



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 08:39 AM BST

PDB ID : 1W1X  
Title : Structure of Neuraminidase from English duck subtype N6 complexed with 30 mM sialic acid (NANA, Neu5Ac), crystal soaked for 3 hours at 277 K.  
Authors : Rudino-Pinera, E.; Tunnah, P.; Crennell, S.J.; Webster, R.G.; Laver, W.G.; Garman, E.F.  
Deposited on : 2004-06-24  
Resolution : 2.00 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 : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

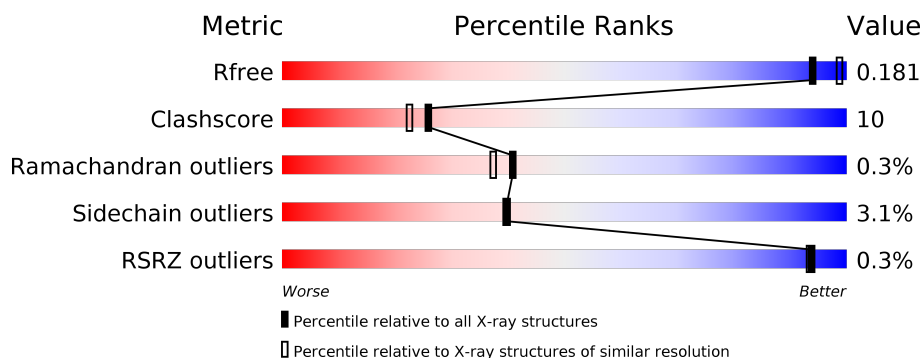
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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.





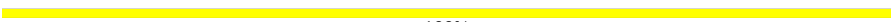
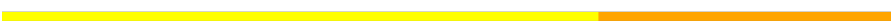
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	389	<div> <div style="width: 84%;"></div> <div style="width: 14%;"></div> <div style="width: 2%;"></div> </div> <div>84% 14% .</div>
1	B	389	<div> <div style="width: 81%;"></div> <div style="width: 17%;"></div> <div style="width: 2%;"></div> </div> <div>81% 17% .</div>
1	C	389	<div> <div style="width: 81%;"></div> <div style="width: 17%;"></div> <div style="width: 2%;"></div> </div> <div>81% 17% .</div>
1	D	389	<div> <div style="width: 83%;"></div> <div style="width: 14%;"></div> <div style="width: 3%;"></div> </div> <div>83% 14% .</div>
2	E	3	<div> <div style="width: 100%;"></div> </div> <div>100%</div>
3	F	2	<div> <div style="width: 100%;"></div> </div> <div>100%</div>

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Mol	Chain	Length	Quality of chain
3	J	2	 100%
4	G	3	 33% 67%
5	H	2	 100%
6	I	3	 67% 33%

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
11	GOL	C	3488	-	X	-	-
11	GOL	D	4483	-	X	-	-
12	PEG	C	3476	-	-	X	-
3	NAG	F	1	-	-	X	-
3	NAG	J	1	-	-	X	-
4	NAG	G	2	-	-	X	-
6	BMA	I	2	-	-	X	-
6	MAN	I	3	-	-	X	-
7	SIA	A	1478	-	-	-	X
7	SIA	C	3478	-	-	-	X

## 2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 14123 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.

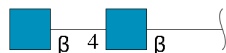
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			3008	1875	535	571	27			
1	B	389	Total	C	N	O	S	0	0	0
			3008	1875	535	571	27			
1	C	389	Total	C	N	O	S	0	0	0
			3008	1875	535	571	27			
1	D	389	Total	C	N	O	S	0	0	0
			3009	1875	535	572	27			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	3	Total	C	O	0	0	0
			33	18	15			

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



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

- 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			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose.



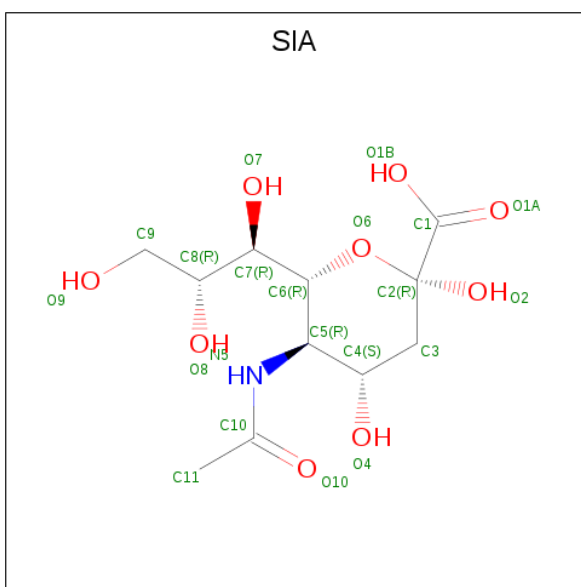
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	H	2	Total	C	O	0	0	0
			22	12	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	3	Total	C	N	O	0	0	0
			36	20	1	15			

- Molecule 7 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: C<sub>11</sub>H<sub>19</sub>NO<sub>9</sub>).

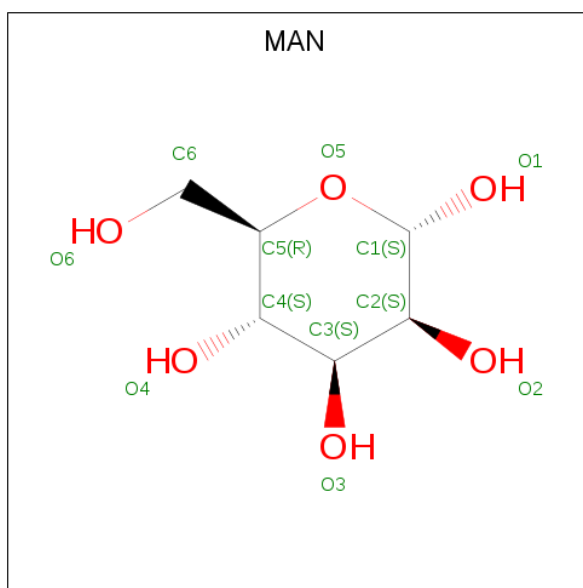


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			21	11	1	9		
7	A	1	Total	C	N	O	0	0
			21	11	1	9		
7	B	1	Total	C	N	O	0	0
			21	11	1	9		
7	B	1	Total	C	N	O	0	0
			21	11	1	9		
7	C	1	Total	C	N	O	0	0
			21	11	1	9		
7	C	1	Total	C	N	O	0	0
			21	11	1	9		
7	D	1	Total	C	N	O	0	0
			21	11	1	9		
7	D	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Ca	0	0
			1	1		
8	A	1	Total	Ca	0	0
			1	1		
8	D	1	Total	Ca	0	0
			1	1		
8	C	1	Total	Ca	0	0
			1	1		

