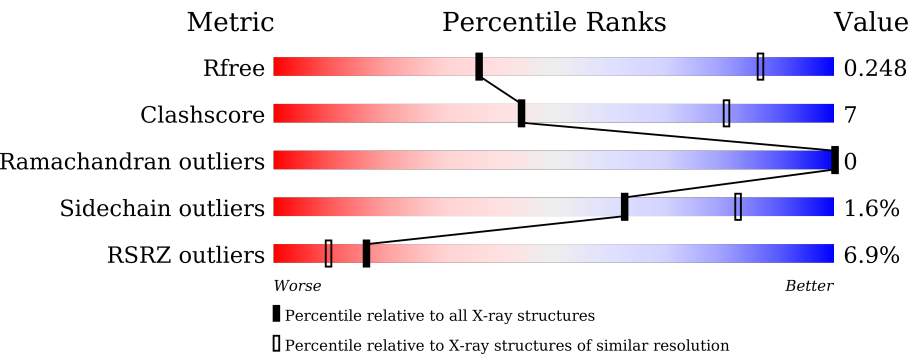
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div><div></div><div>68%14%•17%</div></div>
1	B	469	<div><div></div><div>70%12%•17%</div></div>
1	C	469	<div><div></div><div>70%12%•17%</div></div>
1	D	469	<div><div></div><div>68%13%•17%</div></div>
2	E	237	<div><div>7%</div><div>84%14%•</div></div>
2	H	237	<div><div>8%</div><div>84%14%•</div></div>

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	I	2	-	-	-	X
4	BMA	I	3	-	-	-	X

## 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			

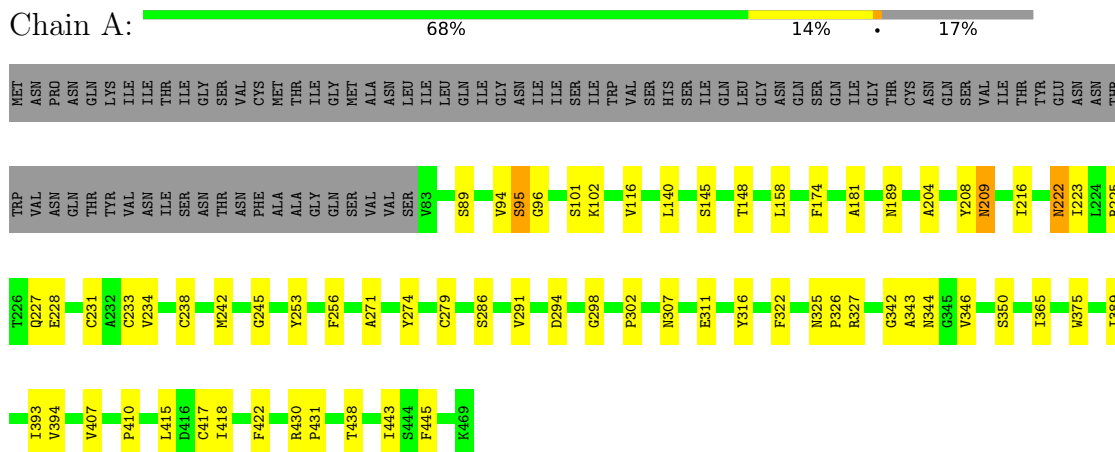
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by author).

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

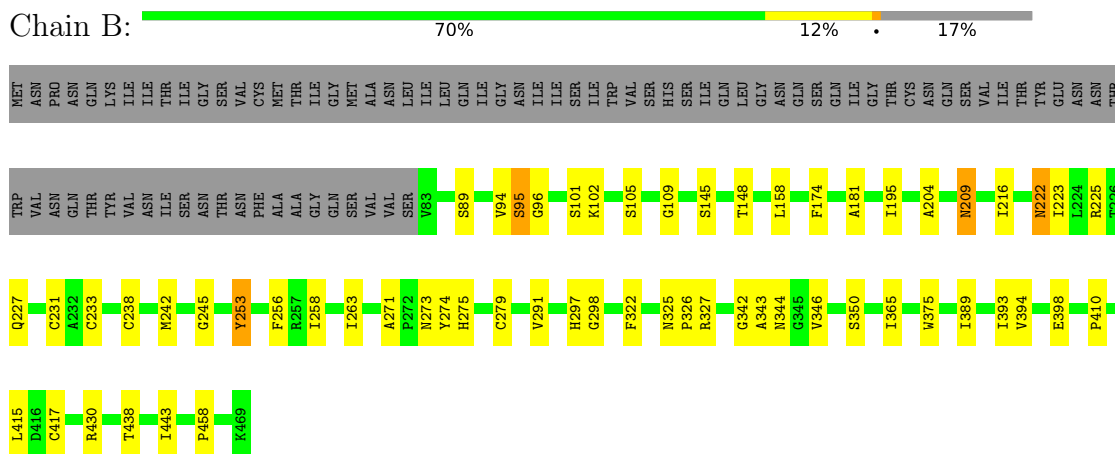
### 3 Residue-property plots

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.

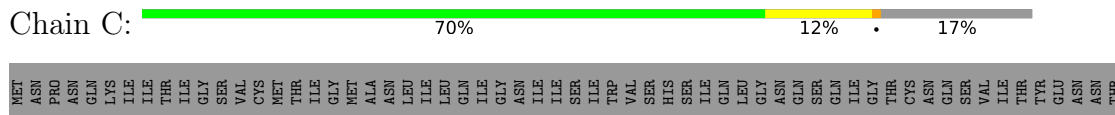
#### • Molecule 1: Neuraminidase

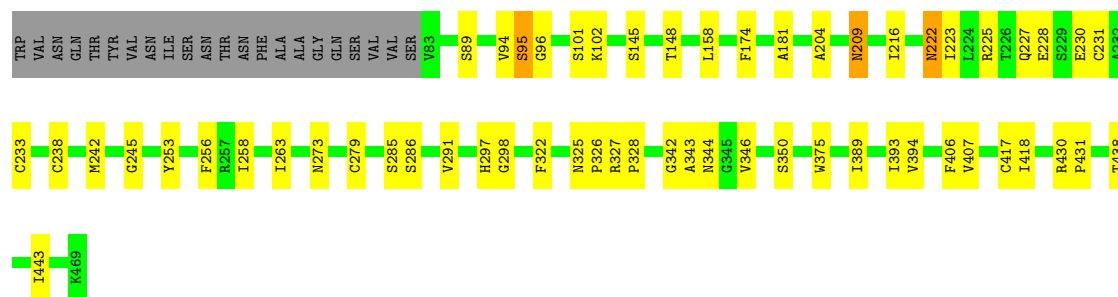


#### • Molecule 1: Neuraminidase



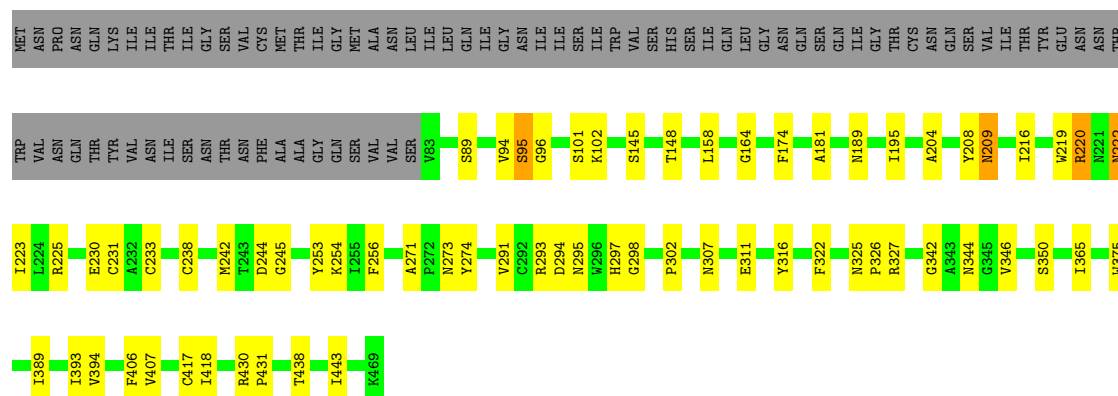
#### • Molecule 1: Neuraminidase





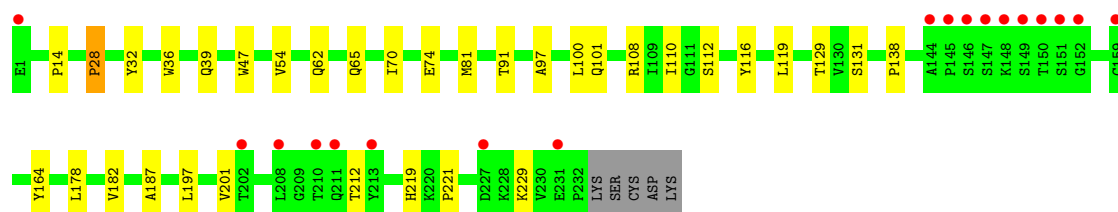
• Molecule 1: Neuraminidase

Chain D: 68% 13% 17%



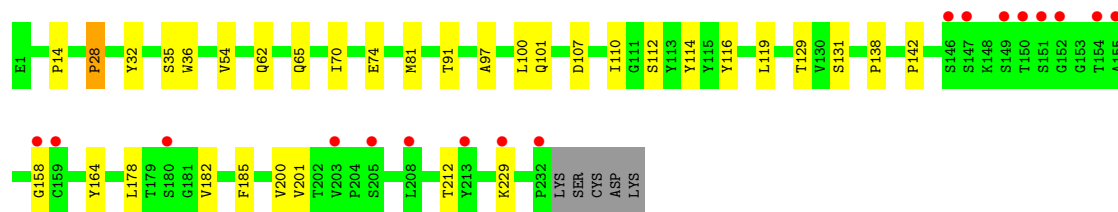
• Molecule 2: Heavy chain of Z2B3-D102R Fab

