



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 04:10 AM JST

PDB ID : 7EQR  
Title : Crystal structure of Truncated (Delta 1-19) Chitoporin VhChiP from *Vibrio harveyi* in complex with chitohexaose  
Authors : Aunkham, A.; Sanram, S.; Suginta, S.  
Deposited on : 2021-05-04  
Resolution : 2.75 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

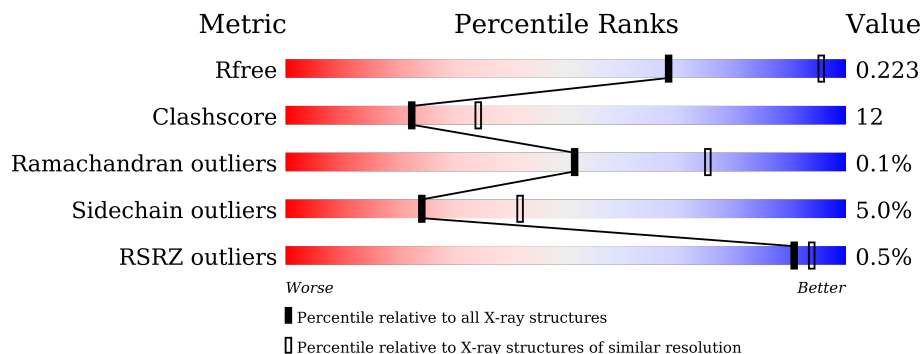
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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  $\geq 3$ , 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	331	76% 23% .
1	B	331	71% 27% .
1	C	331	76% 22% .
1	D	331	80% 18% .
1	E	331	77% 21% .
1	F	331	76% 22% .

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Mol	Chain	Length	Quality of chain	
2	G	2		
3	H	6		
3	L	6		
4	I	4		
5	J	5		
5	K	5		

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
3	NAG	H	1	-	-	-	X
3	NAG	L	1	-	-	-	X
3	NAG	L	6	-	-	-	X
4	NAG	I	4	-	-	-	X

## 2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 16484 atoms, of which 34 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 Chitoporin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	331	2577	1622	427	519	9	0	0	0
1	B	331	2577	1622	427	519	9	0	0	0
1	C	331	2577	1622	427	519	9	0	0	0
1	D	331	2577	1622	427	519	9	0	0	0
1	E	331	2577	1622	427	519	9	0	0	0
1	F	331	2577	1622	427	519	9	0	0	0

- Molecule 2 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
			Total	C	N	O			
2	G	2	28	16	2	10	0	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(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
3	H	6	Total	C	N	O	0	0	0
			85	48	6	31			
3	L	6	Total	C	N	O	0	0	0
			85	48	6	31			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(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	I	4	Total	C	N	O	0	0	0
			56	32	4	20			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



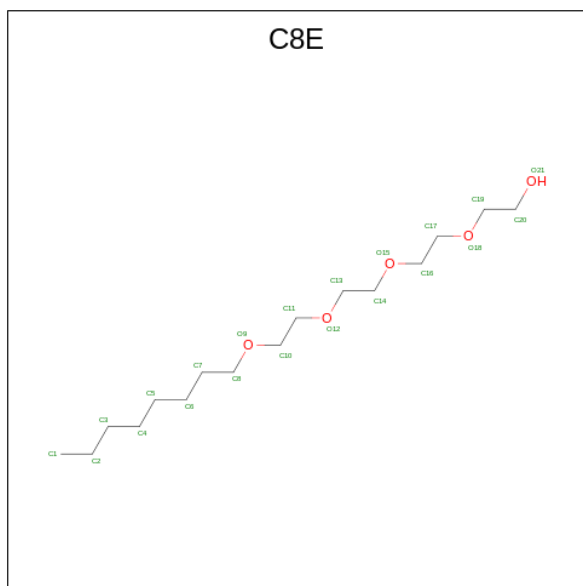
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	J	5	Total	C	N	O	0	0	0
			70	40	5	25			
5	K	5	Total	C	N	O	0	0	0
			70	40	5	25			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula:  $C_{16}H_{34}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	12	10	2	0	0
7	A	1	12	10	2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 12 10 2	0	0
7	A	1	Total C O 9 7 2	0	0
7	B	1	Total C O 12 10 2	0	0
7	B	1	Total C O 12 10 2	0	0
7	B	1	Total C H O 55 16 34 5	0	0
7	C	1	Total C O 12 10 2	0	0
7	C	1	Total C O 12 10 2	0	0
7	C	1	Total C O 12 10 2	0	0
7	C	1	Total C O 12 10 2	0	0
7	C	1	Total C O 8 6 2	0	0
7	C	1	Total C O 8 6 2	0	0
7	C	1	Total C O 12 10 2	0	0
7	D	1	Total C O 12 10 2	0	0
7	D	1	Total C O 12 10 2	0	0
7	E	1	Total C O 12 10 2	0	0
7	E	1	Total C O 12 10 2	0	0
7	E	1	Total C O 12 10 2	0	0
7	E	1	Total C O 8 6 2	0	0
7	E	1	Total C O 12 10 2	0	0
7	F	1	Total C O 12 10 2	0	0

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	4	Total Na 4 4	0	0
8	B	3	Total Na 3 3	0	0
8	C	2	Total Na 2 2	0	0
8	D	3	Total Na 3 3	0	0
8	E	3	Total Na 3 3	0	0
8	F	3	Total Na 3 3	0	0

- Molecule 9 is water.

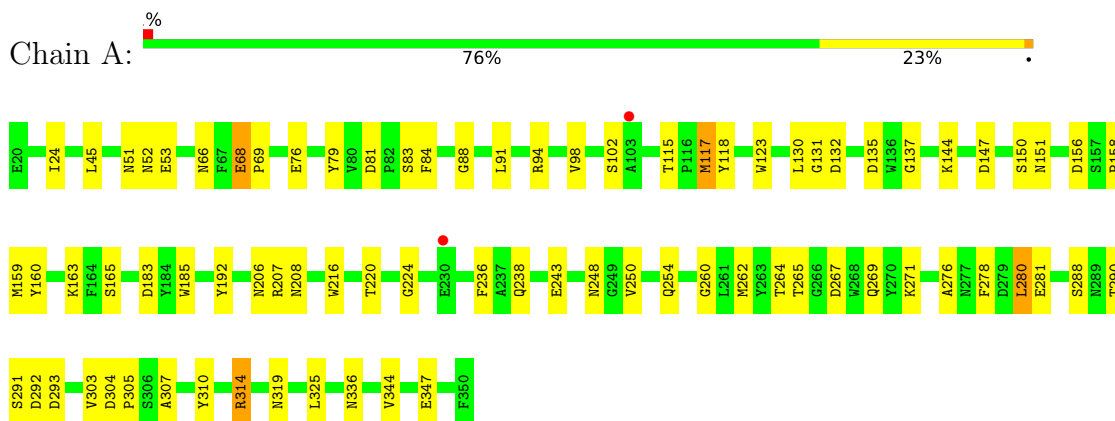
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	71	Total O 71 71	0	0
9	B	32	Total O 32 32	0	0
9	C	51	Total O 51 51	0	0
9	D	47	Total O 47 47	0	0
9	E	49	Total O 49 49	0	0
9	F	54	Total O 54 54	0	0



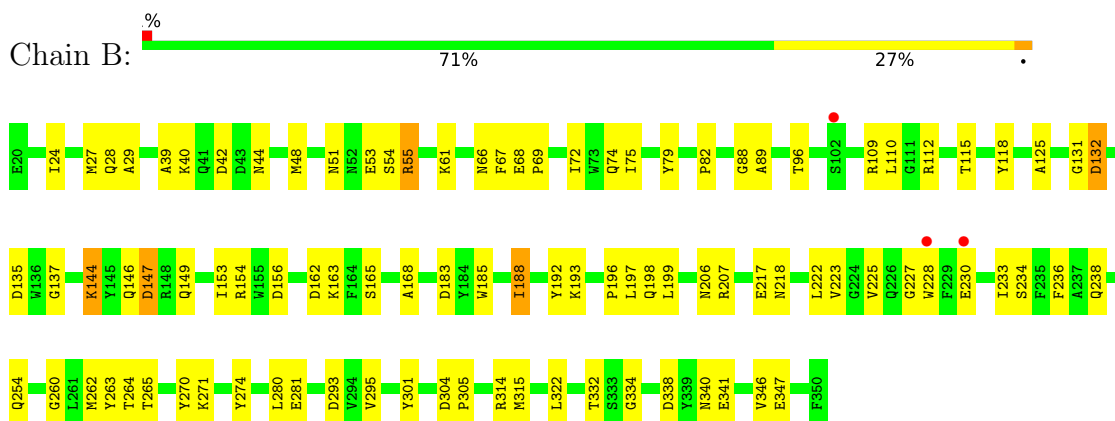
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

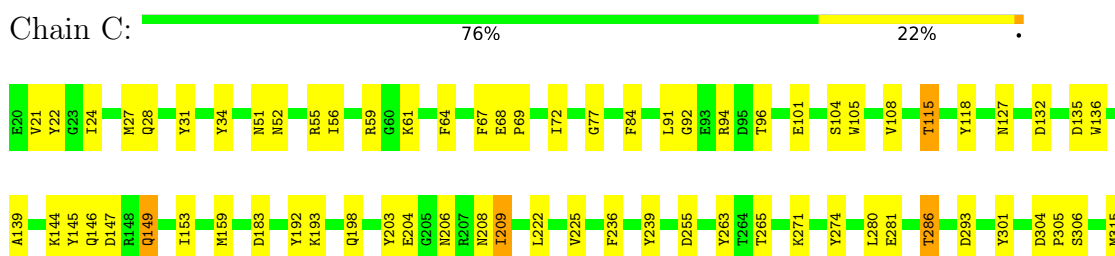
- Molecule 1: Chitoporin

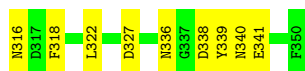


- Molecule 1: Chitoporin

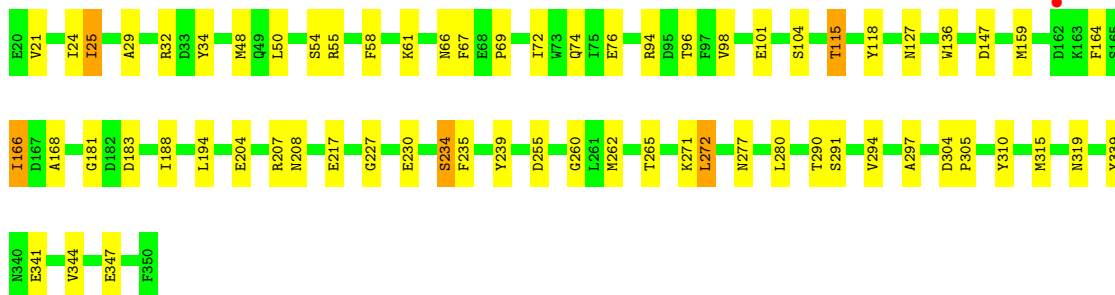
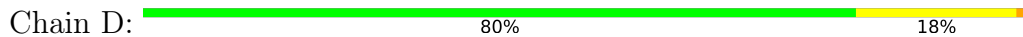


- Molecule 1: Chitoporin

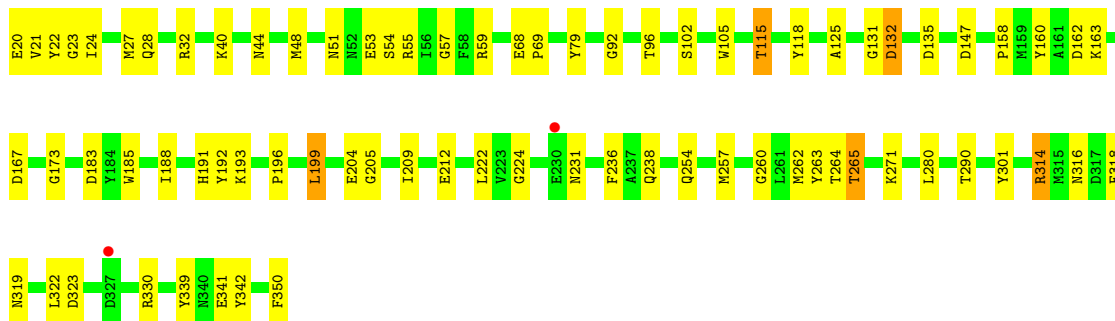
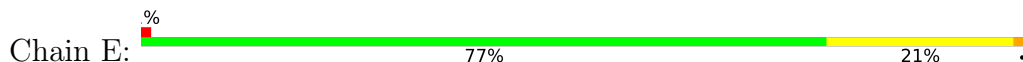




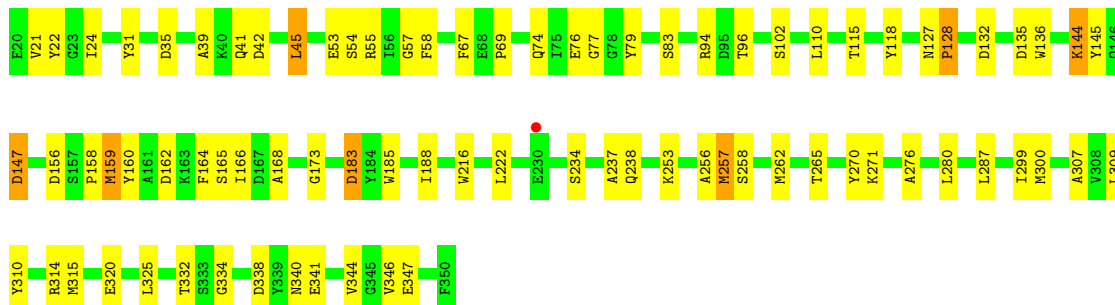
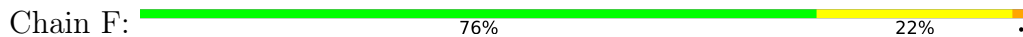
- Molecule 1: Chitoprin



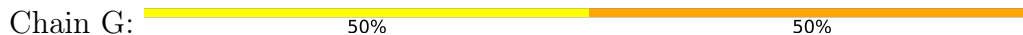
- Molecule 1: Chitoprin



- Molecule 1: Chitoprin



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



MAG1  
MAG2

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

Chain H:  17% 83%

MAG1  
MAG2  
MAG3  
MAG4  
MAG5  
MAG6

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

Chain L:  17% 83%

MAG1  
MAG2  
MAG3  
MAG4  
MAG5  
MAG6

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

Chain I:  50% 50%

MAG1  
MAG2  
MAG3  
MAG4

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  60% 40%

MAG1  
MAG2  
MAG3  
MAG4  
MAG5

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  20% 80%

MAG1  
MAG2  
MAG3  
MAG4  
MAG5

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.00Å 131.23Å 136.59Å 65.80° 87.83° 86.90°	Depositor
Resolution (Å)	19.89 – 2.75 19.89 – 2.75	Depositor EDS
% Data completeness (in resolution range)	90.4 (19.89-2.75) 86.4 (19.89-2.75)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.86 (at 2.75Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.180 , 0.223 0.180 , 0.223	Depositor DCC
$R_{free}$ test set	4784 reflections (5.57%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.0	Xtrriage
Anisotropy	0.077	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 39.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.042 for -h,-l,-k	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	16484	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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: NAG, C8E, NA

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	0.50	0/2643	0.64	0/3581
1	B	0.48	0/2643	0.64	0/3581
1	C	0.49	0/2643	0.64	0/3581
1	D	0.50	0/2643	0.65	0/3581
1	E	0.47	0/2643	0.64	0/3581
1	F	0.48	0/2643	0.64	0/3581
All	All	0.49	0/15858	0.64	0/21486

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2577	0	2342	48	0
1	B	2577	0	2342	66	0
1	C	2577	0	2342	59	1
1	D	2577	0	2342	56	0
1	E	2577	0	2342	52	0
1	F	2577	0	2342	58	0
2	G	28	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	85	0	75	5	0
3	L	85	0	75	10	0
4	I	56	0	49	7	0
5	J	70	0	61	11	0
5	K	70	0	61	6	0
6	A	14	0	13	4	0
7	A	45	0	75	3	0
7	B	45	34	76	3	0
7	C	76	0	125	5	0
7	D	24	0	42	5	0
7	E	56	0	94	6	0
7	F	12	0	21	3	0
8	A	4	0	0	0	0
8	B	3	0	0	0	0
8	C	2	0	0	0	0
8	D	3	0	0	0	0
8	E	3	0	0	0	0
8	F	3	0	0	0	0
9	A	71	0	0	5	0
9	B	32	0	0	2	0
9	C	51	0	0	3	0
9	D	47	0	0	0	0
9	E	49	0	0	5	0
9	F	54	0	0	3	0
All	All	16450	34	14844	360	1

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 12.