- Molecule 9 is alpha-D-mannopyranose (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



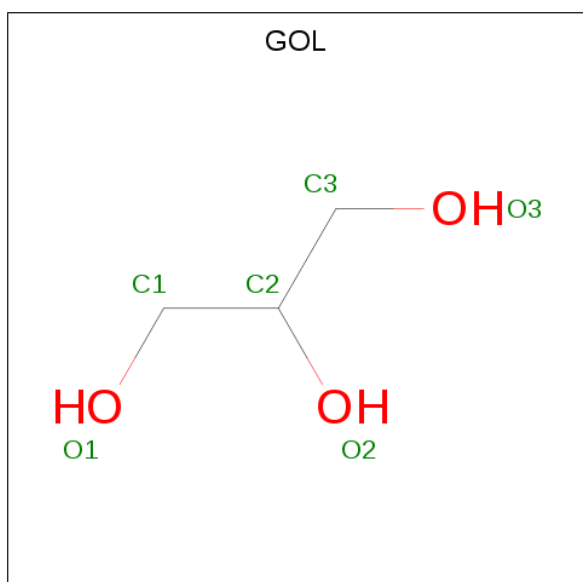
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			11	6	5		
9	B	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

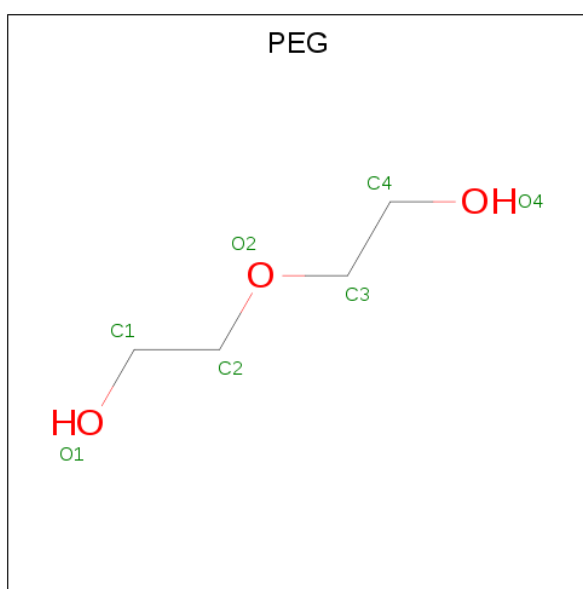
- Molecule 11 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).





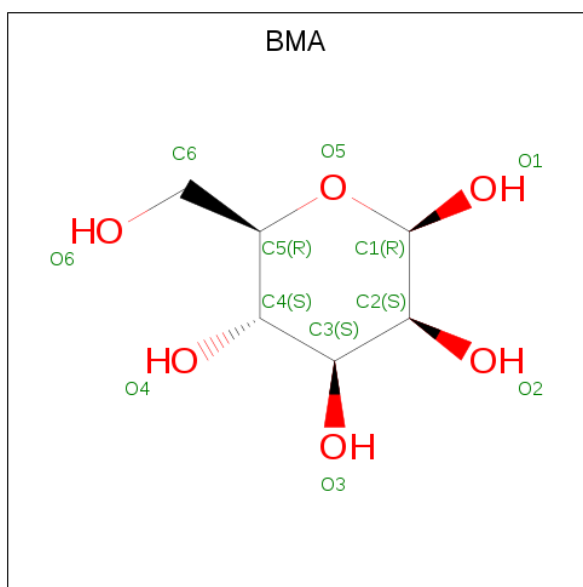
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			6	3	3		
11	B	1	Total	C	O	0	0
			6	3	3		
11	C	1	Total	C	O	0	0
			6	3	3		
11	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 12 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 13 is beta-D-mannopyranose (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	D	1	Total	C	O	0	0
			11	6	5		

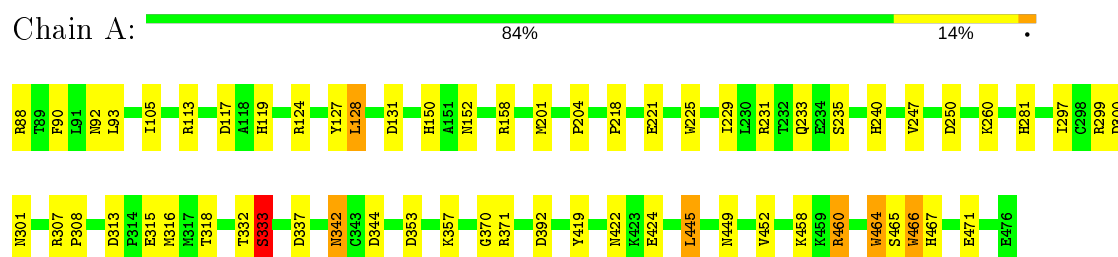
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	397	Total	O	0	0
			397	397		
14	B	385	Total	O	0	0
			385	385		
14	C	375	Total	O	0	0
			375	375		
14	D	408	Total	O	0	0
			408	408		

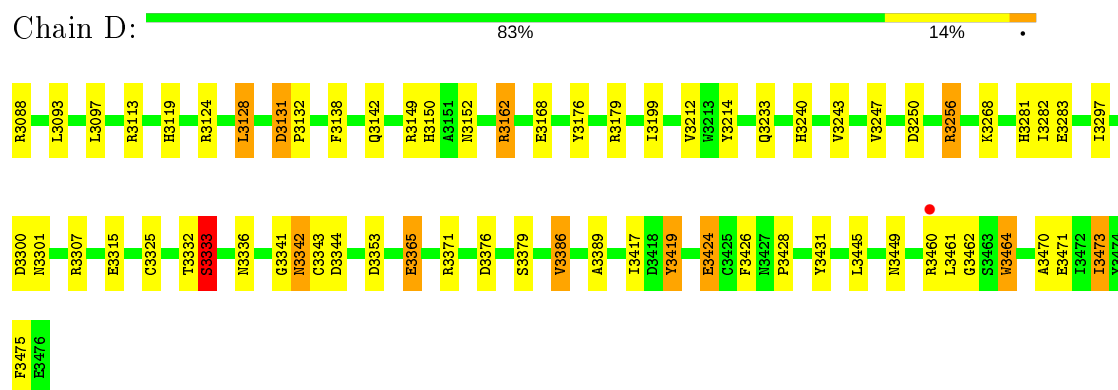
### 3 Residue-property plots

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.