Chain H: 8% 84% 14%



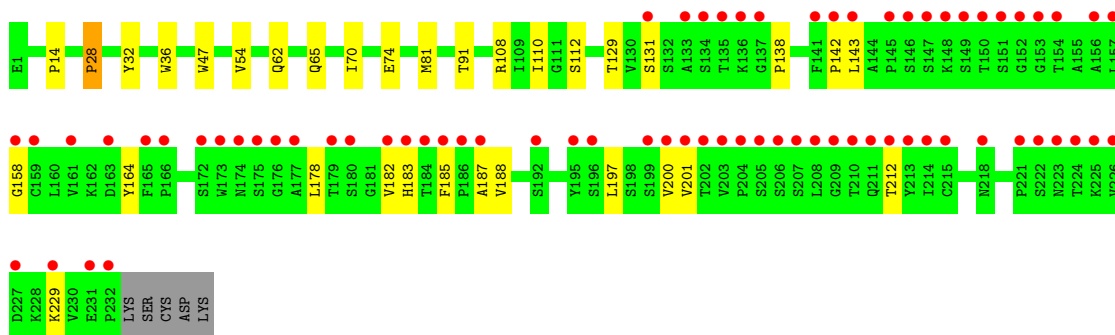
• Molecule 2: Heavy chain of Z2B3-D102R Fab

Chain E: 7% 84% 14%

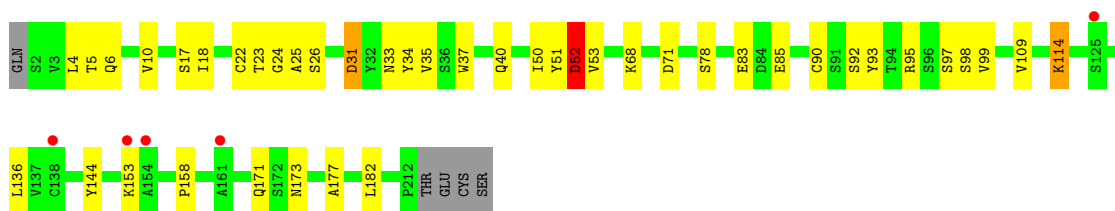
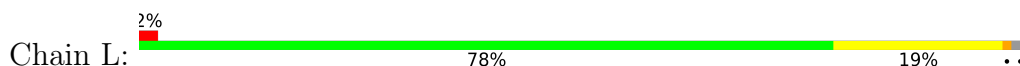


• Molecule 2: Heavy chain of Z2B3-D102R Fab

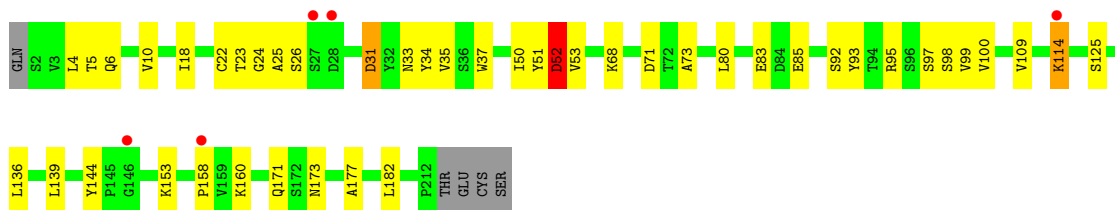
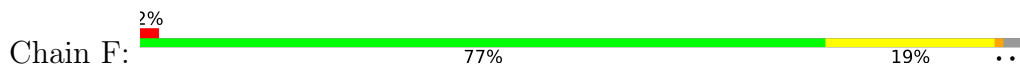
Chain J: 30% 84% 14%



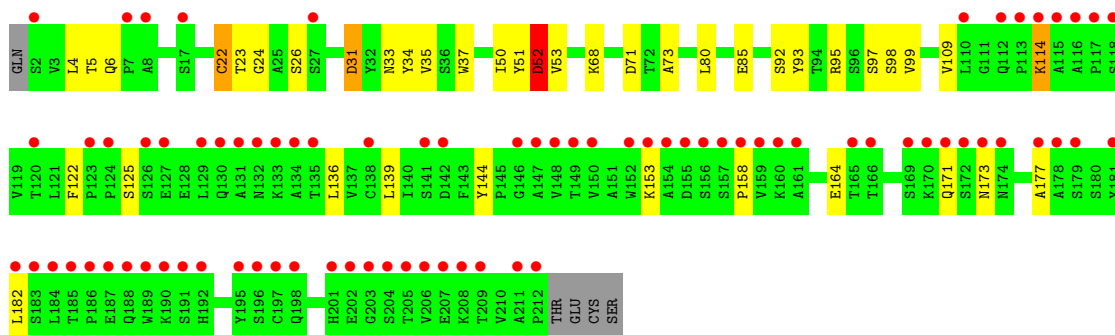
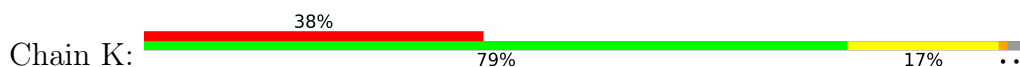
- Molecule 3: Light chain of Z2B3-D102R Fab



- 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

Chain G:  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 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, $\alpha$ , $\beta$ , $\gamma$	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) 99.5 (25.46-3.61)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.50 (at 3.64Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.215 , 0.249 0.214 , 0.248	Depositor DCC
$R_{free}$ test set	2511 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.5	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 40.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, 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	0.26	0/3068	0.47	0/4169
1	B	0.26	0/3068	0.47	0/4169
1	C	0.26	0/3068	0.47	0/4169
1	D	0.26	0/3068	0.48	0/4169
2	E	0.25	0/1772	0.46	0/2416
2	H	0.25	0/1772	0.45	0/2416
2	J	0.25	0/1772	0.46	0/2416
3	F	0.27	0/1600	0.49	0/2183
3	K	0.26	0/1600	0.51	0/2183
3	L	0.28	0/1600	0.50	0/2183
All	All	0.26	0/22388	0.48	0/30473

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.

There are no bond angle outliers.

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	33	0
1	C	2986	0	2809	34	0
1	D	2986	0	2809	40	0
2	E	1730	0	1695	21	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	2	0	0	0	0
5	D	2	0	0	0	0
All	All	21987	0	20972	284	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 (284) 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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:95:SER:O	1:B:95:SER:OG	2.21	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:K:34:TYR:HB2	3:K:93:TYR:HB3	1.87	0.57
3:L:98:SER:O	3:L:99:VAL:HG13	2.05	0.57
1:C:95:SER:O	1:C:95:SER:OG	2.22	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:CD	3:F:114:LYS:H	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:CD	3:K:114:LYS:H	2.19	0.55
3:F:100:VAL:O	3:F:100:VAL:HG23	2.06	0.55
3:L:114:LYS:H	3:L:114:LYS:CD	2.19	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
1:C:94:VAL:HG12	1:C:96:GLY:H	1.73	0.54
3:L:136:LEU:HD12	3:L:182:LEU:HD23	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:182:VAL:HG22	2:E:201:VAL:HG22	1.92	0.51
2:E:36:TRP:CE2	2:E:81:MET:HB2	2.46	0.51
1:A:393:ILE:HG22	1:A:394:VAL:HG23	1.92	0.51
1:C:242:MET:HB2	1:C:256:PHE:HE2	1.76	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: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
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:222:ASN:HB3	1:A:245:GLY:HA2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:SER:OG	1:A:95:SER:O	2.22	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:A:294:ASP:OD2	1:A:316:TYR:OH	2.14	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
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
1:C:204:ALA:HB3	1:C:216:ILE:HG23	1.96	0.47
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
3:L:171:GLN:NE2	3:L:177:ALA:HB2	2.25	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:F:114:LYS:H	3:F:114:LYS:HD2	1.80	0.46
3:L:22:CYS:CB	3:L:90:CYS:SG	3.02	0.46
1:B:258:ILE:HD12	1:B:263:ILE:HG12	1.96	0.46
3:K:114:LYS:HD2	3:K:114:LYS:H	1.81	0.46
3:L:114:LYS:HD2	3:L:114:LYS:H	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:230:GLU:OE2	1:C:406:PHE:HA	2.15	0.46
1:C:102:LYS:HG3	1:C:443:ILE:HG22	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:H:91:THR:HG23	2:H:129:THR:HA	1.97	0.45
3:L:171:GLN:OE1	3:L:173:ASN:ND2	2.48	0.45
3:L:26:SER:HB2	3:L:71:ASP:HA	1.98	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:N	3:L:31:ASP:OD1	2.49	0.45
3:F:153:LYS:HG2	3:F:158:PRO:HA	1.99	0.45
3:F:4:LEU:HD22	3:F:24:GLY:HA3	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
3:L:153:LYS:HG2	3:L:158:PRO:HA	1.98	0.45
1:B:102:LYS:HG3	1:B:443:ILE:HG22	1.98	0.45
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
1:C:298:GLY:N	1:C:342:GLY:O	2.51	0.44
3:L:26:SER:CB	3:L:71:ASP:HA	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:THR:HG23	1:A:438:THR:H	1.83	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:116:TYR:O	3:L:34:TYR:HD1	2.00	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
2:H:187:ALA:HB2	2:H:197:LEU:HD23	1.99	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
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:L:92:SER:O	3:L:99:VAL:HA	2.18	0.43
3:K:37:TRP:HB2	3:K:50:ILE:HB	2.01	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
3:L:4:LEU:HD13	3:L:22:CYS:SG	2.59	0.43
1:C:291:VAL:HG21	1:C:350:SER:HB2	2.01	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:HD3	2:H:108:ARG:HA	1.79	0.43
3:K:92:SER:O	3:K:99:VAL:HA	2.19	0.43
3:L:26:SER:OG	3:L:71:ASP:HA	2.19	0.43
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
1:D:327:ARG:O	1:D:365:ILE:HG22	2.19	0.42
2:H:14:PRO:HD3	2:H:131:SER:O	2.19	0.42
1:A:407:VAL:HG21	1:A:418:ILE:HD11	2.02	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
2:H:62:GLN:HA	2:H:65:GLN:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	3:K:80:LEU:HD23	1.84	0.42
1:A:227:GLN:HB3	1:A:279:CYS:O	2.19	0.42
1:C:430:ARG:HB2	1:C:438:THR:OG1	2.20	0.42
1:B:101:SER:HA	1:D:174:PHE:CZ	2.55	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:L:4:LEU:HD22	3:L:24:GLY:HA3	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
1:C:227:GLN:HB3	1:C:279:CYS:O	2.19	0.41
2:H:219:HIS:CD2	2:H:221:PRO:HD2	2.56	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
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
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
2:E:35:SER:HG	2:E:114:TYR:HH	1.60	0.41
3:F:114:LYS:CD	3:F:114:LYS:N	2.84	0.41
1:B:195:ILE:HG12	1:B:204:ALA:HB2	2.03	0.41
2:H:47:TRP:CG	3:L:99:VAL:CG2	3.04	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
3:F:80:LEU:HD23	3:F:80:LEU:HA	1.84	0.40
2:H:100:LEU:HG	2:H:101:GLN:HG3	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