All (360) 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:F:173:GLY:HA3	1:F:183:ASP:HB3	1.27	1.15
1:E:115:THR:HG22	1:E:118:TYR:H	1.14	1.08
1:D:115:THR:HG22	1:D:118:TYR:H	1.20	1.03
1:C:115:THR:HG22	1:C:118:TYR:H	1.20	1.02
1:D:127:ASN:HD21	5:J:1:NAG:H82	1.19	1.01
1:E:173:GLY:HA3	1:E:183:ASP:HB3	1.43	0.99
5:J:5:NAG:H3	5:J:5:NAG:H83	1.55	0.86
1:C:146:GLN:HB3	1:C:149:GLN:HG2	1.59	0.84
1:E:222:LEU:HD11	1:E:238:GLN:OE1	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:ARG:HD3	1:D:217:GLU:HG2	1.61	0.81
5:J:2:NAG:H62	5:J:3:NAG:C7	2.12	0.78
1:F:309:LEU:CD2	1:F:346:VAL:HG12	2.13	0.77
5:K:1:NAG:O4	5:K:2:NAG:H83	1.84	0.77
1:A:262:MET:HG2	1:A:271:LYS:HG3	1.66	0.76
1:B:61:LYS:HG2	1:B:72:ILE:HG22	1.67	0.76
1:B:137:GLY:O	1:B:144:LYS:HE3	1.85	0.76
1:D:115:THR:HG22	1:D:118:TYR:N	2.01	0.75
1:D:127:ASN:ND2	5:J:1:NAG:H82	1.99	0.75
1:D:136:TRP:HH2	5:J:3:NAG:H82	1.51	0.75
1:F:173:GLY:CA	1:F:183:ASP:HB3	2.14	0.74
1:D:115:THR:CG2	1:D:118:TYR:H	1.98	0.74
1:A:216:TRP:CZ2	1:A:325:LEU:HD22	2.22	0.74
1:F:173:GLY:HA3	1:F:183:ASP:CB	2.15	0.74
1:B:262:MET:HG2	1:B:271:LYS:HG3	1.70	0.73
1:B:29:ALA:HB1	1:B:48:MET:CE	2.19	0.72
1:A:264:THR:OG1	1:A:269:GLN:HG3	1.90	0.72
1:B:199:LEU:HD23	1:B:225:VAL:HG12	1.73	0.71
9:F:534:HOH:O	3:L:6:NAG:O7	2.07	0.71
1:B:146:GLN:HB3	1:B:149:GLN:HG2	1.72	0.70
1:E:115:THR:HG22	1:E:118:TYR:N	1.98	0.70
1:B:314:ARG:HD3	1:B:341:GLU:OE2	1.90	0.70
1:F:314:ARG:HD3	1:F:341:GLU:OE1	1.92	0.70
1:B:315:MET:HG3	1:B:340:ASN:OD1	1.92	0.70
1:F:338:ASP:HB3	7:F:401:C8E:H52	1.74	0.69
1:C:84:PHE:HB3	4:I:4:NAG:H82	1.75	0.69
3:L:2:NAG:O4	3:L:3:NAG:H83	1.93	0.69
1:D:29:ALA:HB1	1:D:48:MET:CE	2.22	0.68
1:D:291:SER:OG	7:D:402:C8E:H71	1.93	0.68
1:B:29:ALA:HB1	1:B:48:MET:HE1	1.75	0.68
1:F:67:PHE:CD2	1:F:69:PRO:HD2	2.28	0.68
1:A:216:TRP:CH2	1:A:325:LEU:HD22	2.29	0.67
9:C:544:HOH:O	4:I:1:NAG:O5	2.12	0.67
6:A:401:NAG:N2	9:A:505:HOH:O	2.26	0.66
1:C:206:ASN:HB3	1:C:209:ILE:CD1	2.26	0.66
1:B:193:LYS:HE2	1:B:228:TRP:CZ3	2.31	0.65
1:C:206:ASN:HB3	1:C:209:ILE:HD13	1.77	0.65
1:E:21:VAL:HG23	7:E:402:C8E:H42	1.77	0.65
1:E:115:THR:CG2	1:E:118:TYR:H	2.00	0.65
1:B:109:ARG:HH21	1:B:154:ARG:HD3	1.60	0.65
1:F:159:MET:CE	1:F:165:SER:HB3	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:LYS:HD2	1:C:145:TYR:CE2	2.32	0.65
9:E:515:HOH:O	5:K:2:NAG:N2	2.30	0.65
1:D:67:PHE:CD2	1:D:69:PRO:HD2	2.33	0.64
7:E:402:C8E:H72	7:E:402:C8E:H13	1.78	0.64
1:E:192:TYR:OH	7:E:405:C8E:H112	1.99	0.63
1:B:233:ILE:HD12	1:B:263:TYR:HD1	1.64	0.63
1:B:66:ASN:HB3	1:C:301:TYR:OH	1.99	0.63
1:C:115:THR:HG22	1:C:118:TYR:N	2.04	0.62
3:L:1:NAG:C3	3:L:2:NAG:O5	2.47	0.62
1:C:149:GLN:OE1	1:C:149:GLN:HA	1.98	0.61
1:E:224:GLY:HA3	1:E:238:GLN:HB3	1.82	0.61
5:J:5:NAG:H3	5:J:5:NAG:C8	2.27	0.61
1:B:338:ASP:HB3	7:B:401:C8E:H81	1.81	0.61
1:D:29:ALA:HB1	1:D:48:MET:HE1	1.82	0.60
1:C:118:TYR:HE1	1:C:135:ASP:OD1	1.84	0.60
1:A:224:GLY:HA3	1:A:238:GLN:HG2	1.83	0.60
1:F:168:ALA:HB2	1:F:188:ILE:HD12	1.84	0.59
3:H:1:NAG:H3	3:H:2:NAG:O5	2.00	0.59
6:A:401:NAG:O6	9:A:501:HOH:O	2.17	0.59
1:C:132:ASP:HB2	9:C:506:HOH:O	2.02	0.59
1:F:159:MET:HE2	1:F:165:SER:HB3	1.84	0.59
2:G:1:NAG:O4	2:G:2:NAG:H83	2.03	0.59
1:C:115:THR:HG21	1:C:204:GLU:OE1	2.02	0.59
1:B:193:LYS:HE2	1:B:228:TRP:HZ3	1.67	0.58
1:F:216:TRP:CZ2	1:F:325:LEU:HD22	2.39	0.58
1:C:21:VAL:HG23	7:C:405:C8E:H72	1.85	0.58
1:C:192:TYR:OH	7:C:404:C8E:H82	2.03	0.58
1:F:216:TRP:CH2	1:F:325:LEU:HD22	2.39	0.58
9:F:526:HOH:O	3:L:3:NAG:O6	2.17	0.58
1:D:76:GLU:HG2	1:D:94:ARG:HB2	1.85	0.58
1:B:110:LEU:HD13	1:B:153:ILE:HG13	1.86	0.57
3:H:1:NAG:H83	3:H:1:NAG:O1	2.04	0.57
1:A:76:GLU:HG2	1:A:94:ARG:HB2	1.86	0.57
1:D:61:LYS:HG2	1:D:72:ILE:HG22	1.86	0.57
5:J:2:NAG:H62	5:J:3:NAG:N2	2.20	0.57
1:D:66:ASN:HB3	1:E:301:TYR:OH	2.05	0.57
1:A:88:GLY:HA2	1:C:91:LEU:O	2.04	0.57
1:B:233:ILE:HD12	1:B:263:TYR:CD1	2.40	0.56
1:B:125:ALA:HA	1:B:236:PHE:CE1	2.40	0.56
1:B:254:GLN:HB2	1:B:280:LEU:HD12	1.86	0.56
1:B:75:ILE:HD12	1:C:56:ILE:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:TRP:CH2	5:J:3:NAG:H82	2.38	0.56
1:B:28:GLN:HB3	1:B:51:ASN:HB3	1.87	0.56
1:F:300:MET:CE	3:L:2:NAG:H81	2.35	0.56
1:C:34:TYR:CD2	1:C:339:TYR:HB3	2.41	0.56
1:D:164:PHE:CZ	1:D:166:ILE:HD11	2.40	0.56
1:D:136:TRP:HH2	5:J:3:NAG:C8	2.17	0.55
1:E:24:ILE:N	1:E:24:ILE:HD12	2.21	0.55
1:A:118:TYR:HE1	1:A:135:ASP:OD1	1.90	0.55
1:D:21:VAL:HG22	1:D:58:PHE:CE2	2.41	0.55
1:E:115:THR:HG21	1:E:204:GLU:OE1	2.07	0.55
1:D:29:ALA:HB1	1:D:48:MET:HE3	1.87	0.55
1:E:23:GLY:C	1:E:24:ILE:HD12	2.26	0.55
1:A:66:ASN:HB3	1:B:301:TYR:OH	2.06	0.55
1:A:118:TYR:CG	1:A:147:ASP:HA	2.42	0.55
1:E:115:THR:CG2	1:E:204:GLU:OE1	2.54	0.55
1:D:277:ASN:O	1:D:291:SER:HB2	2.07	0.55
1:E:262:MET:HG2	1:E:271:LYS:HG3	1.88	0.55
1:B:236:PHE:CE2	1:B:260:GLY:HA3	2.41	0.55
1:D:61:LYS:NZ	1:D:101:GLU:OE2	2.32	0.54
1:E:290:THR:HG21	1:E:322:LEU:HD23	1.89	0.54
1:C:274:TYR:OH	1:C:293:ASP:OD1	2.13	0.54
1:C:192:TYR:CZ	7:C:404:C8E:H82	2.42	0.54
1:D:235:PHE:HA	1:D:260:GLY:O	2.08	0.54
1:E:263:TYR:CE2	1:E:265:THR:HG21	2.43	0.54
1:A:183:ASP:OD1	1:A:183:ASP:N	2.41	0.54
1:D:50:LEU:HD13	1:F:110:LEU:HB3	1.89	0.54
1:D:74:GLN:O	1:D:96:THR:HA	2.08	0.54
1:E:254:GLN:HB2	1:E:280:LEU:HD12	1.90	0.54
5:K:3:NAG:O3	5:K:4:NAG:O5	2.22	0.54
3:L:4:NAG:O3	3:L:5:NAG:O5	2.22	0.53
1:F:24:ILE:O	1:F:54:SER:HA	2.08	0.53
1:F:262:MET:HG2	1:F:271:LYS:HG3	1.90	0.53
1:C:183:ASP:HA	1:C:208:ASN:HB2	1.89	0.53
1:A:304:ASP:CG	1:A:305:PRO:HD2	2.28	0.53
1:E:236:PHE:CE2	1:E:260:GLY:HA3	2.42	0.53
5:K:5:NAG:O7	5:K:5:NAG:H3	2.08	0.53
1:B:340:ASN:ND2	7:B:401:C8E:H52	2.24	0.53
1:B:199:LEU:CD2	1:B:225:VAL:HG12	2.39	0.53
3:L:1:NAG:H3	3:L:2:NAG:O5	2.08	0.53
1:A:53:GLU:HG2	1:A:79:TYR:CD2	2.44	0.52
1:C:84:PHE:CB	4:I:4:NAG:H82	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:GLU:HB3	1:E:69:PRO:HD3	1.92	0.52
1:B:146:GLN:HB3	1:B:149:GLN:CG	2.39	0.52
1:B:338:ASP:CB	7:B:401:C8E:H81	2.40	0.52
1:B:115:THR:HG22	1:B:185:TRP:CH2	2.44	0.52
1:F:118:TYR:HE1	1:F:135:ASP:OD1	1.92	0.52
1:F:21:VAL:HG22	1:F:58:PHE:CE2	2.45	0.52
1:D:297:ALA:HB2	7:D:401:C8E:H111	1.92	0.52
1:F:115:THR:HG22	1:F:185:TRP:CH2	2.45	0.52
1:B:79:TYR:HB2	1:B:82:PRO:HG3	1.92	0.52
1:C:115:THR:CG2	1:C:204:GLU:OE1	2.58	0.52
1:A:51:ASN:HB2	1:A:83:SER:OG	2.10	0.52
1:E:212:GLU:OE1	1:E:330:ARG:NH2	2.36	0.51
1:A:158:PRO:HG2	1:A:160:TYR:CE1	2.46	0.51
1:D:168:ALA:HB2	1:D:188:ILE:HD12	1.91	0.51
1:C:159:MET:HE3	1:C:193:LYS:HE3	1.92	0.51
1:D:32:ARG:HG2	1:D:341:GLU:HG3	1.92	0.51
1:D:98:VAL:HG22	1:E:27:MET:HG2	1.93	0.51
1:F:262:MET:CG	1:F:271:LYS:HG3	2.41	0.51
1:F:309:LEU:HD23	1:F:346:VAL:HG12	1.91	0.51
1:B:132:ASP:HB2	9:B:521:HOH:O	2.11	0.51
1:E:196:PRO:HG3	7:E:401:C8E:H21	1.93	0.51
1:B:332:THR:C	1:B:334:GLY:H	2.13	0.51
1:E:115:THR:HG23	9:E:513:HOH:O	2.11	0.51
9:B:530:HOH:O	3:H:6:NAG:O4	2.19	0.50
1:C:84:PHE:CD2	4:I:4:NAG:H81	2.46	0.50
1:E:290:THR:HA	1:E:319:ASN:HB2	1.92	0.50
1:B:168:ALA:HB2	1:B:188:ILE:HD12	1.92	0.50
1:D:183:ASP:HA	1:D:208:ASN:HB2	1.94	0.50
1:A:91:LEU:O	1:B:88:GLY:HA2	2.12	0.50
1:D:98:VAL:CG2	1:E:27:MET:HG2	2.42	0.50
1:C:24:ILE:N	1:C:24:ILE:HD12	2.27	0.49
1:A:24:ILE:N	1:A:24:ILE:HD12	2.27	0.49
1:C:139:ALA:HB1	1:C:322:LEU:CD1	2.42	0.49
1:E:118:TYR:CG	1:E:147:ASP:HA	2.47	0.49
1:F:118:TYR:CG	1:F:147:ASP:HA	2.47	0.49
1:B:183:ASP:OD1	1:B:183:ASP:N	2.45	0.49
1:C:315:MET:HG3	1:C:340:ASN:OD1	2.12	0.49
1:C:222:LEU:HD23	1:C:222:LEU:C	2.32	0.48
1:C:146:GLN:CB	1:C:149:GLN:HG2	2.38	0.48
1:D:127:ASN:ND2	5:J:1:NAG:H2	2.28	0.48
1:E:24:ILE:O	1:E:54:SER:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:PHE:CD2	6:A:401:NAG:H82	2.49	0.48
1:F:164:PHE:CZ	1:F:166:ILE:HD11	2.49	0.48
1:E:53:GLU:HB3	1:E:79:TYR:CE1	2.48	0.48
1:A:137:GLY:O	1:A:144:LYS:HE3	2.14	0.48
1:A:267:ASP:OD2	9:A:502:HOH:O	2.19	0.48
7:E:402:C8E:H13	7:E:402:C8E:H41	1.65	0.48
1:A:303:VAL:HG22	1:C:64:PHE:HB3	1.96	0.48
1:B:274:TYR:HD1	1:B:295:VAL:HG22	1.78	0.48
1:A:150:SER:O	1:A:151:ASN:HB2	2.14	0.47
1:A:183:ASP:HA	1:A:208:ASN:HB2	1.97	0.47
1:A:248:ASN:OD1	1:A:250:VAL:HG23	2.14	0.47
1:B:131:GLY:HA2	1:B:135:ASP:HB2	1.96	0.47
1:E:125:ALA:HA	1:E:236:PHE:CE1	2.49	0.47
1:F:24:ILE:N	1:F:24:ILE:HD12	2.29	0.47
1:B:29:ALA:HB1	1:B:48:MET:HE3	1.97	0.47
1:C:22:TYR:CD1	1:C:59:ARG:HG2	2.49	0.47
1:E:158:PRO:HD2	1:E:160:TYR:CZ	2.49	0.47
1:F:110:LEU:HD12	1:F:110:LEU:N	2.29	0.47
1:F:309:LEU:HD22	1:F:346:VAL:HG12	1.94	0.47
7:F:401:C8E:H41	7:F:401:C8E:H71	1.41	0.47
3:L:1:NAG:O3	3:L:2:NAG:O5	2.33	0.47
1:A:117:MET:HE1	1:A:220:THR:HG22	1.96	0.47
1:E:22:TYR:CE1	1:E:57:GLY:HA3	2.49	0.47
1:F:310:TYR:O	1:F:344:VAL:HA	2.14	0.47
1:B:222:LEU:C	1:B:222:LEU:HD23	2.35	0.47
1:F:74:GLN:O	1:F:96:THR:HA	2.15	0.47
1:A:52:ASN:HB3	1:A:81:ASP:HB3	1.96	0.47
1:A:291:SER:OG	7:A:404:C8E:H61	2.14	0.47
1:B:74:GLN:O	1:B:96:THR:HA	2.15	0.47
1:D:24:ILE:O	1:D:54:SER:HA	2.15	0.47
1:E:183:ASP:OD1	1:E:209:ILE:HD13	2.15	0.47
5:K:5:NAG:O7	5:K:5:NAG:C3	2.62	0.47
1:A:307:ALA:HA	1:A:347:GLU:O	2.15	0.46
1:A:310:TYR:O	1:A:344:VAL:HA	2.16	0.46
1:C:139:ALA:HB1	1:C:322:LEU:HD13	1.98	0.46
1:E:59:ARG:HD2	9:E:536:HOH:O	2.15	0.46
1:E:173:GLY:HA3	1:E:183:ASP:CB	2.31	0.46
1:D:168:ALA:HB2	1:D:188:ILE:CD1	2.45	0.46
1:B:39:ALA:O	1:B:42:ASP:HB2	2.16	0.46
1:B:146:GLN:HG3	1:B:149:GLN:HG3	1.96	0.46
1:E:263:TYR:CE2	1:E:265:THR:CG2	2.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:PHE:CE2	7:A:402:C8E:H42	2.50	0.46
1:D:304:ASP:CG	1:D:305:PRO:HD2	2.36	0.46
1:C:67:PHE:CD2	1:C:69:PRO:HD2	2.51	0.46
1:B:304:ASP:CG	1:B:305:PRO:HD2	2.36	0.46
1:A:45:LEU:HD13	1:A:336:ASN:HB3	1.98	0.46
1:B:112:ARG:HA	1:B:149:GLN:O	2.15	0.46
3:H:2:NAG:O4	3:H:3:NAG:O7	2.34	0.46
1:C:64:PHE:N	9:C:501:HOH:O	2.37	0.46
1:F:253:LYS:O	1:F:280:LEU:HD12	2.16	0.45
1:A:236:PHE:CE2	1:A:260:GLY:HA3	2.51	0.45
1:B:118:TYR:CG	1:B:147:ASP:HA	2.52	0.45
1:C:144:LYS:HD2	1:C:145:TYR:CZ	2.51	0.45
1:F:222:LEU:HD11	1:F:238:GLN:OE1	2.17	0.45
1:F:262:MET:HA	1:F:270:TYR:O	2.15	0.45
1:A:304:ASP:OD1	1:A:305:PRO:HD2	2.16	0.45
7:D:402:C8E:H13	7:D:402:C8E:H42	1.77	0.45
1:B:196:PRO:O	1:B:227:GLY:HA2	2.16	0.45
1:E:20:GLU:N	7:E:402:C8E:H41	2.31	0.45
1:E:314:ARG:HD3	1:E:341:GLU:OE2	2.16	0.45
1:A:276:ALA:HA	1:A:292:ASP:O	2.17	0.45
1:C:77:GLY:O	1:C:94:ARG:HD3	2.17	0.45
1:F:159:MET:HE3	1:F:165:SER:HB3	1.95	0.45
3:L:6:NAG:O7	3:L:6:NAG:H3	2.16	0.45
1:D:265:THR:HG23	1:D:265:THR:O	2.16	0.45
1:A:163:LYS:O	1:A:192:TYR:HA	2.17	0.45
1:D:34:TYR:CD2	1:D:339:TYR:HB3	2.52	0.45
1:E:105:TRP:HA	9:E:512:HOH:O	2.17	0.45
1:A:68:GLU:N	1:A:69:PRO:CD	2.80	0.44
1:F:307:ALA:HA	1:F:347:GLU:O	2.16	0.44
1:D:136:TRP:CZ3	5:J:3:NAG:H4	2.52	0.44
9:E:515:HOH:O	5:K:2:NAG:C7	2.64	0.44
1:F:21:VAL:HG22	1:F:58:PHE:CD2	2.52	0.44
1:C:255:ASP:OD1	1:C:255:ASP:N	2.48	0.44
1:D:25:ILE:O	1:D:347:GLU:HA	2.17	0.44
1:F:315:MET:HG3	1:F:340:ASN:OD1	2.17	0.44
1:E:162:ASP:C	1:E:163:LYS:HG2	2.38	0.44
1:C:135:ASP:HB3	1:C:136:TRP:CE3	2.53	0.44
1:E:191:HIS:HA	1:E:199:LEU:O	2.18	0.44
1:A:290:THR:HA	1:A:319:ASN:HB2	1.99	0.44
1:D:164:PHE:HZ	1:D:166:ILE:HD11	1.79	0.44
1:D:207:ARG:CD	1:D:217:GLU:HG2	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:4:NAG:HO3	3:H:5:NAG:C1	2.30	0.44
1:B:53:GLU:O	1:B:55:ARG:HD3	2.18	0.44
1:C:118:TYR:CG	1:C:147:ASP:HA	2.53	0.44
1:C:27:MET:CE	1:C:52:ASN:HB2	2.48	0.44
1:C:281:GLU:HA	1:C:286:THR:HA	1.99	0.44
1:D:239:TYR:CE1	1:D:255:ASP:HB2	2.52	0.44
1:D:310:TYR:O	1:D:344:VAL:HA	2.17	0.44
1:F:257:MET:O	1:F:257:MET:HG3	2.18	0.44
1:F:332:THR:C	1:F:334:GLY:H	2.21	0.44
1:A:293:ASP:OD1	7:A:404:C8E:H82	2.18	0.44
1:D:115:THR:CG2	1:D:204:GLU:OE1	2.66	0.44
1:C:239:TYR:HB2	7:C:402:C8E:H52	2.00	0.43
1:F:31:TYR:O	1:F:341:GLU:HA	2.18	0.43
1:B:280:LEU:HG	1:B:281:GLU:N	2.32	0.43
1:B:24:ILE:O	1:B:54:SER:HA	2.18	0.43
1:B:40:LYS:HE2	1:B:44:ASN:OD1	2.19	0.43
1:C:68:GLU:HB3	1:C:69:PRO:HD3	2.00	0.43
1:B:67:PHE:CD2	1:B:69:PRO:HD2	2.53	0.43
1:D:291:SER:HB2	7:D:402:C8E:H72	2.00	0.43
1:F:135:ASP:HB3	1:F:136:TRP:CE3	2.53	0.43
1:F:299:ILE:O	1:F:299:ILE:HG13	2.17	0.43
1:A:132:ASP:OD1	1:A:314:ARG:NH2	2.51	0.43
1:C:105:TRP:HZ3	1:C:108:VAL:HG23	1.82	0.43
1:D:234:SER:HB2	1:D:262:MET:HE1	2.01	0.43
1:D:290:THR:HA	1:D:319:ASN:HB2	2.00	0.43
1:B:68:GLU:N	1:B:69:PRO:CD	2.82	0.43
1:C:203:TYR:CZ	7:C:403:C8E:H81	2.53	0.43
1:F:35:ASP:HB2	7:F:401:C8E:H81	2.00	0.43
1:D:227:GLY:HA3	1:D:235:PHE:CE1	2.53	0.43
1:F:22:TYR:CZ	1:F:57:GLY:HA3	2.54	0.43
1:E:23:GLY:HA3	1:E:350:PHE:CE2	2.54	0.43
1:F:158:PRO:HG2	1:F:160:TYR:CE1	2.53	0.43
1:A:265:THR:HG23	1:A:265:THR:O	2.19	0.43
1:F:159:MET:HG2	1:F:162:ASP:HA	2.00	0.43
1:B:314:ARG:HH11	1:B:341:GLU:CD	2.21	0.43
1:C:61:LYS:NZ	1:C:101:GLU:OE2	2.37	0.43
1:A:243:GLU:OE1	9:A:503:HOH:O	2.22	0.42
1:C:159:MET:HE3	1:C:193:LYS:HG3	2.01	0.42
1:C:304:ASP:CG	1:C:305:PRO:HD2	2.39	0.42
1:B:207:ARG:HD3	1:B:217:GLU:HG2	2.01	0.42
1:E:262:MET:CG	1:E:271:LYS:HG3	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:MET:HA	1:B:270:TYR:O	2.18	0.42
1:C:84:PHE:CD2	4:I:4:NAG:C8	3.03	0.42
1:C:236:PHE:CD1	1:C:236:PHE:C	2.92	0.42
1:C:316:ASN:HB3	1:C:318:PHE:CE2	2.54	0.42
1:E:316:ASN:HB3	1:E:318:PHE:CE2	2.54	0.42
1:D:272:LEU:HA	1:D:272:LEU:HD12	1.70	0.42
1:F:280:LEU:HD23	1:F:287:LEU:HD12	2.02	0.42
1:A:206:ASN:O	1:A:207:ARG:NH1	2.45	0.42
6:A:401:NAG:H82	9:A:505:HOH:O	2.19	0.42
1:B:40:LYS:HD2	1:B:40:LYS:HA	1.82	0.42
1:F:257:MET:HE1	9:F:554:HOH:O	2.19	0.42
1:A:123:TRP:CE3	2:G:1:NAG:H61	2.54	0.42
1:E:167:ASP:O	1:E:188:ILE:HA	2.19	0.42
1:C:318:PHE:N	1:C:338:ASP:OD1	2.40	0.42
1:A:98:VAL:CG2	1:B:27:MET:HG2	2.50	0.42
1:A:131:GLY:O	1:A:135:ASP:HB3	2.20	0.41
1:C:127:ASN:OD1	1:C:271:LYS:NZ	2.35	0.41
1:D:262:MET:SD	1:D:271:LYS:HE3	2.60	0.41
1:D:291:SER:OG	7:D:402:C8E:C7	2.65	0.41
1:F:39:ALA:O	1:F:42:ASP:HB2	2.19	0.41
1:B:332:THR:C	1:B:334:GLY:N	2.73	0.41
1:D:262:MET:CG	1:D:271:LYS:HG3	2.50	0.41
1:F:77:GLY:O	1:F:94:ARG:HD3	2.20	0.41
1:F:332:THR:C	1:F:334:GLY:N	2.74	0.41
1:A:254:GLN:HB2	1:A:280:LEU:HD12	2.02	0.41
1:B:79:TYR:O	1:B:89:ALA:HB2	2.21	0.41
1:C:28:GLN:HB3	1:C:51:ASN:HB3	2.02	0.41
1:D:67:PHE:CE2	1:D:69:PRO:HD2	2.56	0.41
1:D:262:MET:HG3	1:D:271:LYS:HG3	2.02	0.41
1:B:79:TYR:CB	1:B:82:PRO:HG3	2.50	0.41
1:B:206:ASN:HB2	1:B:218:ASN:HB2	2.02	0.41
1:B:314:ARG:HG2	1:B:341:GLU:HB3	2.03	0.41
1:E:342:TYR:CD1	1:E:342:TYR:N	2.89	0.41
1:A:115:THR:HG22	1:A:185:TRP:CH2	2.56	0.41
1:E:28:GLN:HB3	1:E:51:ASN:HB3	2.02	0.41
1:B:118:TYR:HE1	1:B:135:ASP:OD1	2.03	0.41
1:B:163:LYS:O	1:B:192:TYR:HA	2.21	0.41
1:E:32:ARG:HD3	1:E:339:TYR:CD1	2.56	0.41
3:L:2:NAG:H62	3:L:3:NAG:C7	2.51	0.41
1:C:92:GLY:HA2	1:C:96:THR:OG1	2.20	0.41
1:F:127:ASN:HA	1:F:128:PRO:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:144:LYS:HD2	1:F:145:TYR:CZ	2.56	0.41
1:F:234:SER:OG	1:F:262:MET:HB2	2.20	0.41
1:F:237:ALA:HA	1:F:258:SER:O	2.21	0.41
1:E:132:ASP:OD1	1:E:314:ARG:NH2	2.54	0.40
1:F:53:GLU:HG2	1:F:79:TYR:CD2	2.55	0.40
1:C:84:PHE:HB3	4:I:4:NAG:C8	2.47	0.40
1:C:198:GLN:O	1:C:225:VAL:HA	2.21	0.40
1:F:41:GLN:HG3	1:F:45:LEU:HD23	2.02	0.40
1:F:256:ALA:HB1	1:F:276:ALA:O	2.21	0.40
1:E:185:TRP:HA	1:E:205:GLY:O	2.21	0.40
1:F:41:GLN:HG3	1:F:45:LEU:CD2	2.52	0.40
1:F:76:GLU:HG2	1:F:94:ARG:HB2	2.03	0.40
1:B:198:GLN:OE1	1:B:228:TRP:HH2	2.04	0.40
1:B:222:LEU:HD11	1:B:238:GLN:OE1	2.22	0.40
1:D:294:VAL:HA	1:D:315:MET:O	2.22	0.40
1:A:83:SER:HB3	1:A:84:PHE:CD1	2.57	0.40
1:B:346:VAL:HG22	1:B:347:GLU:N	2.36	0.40
1:C:31:TYR:O	1:C:341:GLU:HA	2.21	0.40
1:C:336:ASN:ND2	4:I:4:NAG:O7	2.54	0.40
1:D:118:TYR:CG	1:D:147:ASP:HA	2.56	0.40
1:D:181:GLY:HA2	1:E:44:ASN:OD1	2.21	0.40
1:E:92:GLY:HA2	1:E:96:THR:OG1	2.21	0.40
1:E:131:GLY:O	1:E:135:ASP:HB3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:TYR:OH	1:C:327:ASP:OD2[1_455]	2.13	0.07