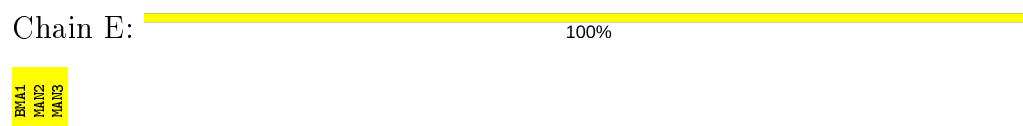
#### • Molecule 1: NEURAMINIDASE



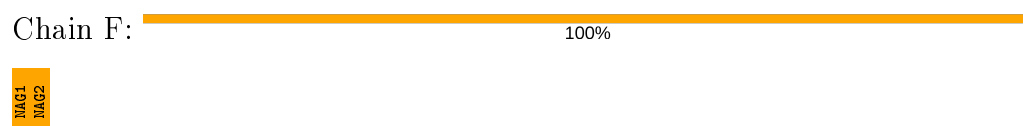
- Molecule 1: NEURAMINIDASE



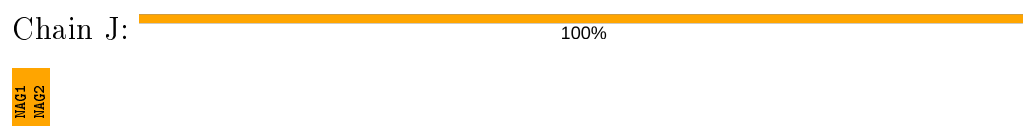
- Molecule 2: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose



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



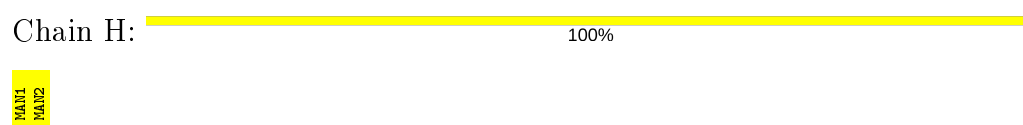
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 5: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose



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

Chain I: 

MAG1  
BMA2  
MAN3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.99Å 73.46Å 107.41Å 90.00° 90.38° 90.00°	Depositor
Resolution (Å)	33.71 – 2.00 33.78 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (33.71-2.00) 99.3 (33.78-2.00)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.70 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.164 , 0.207 0.174 , 0.181	Depositor DCC
$R_{free}$ test set	5604 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.2	Xtriage
Anisotropy	1.507	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 59.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for l,k,-h 0.019 for h,-k,-l 0.017 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14123	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: GOL, BMA, NAG, CA, SIA, PEG, MAN

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	1.30	7/3083 (0.2%)	1.04	14/4185 (0.3%)
1	B	1.31	10/3083 (0.3%)	1.01	14/4185 (0.3%)
1	C	1.28	7/3083 (0.2%)	1.01	8/4185 (0.2%)
1	D	1.28	10/3084 (0.3%)	1.03	15/4185 (0.4%)
All	All	1.29	34/12333 (0.3%)	1.02	51/16740 (0.3%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	3475	PHE	CD1-CE1	7.32	1.53	1.39
1	C	2474	TYR	CE1-CZ	6.49	1.47	1.38
1	D	3268	LYS	CE-NZ	6.49	1.65	1.49
1	D	3176	TYR	CD2-CE2	6.48	1.49	1.39
1	B	1475	PHE	CD2-CE2	6.31	1.51	1.39
1	A	464	TRP	CE3-CZ3	6.26	1.49	1.38
1	B	1286	SER	CB-OG	6.25	1.50	1.42
1	D	3419	TYR	CE1-CZ	6.15	1.46	1.38
1	B	1452	VAL	CB-CG1	6.03	1.65	1.52
1	C	2238	VAL	CB-CG2	6.02	1.65	1.52
1	D	3214	TYR	CE1-CZ	5.88	1.46	1.38
1	B	1180	VAL	CB-CG2	5.84	1.65	1.52
1	B	1416	PHE	CE2-CZ	5.84	1.48	1.37
1	B	1183	ILE	CB-CG2	5.82	1.70	1.52
1	B	1127	TYR	CE1-CZ	5.69	1.46	1.38
1	C	2333	SER	CA-CB	-5.62	1.44	1.52
1	C	2426	PHE	CD1-CE1	5.58	1.50	1.39
1	A	424	GLU	CG-CD	5.51	1.60	1.51
1	D	3365	GLU	CD-OE1	5.46	1.31	1.25
1	B	1127	TYR	CD2-CE2	5.42	1.47	1.39
1	C	2317	MET	SD-CE	5.40	2.08	1.77
1	D	3243	VAL	CB-CG2	5.36	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2139	ALA	CA-CB	5.34	1.63	1.52
1	D	3431	TYR	CE2-CZ	5.33	1.45	1.38
1	A	471	GLU	CD-OE2	5.32	1.31	1.25
1	A	466	TRP	CB-CG	5.30	1.59	1.50
1	B	1176	TYR	CD2-CE2	5.30	1.47	1.39
1	A	90	PHE	CE1-CZ	5.29	1.47	1.37
1	D	3162	ARG	CB-CG	5.26	1.66	1.52
1	A	419	TYR	CD2-CE2	5.24	1.47	1.39
1	A	299	ARG	CZ-NH2	5.23	1.39	1.33
1	C	2475	PHE	CE2-CZ	5.22	1.47	1.37
1	B	1359	PHE	CE1-CZ	5.21	1.47	1.37
1	D	3138	PHE	CD1-CE1	5.09	1.49	1.39