### 5.3.1 Protein backbone

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
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%)	328 (99%)	4 (1%)	71	87
1	B	332/407 (82%)	328 (99%)	4 (1%)	71	87
1	C	332/407 (82%)	328 (99%)	4 (1%)	71	87
1	D	332/407 (82%)	327 (98%)	5 (2%)	65	84
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%)	194 (100%)	1 (0%)	88	95
3	F	178/183 (97%)	170 (96%)	8 (4%)	27	62
3	K	178/183 (97%)	171 (96%)	7 (4%)	32	65
3	L	178/183 (97%)	171 (96%)	7 (4%)	32	65
All	All	2447/2777 (88%)	2407 (98%)	40 (2%)	62	83

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	SER
1	A	209	ASN
1	A	231	CYS
1	A	253	TYR
3	L	6	GLN
3	L	31	ASP
3	L	52	ASP
3	L	83	GLU
3	L	97	SER
3	L	114	LYS
3	L	144	TYR
1	B	95	SER
1	B	209	ASN
1	B	231	CYS
1	B	253	TYR
1	C	95	SER

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Mol	Chain	Res	Type
1	C	209	ASN
1	C	231	CYS
1	C	253	TYR
1	D	95	SER
1	D	209	ASN
1	D	220	ARG
1	D	231	CYS
1	D	253	TYR
3	F	6	GLN
3	F	31	ASP
3	F	52	ASP
3	F	83	GLU
3	F	97	SER
3	F	114	LYS
3	F	144	TYR
3	F	160	LYS
2	J	183	HIS
3	K	6	GLN
3	K	22	CYS
3	K	31	ASP
3	K	52	ASP
3	K	97	SER
3	K	114	LYS
3	K	144	TYR

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

Mol	Chain	Res	Type
3	L	171	GLN
3	L	173	ASN
1	C	325	ASN
3	F	171	GLN
3	F	173	ASN
2	J	39	GLN
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	1,4	14,14,15	0.22	0	17,19,21	0.37	0
4	NAG	G	2	4	14,14,15	0.19	0	17,19,21	0.44	0
4	BMA	G	3	4	11,11,12	0.64	0	15,15,17	0.75	0
4	NAG	I	1	1,4	14,14,15	0.23	0	17,19,21	0.36	0
4	NAG	I	2	4	14,14,15	0.20	0	17,19,21	0.40	0
4	BMA	I	3	4	11,11,12	0.61	0	15,15,17	0.76	0
4	NAG	M	1	1,4	14,14,15	0.21	0	17,19,21	0.38	0
4	NAG	M	2	4	14,14,15	0.20	0	17,19,21	0.43	0
4	BMA	M	3	4	11,11,12	0.63	0	15,15,17	0.78	0
4	NAG	N	1	1,4	14,14,15	0.20	0	17,19,21	0.38	0
4	NAG	N	2	4	14,14,15	0.19	0	17,19,21	0.42	0
4	BMA	N	3	4	11,11,12	0.65	0	15,15,17	0.75	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	1,4	-	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	1,4	-	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	1,4	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	M	3	4	-	0/2/19/22	0/1/1/1
4	NAG	N	1	1,4	-	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.

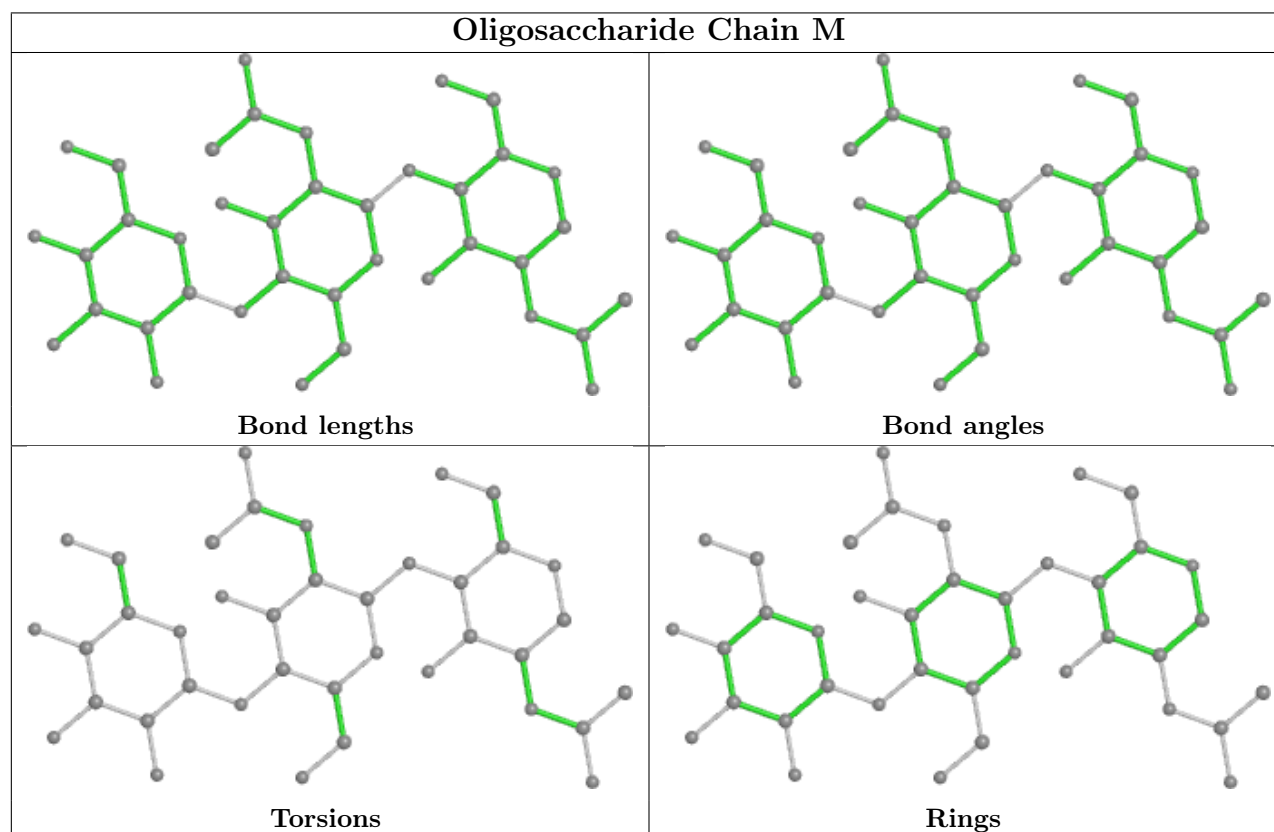
There are no chirality outliers.