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	329/331 (99%)	315 (96%)	14 (4%)	0	100	100
1	B	329/331 (99%)	315 (96%)	14 (4%)	0	100	100
1	C	329/331 (99%)	314 (95%)	15 (5%)	0	100	100
1	D	329/331 (99%)	314 (95%)	15 (5%)	0	100	100
1	E	329/331 (99%)	317 (96%)	12 (4%)	0	100	100
1	F	329/331 (99%)	319 (97%)	8 (2%)	2 (1%)	25	42
All	All	1974/1986 (99%)	1894 (96%)	78 (4%)	2 (0%)	51	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	183	ASP
1	F	128	PRO

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	252/252 (100%)	241 (96%)	11 (4%)	28	47
1	B	252/252 (100%)	236 (94%)	16 (6%)	18	31
1	C	252/252 (100%)	241 (96%)	11 (4%)	28	47
1	D	252/252 (100%)	241 (96%)	11 (4%)	28	47
1	E	252/252 (100%)	238 (94%)	14 (6%)	21	36
1	F	252/252 (100%)	240 (95%)	12 (5%)	25	44
All	All	1512/1512 (100%)	1437 (95%)	75 (5%)	24	42

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	GLU
1	A	102	SER
1	A	117	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	130	LEU
1	A	156	ASP
1	A	159	MET
1	A	165	SER
1	A	280	LEU
1	A	281	GLU
1	A	288	SER
1	A	314	ARG
1	B	55	ARG
1	B	132	ASP
1	B	144	LYS
1	B	147	ASP
1	B	156	ASP
1	B	162	ASP
1	B	165	SER
1	B	188	ILE
1	B	197	LEU
1	B	223	VAL
1	B	230	GLU
1	B	234	SER
1	B	264	THR
1	B	265	THR
1	B	293	ASP
1	B	322	LEU
1	C	55	ARG
1	C	72	ILE
1	C	104	SER
1	C	115	THR
1	C	149	GLN
1	C	153	ILE
1	C	209	ILE
1	C	265	THR
1	C	280	LEU
1	C	286	THR
1	C	306	SER
1	D	25	ILE
1	D	55	ARG
1	D	104	SER
1	D	115	THR
1	D	159	MET
1	D	166	ILE
1	D	194	LEU

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Mol	Chain	Res	Type
1	D	230	GLU
1	D	234	SER
1	D	272	LEU
1	D	280	LEU
1	E	40	LYS
1	E	48	MET
1	E	55	ARG
1	E	102	SER
1	E	115	THR
1	E	132	ASP
1	E	193	LYS
1	E	199	LEU
1	E	231	ASN
1	E	257	MET
1	E	264	THR
1	E	265	THR
1	E	314	ARG
1	E	323	ASP
1	F	45	LEU
1	F	55	ARG
1	F	83	SER
1	F	102	SER
1	F	132	ASP
1	F	144	LYS
1	F	147	ASP
1	F	156	ASP
1	F	159	MET
1	F	257	MET
1	F	265	THR
1	F	320	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	127	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

28 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	G	1	2	14,14,15	0.71	1 (7%)	17,19,21	0.88	1 (5%)
2	NAG	G	2	2	14,14,15	0.65	0	17,19,21	0.76	0
3	NAG	H	1	3	15,15,15	0.93	1 (6%)	21,21,21	1.32	2 (9%)
3	NAG	H	2	3	14,14,15	0.63	0	17,19,21	0.60	0
3	NAG	H	3	3	14,14,15	0.72	1 (7%)	17,19,21	1.10	1 (5%)
3	NAG	H	4	3	14,14,15	0.95	1 (7%)	17,19,21	1.34	1 (5%)
3	NAG	H	5	3	14,14,15	0.82	1 (7%)	17,19,21	0.82	1 (5%)
3	NAG	H	6	3	14,14,15	1.25	1 (7%)	17,19,21	1.05	2 (11%)
4	NAG	I	1	4	14,14,15	0.86	1 (7%)	17,19,21	0.86	1 (5%)
4	NAG	I	2	4	14,14,15	0.98	1 (7%)	17,19,21	1.13	1 (5%)
4	NAG	I	3	4	14,14,15	0.99	2 (14%)	17,19,21	0.80	1 (5%)
4	NAG	I	4	4	14,14,15	0.85	1 (7%)	17,19,21	0.77	1 (5%)
5	NAG	J	1	5	14,14,15	0.36	0	17,19,21	0.83	1 (5%)
5	NAG	J	2	5	14,14,15	0.57	0	17,19,21	0.68	0
5	NAG	J	3	5	14,14,15	0.63	1 (7%)	17,19,21	1.04	1 (5%)
5	NAG	J	4	5	14,14,15	0.47	0	17,19,21	0.81	1 (5%)
5	NAG	J	5	5	14,14,15	0.38	0	17,19,21	0.77	0
5	NAG	K	1	5	14,14,15	0.42	0	17,19,21	0.59	0
5	NAG	K	2	5	14,14,15	0.41	0	17,19,21	0.80	1 (5%)
5	NAG	K	3	5	14,14,15	0.98	1 (7%)	17,19,21	1.12	1 (5%)
5	NAG	K	4	5	14,14,15	1.18	2 (14%)	17,19,21	0.81	1 (5%)
5	NAG	K	5	5	14,14,15	0.57	0	17,19,21	0.76	1 (5%)
3	NAG	L	1	3	15,15,15	0.31	0	21,21,21	0.80	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	L	2	3	14,14,15	0.88	2 (14%)	17,19,21	0.77	0
3	NAG	L	3	3	14,14,15	0.32	0	17,19,21	0.81	1 (5%)
3	NAG	L	4	3	14,14,15	1.01	1 (7%)	17,19,21	1.05	1 (5%)
3	NAG	L	5	3	14,14,15	1.19	2 (14%)	17,19,21	0.77	1 (5%)
3	NAG	L	6	3	14,14,15	0.46	0	17,19,21	0.90	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
2	NAG	G	1	2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3	-	4/6/26/26	0/1/1/1
3	NAG	H	2	3	-	1/6/23/26	0/1/1/1
3	NAG	H	3	3	-	3/6/23/26	0/1/1/1
3	NAG	H	4	3	-	2/6/23/26	0/1/1/1
3	NAG	H	5	3	-	2/6/23/26	0/1/1/1
3	NAG	H	6	3	-	2/6/23/26	0/1/1/1
4	NAG	I	1	4	-	4/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	NAG	I	3	4	-	0/6/23/26	0/1/1/1
4	NAG	I	4	4	-	2/6/23/26	0/1/1/1
5	NAG	J	1	5	-	4/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1
5	NAG	J	3	5	-	4/6/23/26	0/1/1/1
5	NAG	J	4	5	-	1/6/23/26	0/1/1/1
5	NAG	J	5	5	-	5/6/23/26	0/1/1/1
5	NAG	K	1	5	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	4/6/23/26	0/1/1/1
5	NAG	K	3	5	-	2/6/23/26	0/1/1/1
5	NAG	K	4	5	-	2/6/23/26	0/1/1/1
5	NAG	K	5	5	-	3/6/23/26	0/1/1/1
3	NAG	L	1	3	-	4/6/26/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	NAG	L	3	3	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	L	4	3	-	2/6/23/26	0/1/1/1
3	NAG	L	5	3	-	2/6/23/26	0/1/1/1
3	NAG	L	6	3	-	3/6/23/26	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	6	NAG	C1-C2	4.00	1.58	1.52
3	L	4	NAG	O5-C1	3.67	1.49	1.43
3	L	5	NAG	O5-C1	3.62	1.49	1.43
5	K	3	NAG	O5-C1	3.55	1.49	1.43
5	K	4	NAG	O5-C1	3.52	1.49	1.43
4	I	2	NAG	O5-C1	3.45	1.49	1.43
3	H	4	NAG	O5-C1	3.35	1.49	1.43
4	I	3	NAG	O5-C1	2.90	1.48	1.43
3	H	1	NAG	O5-C1	-2.86	1.35	1.42
4	I	1	NAG	O5-C1	2.85	1.48	1.43
4	I	4	NAG	C1-C2	2.74	1.56	1.52
5	K	4	NAG	C1-C2	2.58	1.56	1.52
3	L	5	NAG	C1-C2	2.50	1.56	1.52
3	H	3	NAG	O5-C1	2.39	1.47	1.43
3	L	2	NAG	O5-C1	2.37	1.47	1.43
3	H	5	NAG	O5-C1	2.19	1.47	1.43
2	G	1	NAG	C1-C2	2.15	1.55	1.52
5	J	3	NAG	O5-C1	2.11	1.47	1.43
3	L	2	NAG	C1-C2	2.05	1.55	1.52
4	I	3	NAG	C1-C2	2.05	1.55	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	4	NAG	C1-O5-C5	4.83	118.73	112.19
3	H	1	NAG	C3-C4-C5	3.86	117.13	110.24
5	J	3	NAG	C1-O5-C5	3.65	117.14	112.19
4	I	2	NAG	C1-O5-C5	3.64	117.13	112.19
3	H	1	NAG	C4-C3-C2	3.63	115.66	110.34
5	K	3	NAG	C1-O5-C5	3.59	117.06	112.19
3	H	3	NAG	C1-O5-C5	3.48	116.91	112.19
3	L	4	NAG	C1-O5-C5	3.45	116.87	112.19
2	G	1	NAG	C1-O5-C5	3.26	116.61	112.19
3	L	3	NAG	C1-O5-C5	2.64	115.77	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	4	NAG	C1-O5-C5	2.59	115.70	112.19
5	J	4	NAG	C1-O5-C5	2.57	115.67	112.19
4	I	3	NAG	C1-O5-C5	2.56	115.67	112.19
4	I	1	NAG	C1-O5-C5	2.51	115.59	112.19
3	H	6	NAG	C4-C3-C2	2.38	114.51	111.02
3	H	6	NAG	C1-O5-C5	2.37	115.41	112.19
4	I	4	NAG	C1-O5-C5	2.35	115.37	112.19
3	L	1	NAG	C4-C3-C2	2.32	113.75	110.34
3	H	5	NAG	C1-O5-C5	2.25	115.24	112.19
5	K	2	NAG	C1-O5-C5	2.22	115.19	112.19
5	K	5	NAG	C2-N2-C7	2.15	125.96	122.90
3	L	5	NAG	C1-O5-C5	2.08	115.00	112.19
5	J	1	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L	6	NAG	C3-C2-N2-C7
5	K	5	NAG	C3-C2-N2-C7
4	I	2	NAG	O5-C5-C6-O6
3	H	6	NAG	C4-C5-C6-O6
4	I	4	NAG	C4-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	L	5	NAG	O5-C5-C6-O6
5	K	3	NAG	O5-C5-C6-O6
3	H	4	NAG	C4-C5-C6-O6
3	L	4	NAG	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
4	I	4	NAG	O5-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
5	K	5	NAG	C4-C5-C6-O6
3	H	4	NAG	O5-C5-C6-O6
3	H	6	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
5	K	3	NAG	C4-C5-C6-O6
3	H	3	NAG	O5-C5-C6-O6
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
3	H	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	H	1	NAG	O7-C7-N2-C2
3	L	1	NAG	C8-C7-N2-C2
3	L	1	NAG	O7-C7-N2-C2
3	L	3	NAG	C8-C7-N2-C2
3	L	3	NAG	O7-C7-N2-C2
4	I	1	NAG	C8-C7-N2-C2
4	I	1	NAG	O7-C7-N2-C2
5	J	1	NAG	C8-C7-N2-C2
5	J	1	NAG	O7-C7-N2-C2
5	J	3	NAG	C8-C7-N2-C2
5	J	3	NAG	O7-C7-N2-C2
5	J	5	NAG	C8-C7-N2-C2
5	J	5	NAG	O7-C7-N2-C2
5	K	2	NAG	C8-C7-N2-C2
5	K	2	NAG	O7-C7-N2-C2
3	L	4	NAG	C4-C5-C6-O6
3	H	5	NAG	O5-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
3	L	3	NAG	O5-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
5	J	5	NAG	C4-C5-C6-O6
5	K	4	NAG	O5-C5-C6-O6
5	J	3	NAG	O5-C5-C6-O6
3	L	5	NAG	C4-C5-C6-O6
3	L	6	NAG	C4-C5-C6-O6
5	K	5	NAG	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
5	J	5	NAG	O5-C5-C6-O6
3	H	3	NAG	C4-C5-C6-O6
5	K	1	NAG	C4-C5-C6-O6
3	L	3	NAG	C4-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
3	L	6	NAG	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
5	J	4	NAG	O5-C5-C6-O6
5	J	3	NAG	C4-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
3	H	5	NAG	C4-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
3	H	3	NAG	C3-C2-N2-C7
5	J	5	NAG	C3-C2-N2-C7
5	K	4	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	J	1	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6

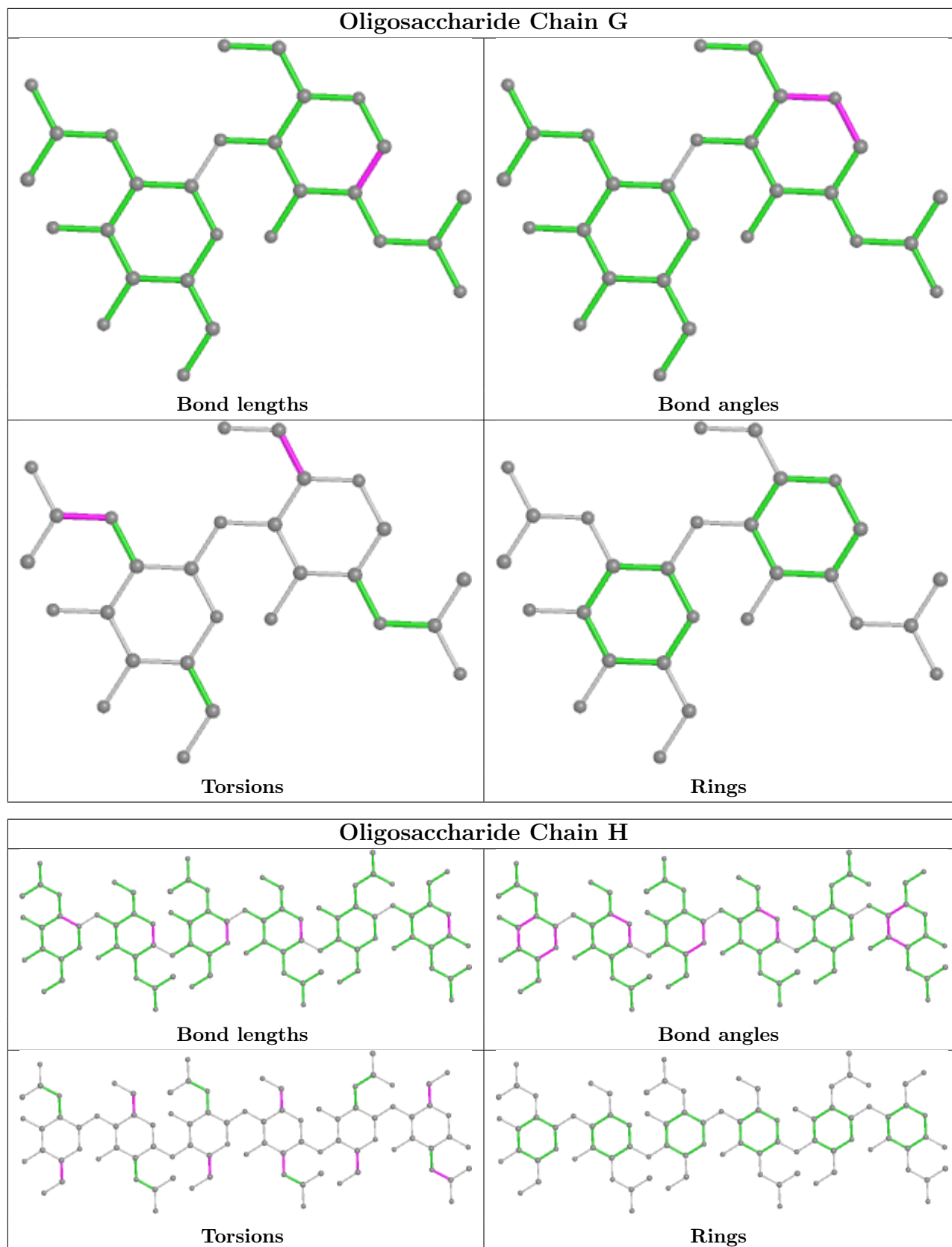
There are no ring outliers.