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3250	ASP	CB-CG-OD2	8.72	126.15	118.30
1	B	1117	ASP	CB-CG-OD2	7.89	125.40	118.30
1	C	2313	ASP	CB-CG-OD2	7.86	125.38	118.30
1	B	1337	ASP	CB-CG-OD2	7.72	125.25	118.30
1	A	231	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	A	300	ASP	CB-CG-OD2	7.22	124.80	118.30
1	D	3333	SER	N-CA-C	-7.11	91.81	111.00
1	A	131	ASP	CB-CG-OD2	7.09	124.69	118.30
1	A	128	LEU	CA-CB-CG	7.08	131.59	115.30
1	B	1128	LEU	CA-CB-CG	7.06	131.53	115.30
1	A	392	ASP	CB-CG-OD1	6.96	124.56	118.30
1	C	2128	LEU	CA-CB-CG	6.96	131.29	115.30
1	B	1250	ASP	CB-CG-OD2	6.87	124.48	118.30
1	D	3376	ASP	CB-CG-OD1	6.61	124.25	118.30
1	B	1333	SER	CB-CA-C	6.55	122.54	110.10
1	D	3128	LEU	CA-CB-CG	6.35	129.91	115.30
1	D	3131	ASP	CB-CG-OD2	6.24	123.92	118.30
1	C	2131	ASP	CB-CG-OD2	6.16	123.85	118.30
1	B	1468	ASP	CB-CG-OD2	6.12	123.81	118.30
1	D	3307	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	B	1333	SER	N-CA-C	-6.09	94.56	111.00
1	A	231	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	C	2337	ASP	CB-CG-OD2	6.02	123.72	118.30
1	D	3256	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	C	2250	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	128	LEU	CB-CG-CD2	5.85	120.95	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1344	ASP	CB-CG-OD2	5.82	123.54	118.30
1	D	3473	ILE	CG1-CB-CG2	-5.81	98.62	111.40
1	C	2344	ASP	CB-CG-OD2	5.79	123.51	118.30
1	C	2124	ARG	NE-CZ-NH2	5.79	123.19	120.30
1	D	3371	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	C	2333	SER	N-CA-C	-5.69	95.65	111.00
1	A	250	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	333	SER	N-CA-C	-5.65	95.74	111.00
1	B	1332	THR	O-C-N	5.62	131.70	122.70
1	D	3307	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	A	117	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	313	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	333	SER	CB-CA-C	5.50	120.55	110.10
1	B	1332	THR	CA-C-N	-5.47	105.16	117.20
1	B	1313	ASP	CB-CG-OD2	5.45	123.21	118.30
1	A	337	ASP	CB-CG-OD2	5.42	123.18	118.30
1	D	3300	ASP	CB-CG-OD2	5.37	123.13	118.30
1	B	1128	LEU	CB-CG-CD2	5.32	120.05	111.00
1	D	3333	SER	CB-CA-C	5.31	120.18	110.10
1	B	1332	THR	C-N-CA	5.27	134.87	121.70
1	B	1256	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	158	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	D	3332	THR	C-N-CA	5.03	134.26	121.70
1	D	3149	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	D	3179	ARG	NE-CZ-NH1	5.01	122.81	120.30

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	3008	0	2888	47	0
1	B	3008	0	2888	50	0
1	C	3008	0	2888	65	0
1	D	3009	0	2887	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	33	0	30	8	0
3	F	28	0	25	11	0
3	J	28	0	26	9	0
4	G	39	0	36	11	0
5	H	22	0	20	5	0
6	I	36	0	33	13	0
7	A	42	0	36	4	0
7	B	42	0	36	2	0
7	C	42	0	36	5	0
7	D	42	0	36	3	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	11	0	10	2	0
9	B	11	0	10	2	0
9	C	33	0	30	9	0
10	A	28	0	26	4	0
10	B	14	0	13	2	0
10	C	14	0	13	2	0
10	D	14	0	13	1	0
11	A	6	0	8	2	0
11	B	6	0	8	2	0
11	C	6	0	8	1	0
11	D	6	0	8	2	0
12	C	7	0	10	8	0
13	D	11	0	10	2	0
14	A	397	0	0	2	0
14	B	385	0	0	4	0
14	C	375	0	0	7	0
14	D	408	0	0	10	0
All	All	14123	0	12032	243	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 10.