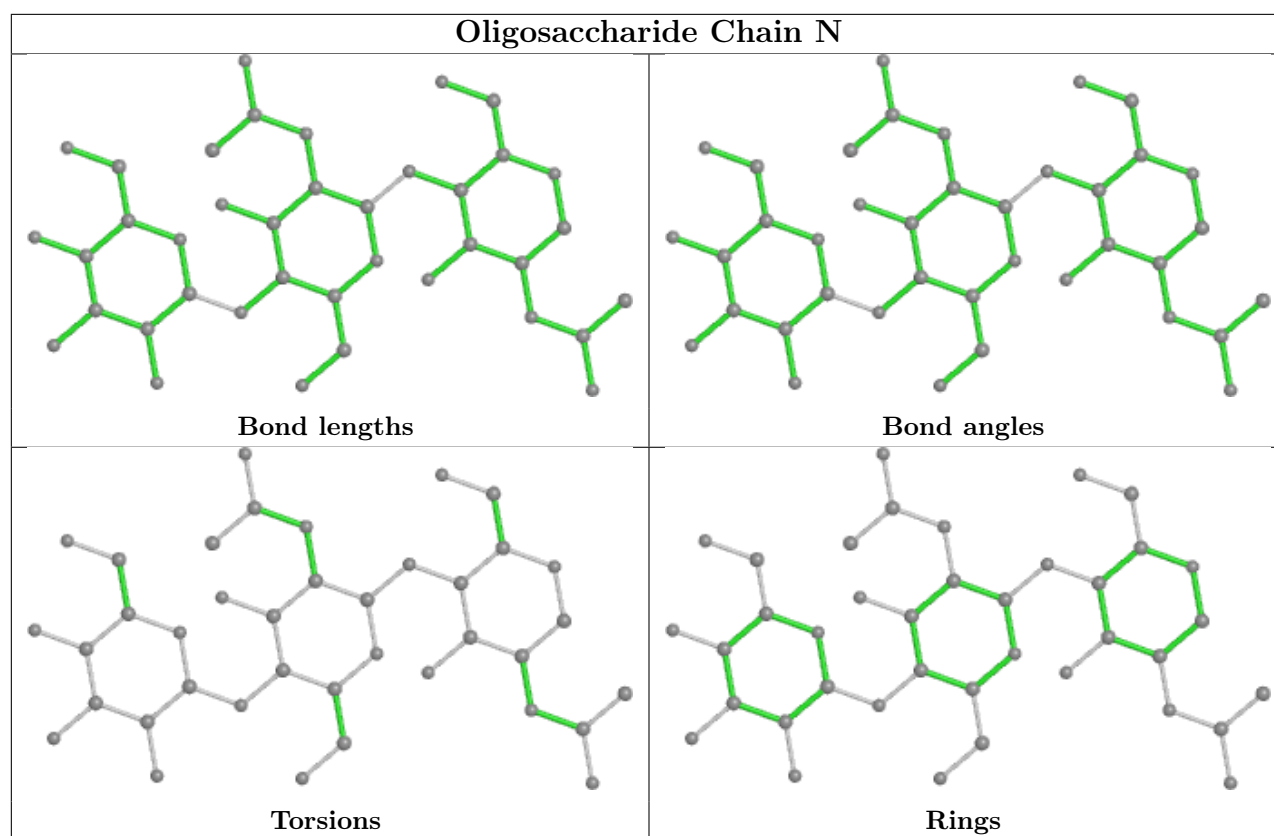
There are no torsion outliers.

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 [i](#)

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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	387/469 (82%)	-0.70	0	100	100	21, 49, 77, 106	0
1	B	387/469 (82%)	-0.68	0	100	100	22, 48, 77, 144	0
1	C	387/469 (82%)	-0.67	0	100	100	32, 53, 84, 101	0
1	D	387/469 (82%)	-0.69	0	100	100	24, 52, 81, 145	0
2	E	232/237 (97%)	0.11	17 (7%)	15	9	43, 104, 224, 361	0
2	H	232/237 (97%)	0.13	18 (7%)	13	8	41, 101, 234, 393	0
2	J	232/237 (97%)	1.52	72 (31%)	0	0	50, 156, 399, 524	0
3	F	211/216 (97%)	0.11	5 (2%)	59	42	64, 124, 178, 224	0
3	K	211/216 (97%)	1.85	81 (38%)	0	0	101, 210, 388, 547	0
3	L	211/216 (97%)	-0.00	5 (2%)	59	42	44, 101, 199, 264	0
All	All	2877/3235 (88%)	-0.08	198 (6%)	16	10	21, 66, 260, 547	0

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	149	THR	11.5
2	E	150	THR	10.4
2	J	202	THR	10.3
2	J	232	PRO	8.3
2	J	150	THR	8.2
2	J	145	PRO	8.2
2	J	149	SER	8.1
3	K	156	SER	8.0
3	K	179	SER	7.6
2	H	147	SER	7.2
2	J	212	THR	7.2
3	K	113	PRO	7.2
3	K	196	SER	6.9

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Mol	Chain	Res	Type	RSRZ
2	J	210	THR	6.8
2	H	145	PRO	6.6
3	K	209	THR	6.6
2	J	227	ASP	6.5
2	J	186	PRO	6.5
2	J	151	SER	6.3
2	J	146	SER	6.2
2	J	225	LYS	6.1
2	J	152	GLY	6.1
3	K	132	ASN	6.0
3	K	183	SER	5.9
2	J	224	THR	5.8
3	K	172	SER	5.8
2	J	213	TYR	5.6
2	H	151	SER	5.6
3	K	134	ALA	5.4
2	H	150	THR	5.4
2	J	176	GLY	5.4
3	K	124	PRO	5.4
3	K	165	THR	5.4
2	E	158	GLY	5.3
2	J	183	HIS	5.3
3	K	187	GLU	5.3
3	K	189	TRP	5.2
2	E	149	SER	5.2
3	K	191	SER	5.2
3	K	173	ASN	5.1
2	H	144	ALA	5.1
2	J	207	SER	5.1
3	K	188	GLN	5.1
2	J	209	GLY	5.0
2	J	165	PHE	5.0
3	K	197	CYS	5.0
2	J	184	THR	4.9
2	J	206	SER	4.8
2	J	179	THR	4.8
2	J	205	SER	4.8
2	J	147	SER	4.7
2	H	146	SER	4.7
3	K	174	ASN	4.6
2	J	203	VAL	4.6
2	J	226	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
2	J	231	GLU	4.6
2	J	153	GLY	4.5
2	J	211	GLN	4.5
2	J	185	PHE	4.5
3	K	116	ALA	4.4
3	K	192	HIS	4.3
3	K	148	VAL	4.3
2	J	156	ALA	4.3
2	J	157	LEU	4.2
3	K	182	LEU	4.2
2	J	177	ALA	4.2
2	J	215	CYS	4.1
3	K	171	GLN	4.1
2	J	187	ALA	4.1
2	E	213	TYR	4.1
2	J	175	SER	4.0
3	K	155	ASP	4.0
2	J	158	GLY	4.0
3	K	154	ALA	4.0
3	K	146	GLY	4.0
3	K	123	PRO	3.9
3	K	150	VAL	3.9
2	J	159	CYS	3.9
3	K	202	GLU	3.9
2	E	159	CYS	3.9
2	H	211	GLN	3.9
2	J	166	PRO	3.9
3	K	160	LYS	3.9
3	K	190	LYS	3.8
2	E	208	LEU	3.7
2	J	192	SER	3.7
3	K	204	SER	3.7
2	J	201	VAL	3.7
3	K	157	SER	3.6
3	K	147	ALA	3.6
3	K	131	ALA	3.6
2	J	134	SER	3.5
3	K	126	SER	3.5
3	K	120	THR	3.5
3	K	115	ALA	3.5
2	J	223	ASN	3.4
3	F	27	SER	3.4

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Mol	Chain	Res	Type	RSRZ
2	J	148	LYS	3.4
2	H	159	CYS	3.4
2	J	204	PRO	3.4
2	E	151	SER	3.4
3	K	186	PRO	3.4
2	J	142	PRO	3.4
3	K	177	ALA	3.3
3	K	153	LYS	3.3
3	K	114	LYS	3.3
2	E	147	SER	3.3
3	K	133	LYS	3.3
2	J	196	SER	3.3
3	K	195	TYR	3.2
3	K	203	GLY	3.2
3	F	114	LYS	3.2
3	K	212	PRO	3.2
3	K	110	LEU	3.2
3	K	141	SER	3.2
3	K	198	GLN	3.2
3	K	166	THR	3.2
3	K	112	GLN	3.1
2	J	143	LEU	3.1
3	K	178	ALA	3.1
3	K	170	LYS	3.1
2	J	136	LYS	3.0
2	J	208	LEU	3.0
2	J	214	ILE	3.0
3	F	28	ASP	2.9
3	K	117	PRO	2.9
3	K	161	ALA	2.9
3	K	130	GLN	2.9
3	K	158	PRO	2.9
2	H	213	TYR	2.9
2	J	180	SER	2.9
3	K	211	ALA	2.8
2	J	131	SER	2.8
2	E	155	ALA	2.8
3	L	153	LYS	2.8
3	K	207	GLU	2.8
2	J	172	SER	2.7
2	J	222	SER	2.7
3	K	184	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	J	154	THR	2.7
3	L	161	ALA	2.7
3	K	169	SER	2.6
2	H	231	GLU	2.6
2	J	218	ASN	2.6
2	H	152	GLY	2.6
2	J	141	PHE	2.6
3	K	181	TYR	2.6
3	L	138	CYS	2.5
3	K	159	VAL	2.5
2	J	161	VAL	2.5
3	K	129	LEU	2.4
3	K	208	LYS	2.4
2	E	152	GLY	2.4
3	L	154	ALA	2.4
2	J	229	LYS	2.4
3	K	17	SER	2.4
2	H	148	LYS	2.4
2	E	154	THR	2.4
2	H	210	THR	2.4
2	J	137	GLY	2.3
3	K	118	SER	2.3
3	K	135	THR	2.3
2	E	203	VAL	2.3
2	E	146	SER	2.3
3	F	146	GLY	2.3
2	E	180	SER	2.3
2	J	182	VAL	2.3
2	J	200	VAL	2.3
3	K	206	VAL	2.3
2	H	202	THR	2.3
2	J	173	TRP	2.3
2	E	232	PRO	2.3
2	J	174	ASN	2.2
3	F	158	PRO	2.2
3	K	27	SER	2.2
2	J	133	ALA	2.2
2	H	1	GLU	2.2
3	K	185	THR	2.2
3	K	8	ALA	2.2
3	K	152	TRP	2.2
2	H	208	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	229	LYS	2.2
3	K	201	HIS	2.2
2	H	149	SER	2.2
2	J	195	TYR	2.1
3	K	7	PRO	2.1
3	K	127	GLU	2.1
2	E	205	SER	2.1
2	J	199	SER	2.1
3	K	138	CYS	2.1
3	K	142	ASP	2.1
3	K	2	SER	2.1
3	L	125	SER	2.1
3	K	205	THR	2.0
2	H	227	ASP	2.0
2	J	163	ASP	2.0
2	J	135	THR	2.0
2	J	221	PRO	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