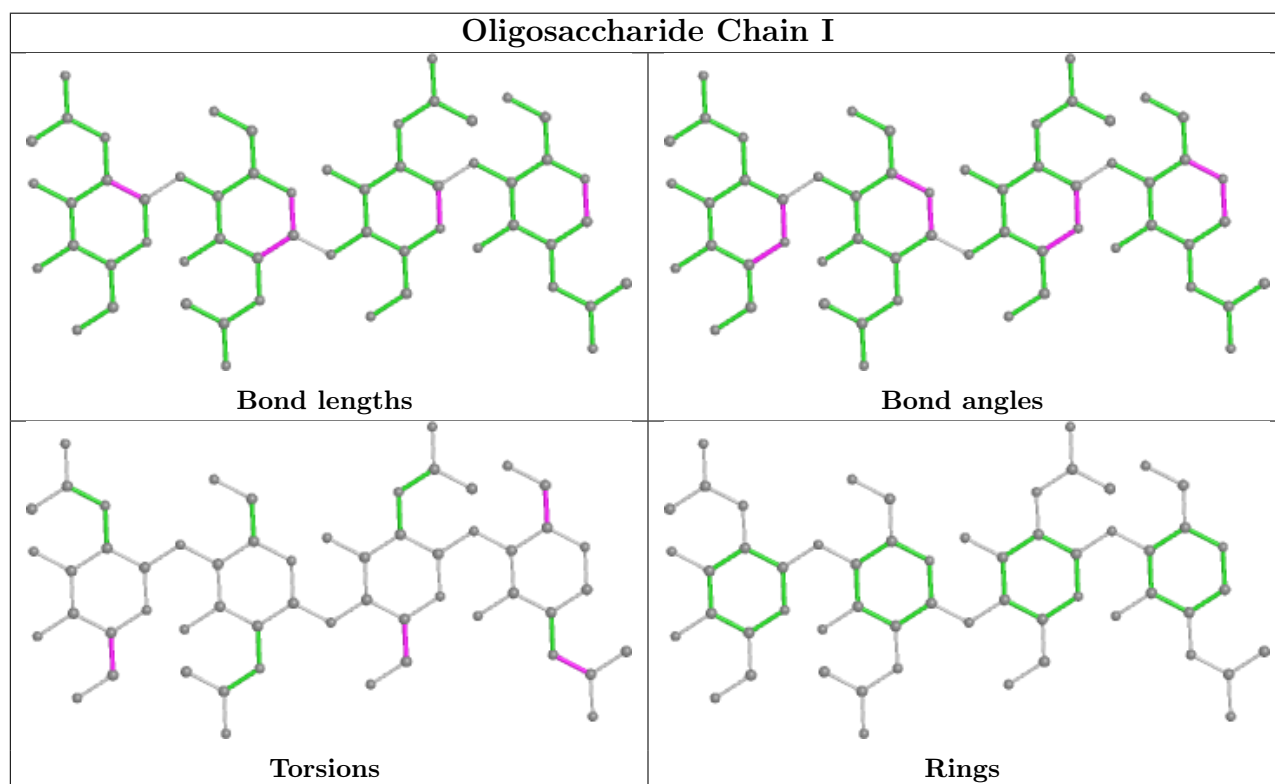
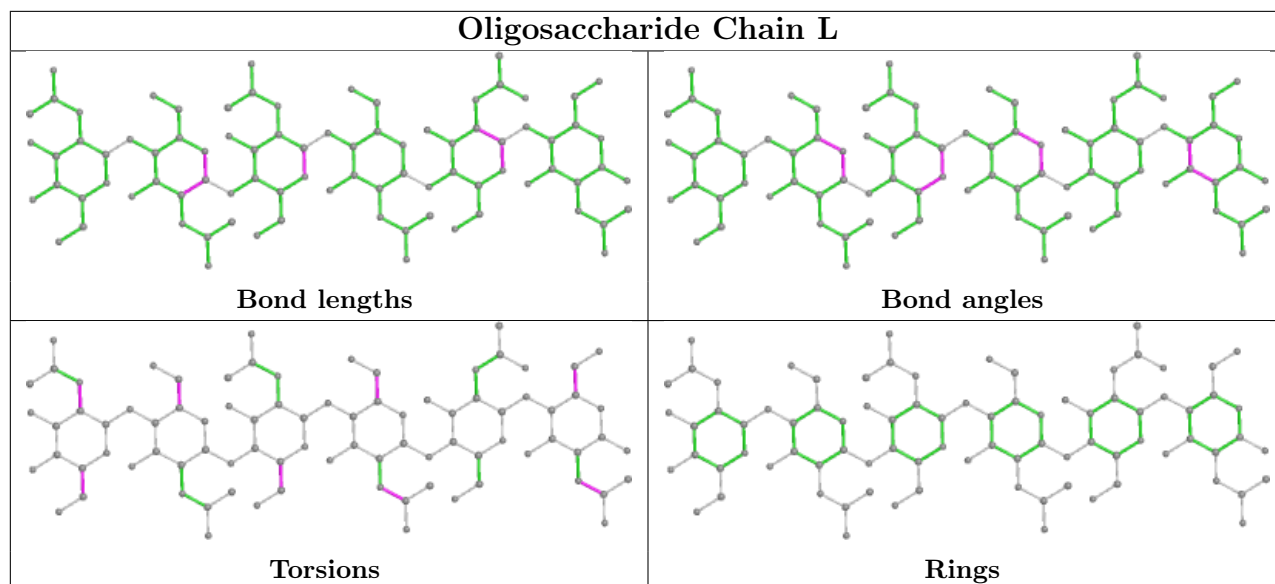
25 monomers are involved in 41 short contacts:

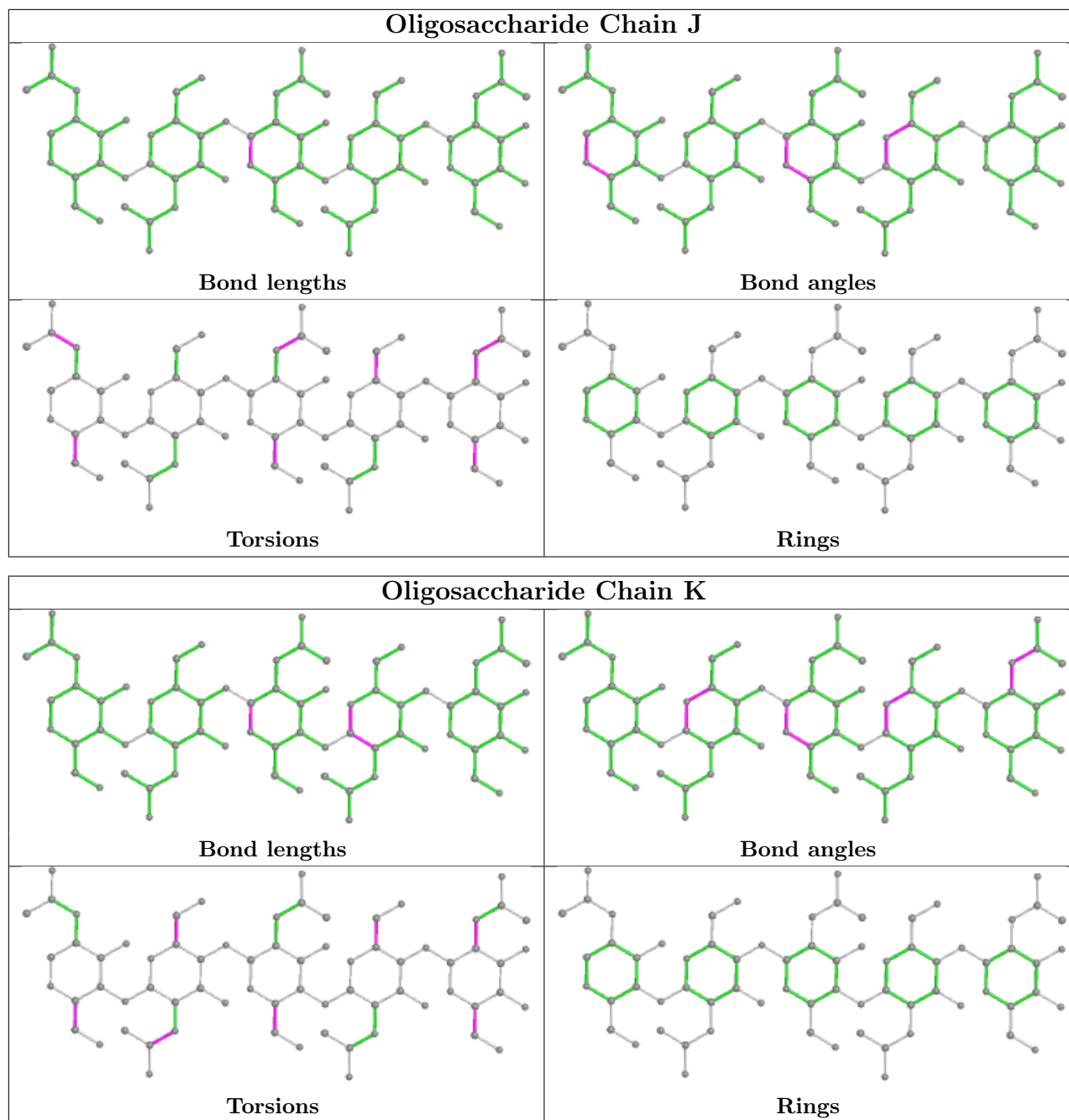
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	2	NAG	2	0
5	K	1	NAG	1	0
3	L	6	NAG	2	0
2	G	1	NAG	2	0
3	L	1	NAG	3	0
4	I	1	NAG	1	0
3	H	2	NAG	2	0
3	H	1	NAG	2	0
3	L	2	NAG	6	0
5	J	5	NAG	2	0
3	L	4	NAG	1	0
3	H	4	NAG	1	0
3	L	5	NAG	1	0
5	K	3	NAG	1	0
3	H	6	NAG	1	0
3	H	5	NAG	1	0
3	H	3	NAG	1	0
2	G	2	NAG	1	0
5	K	2	NAG	3	0
5	K	5	NAG	2	0
4	I	4	NAG	6	0
5	J	3	NAG	6	0
5	J	1	NAG	3	0
5	K	4	NAG	1	0
3	L	3	NAG	3	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 41 ligands modelled in this entry, 18 are monoatomic - leaving 23 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
7	C8E	F	401	-	11,11,20	0.38	0	10,10,19	0.52	0
7	C8E	A	402	-	11,11,20	0.48	0	10,10,19	0.49	0
7	C8E	B	402	-	11,11,20	0.39	0	10,10,19	0.49	0
7	C8E	A	405	-	8,8,20	0.39	0	7,7,19	0.49	0
7	C8E	A	404	-	11,11,20	0.35	0	10,10,19	0.39	0
7	C8E	E	404	-	7,7,20	0.39	0	6,6,19	0.46	0
7	C8E	D	402	-	11,11,20	0.36	0	10,10,19	0.41	0
7	C8E	B	401	-	11,11,20	0.35	0	10,10,19	0.56	0
7	C8E	A	403	-	11,11,20	0.51	0	10,10,19	0.47	0
7	C8E	E	405	-	11,11,20	0.40	0	10,10,19	0.44	0
7	C8E	D	401	-	11,11,20	0.38	0	10,10,19	0.40	0
7	C8E	C	401	-	11,11,20	0.51	0	10,10,19	0.31	0
7	C8E	E	403	-	11,11,20	0.45	0	10,10,19	0.44	0
7	C8E	B	403	-	20,20,20	0.50	0	19,19,19	0.65	0
7	C8E	C	405	-	7,7,20	0.42	0	6,6,19	0.41	0
6	NAG	A	401	-	14,14,15	0.47	0	17,19,21	0.60	0
7	C8E	C	403	-	11,11,20	0.42	0	10,10,19	0.32	0
7	C8E	C	402	-	11,11,20	0.47	0	10,10,19	0.49	0
7	C8E	E	401	-	11,11,20	0.55	0	10,10,19	0.35	0
7	C8E	C	404	-	11,11,20	0.39	0	10,10,19	0.56	0
7	C8E	C	406	-	7,7,20	0.38	0	6,6,19	0.50	0
7	C8E	C	407	-	11,11,20	0.43	0	10,10,19	0.43	0
7	C8E	E	402	-	11,11,20	0.33	0	10,10,19	0.48	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
7	C8E	F	401	-	-	8/9/9/18	-
7	C8E	A	402	-	-	5/9/9/18	-
7	C8E	B	402	-	-	3/9/9/18	-
7	C8E	A	405	-	-	1/6/6/18	-
7	C8E	A	404	-	-	5/9/9/18	-
7	C8E	E	404	-	-	2/5/5/18	-
7	C8E	D	402	-	-	6/9/9/18	-
7	C8E	B	401	-	-	5/9/9/18	-
7	C8E	A	403	-	-	3/9/9/18	-
7	C8E	E	405	-	-	3/9/9/18	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	C8E	D	401	-	-	6/9/9/18	-
7	C8E	C	401	-	-	2/9/9/18	-
7	C8E	E	403	-	-	4/9/9/18	-
7	C8E	B	403	-	-	10/18/18/18	-
7	C8E	C	405	-	-	2/5/5/18	-
6	NAG	A	401	-	-	3/6/23/26	0/1/1/1
7	C8E	C	403	-	-	7/9/9/18	-
7	C8E	C	402	-	-	5/9/9/18	-
7	C8E	E	401	-	-	5/9/9/18	-
7	C8E	C	404	-	-	3/9/9/18	-
7	C8E	C	406	-	-	5/5/5/18	-
7	C8E	C	407	-	-	3/9/9/18	-
7	C8E	E	402	-	-	3/9/9/18	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (99) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	401	NAG	C4-C5-C6-O6
7	D	401	C8E	C2-C3-C4-C5
7	F	401	C8E	C4-C5-C6-C7
6	A	401	NAG	O5-C5-C6-O6
6	A	401	NAG	C1-C2-N2-C7
7	B	403	C8E	O12-C13-C14-O15
7	D	402	C8E	C6-C7-C8-O9
7	E	401	C8E	C6-C7-C8-O9
7	F	401	C8E	C6-C7-C8-O9
7	A	402	C8E	C6-C7-C8-O9
7	D	401	C8E	C6-C7-C8-O9
7	A	402	C8E	O9-C10-C11-O12
7	B	401	C8E	O9-C10-C11-O12
7	E	403	C8E	O9-C10-C11-O12
7	B	401	C8E	C3-C4-C5-C6
7	E	402	C8E	C2-C3-C4-C5
7	E	405	C8E	C4-C5-C6-C7
7	D	402	C8E	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
7	A	402	C8E	C2-C3-C4-C5
7	A	404	C8E	C3-C4-C5-C6
7	C	402	C8E	C2-C3-C4-C5
7	F	401	C8E	C2-C3-C4-C5
7	F	401	C8E	C5-C6-C7-C8
7	F	401	C8E	C3-C4-C5-C6
7	E	401	C8E	C4-C5-C6-C7
7	A	404	C8E	C4-C5-C6-C7
7	B	401	C8E	C2-C3-C4-C5
7	A	402	C8E	C3-C4-C5-C6
7	C	402	C8E	C6-C7-C8-O9
7	A	404	C8E	C2-C3-C4-C5
7	D	402	C8E	C3-C4-C5-C6
7	B	401	C8E	C4-C5-C6-C7
7	C	403	C8E	C3-C4-C5-C6
7	D	401	C8E	O9-C10-C11-O12
7	E	402	C8E	C1-C2-C3-C4
7	D	402	C8E	C2-C3-C4-C5
7	C	403	C8E	C5-C6-C7-C8
7	D	402	C8E	C1-C2-C3-C4
7	C	404	C8E	C3-C4-C5-C6
7	C	405	C8E	C5-C6-C7-C8
7	C	401	C8E	C3-C4-C5-C6
7	C	403	C8E	O9-C10-C11-O12
7	C	406	C8E	O9-C10-C11-O12
7	B	403	C8E	C14-C13-O12-C11
7	E	405	C8E	C5-C6-C7-C8
7	E	403	C8E	C3-C4-C5-C6
7	C	403	C8E	C4-C5-C6-C7
7	B	402	C8E	O9-C10-C11-O12
7	B	403	C8E	O18-C19-C20-O21
7	A	402	C8E	C1-C2-C3-C4
7	E	402	C8E	C3-C4-C5-C6
7	C	402	C8E	C3-C4-C5-C6
7	F	401	C8E	C1-C2-C3-C4
7	C	402	C8E	C4-C5-C6-C7
7	E	401	C8E	C2-C3-C4-C5
7	D	402	C8E	O9-C10-C11-O12
7	E	405	C8E	C3-C4-C5-C6
7	D	401	C8E	C3-C4-C5-C6
7	C	406	C8E	C5-C6-C7-C8
7	B	403	C8E	C2-C3-C4-C5

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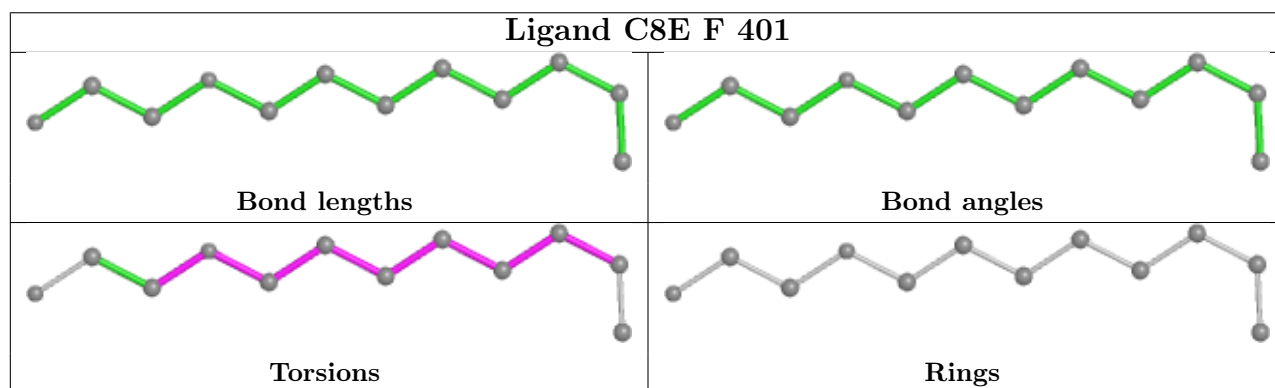
Mol	Chain	Res	Type	Atoms
7	C	404	C8E	C7-C8-O9-C10
7	D	401	C8E	C1-C2-C3-C4
7	C	405	C8E	C6-C7-C8-O9
7	C	403	C8E	C6-C7-C8-O9
7	E	404	C8E	O9-C10-C11-O12
7	A	404	C8E	C7-C8-O9-C10
7	B	403	C8E	C13-C14-O15-C16
7	C	407	C8E	C2-C3-C4-C5
7	C	401	C8E	C7-C8-O9-C10
7	F	401	C8E	C7-C8-O9-C10
7	A	403	C8E	C6-C7-C8-O9
7	C	407	C8E	C1-C2-C3-C4
7	F	401	C8E	C11-C10-O9-C8
7	B	401	C8E	C7-C8-O9-C10
7	E	403	C8E	C7-C8-O9-C10
7	A	405	C8E	C7-C8-O9-C10
7	B	403	C8E	C16-C17-O18-C19
7	A	404	C8E	O9-C10-C11-O12
7	D	401	C8E	C11-C10-O9-C8
7	C	406	C8E	C11-C10-O9-C8
7	B	402	C8E	C3-C4-C5-C6
7	C	403	C8E	C7-C8-O9-C10
7	A	403	C8E	O9-C10-C11-O12
7	A	403	C8E	C5-C6-C7-C8
7	B	403	C8E	O15-C16-C17-O18
7	B	402	C8E	C4-C5-C6-C7
7	C	406	C8E	C6-C7-C8-O9
7	C	402	C8E	C7-C8-O9-C10
7	C	403	C8E	C2-C3-C4-C5
7	E	401	C8E	C1-C2-C3-C4
7	C	407	C8E	C3-C4-C5-C6
7	E	404	C8E	C7-C8-O9-C10
7	E	401	C8E	C5-C6-C7-C8
7	B	403	C8E	C17-C16-O15-C14
7	B	403	C8E	C4-C5-C6-C7
7	C	406	C8E	C7-C8-O9-C10
7	B	403	C8E	O9-C10-C11-O12
7	C	404	C8E	C11-C10-O9-C8
7	E	403	C8E	C4-C5-C6-C7

There are no ring outliers.