All (243) 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:92:ASN:HD21	10:A:1484:NAG:C1	1.01	1.62
1:A:152:ASN:HD21	10:A:1485:NAG:C1	1.01	1.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3152:ASN:HD21	10:D:4482:NAG:C1	1.08	1.54
1:B:1152:ASN:HD21	10:B:2484:NAG:C1	1.24	1.49
1:C:2152:ASN:HD21	10:C:3486:NAG:C1	1.27	1.46
1:C:2317:MET:SD	1:C:2317:MET:CE	2.08	1.42
1:B:1207:ASN:ND2	3:F:1:NAG:H2	1.47	1.28
1:B:1207:ASN:HD21	3:F:1:NAG:C2	1.45	1.28
1:C:2207:ASN:HD21	3:J:1:NAG:C1	1.45	1.26
1:C:2152:ASN:ND2	10:C:3486:NAG:C1	2.08	1.14
1:B:1207:ASN:HD21	3:F:1:NAG:C1	1.65	1.08
1:B:1207:ASN:HD21	3:F:1:NAG:H2	0.99	1.02
3:J:1:NAG:HO4	3:J:2:NAG:C1	1.56	1.01
9:C:3483:MAN:C1	6:I:3:MAN:O6	2.09	1.00
4:G:3:BMA:O6	5:H:1:MAN:C1	2.11	0.98
1:B:1207:ASN:ND2	3:F:1:NAG:C2	2.17	0.96
2:E:1:BMA:C1	3:F:2:NAG:O4	2.14	0.94
1:D:3386:VAL:HG22	1:D:3389:ALA:HB2	1.51	0.92
9:A:1483:MAN:C1	2:E:2:MAN:O3	2.18	0.92
13:D:4480:BMA:C1	3:J:2:NAG:O4	2.18	0.91
1:A:218:PRO:HG2	12:C:3476:PEG:H11	1.52	0.91
1:D:3093:LEU:H	1:D:3240:HIS:HD2	1.14	0.90
1:A:221:GLU:OE1	12:C:3476:PEG:H42	1.71	0.90
9:C:3484:MAN:C1	6:I:3:MAN:O3	2.21	0.88
1:C:2093:LEU:H	1:C:2240:HIS:HD2	1.20	0.85
1:A:460:ARG:HD2	14:A:2345:HOH:O	1.77	0.84
1:A:150:HIS:HE1	1:C:2471:GLU:H	1.21	0.84
1:B:1471:GLU:H	1:D:3150:HIS:HE1	1.23	0.83
1:B:1093:LEU:H	1:B:1240:HIS:HD2	1.23	0.82
4:G:2:NAG:HO4	4:G:3:BMA:C1	1.88	0.82
9:C:3481:MAN:C1	6:I:2:BMA:H3	2.11	0.81
1:B:1405:ASN:C	1:B:1405:ASN:HD22	1.82	0.81
1:C:2150:HIS:HE1	1:D:3471:GLU:H	1.29	0.81
4:G:1:NAG:HO4	4:G:2:NAG:C1	1.92	0.80
1:D:3088:ARG:N	14:D:2033:HOH:O	2.14	0.80
1:A:93:LEU:H	1:A:240:HIS:HD2	1.30	0.80
9:C:3484:MAN:C1	6:I:3:MAN:C3	2.60	0.80
1:B:1207:ASN:ND2	3:F:1:NAG:C1	2.43	0.78
1:D:3233:GLN:HE21	1:D:3247:VAL:H	1.28	0.78
1:A:233:GLN:HE21	1:A:247:VAL:H	1.30	0.77
1:D:3333:SER:HB2	1:D:3353:ASP:O	1.87	0.73
1:C:2233:GLN:HE21	1:C:2247:VAL:H	1.36	0.73
3:J:1:NAG:C4	3:J:2:NAG:C1	2.67	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1233:GLN:HE21	1:B:1247:VAL:H	1.38	0.72
1:C:2093:LEU:H	1:C:2240:HIS:CD2	2.06	0.71
1:B:1333:SER:HB3	1:B:1353:ASP:O	1.91	0.71
4:G:2:NAG:C4	4:G:3:BMA:C1	2.69	0.70
6:I:2:BMA:HO6	6:I:3:MAN:C1	1.99	0.69
1:D:3461:LEU:O	3:J:1:NAG:H62	1.93	0.69
1:C:2207:ASN:HD21	3:J:1:NAG:C2	2.05	0.69
9:B:2483:MAN:C1	5:H:1:MAN:O3	2.40	0.68
2:E:2:MAN:HO6	2:E:3:MAN:C1	2.03	0.68
4:G:1:NAG:C4	4:G:2:NAG:C1	2.71	0.67
1:A:218:PRO:CG	12:C:3476:PEG:H11	2.24	0.67
1:D:3093:LEU:H	1:D:3240:HIS:CD2	2.06	0.67
1:D:3283:GLU:OE1	14:D:2216:HOH:O	2.13	0.67
1:B:1342:ASN:HD22	1:B:1344:ASP:H	1.42	0.66
2:E:1:BMA:C1	3:F:2:NAG:HO4	2.08	0.66
1:A:458:LYS:HE2	14:A:2012:HOH:O	1.94	0.66
9:C:3481:MAN:C1	6:I:2:BMA:C3	2.75	0.65
9:A:1483:MAN:C1	2:E:2:MAN:C3	2.74	0.65
11:A:1487:GOL:H32	1:C:2113:ARG:NH2	2.12	0.65
1:C:2207:ASN:CG	3:J:1:NAG:C1	2.65	0.65
2:E:1:BMA:C1	3:F:2:NAG:C4	2.75	0.65
1:B:1342:ASN:ND2	1:B:1344:ASP:H	1.93	0.65
1:C:2131:ASP:HB2	1:C:2132:PRO:HD2	1.77	0.65
1:B:1333:SER:CB	1:B:1353:ASP:O	2.45	0.64
11:A:1487:GOL:H32	1:C:2113:ARG:HH22	1.62	0.64
1:B:1131:ASP:HB2	1:B:1132:PRO:CD	2.26	0.64
1:C:2102:SER:HB2	1:C:2459:LYS:O	1.99	0.63
1:D:3097:LEU:HD22	1:D:3428:PRO:HG3	1.81	0.62
1:C:2465:SER:OG	1:C:2467:HIS:HD2	1.81	0.62
1:B:1093:LEU:H	1:B:1240:HIS:CD2	2.12	0.62
1:C:2473:ILE:HG12	14:C:3346:HOH:O	1.98	0.62
1:B:1473:ILE:HG22	14:B:2356:HOH:O	1.99	0.61
1:C:2283:GLU:HG3	14:C:3186:HOH:O	1.99	0.61
13:D:4480:BMA:C1	3:J:2:NAG:C4	2.79	0.60
1:C:2131:ASP:HB2	1:C:2132:PRO:CD	2.31	0.60
1:D:3342:ASN:HD22	1:D:3342:ASN:C	2.05	0.60
1:A:124:ARG:HA	1:A:449:ASN:ND2	2.15	0.60
1:A:342:ASN:HD22	1:A:344:ASP:H	1.48	0.59
1:D:3471:GLU:HG3	1:D:3473:ILE:HG22	1.83	0.59
9:C:3484:MAN:C1	6:I:3:MAN:H3	2.31	0.59
1:A:150:HIS:CE1	1:C:2471:GLU:H	2.12	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2150:HIS:CE1	1:D:3471:GLU:H	2.15	0.59
1:A:221:GLU:OE1	12:C:3476:PEG:C4	2.49	0.58
6:I:1:NAG:HO4	6:I:2:BMA:C1	2.14	0.58
1:B:1247:VAL:HG22	1:B:1261:ILE:HD12	1.84	0.58
2:E:1:BMA:C6	2:E:2:MAN:C1	2.81	0.58
1:B:1423:LYS:HE2	14:D:2162:HOH:O	2.03	0.58
1:D:3281:HIS:HD2	1:D:3301:ASN:H	1.51	0.58
1:A:333:SER:HB2	1:A:353:ASP:O	2.04	0.57
1:C:2092:ASN:ND2	14:C:3017:HOH:O	2.38	0.57
1:B:1156:HIS:HB2	14:B:2067:HOH:O	2.04	0.57
1:C:2455:CYS:HB3	12:C:3476:PEG:H22	1.86	0.56
7:D:4478:SIA:O1A	7:D:4478:SIA:H6	2.05	0.56
1:A:113:ARG:NH2	11:B:2486:GOL:H32	2.20	0.56
1:C:2204:PRO:HD3	1:D:3464:TRP:HB3	1.87	0.56
7:C:3477:SIA:O2	7:C:3477:SIA:H5	2.05	0.56
1:B:1207:ASN:HD22	3:F:1:NAG:H2	1.61	0.56
1:B:1461:LEU:O	4:G:1:NAG:H62	2.05	0.56
7:D:4477:SIA:O2	7:D:4477:SIA:H5	2.05	0.55
1:A:235:SER:HB3	1:A:357:LYS:HE2	1.89	0.55
1:A:465:SER:OG	1:A:467:HIS:HD2	1.90	0.55
1:C:2150:HIS:HE1	1:D:3471:GLU:N	2.02	0.54
1:C:2233:GLN:NE2	1:C:2247:VAL:H	2.02	0.54
1:C:2281:HIS:HD2	1:C:2301:ASN:H	1.53	0.54
1:D:3424:GLU:CD	1:D:3424:GLU:H	2.11	0.54
1:B:1088:ARG:NH1	1:B:1088:ARG:HB2	2.23	0.54
1:C:2115:GLY:HA2	1:C:2120:ILE:CG1	2.38	0.54
1:C:2399:SER:CA	6:I:2:BMA:H62	2.38	0.54
1:C:2150:HIS:CE1	1:D:3470:ALA:HA	2.44	0.53
1:C:2283:GLU:CG	14:C:3186:HOH:O	2.57	0.53
1:A:233:GLN:NE2	1:A:247:VAL:H	2.05	0.52
1:C:2333:SER:HB3	1:C:2353:ASP:O	2.09	0.52
1:A:445:LEU:HD21	10:A:1485:NAG:H82	1.91	0.52
1:B:1119:HIS:CE1	1:D:3119:HIS:CE1	2.97	0.52
1:D:3168:GLU:OE1	14:D:2118:HOH:O	2.19	0.52
1:D:3142:GLN:NE2	1:D:3162:ARG:CZ	2.73	0.51
1:B:1113:ARG:HH22	11:D:4483:GOL:H32	1.75	0.51
1:B:1127:TYR:CG	1:B:1235:SER:HA	2.45	0.51
1:D:3233:GLN:NE2	1:D:3247:VAL:H	2.01	0.51
1:D:3124:ARG:HA	1:D:3449:ASN:ND2	2.26	0.51
1:C:2333:SER:CB	1:C:2353:ASP:O	2.59	0.51
1:A:467:HIS:CD2	1:A:467:HIS:H	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:2:NAG:O4	4:G:3:BMA:O5	2.11	0.51