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<sup>th</sup> 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.

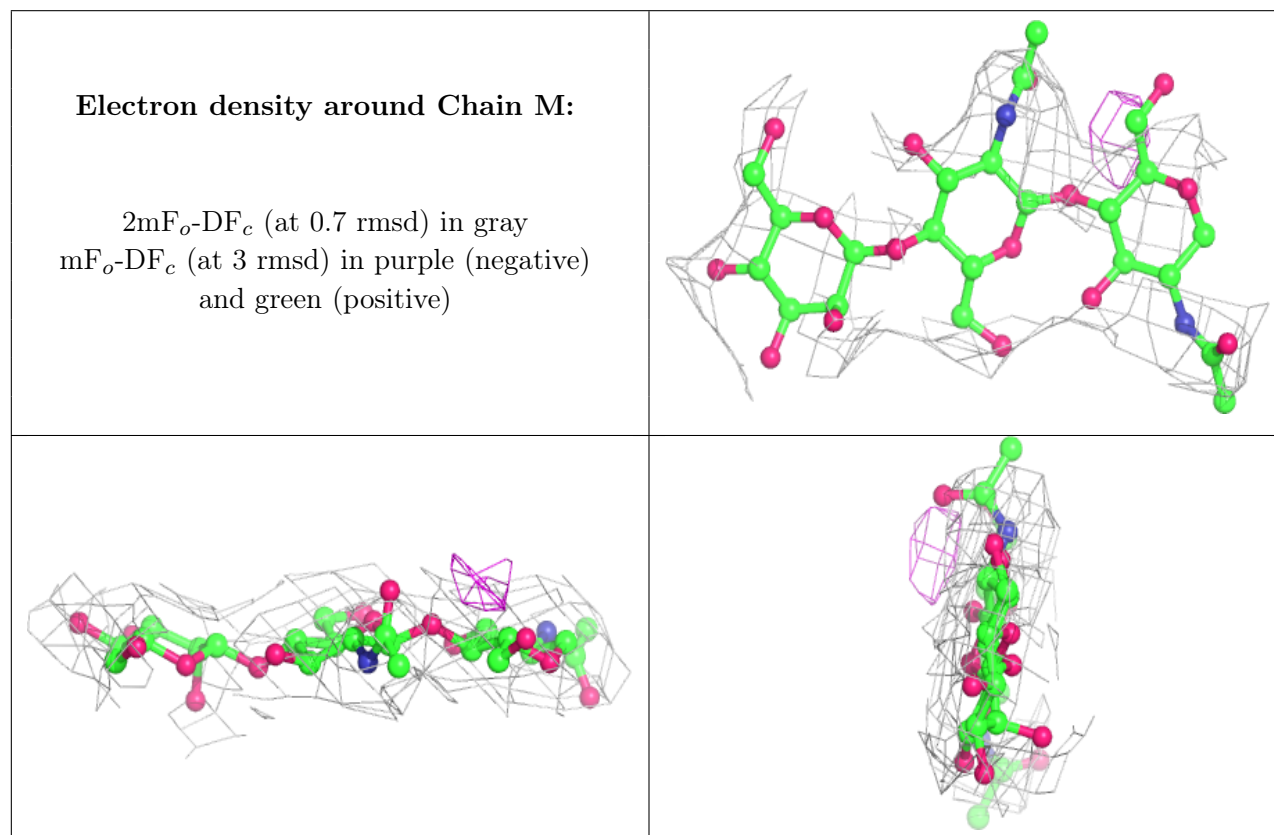
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	BMA	I	3	11/12	0.55	0.63	183,185,194,206	0
4	NAG	I	2	14/15	0.59	0.55	188,208,226,230	0
4	BMA	G	3	11/12	0.70	0.36	138,154,164,167	0
4	NAG	I	1	14/15	0.70	0.35	89,119,162,183	0
4	BMA	M	3	11/12	0.79	0.35	120,139,150,153	0
4	NAG	G	1	14/15	0.82	0.24	71,90,107,122	0
4	BMA	N	3	11/12	0.83	0.46	121,143,160,164	0
4	NAG	N	1	14/15	0.85	0.26	73,83,103,115	0
4	NAG	M	2	14/15	0.87	0.33	124,139,150,159	0
4	NAG	G	2	14/15	0.88	0.25	94,102,114,120	0
4	NAG	N	2	14/15	0.88	0.36	94,109,124,129	0

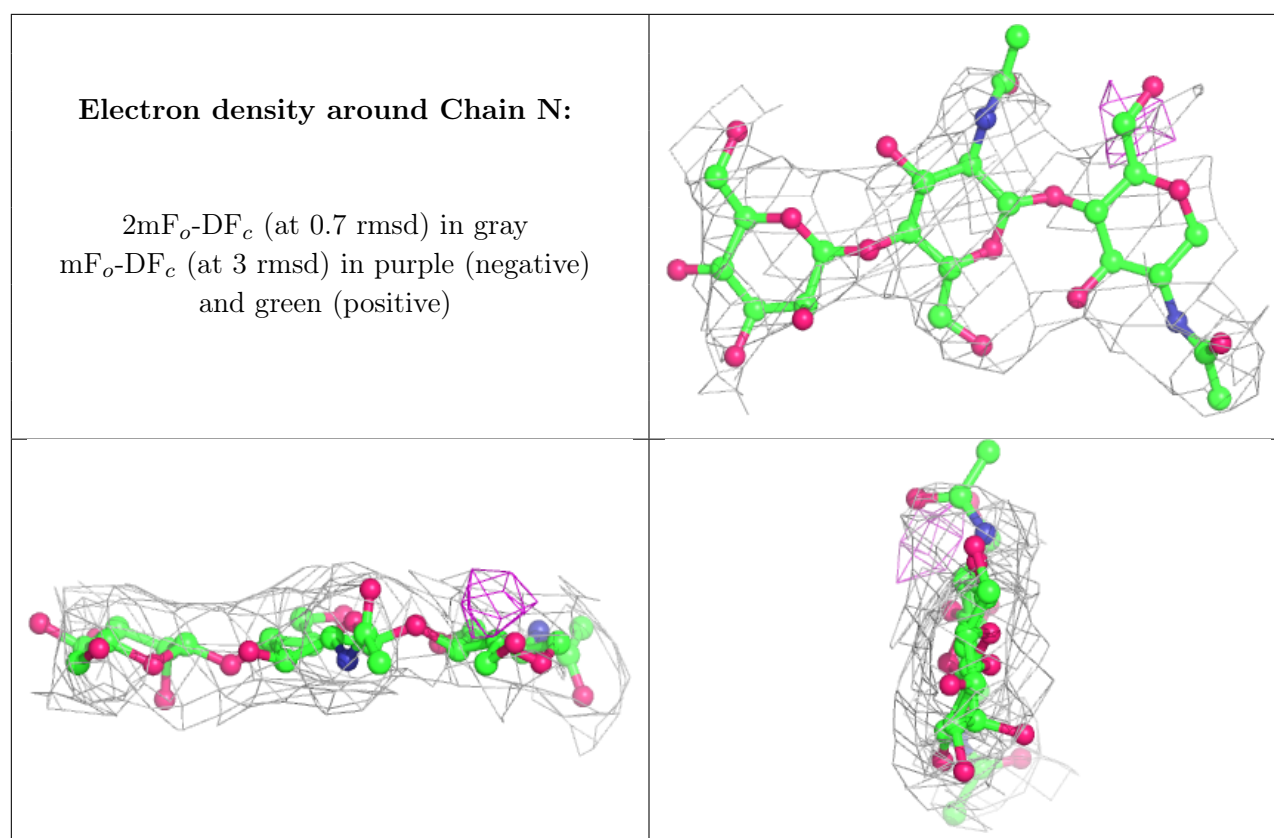
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	M	1	14/15	0.88	0.29	72,89,113,120	0

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.