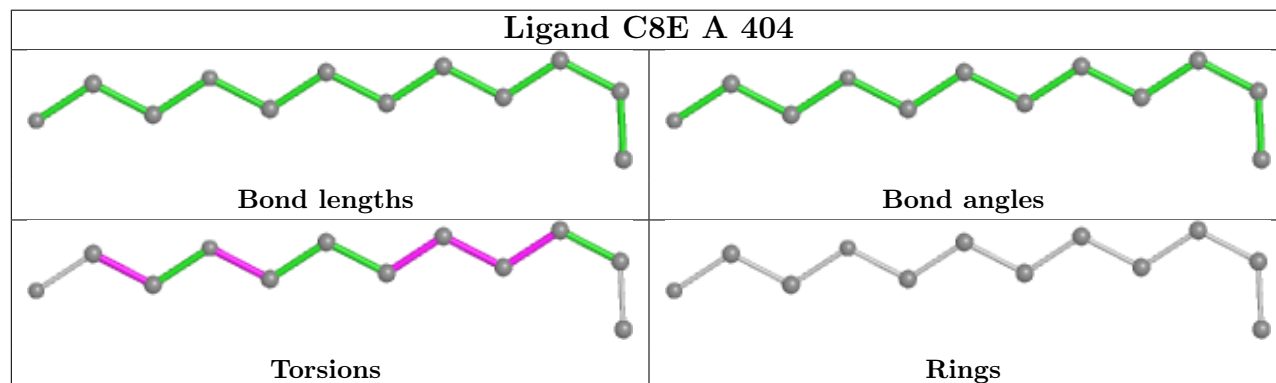
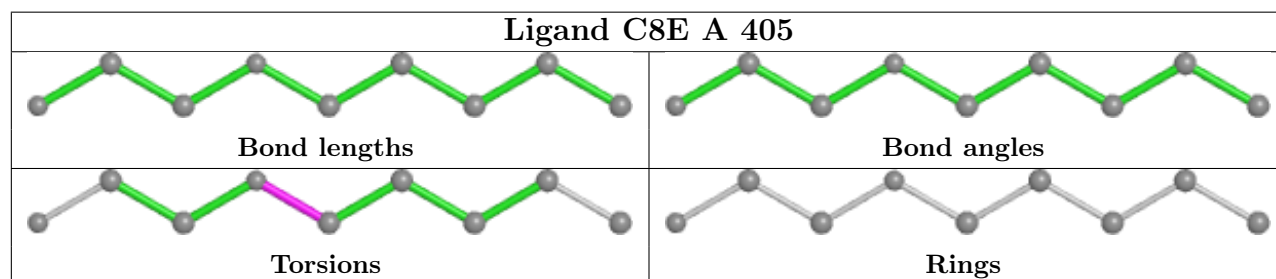
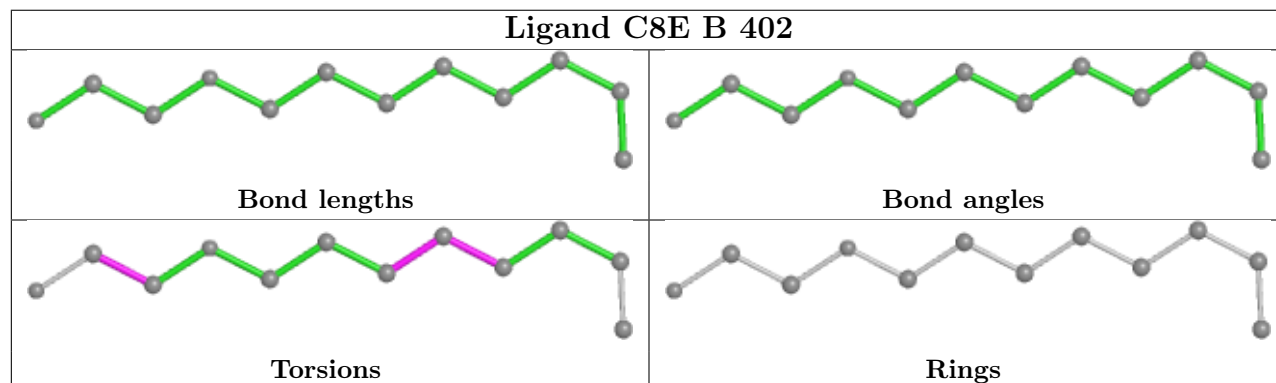
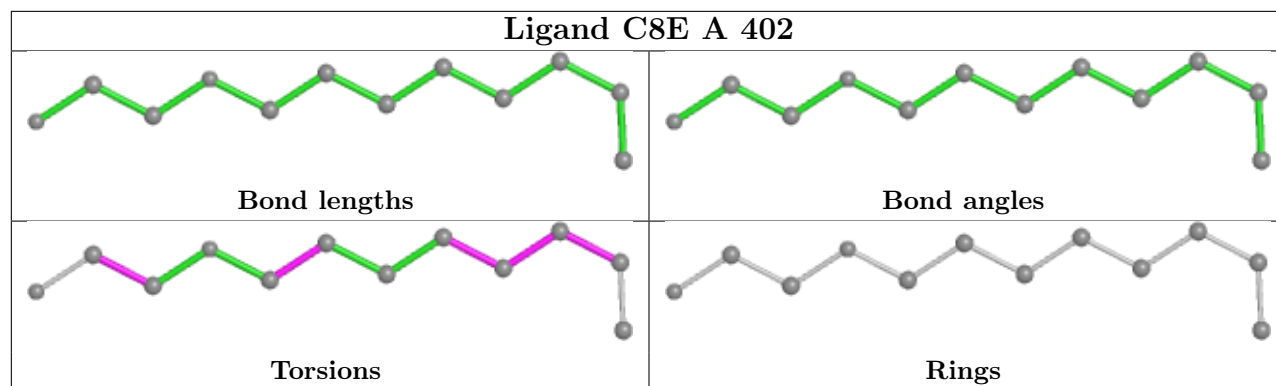
14 monomers are involved in 29 short contacts:

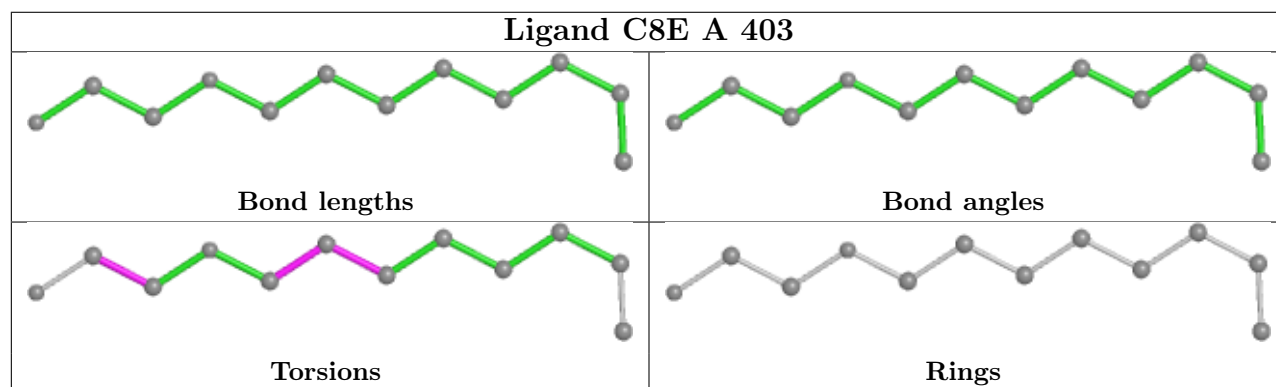
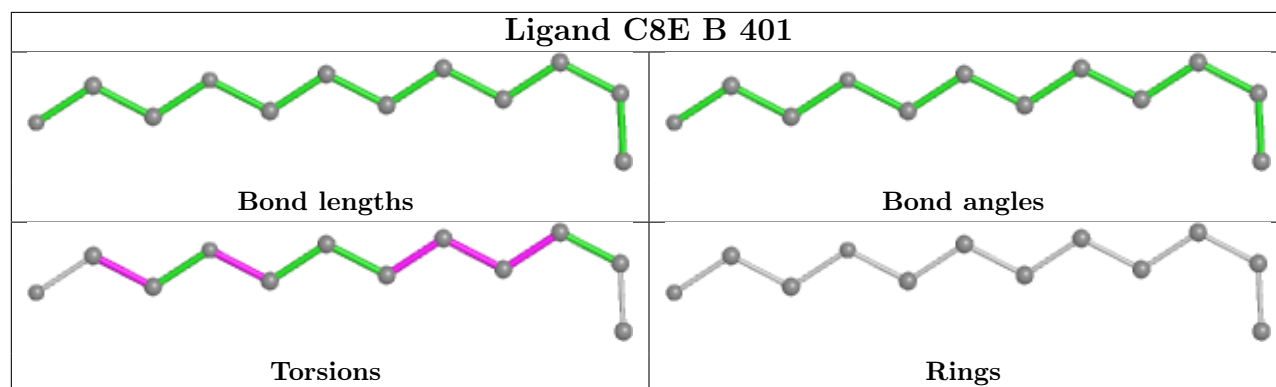
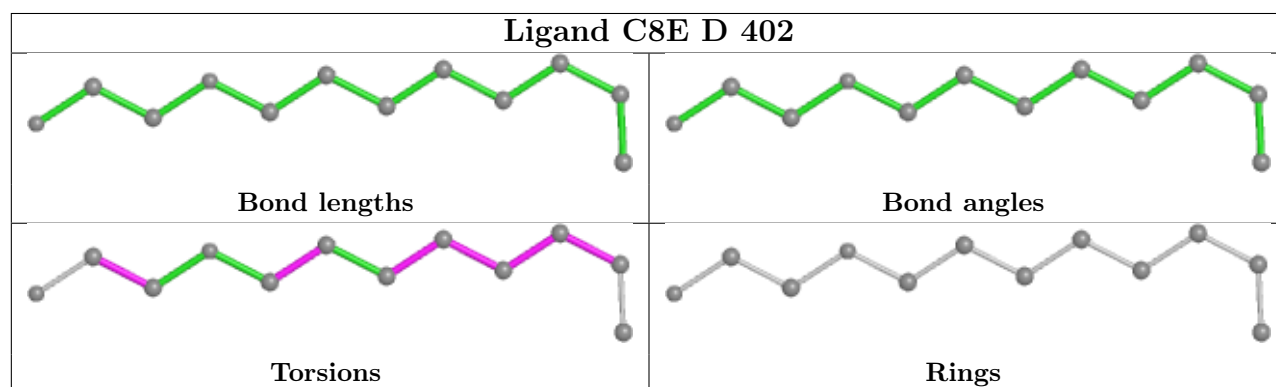
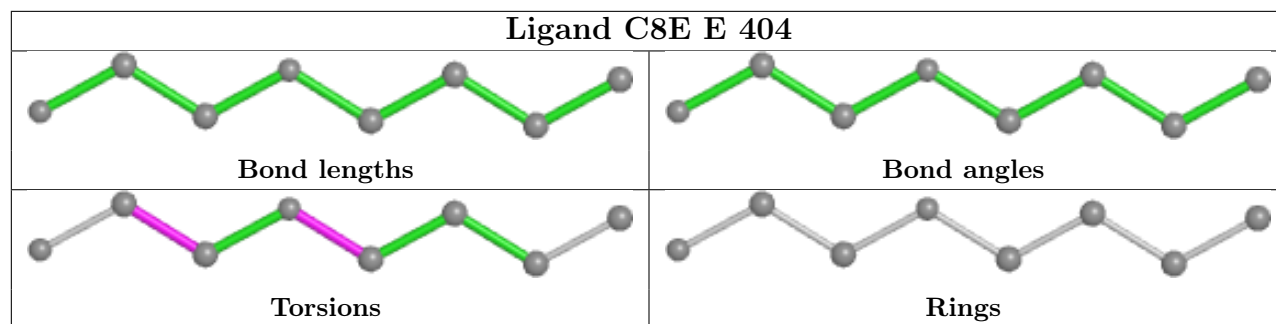
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	401	C8E	3	0
7	A	402	C8E	1	0
7	A	404	C8E	2	0
7	D	402	C8E	4	0
7	B	401	C8E	3	0
7	E	405	C8E	1	0
7	D	401	C8E	1	0
7	C	405	C8E	1	0
6	A	401	NAG	4	0
7	C	403	C8E	1	0
7	C	402	C8E	1	0
7	E	401	C8E	1	0
7	C	404	C8E	2	0
7	E	402	C8E	4	0

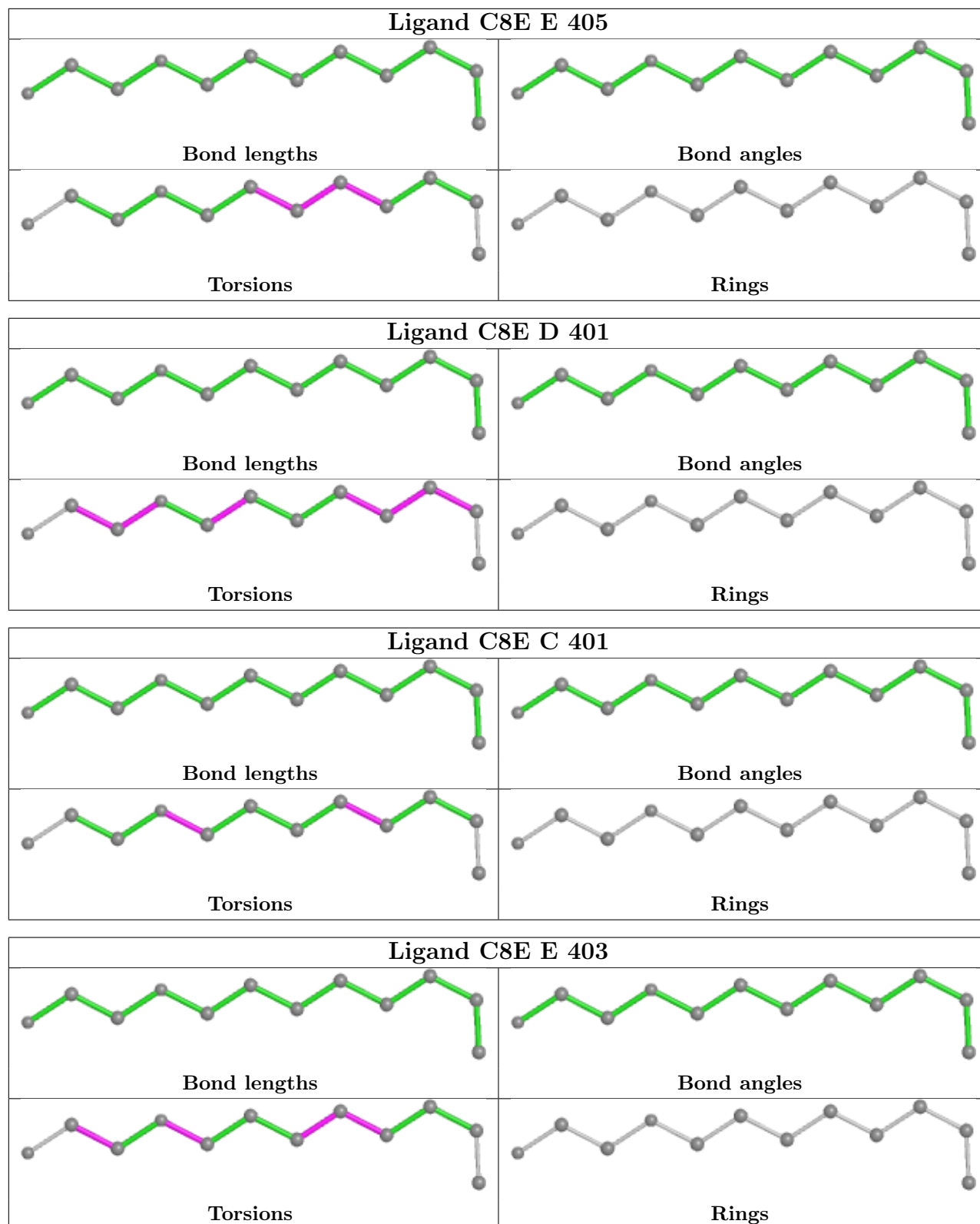
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

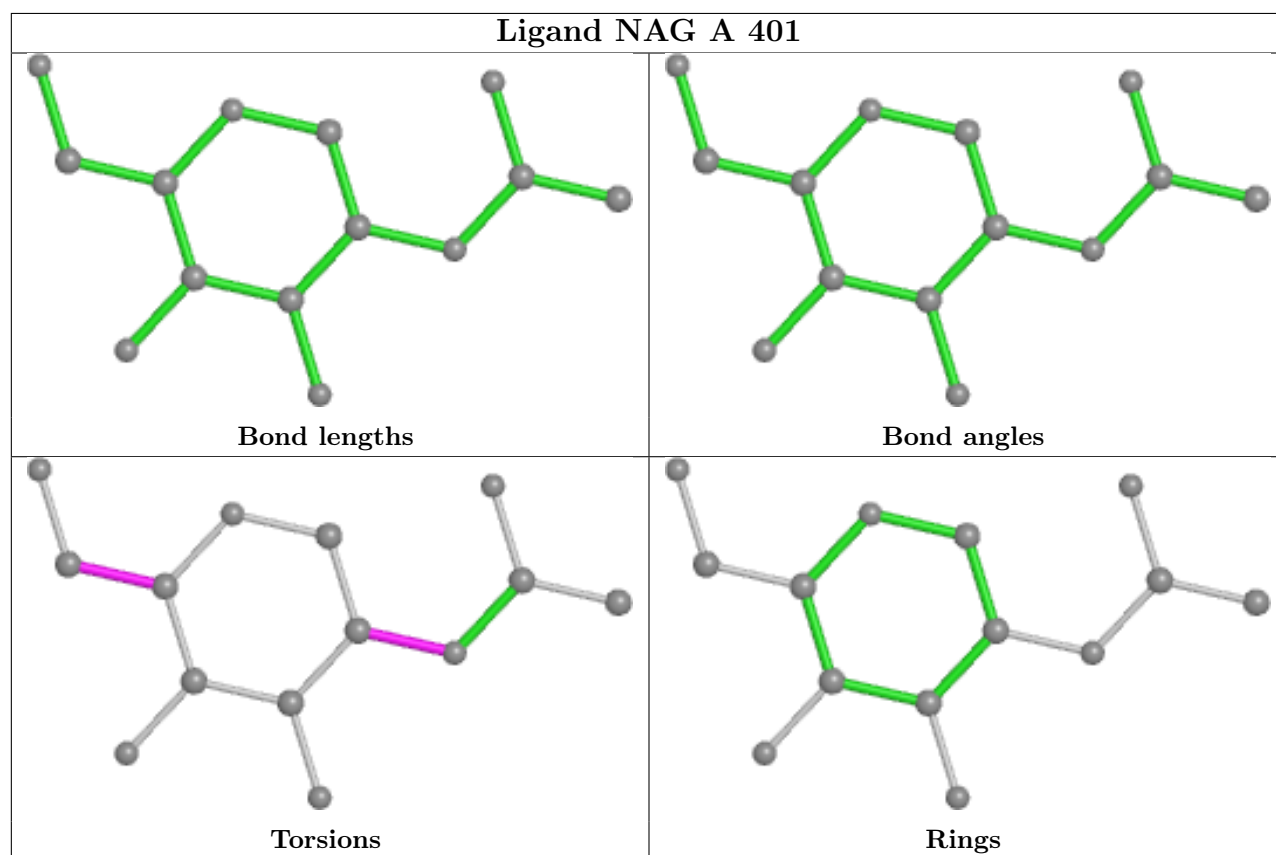
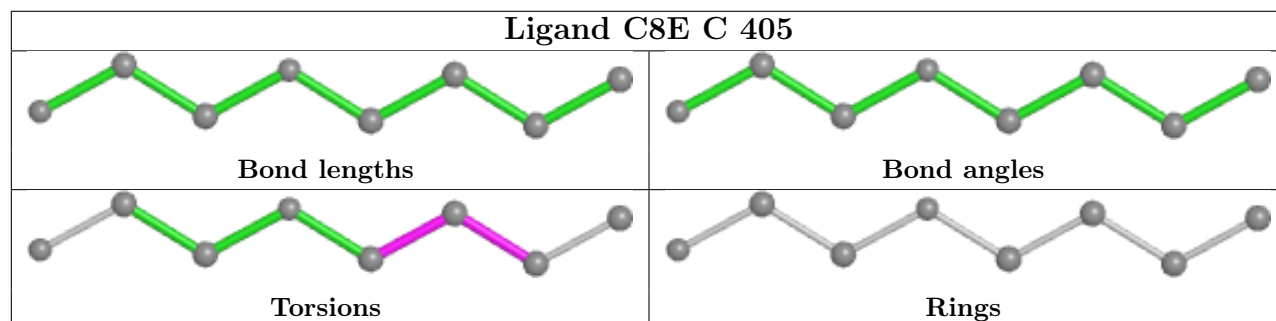
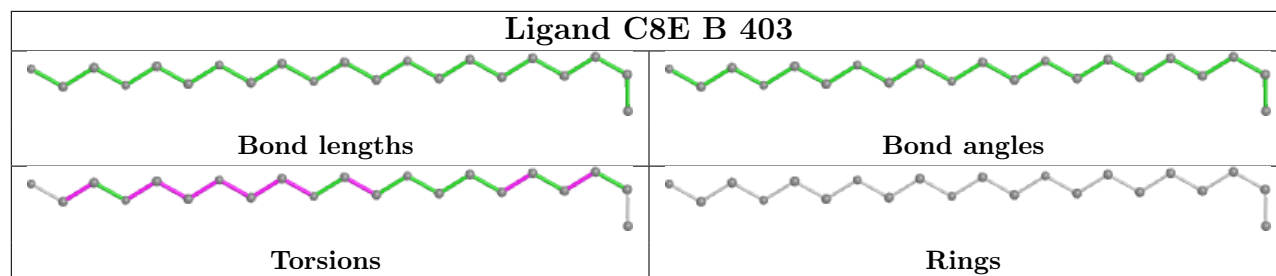