1:A:150:HIS:HE1	1:C:2471:GLU:N	1.99	0.51
1:D:3471:GLU:CG	1:D:3473:ILE:HG22	2.41	0.51
1:D:3283:GLU:CG	14:D:2216:HOH:O	2.59	0.51
1:D:3333:SER:CB	1:D:3353:ASP:O	2.55	0.51
1:B:1131:ASP:HB2	1:B:1132:PRO:HD3	1.92	0.50
1:D:3131:ASP:HB2	1:D:3132:PRO:CD	2.41	0.50
1:C:2240:HIS:HE1	1:C:2315:GLU:OE1	1.95	0.50
1:B:1462:GLY:HA2	4:G:1:NAG:O5	2.11	0.50
1:C:2334:ARG:CZ	1:C:2371:ARG:HD2	2.41	0.50
1:B:1113:ARG:NH2	11:D:4483:GOL:H32	2.26	0.50
1:C:2297:ILE:HD12	1:C:2297:ILE:N	2.26	0.50
1:B:1281:HIS:HD2	1:B:1301:ASN:H	1.59	0.50
7:D:4477:SIA:O2	7:D:4477:SIA:C5	2.59	0.49
1:A:119:HIS:CE1	1:C:2119:HIS:CE1	2.99	0.49
1:A:281:HIS:HD2	1:A:301:ASN:H	1.61	0.49
1:A:342:ASN:ND2	1:A:344:ASP:H	2.09	0.49
1:C:2158:ARG:HB3	1:C:2185:TRP:CD1	2.48	0.49
7:C:3477:SIA:O2	7:C:3477:SIA:C5	2.59	0.49
1:A:229:ILE:O	1:A:229:ILE:HG22	2.12	0.49
6:I:1:NAG:C4	6:I:2:BMA:C1	2.89	0.49
1:C:2424:GLU:CD	1:C:2424:GLU:H	2.17	0.48
5:H:1:MAN:C6	5:H:2:MAN:C1	2.87	0.48
1:B:1297:ILE:HD12	1:B:1297:ILE:N	2.29	0.48
1:C:2088:ARG:N	14:C:3012:HOH:O	2.46	0.48
1:C:2332:THR:O	1:C:2333:SER:HB2	2.13	0.48
1:D:3426:PHE:O	1:D:3428:PRO:HD3	2.14	0.48
1:A:93:LEU:H	1:A:240:HIS:CD2	2.21	0.48
1:A:119:HIS:HE1	1:C:2119:HIS:CE1	2.32	0.48
11:C:3488:GOL:H32	1:D:3113:ARG:NH2	2.29	0.47
1:A:240:HIS:HE1	1:A:315:GLU:OE2	1.96	0.47
7:B:2477:SIA:O2	7:B:2477:SIA:H5	2.14	0.47
2:E:1:BMA:C1	3:F:2:NAG:H4	2.45	0.47
1:D:3131:ASP:HB2	1:D:3132:PRO:HD2	1.95	0.47
9:C:3483:MAN:C1	6:I:3:MAN:HO6	2.25	0.47
1:D:3281:HIS:CD2	1:D:3301:ASN:H	2.30	0.47
1:B:1195:SER:HB2	1:B:1214:TYR:CZ	2.50	0.47
1:B:1445:LEU:CD1	10:B:2484:NAG:H82	2.45	0.47
9:C:3481:MAN:C1	6:I:2:BMA:O3	2.63	0.47
1:B:1460:ARG:NH2	14:B:2345:HOH:O	2.47	0.47
9:C:3481:MAN:H5	6:I:2:BMA:H2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1233:GLN:NE2	1:B:1247:VAL:H	2.11	0.46
4:G:1:NAG:O4	4:G:2:NAG:H83	2.15	0.46
1:D:3199:ILE:HG12	1:D:3212:VAL:HG13	1.96	0.46
7:A:1477:SIA:H5	7:A:1477:SIA:O2	2.15	0.46
1:A:333:SER:CB	1:A:353:ASP:O	2.63	0.46
1:D:3336:ASN:ND2	14:D:2259:HOH:O	2.39	0.46
1:B:1405:ASN:C	1:B:1405:ASN:ND2	2.58	0.46
1:C:2204:PRO:HG2	1:C:2207:ASN:HB2	1.96	0.46
12:C:3476:PEG:H12	14:C:3355:HOH:O	2.14	0.46
7:A:1477:SIA:O7	7:A:1477:SIA:O2	2.34	0.46
1:B:1336:ASN:OD1	1:B:1375:LYS:HE3	2.16	0.45
1:C:2374:SER:HB2	7:C:3478:SIA:O1B	2.17	0.45
1:D:3283:GLU:HG3	14:D:2216:HOH:O	2.16	0.45
1:A:113:ARG:HH22	11:B:2486:GOL:H32	1.79	0.45
5:H:1:MAN:O6	5:H:2:MAN:C2	2.59	0.45
1:A:127:TYR:CG	1:A:235:SER:HA	2.51	0.45
1:C:2235:SER:HB3	1:C:2357:LYS:HE2	1.98	0.45
1:C:2333:SER:HB2	1:C:2353:ASP:HB2	1.97	0.45
1:C:2127:TYR:CG	1:C:2235:SER:HA	2.52	0.45
1:C:2467:HIS:H	1:C:2467:HIS:CD2	2.34	0.45
1:A:307:ARG:HA	1:A:308:PRO:HD3	1.84	0.45
7:A:1478:SIA:H6	7:A:1478:SIA:O1A	2.16	0.45
1:C:2340:ASN:ND2	1:C:2394:GLN:HG2	2.31	0.45
1:C:2115:GLY:HA2	1:C:2120:ILE:HG12	1.99	0.45
1:A:316:MET:HE2	1:A:318:THR:OG1	2.16	0.44
1:C:2332:THR:CG2	1:C:2333:SER:N	2.80	0.44
7:A:1477:SIA:C5	7:A:1477:SIA:O2	2.64	0.44
1:A:218:PRO:HG2	12:C:3476:PEG:C1	2.35	0.44
1:D:3297:ILE:HD12	1:D:3297:ILE:N	2.33	0.44
1:A:225:TRP:CD2	1:A:260:LYS:HE2	2.54	0.43
4:G:2:NAG:H4	4:G:3:BMA:C1	2.47	0.43
1:B:1138:PHE:O	1:B:1139:ALA:HB2	2.17	0.43
1:B:1339:THR:C	1:B:1340:ASN:HD22	2.21	0.43
1:B:1334:ARG:CZ	1:B:1371:ARG:HD2	2.47	0.43
4:G:1:NAG:H4	4:G:2:NAG:C1	2.48	0.43
1:C:2130:CYS:HA	1:C:2135:CYS:HA	2.01	0.43
1:B:1393:ILE:HG12	14:B:2289:HOH:O	2.19	0.42
1:D:3342:ASN:HD22	1:D:3343:CYS:N	2.16	0.42
9:B:2483:MAN:C1	5:H:1:MAN:C3	2.98	0.42
1:B:1124:ARG:HA	1:B:1449:ASN:ND2	2.34	0.42
1:D:3168:GLU:HG3	14:D:2084:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3283:GLU:CD	14:D:2216:HOH:O	2.56	0.42
1:C:2296:CYS:C	1:C:2297:ILE:HD12	2.39	0.42
1:A:452:VAL:HG21	1:A:466:TRP:CB	2.49	0.42
1:B:1465:SER:OG	1:B:1467:HIS:HD2	2.02	0.42
1:B:1240:HIS:HE1	1:B:1315:GLU:OE2	2.02	0.42
1:C:2137:MET:HG3	1:C:2169:MET:HA	2.02	0.42
1:C:2325:CYS:O	1:C:2393:ILE:HA	2.19	0.42
7:C:3478:SIA:H6	7:C:3478:SIA:O1A	2.19	0.42
1:C:2324:LEU:HD21	1:C:2362:LEU:HD21	2.02	0.42
1:A:92:ASN:ND2	10:A:1484:NAG:C2	2.72	0.42
1:B:1138:PHE:CE2	1:B:1166:SER:HB3	2.55	0.42
7:B:2477:SIA:O2	7:B:2477:SIA:C5	2.64	0.41
1:C:2406:ASN:O	7:C:3478:SIA:O4	2.27	0.41
1:C:2427:ASN:OD1	12:C:3476:PEG:C2	2.68	0.41
1:D:3325:CYS:O	1:D:3341:GLY:HA3	2.20	0.41
1:A:124:ARG:HA	1:A:449:ASN:HD22	1.81	0.41
1:D:3240:HIS:HE1	1:D:3315:GLU:OE1	2.03	0.41
1:A:119:HIS:HE1	1:C:2119:HIS:HE1	1.66	0.41
1:D:3462:GLY:HA2	3:J:1:NAG:O5	2.20	0.41
1:C:2150:HIS:HD2	14:D:2068:HOH:O	2.04	0.41
1:D:3417:ILE:HB	1:D:3419:TYR:CZ	2.56	0.41
1:B:1263:TYR:CE2	1:B:1317:MET:HA	2.56	0.41
1:C:2427:ASN:HA	1:C:2428:PRO:HD3	1.97	0.41
1:D:3282:ILE:C	1:D:3283:GLU:HG2	2.40	0.41
1:B:1417:ILE:HB	1:B:1419:TYR:CZ	2.56	0.41
1:A:452:VAL:HG21	1:A:466:TRP:HB3	2.01	0.41
1:B:1131:ASP:CB	1:B:1132:PRO:CD	2.97	0.41
1:B:1359:PHE:HE1	1:B:1381:TYR:HH	1.65	0.41
1:A:105:ILE:HD13	1:A:466:TRP:CE2	2.56	0.41
1:A:150:HIS:CE1	1:C:2470:ALA:HA	2.56	0.41
1:A:297:ILE:N	1:A:297:ILE:HD12	2.36	0.40
1:C:2156:HIS:CE1	14:C:3088:HOH:O	2.74	0.40
1:A:332:THR:O	1:A:333:SER:HB2	2.21	0.40
1:A:370:GLY:O	1:A:371:ARG:HB3	2.21	0.40
1:D:3342:ASN:ND2	1:D:3344:ASP:H	2.19	0.40
1:A:204:PRO:HD3	1:C:2464:TRP:HB3	2.03	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	387/389 (100%)	370 (96%)	16 (4%)	1 (0%)	41	37
1	B	387/389 (100%)	367 (95%)	19 (5%)	1 (0%)	41	37
1	C	387/389 (100%)	368 (95%)	18 (5%)	1 (0%)	41	37
1	D	387/389 (100%)	371 (96%)	15 (4%)	1 (0%)	41	37
All	All	1548/1556 (100%)	1476 (95%)	68 (4%)	4 (0%)	41	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	2333	SER
1	A	333	SER
1	B	1333	SER
1	D	3333	SER