## 6.4 Ligands [i](#)

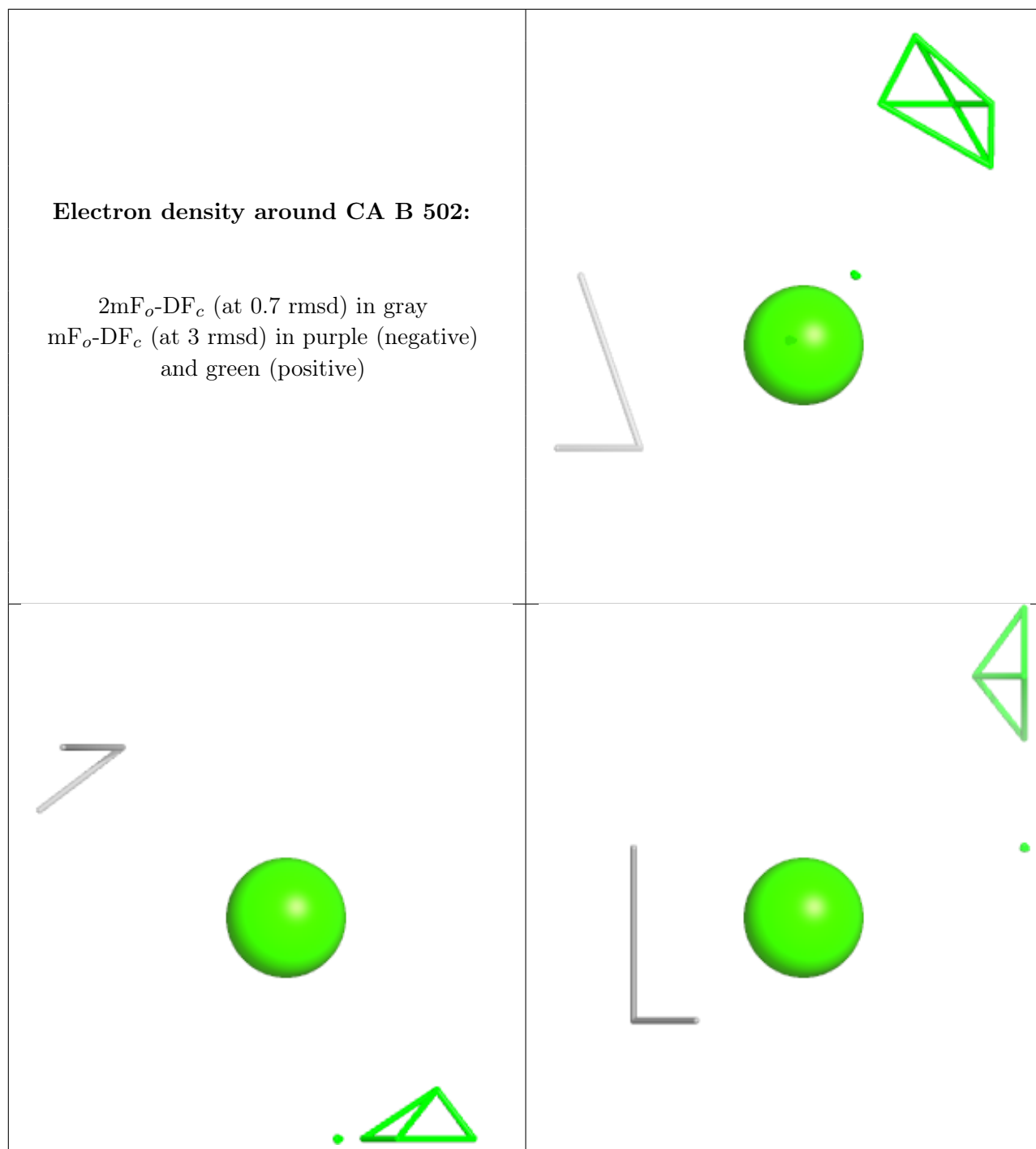
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

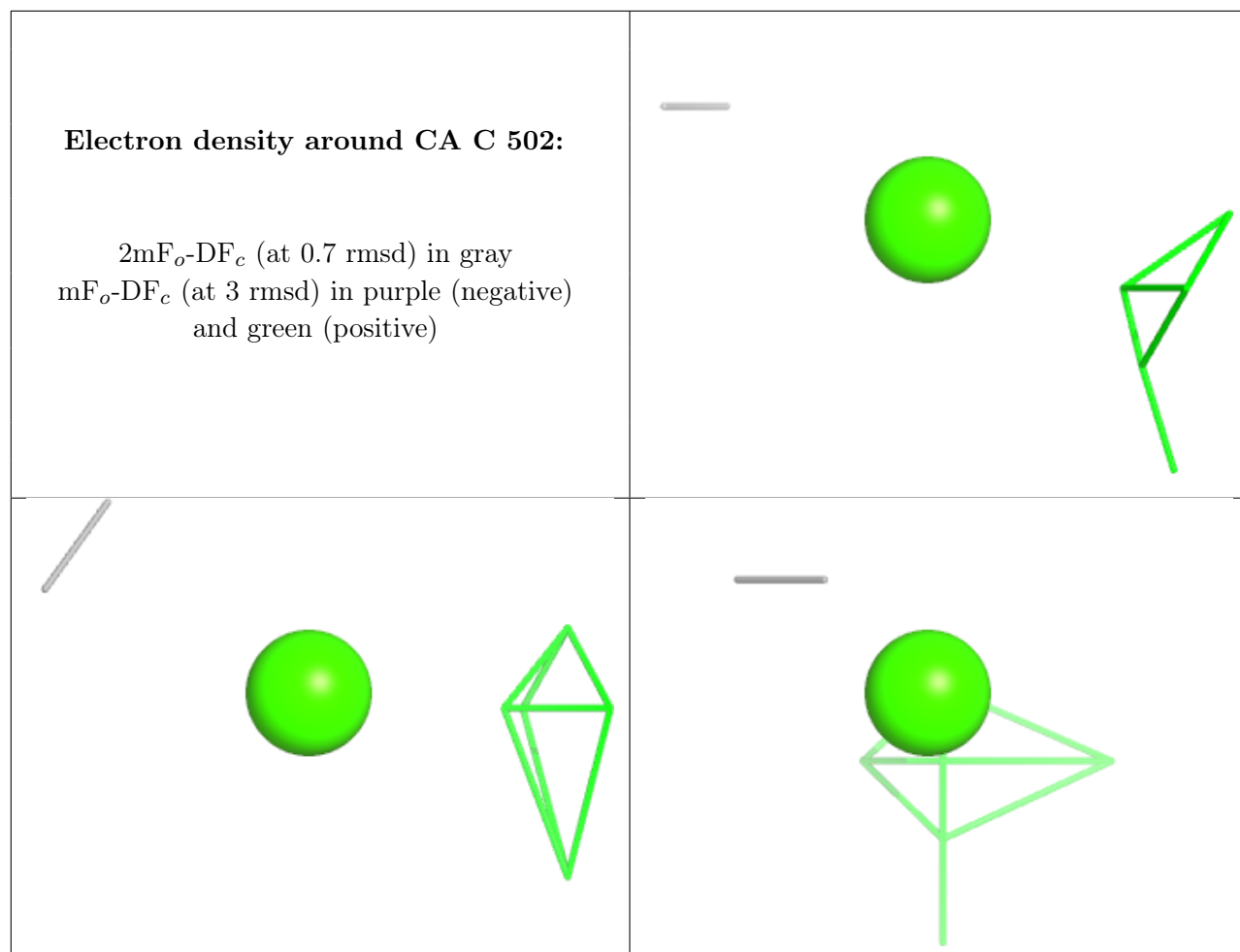
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CA	B	502	1/1	0.64	0.11	96,96,96,96	0
5	CA	C	502	1/1	0.68	0.12	70,70,70,70	0
5	CA	D	502	1/1	0.86	0.11	81,81,81,81	0
5	CA	B	501	1/1	0.89	0.10	54,54,54,54	0
5	CA	A	502	1/1	0.89	0.06	72,72,72,72	0
5	CA	D	501	1/1	0.94	0.18	45,45,45,45	0
5	CA	A	501	1/1	0.95	0.20	36,36,36,36	0
5	CA	C	501	1/1	0.98	0.16	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 B 502:**