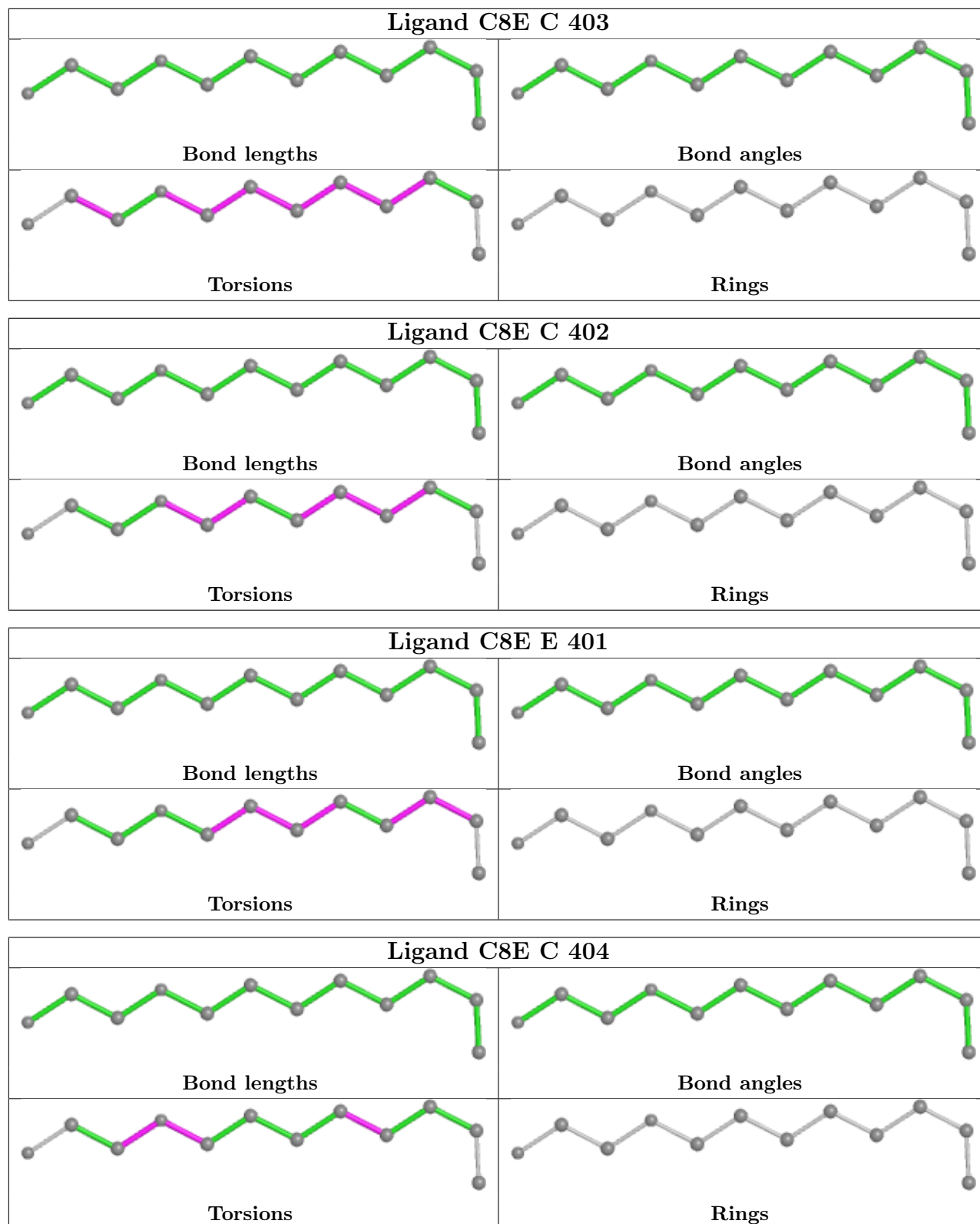


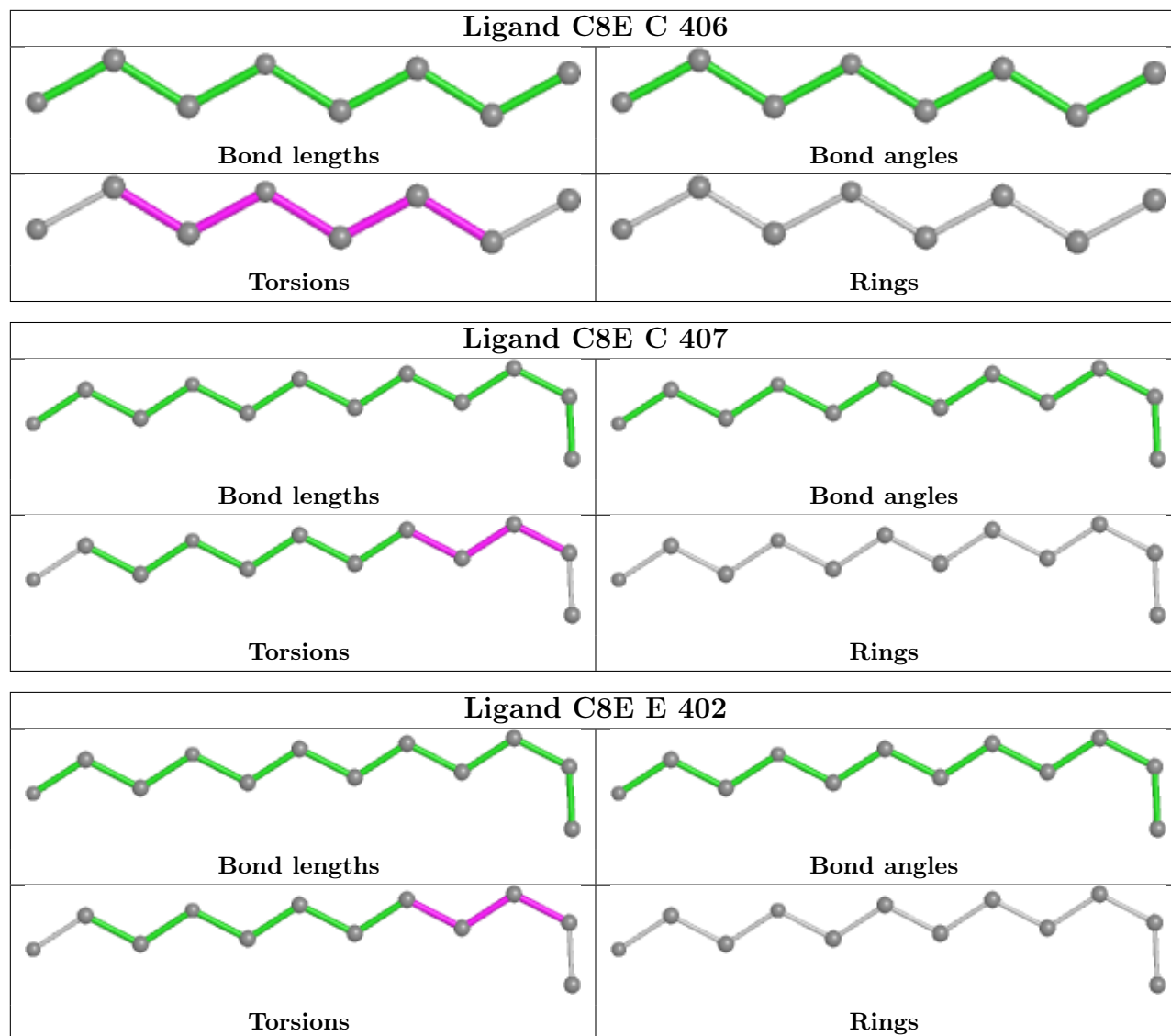












## 5.7 Other polymers [i](#)

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, 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	331/331 (100%)	-0.48	2 (0%) 89 92	29, 40, 59, 84	0
1	B	331/331 (100%)	-0.33	3 (0%) 84 89	30, 43, 68, 91	0
1	C	331/331 (100%)	-0.54	0 100 100	27, 39, 56, 64	0
1	D	331/331 (100%)	-0.54	1 (0%) 94 96	26, 37, 53, 76	0
1	E	331/331 (100%)	-0.45	2 (0%) 89 92	28, 42, 60, 85	0
1	F	331/331 (100%)	-0.53	1 (0%) 94 96	29, 41, 54, 79	0
All	All	1986/1986 (100%)	-0.48	9 (0%) 91 94	26, 41, 59, 91	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	230	GLU	3.3
1	E	327	ASP	3.1
1	D	162	ASP	3.1
1	A	103	ALA	2.4
1	E	230	GLU	2.4
1	B	230	GLU	2.4
1	F	230	GLU	2.3
1	B	102	SER	2.2
1	B	228	TRP	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates i

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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.

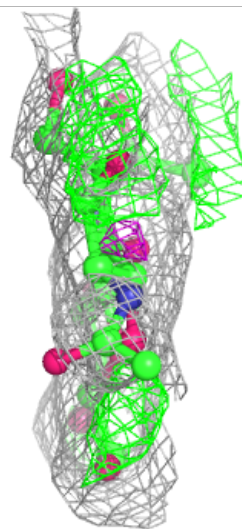
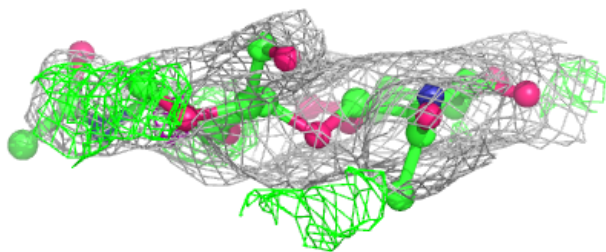
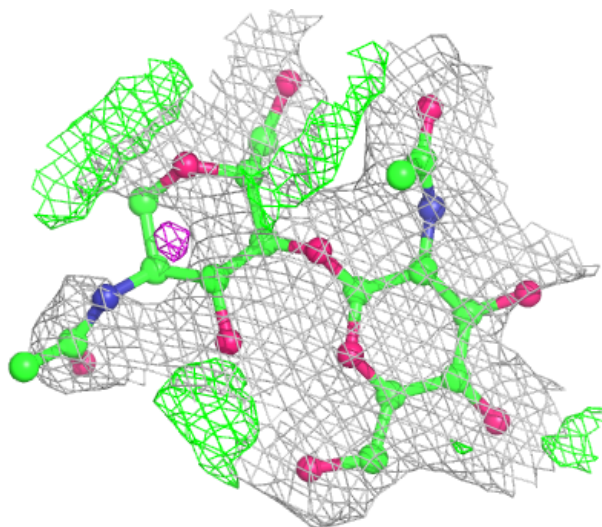
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	L	1	15/15	0.63	0.54	68,78,87,91	15
5	NAG	J	5	14/15	0.63	0.34	40,57,60,60	14
3	NAG	L	2	14/15	0.69	0.34	55,74,79,81	14
5	NAG	K	5	14/15	0.73	0.35	42,54,58,59	14
3	NAG	L	6	14/15	0.74	0.41	48,63,68,68	14
4	NAG	I	4	14/15	0.74	0.41	64,70,73,75	14
3	NAG	H	6	14/15	0.75	0.35	50,56,59,60	14
4	NAG	I	1	14/15	0.78	0.21	47,62,68,68	14
2	NAG	G	1	14/15	0.78	0.29	60,68,75,76	14
2	NAG	G	2	14/15	0.80	0.22	57,67,71,72	14
3	NAG	H	1	15/15	0.80	0.51	69,75,79,81	15
5	NAG	J	1	14/15	0.82	0.23	55,62,67,69	14
5	NAG	J	3	14/15	0.83	0.26	52,58,65,69	14
3	NAG	L	3	14/15	0.83	0.21	64,68,71,74	14
4	NAG	I	2	14/15	0.83	0.26	60,64,69,74	14
3	NAG	L	5	14/15	0.84	0.32	58,62,68,72	14
5	NAG	K	1	14/15	0.85	0.22	54,61,64,67	14
5	NAG	J	2	14/15	0.85	0.19	42,58,63,68	14
5	NAG	K	2	14/15	0.86	0.17	53,58,62,63	14
3	NAG	H	2	14/15	0.86	0.24	63,70,76,77	14
5	NAG	K	3	14/15	0.87	0.24	54,57,62,64	14
4	NAG	I	3	14/15	0.87	0.34	55,61,70,71	14
3	NAG	H	3	14/15	0.88	0.17	53,63,70,71	0
3	NAG	L	4	14/15	0.88	0.25	60,65,71,74	14
5	NAG	K	4	14/15	0.89	0.33	48,54,58,60	14
3	NAG	H	5	14/15	0.89	0.32	50,54,57,58	14
5	NAG	J	4	14/15	0.91	0.29	47,52,57,57	14
3	NAG	H	4	14/15	0.92	0.21	55,59,62,63	14

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.



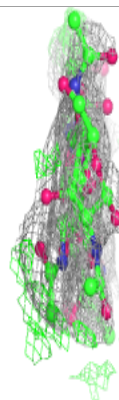
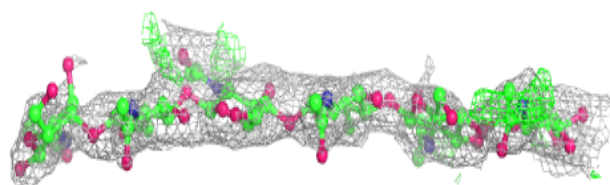
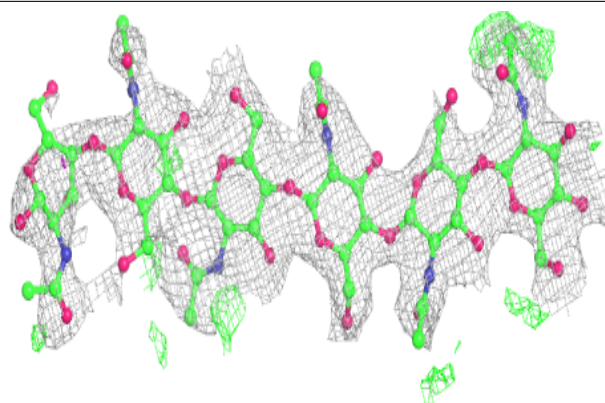
**Electron density around Chain G:**

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

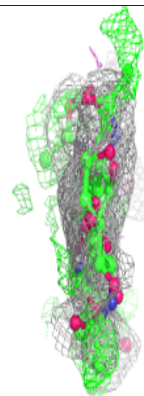
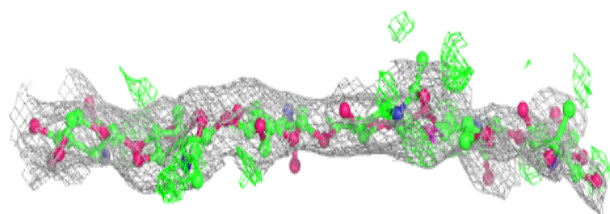
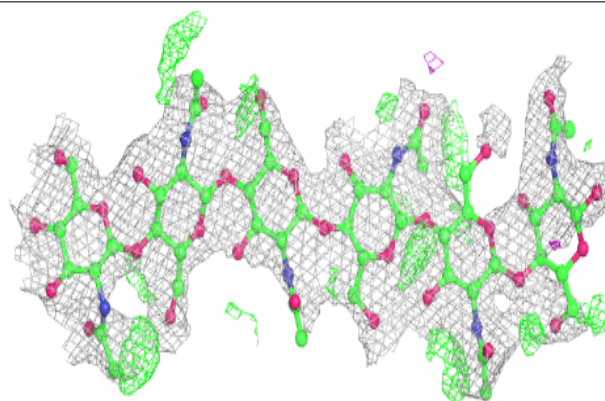


**Electron density around Chain H:**

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

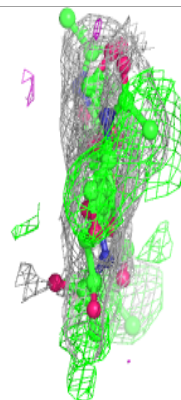
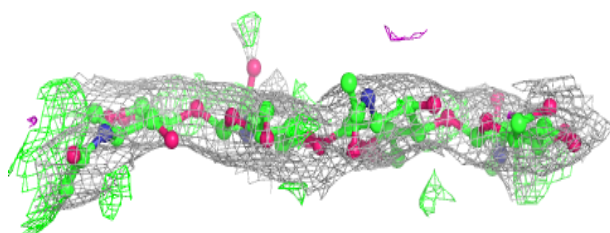
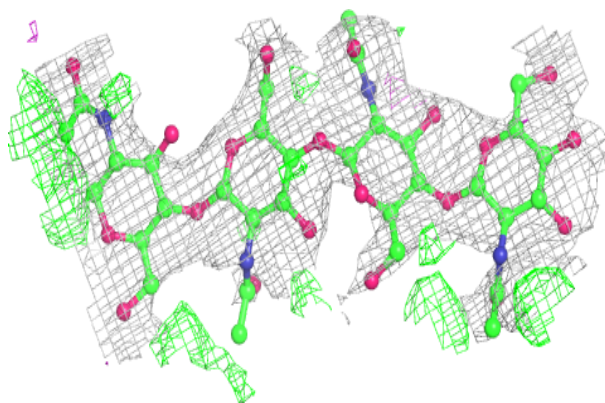
**Electron density around Chain L:**

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

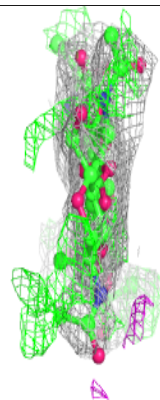
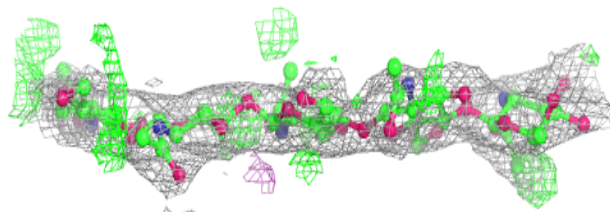
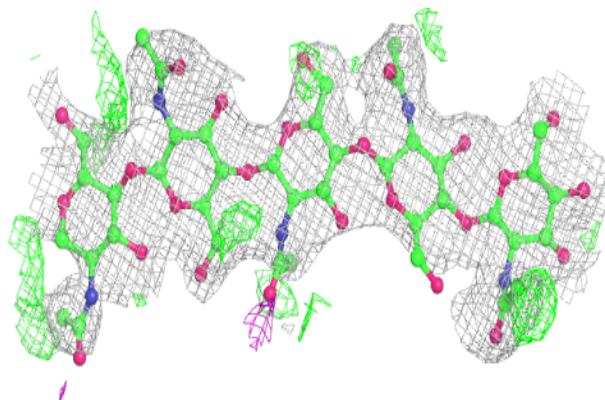


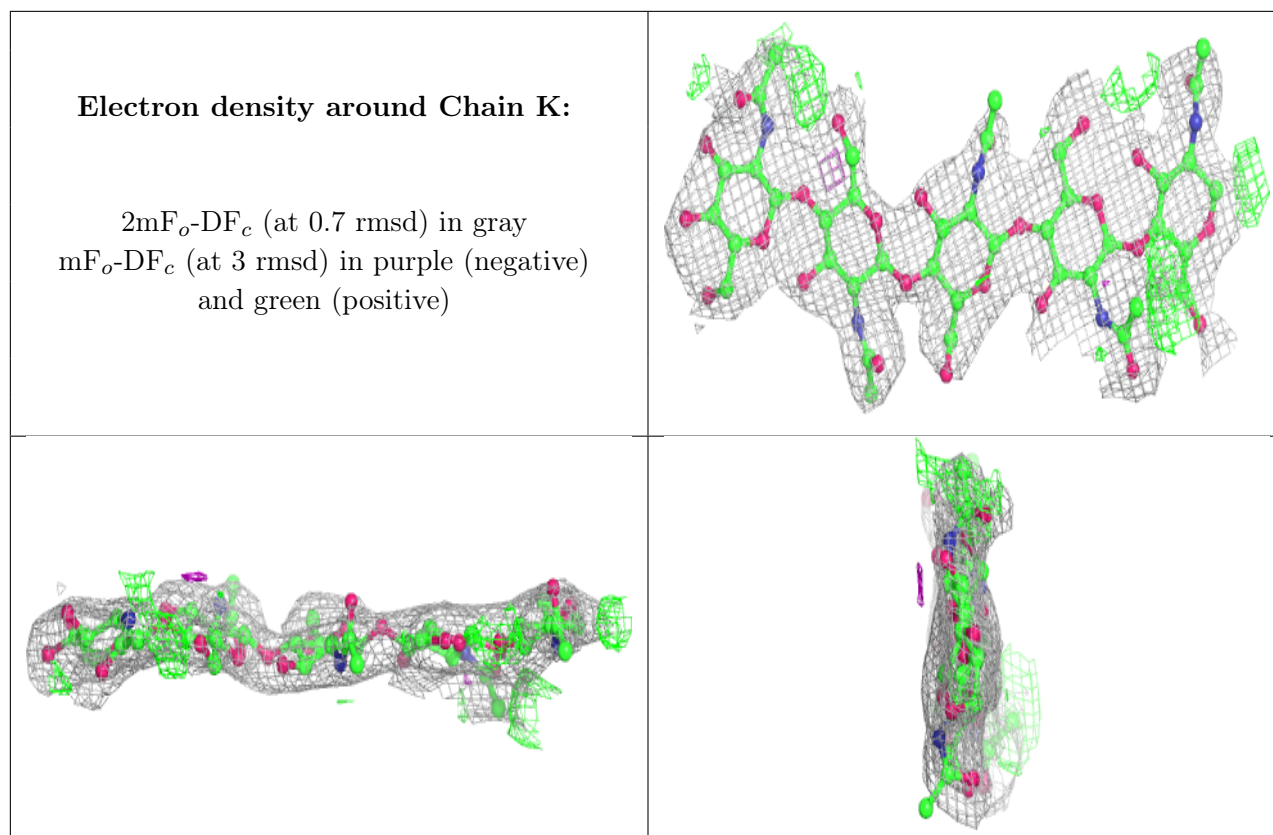
**Electron density around Chain I:**

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

**Electron density around Chain J:**

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





## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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
6	NAG	A	401	14/15	0.76	0.33	35,56,60,61	14
7	C8E	B	401	12/21	0.76	0.30	42,50,77,98	0
7	C8E	F	401	12/21	0.81	0.33	46,61,70,73	0
8	NA	A	409	1/1	0.81	0.19	57,57,57,57	0
7	C8E	E	403	12/21	0.82	0.39	40,50,58,62	0
7	C8E	A	404	12/21	0.84	0.37	48,58,70,73	0
8	NA	B	405	1/1	0.86	0.15	47,47,47,47	0
7	C8E	E	405	12/21	0.89	0.18	45,54,57,61	0
7	C8E	B	403	21/21	0.89	0.35	51,67,84,90	0
7	C8E	E	402	12/21	0.89	0.16	42,47,62,65	0
7	C8E	A	405	9/21	0.89	0.37	42,51,61,63	0
8	NA	F	404	1/1	0.89	0.34	55,55,55,55	0
7	C8E	D	401	12/21	0.90	0.28	38,49,56,56	0
8	NA	F	403	1/1	0.90	0.14	38,38,38,38	0