### 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	331/331 (100%)	322 (97%)	9 (3%)	44	46
1	B	331/331 (100%)	320 (97%)	11 (3%)	38	37
1	C	331/331 (100%)	320 (97%)	11 (3%)	38	37
1	D	331/331 (100%)	321 (97%)	10 (3%)	41	41
All	All	1324/1324 (100%)	1283 (97%)	41 (3%)	40	40

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	ARG
1	A	128	LEU
1	A	201	MET
1	A	333	SER
1	A	342	ASN
1	A	422	ASN
1	A	445	LEU
1	A	460	ARG
1	A	464	TRP
1	B	1088	ARG
1	B	1089	THR
1	B	1128	LEU
1	B	1142	GLN
1	B	1147	ARG
1	B	1283	GLU
1	B	1333	SER
1	B	1342	ASN
1	B	1400	ASN
1	B	1405	ASN
1	B	1464	TRP
1	C	2102	SER
1	C	2128	LEU
1	C	2156	HIS
1	C	2182	CYS
1	C	2201	MET
1	C	2256	ARG
1	C	2333	SER
1	C	2423	LYS
1	C	2424	GLU
1	C	2445	LEU
1	C	2464	TRP
1	D	3128	LEU
1	D	3256	ARG
1	D	3342	ASN
1	D	3365	GLU
1	D	3379	SER
1	D	3386	VAL
1	D	3424	GLU
1	D	3445	LEU
1	D	3460	ARG
1	D	3464	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	119	HIS
1	A	150	HIS
1	A	152	ASN
1	A	233	GLN
1	A	240	HIS
1	A	281	HIS
1	A	340	ASN
1	A	342	ASN
1	A	400	ASN
1	A	406	ASN
1	A	408	ASN
1	A	422	ASN
1	A	427	ASN
1	A	449	ASN
1	A	467	HIS
1	B	1119	HIS
1	B	1142	GLN
1	B	1152	ASN
1	B	1207	ASN
1	B	1233	GLN
1	B	1240	HIS
1	B	1281	HIS
1	B	1340	ASN
1	B	1342	ASN
1	B	1400	ASN
1	B	1405	ASN
1	B	1406	ASN
1	B	1408	ASN
1	B	1427	ASN
1	B	1449	ASN
1	B	1467	HIS
1	C	2119	HIS
1	C	2150	HIS
1	C	2152	ASN
1	C	2207	ASN
1	C	2233	GLN
1	C	2240	HIS
1	C	2281	HIS
1	C	2340	ASN
1	C	2406	ASN