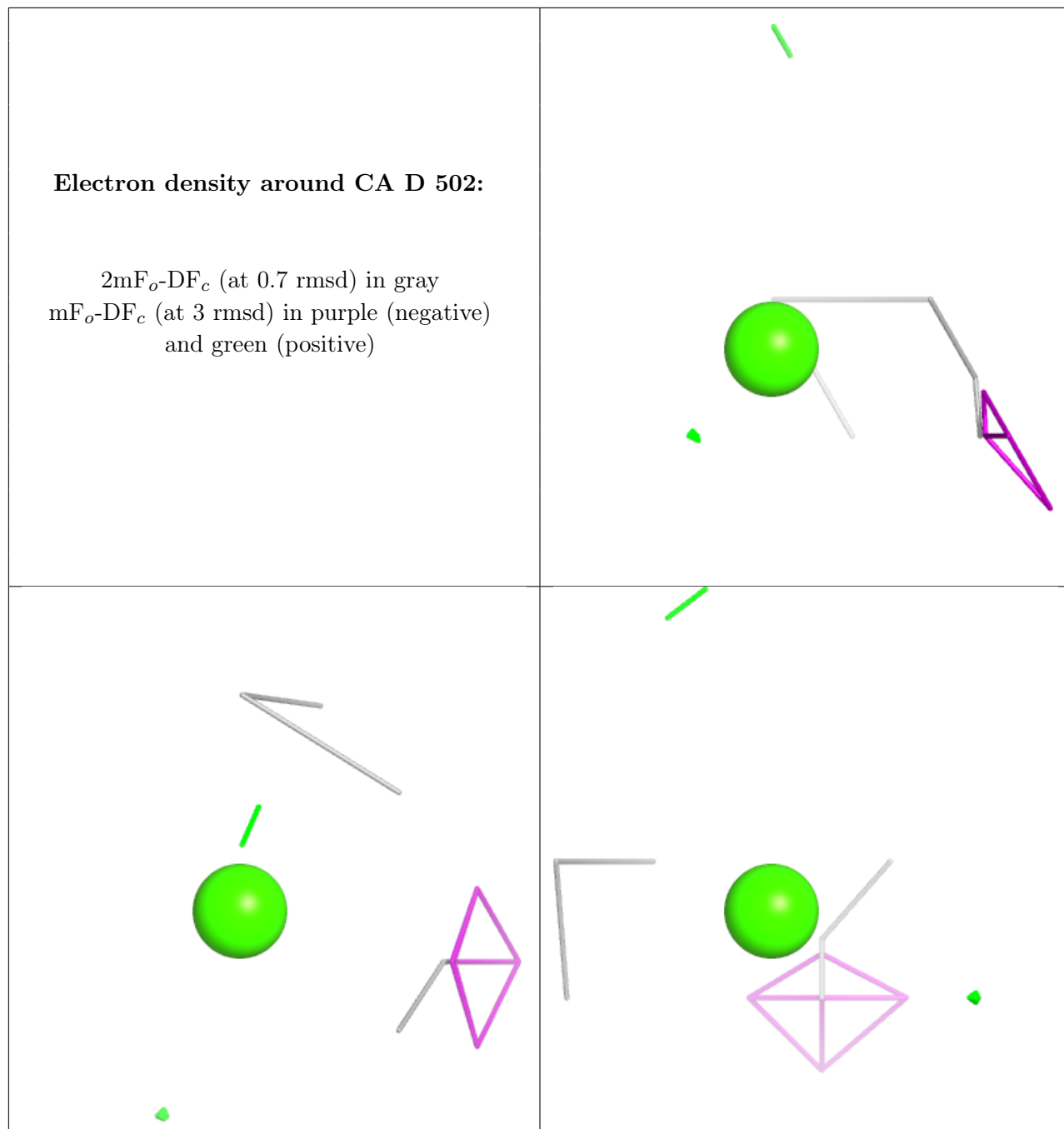
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

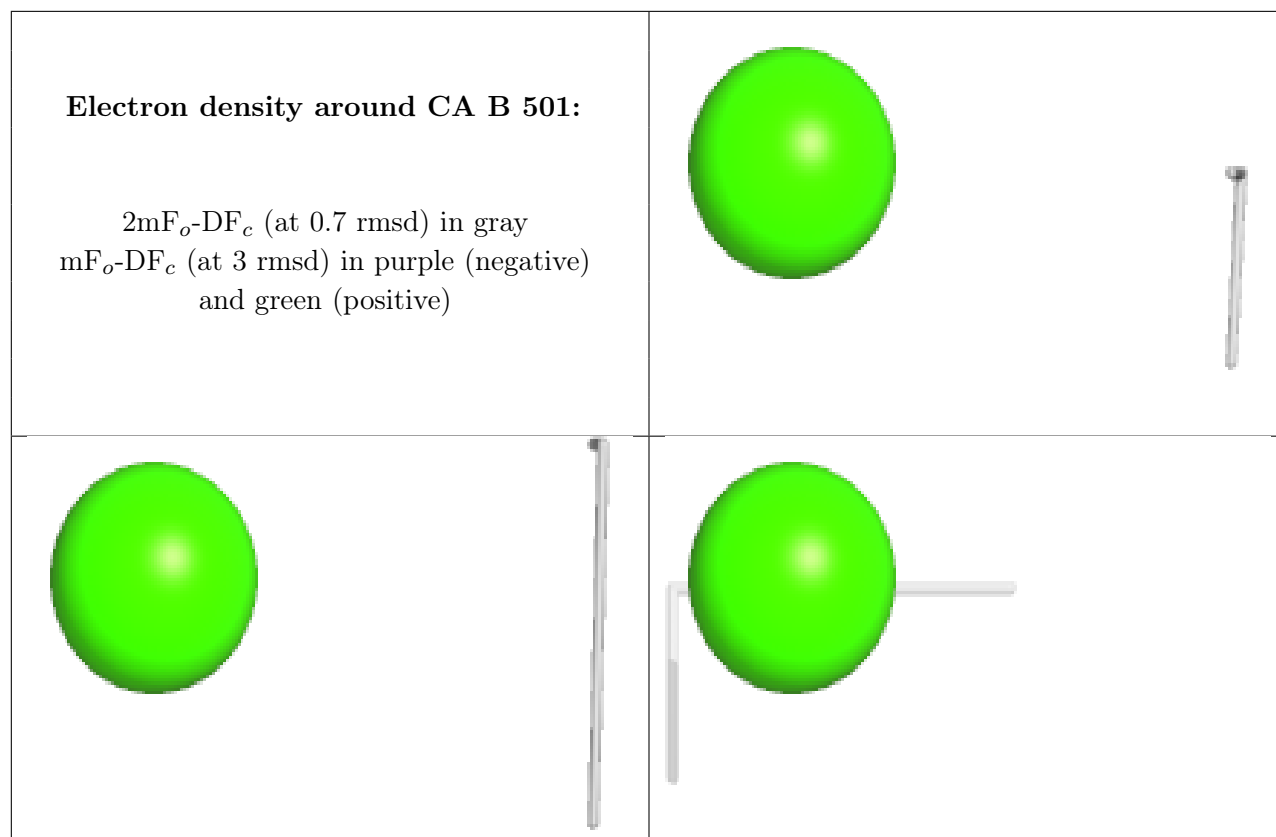




**Electron density around CA D 502:**

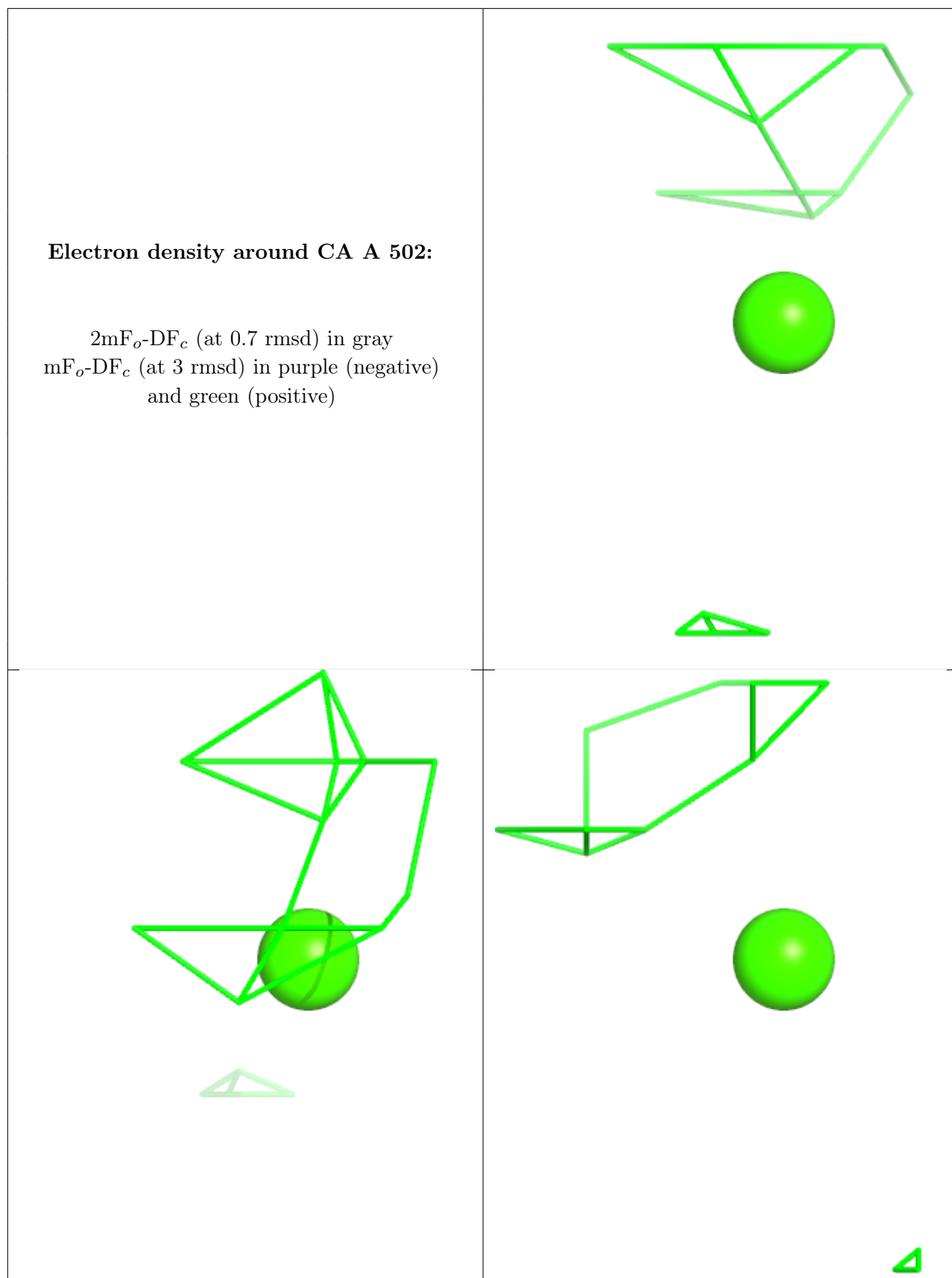
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