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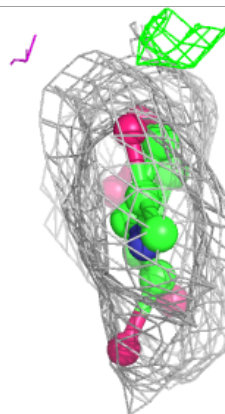
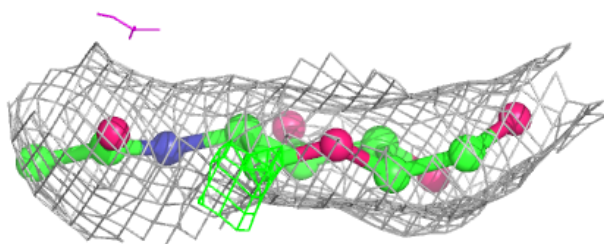
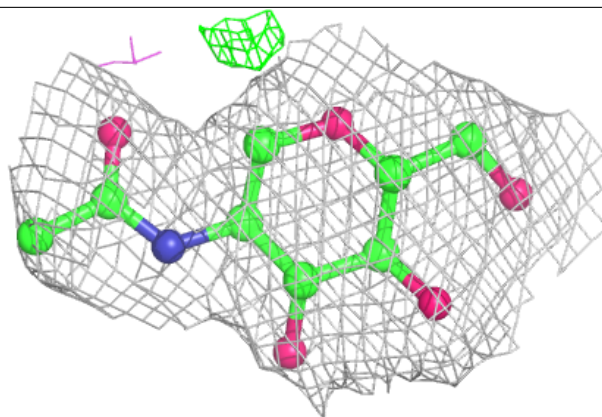
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	C8E	C	404	12/21	0.90	0.17	38,50,58,67	0
7	C8E	C	406	8/21	0.91	0.30	35,49,58,59	0
7	C8E	A	402	12/21	0.91	0.17	37,41,49,50	0
7	C8E	B	402	12/21	0.92	0.31	40,50,57,60	0
7	C8E	E	401	12/21	0.92	0.18	40,46,51,52	0
7	C8E	C	405	8/21	0.92	0.17	41,48,58,60	0
7	C8E	C	402	12/21	0.92	0.17	35,38,45,48	0
7	C8E	C	407	12/21	0.92	0.13	43,50,56,59	0
7	C8E	C	403	12/21	0.93	0.24	32,41,43,54	0
8	NA	D	404	1/1	0.93	0.07	34,34,34,34	0
8	NA	A	407	1/1	0.93	0.14	40,40,40,40	0
7	C8E	D	402	12/21	0.93	0.19	36,49,53,57	0
8	NA	E	408	1/1	0.94	0.10	41,41,41,41	0
8	NA	A	408	1/1	0.94	0.28	43,43,43,43	0
8	NA	D	405	1/1	0.94	0.14	42,42,42,42	0
8	NA	C	409	1/1	0.95	0.07	39,39,39,39	0
7	C8E	C	401	12/21	0.95	0.12	31,33,39,39	0
7	C8E	E	404	8/21	0.95	0.26	38,44,51,53	0
7	C8E	A	403	12/21	0.96	0.12	37,42,46,52	0
8	NA	D	403	1/1	0.97	0.05	31,31,31,31	0
8	NA	F	402	1/1	0.97	0.08	25,25,25,25	0
8	NA	B	406	1/1	0.97	0.07	37,37,37,37	0
8	NA	A	406	1/1	0.97	0.08	33,33,33,33	0
8	NA	B	404	1/1	0.98	0.05	29,29,29,29	0
8	NA	E	406	1/1	0.98	0.10	21,21,21,21	0
8	NA	C	408	1/1	0.99	0.04	27,27,27,27	0
8	NA	E	407	1/1	0.99	0.04	39,39,39,39	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.

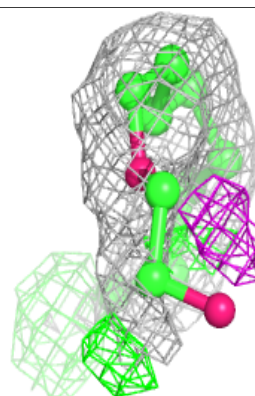
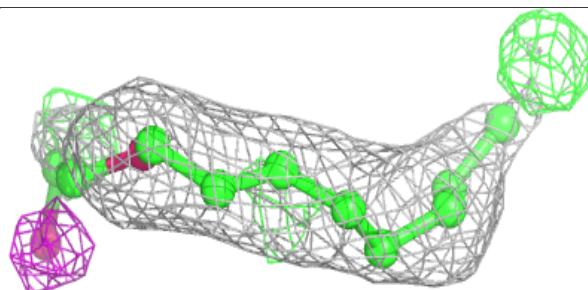
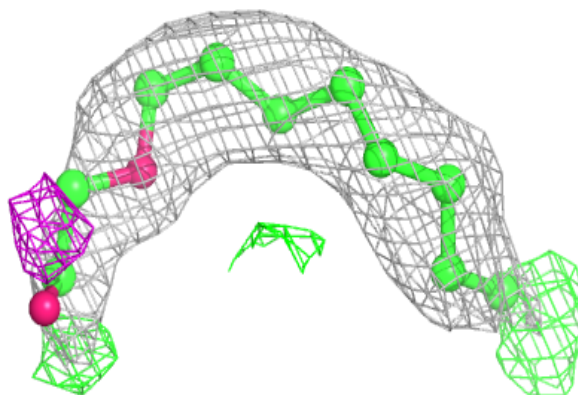


**Electron density around NAG A 401:**

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

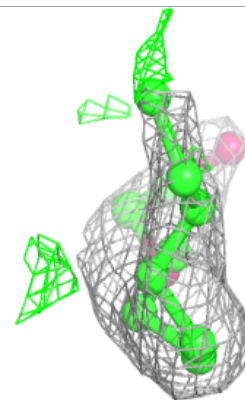
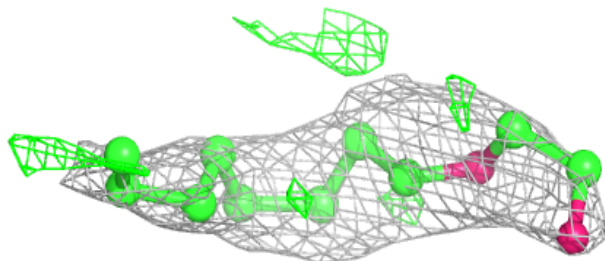
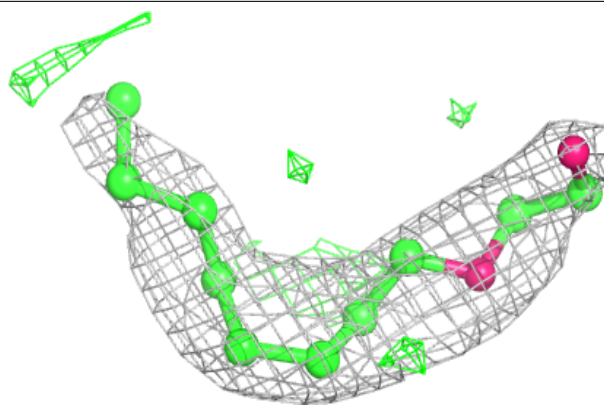
**Electron density around C8E B 401:**

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

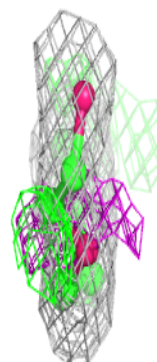
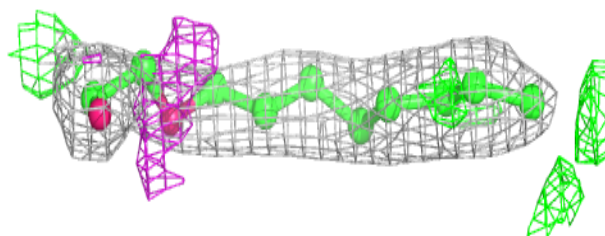
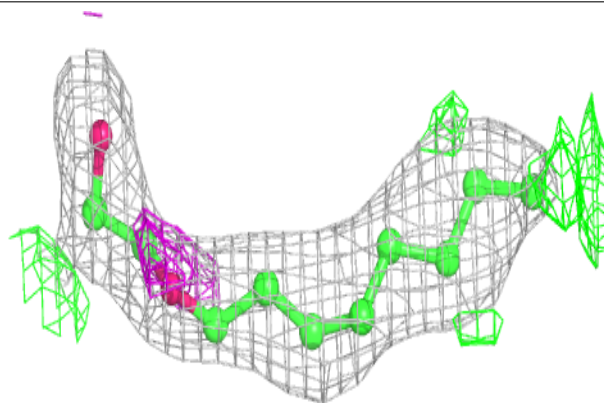


**Electron density around C8E F 401:**

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

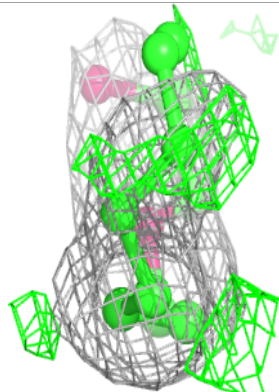
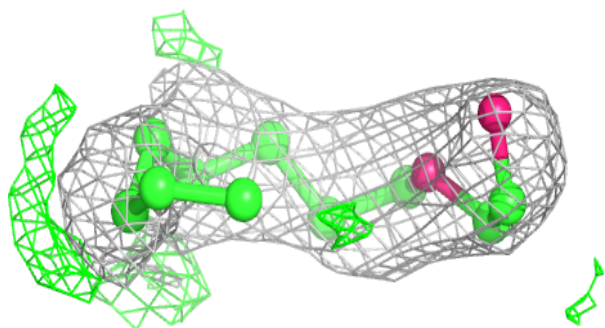
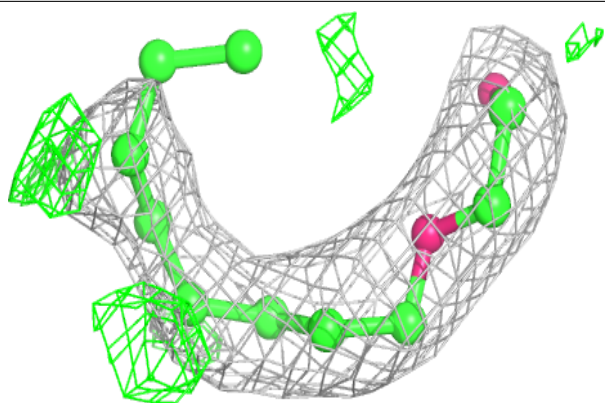
**Electron density around C8E E 403:**

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and green (positive)

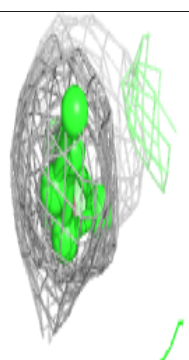
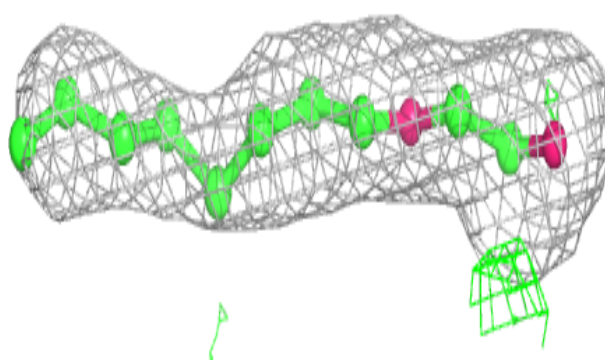
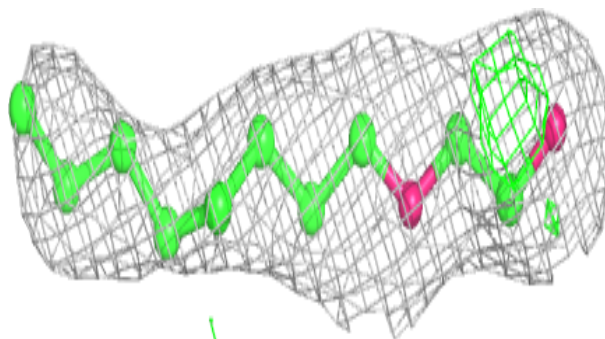


**Electron density around C8E A 404:**

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

**Electron density around C8E E 405:**

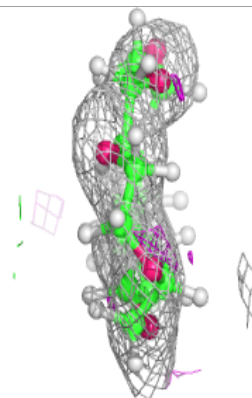
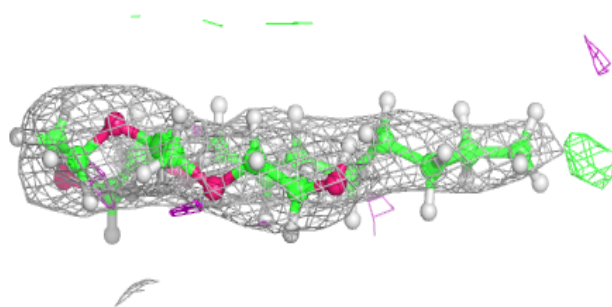
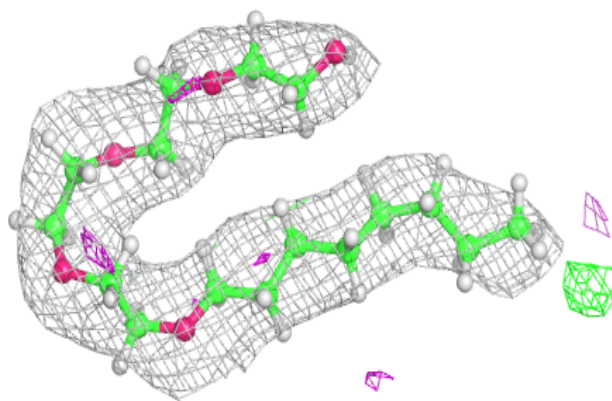
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



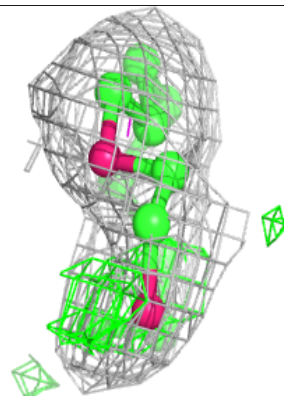
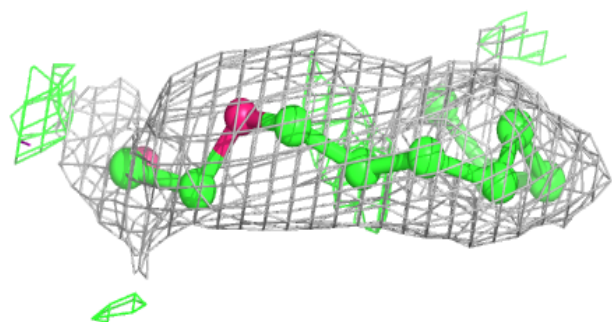
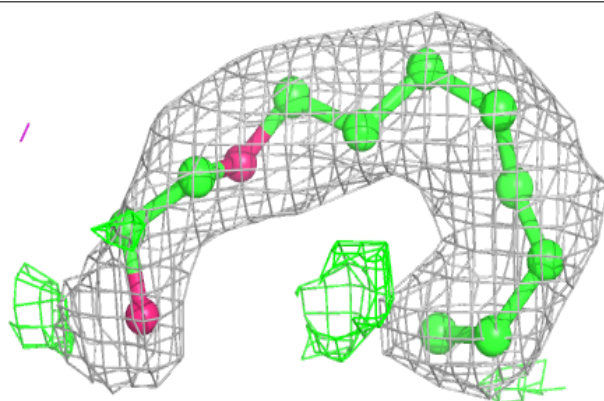


**Electron density around C8E B 403:**

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

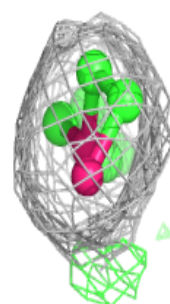
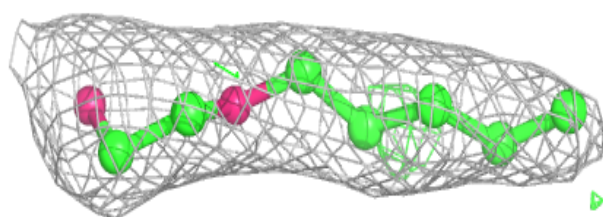
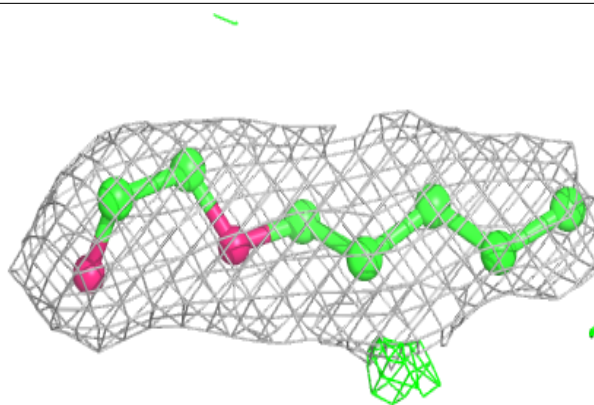
**Electron density around C8E E 402:**

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

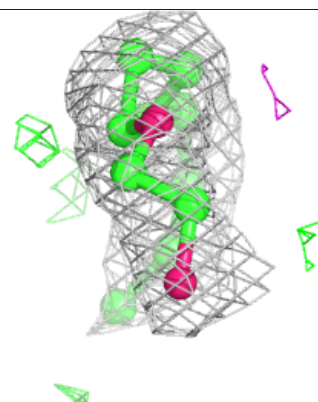
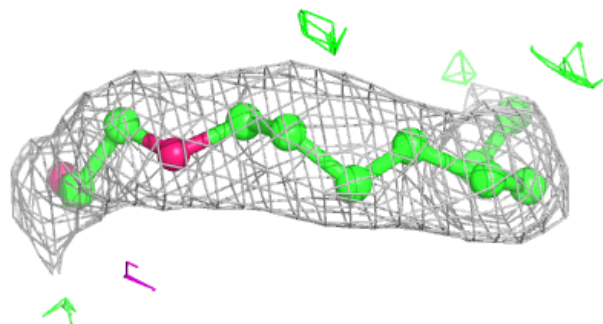
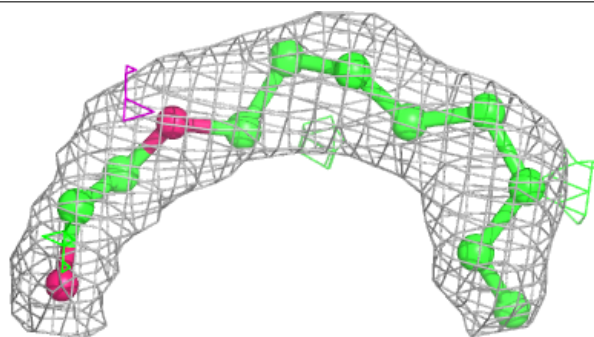


**Electron density around C8E A 405:**

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

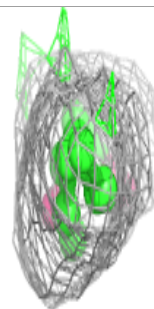
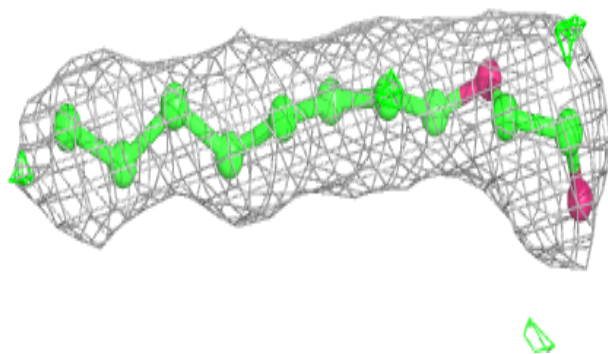
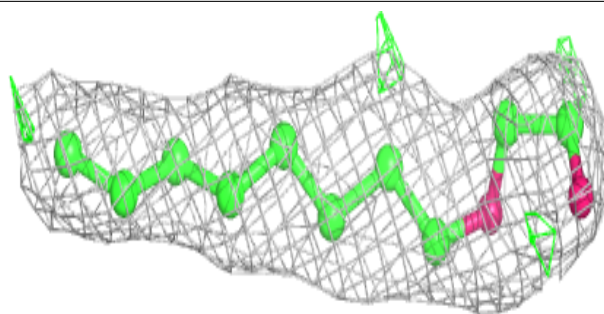
**Electron density around C8E D 401:**