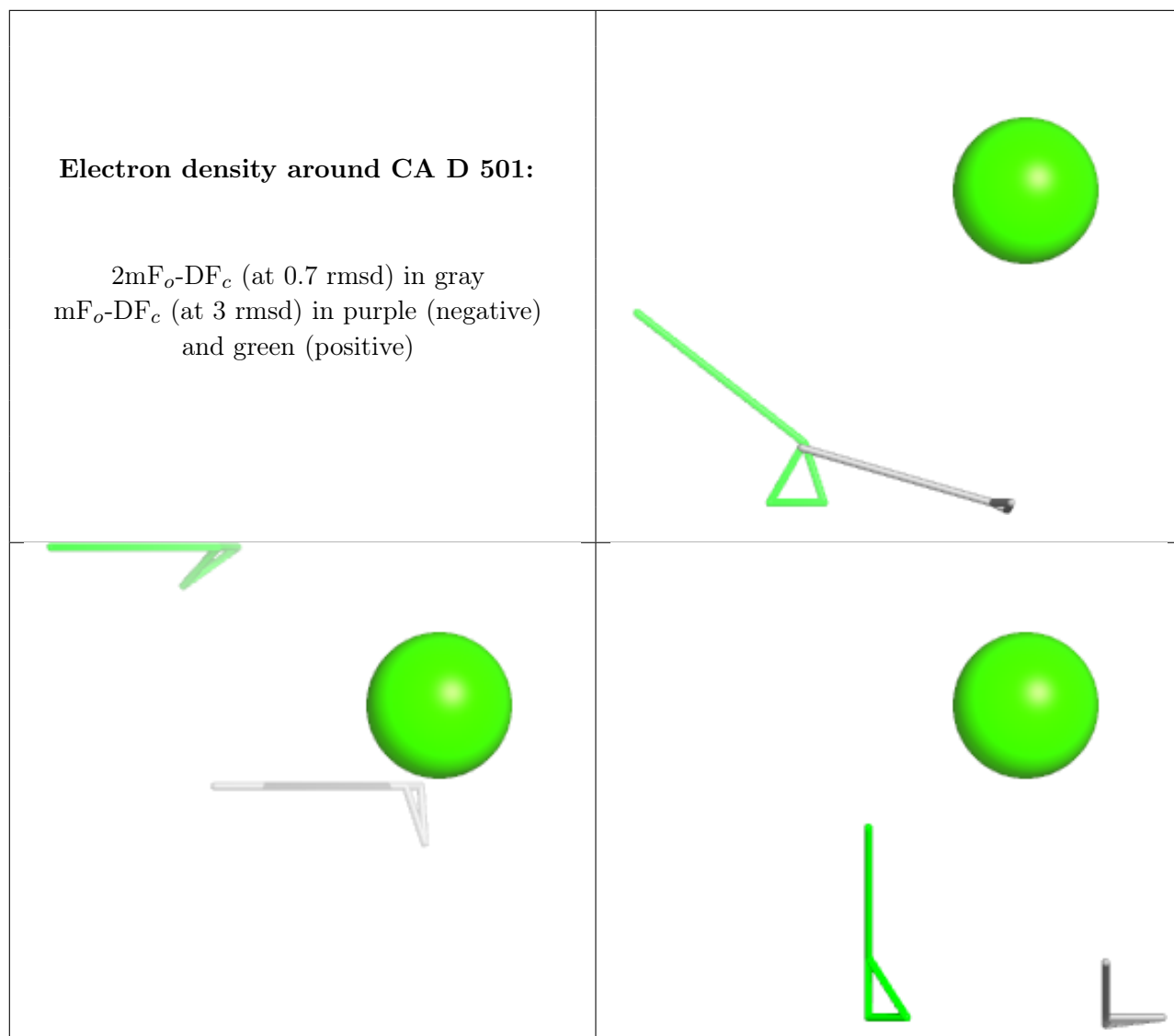
**Electron density around CA A 502:**

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



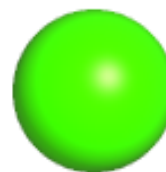
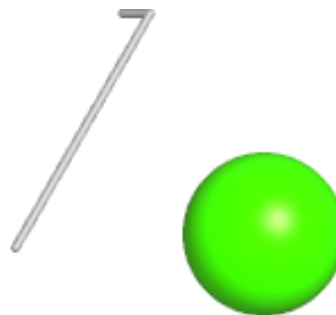
**Electron density around CA D 501:**

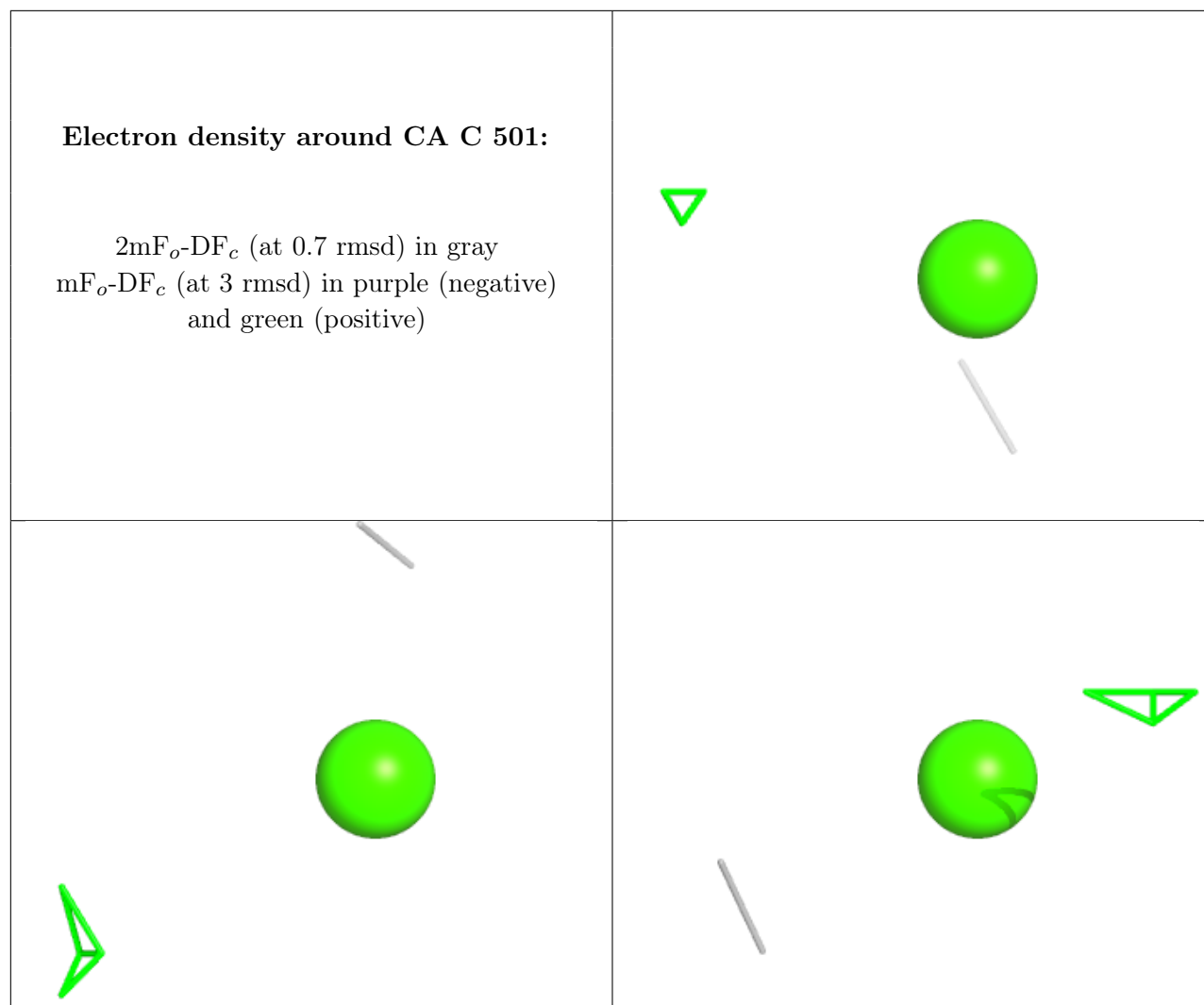
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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 [i](#)

There are no such residues in this entry.