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

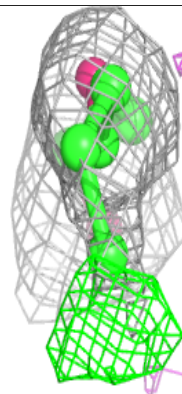
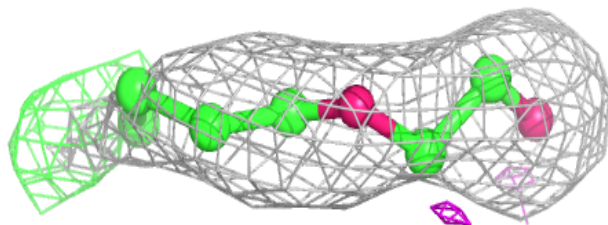
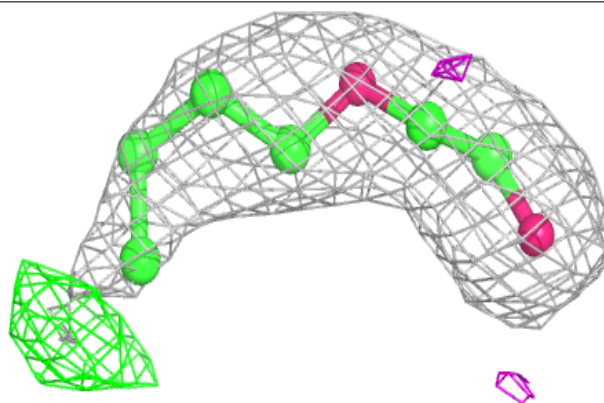


**Electron density around C8E C 404:**

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

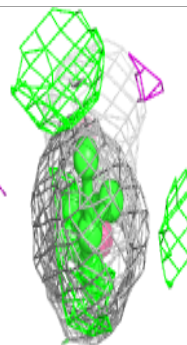
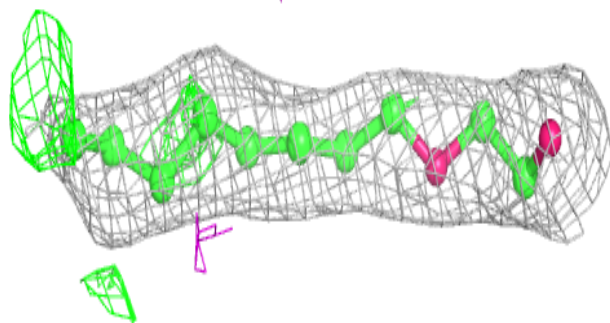
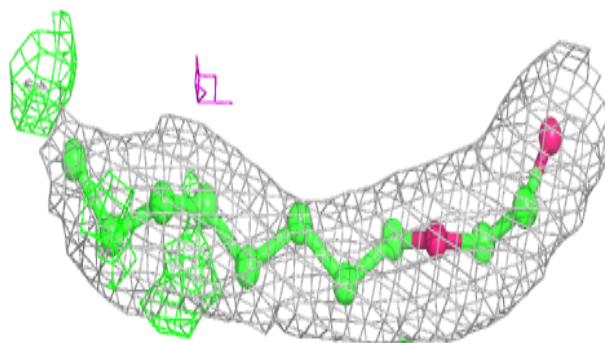
**Electron density around C8E C 406:**

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

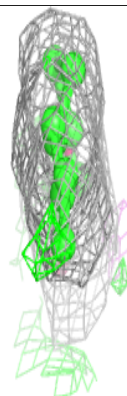
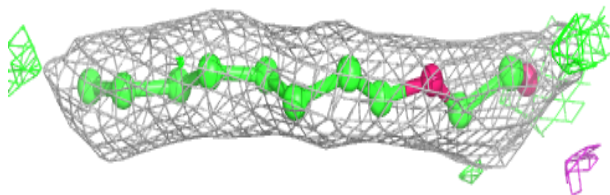
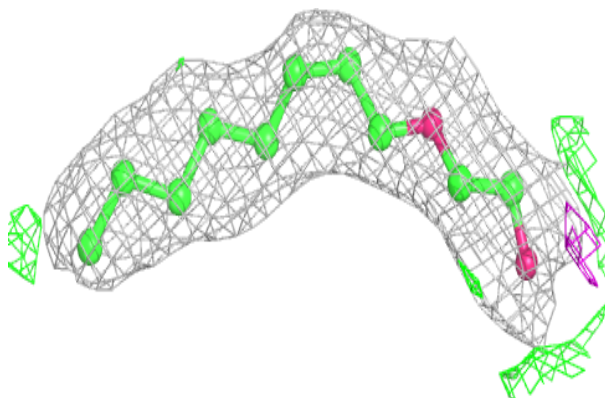


**Electron density around C8E A 402:**

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

**Electron density around C8E B 402:**

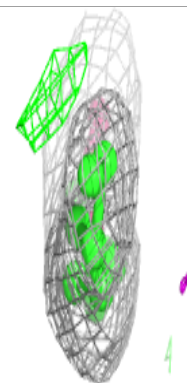
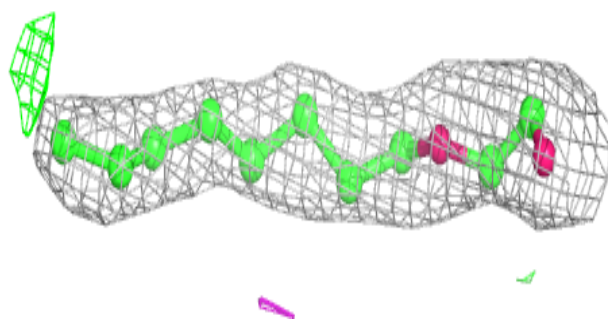
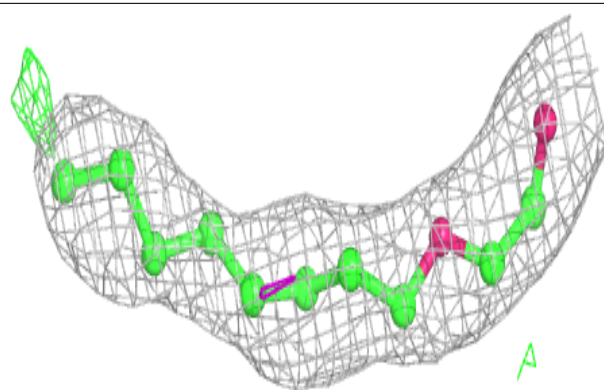
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





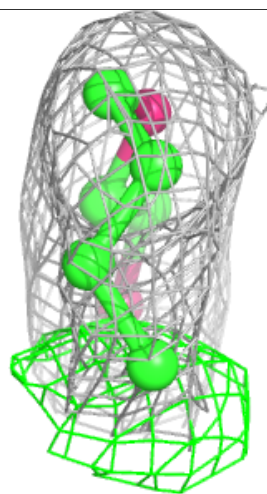
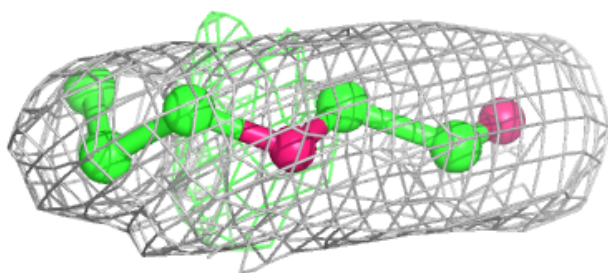
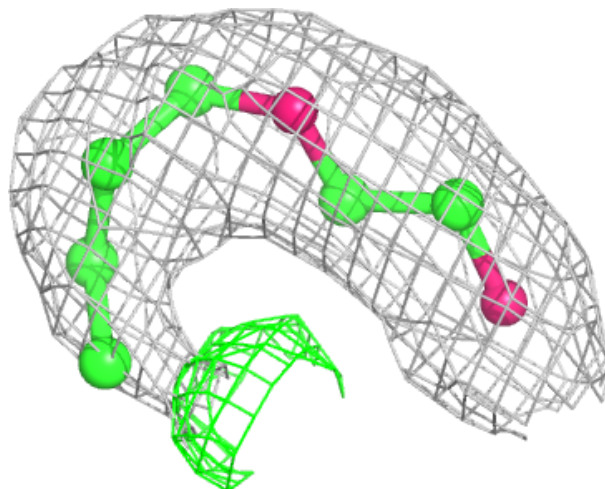
**Electron density around C8E E 401:**

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



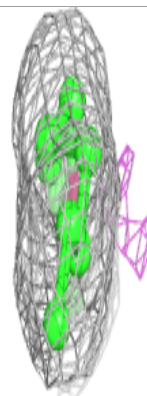
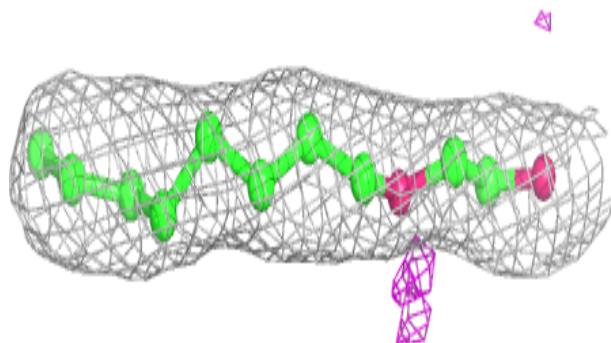
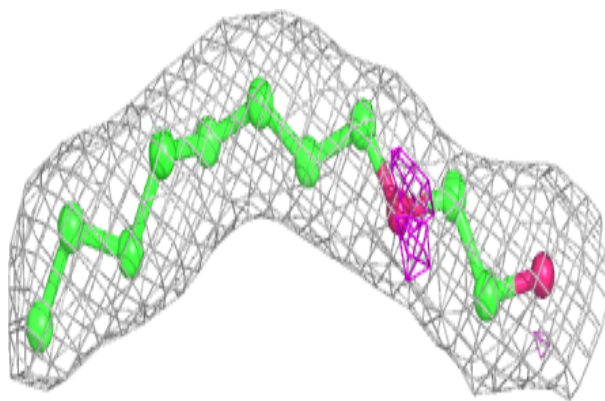
**Electron density around C8E C 405:**

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

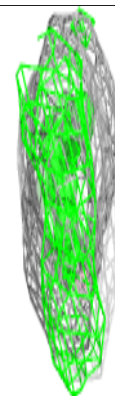
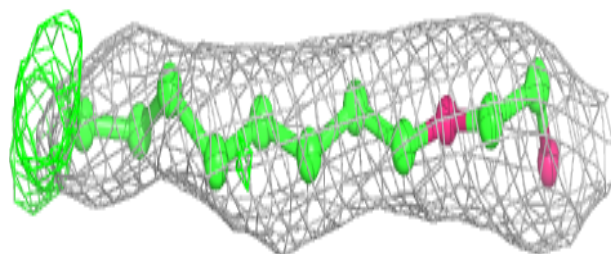
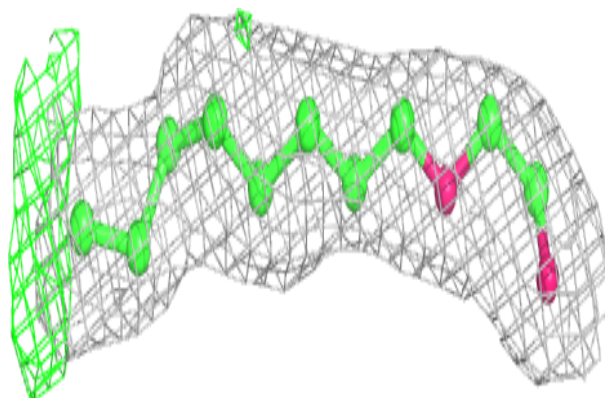


**Electron density around C8E C 402:**

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

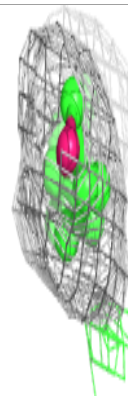
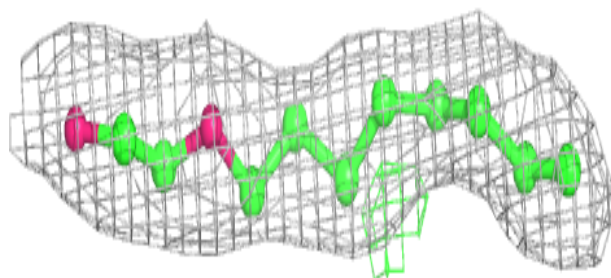
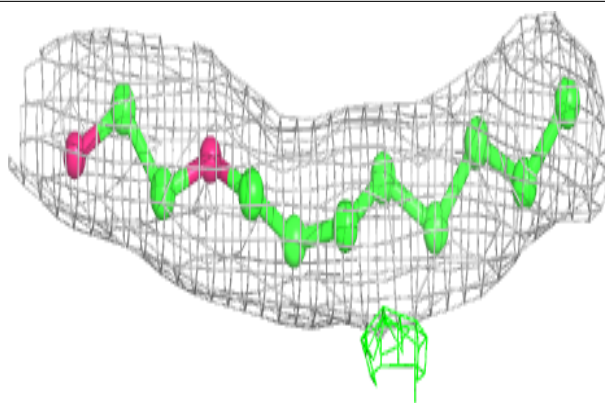
**Electron density around C8E C 407:**

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

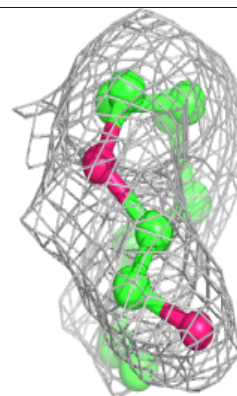
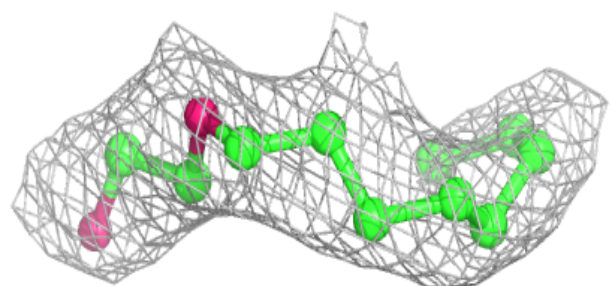
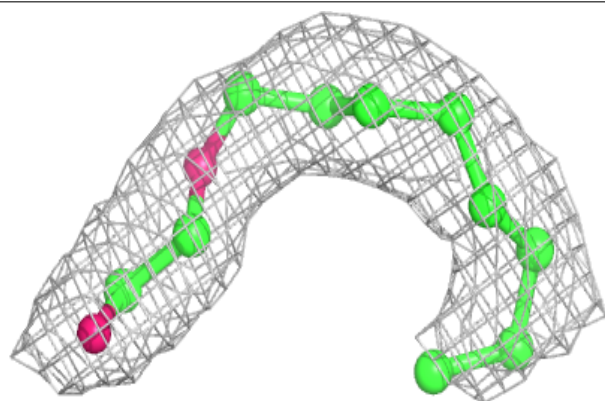


**Electron density around C8E C 403:**

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

**Electron density around C8E D 402:**

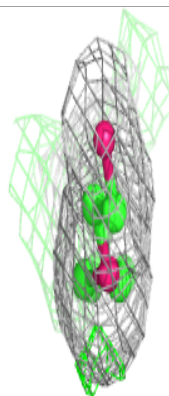
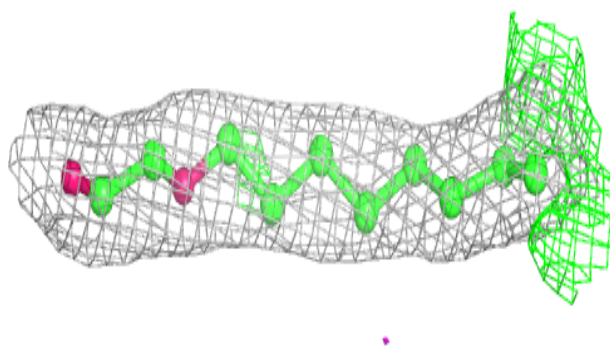
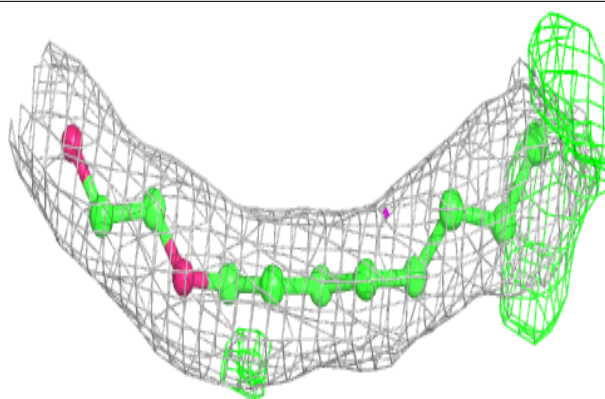
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



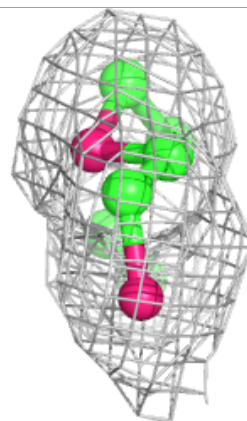
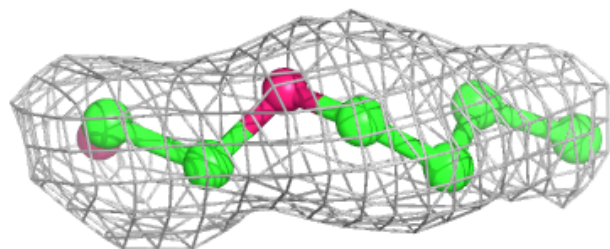
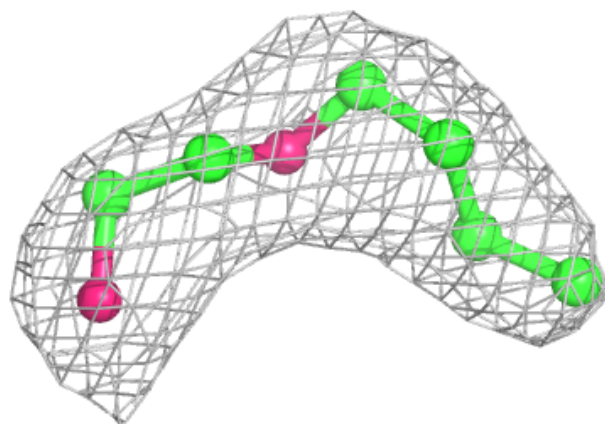


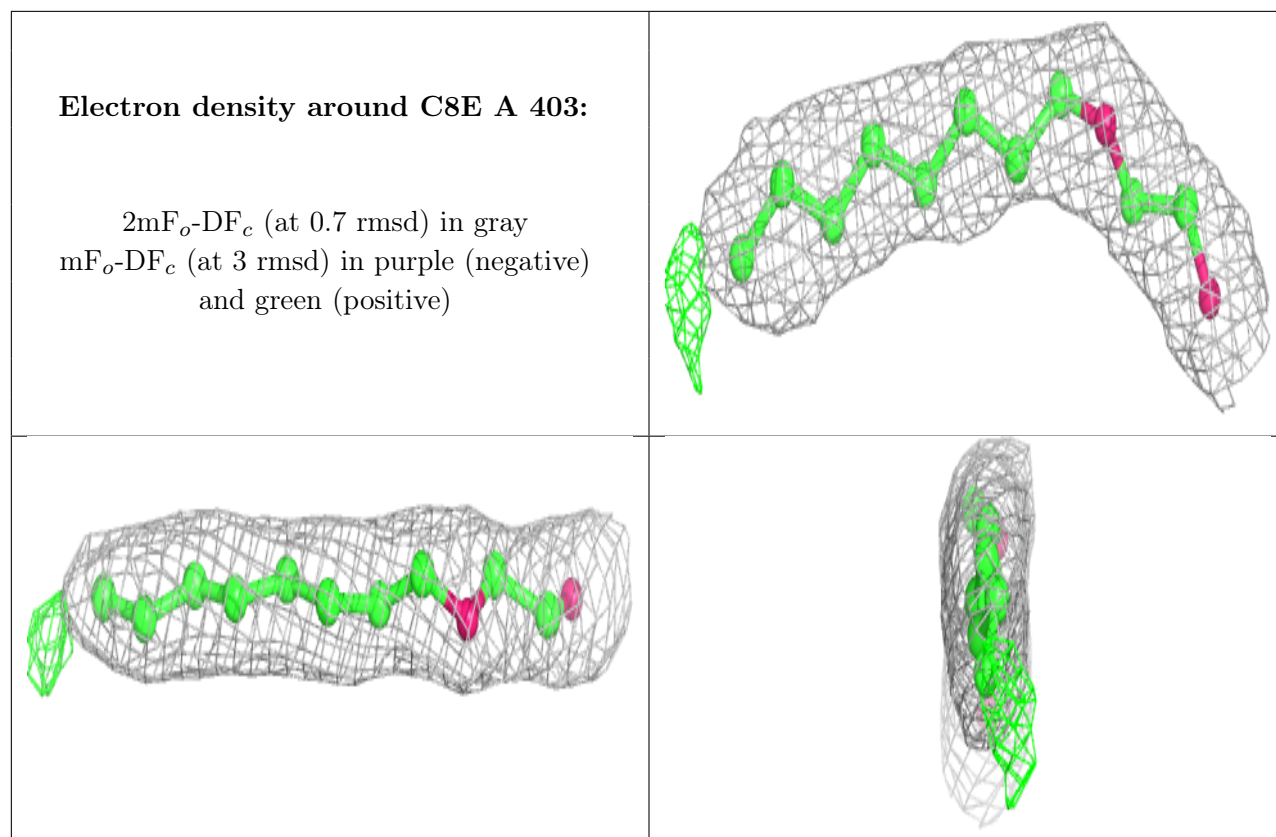
**Electron density around C8E C 401:**

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

**Electron density around C8E E 404:**

$2mF_o-DF_c$  (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.