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Mol	Chain	Res	Type
1	C	2408	ASN
1	C	2422	ASN
1	C	2449	ASN
1	C	2467	HIS
1	D	3119	HIS
1	D	3150	HIS
1	D	3152	ASN
1	D	3233	GLN
1	D	3240	HIS
1	D	3281	HIS
1	D	3340	ASN
1	D	3342	ASN
1	D	3406	ASN
1	D	3427	ASN
1	D	3449	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](#)

15 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	BMA	E	1	2	11,11,12	0.26	0	15,15,17	0.64	0
2	MAN	E	2	2	11,11,12	0.26	0	15,15,17	0.65	0
2	MAN	E	3	2	11,11,12	0.27	0	15,15,17	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	F	1	3	14,14,15	0.27	0	17,19,21	1.01	1 (5%)
3	NAG	F	2	3	14,14,15	0.26	0	17,19,21	1.01	1 (5%)
4	NAG	G	1	1,4	14,14,15	0.26	0	17,19,21	1.01	1 (5%)
4	NAG	G	2	4	14,14,15	0.26	0	17,19,21	1.01	1 (5%)
4	BMA	G	3	4	11,11,12	0.27	0	15,15,17	0.64	0
5	MAN	H	1	5	11,11,12	0.25	0	15,15,17	0.64	0
5	MAN	H	2	5	11,11,12	0.26	0	15,15,17	0.64	0
6	NAG	I	1	6	14,14,15	0.26	0	17,19,21	1.01	1 (5%)
6	BMA	I	2	6	11,11,12	0.26	0	15,15,17	0.64	0
6	MAN	I	3	6	11,11,12	0.26	0	15,15,17	0.64	0
3	NAG	J	1	1,3	14,14,15	0.27	0	17,19,21	1.02	1 (5%)
3	NAG	J	2	3	14,14,15	0.26	0	17,19,21	1.01	1 (5%)

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	BMA	E	1	2	-	2/2/19/22	0/1/1/1
2	MAN	E	2	2	-	0/2/19/22	0/1/1/1
2	MAN	E	3	2	-	2/2/19/22	0/1/1/1
3	NAG	F	1	3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	1/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	4/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
5	MAN	H	1	5	-	0/2/19/22	0/1/1/1
5	MAN	H	2	5	-	1/2/19/22	0/1/1/1
6	NAG	I	1	6	-	2/6/23/26	0/1/1/1
6	BMA	I	2	6	-	0/2/19/22	0/1/1/1
6	MAN	I	3	6	-	2/2/19/22	0/1/1/1
3	NAG	J	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	J	1	NAG	C1-C2-N2	-3.23	104.97	110.49
3	J	2	NAG	C1-C2-N2	-3.22	104.99	110.49
6	I	1	NAG	C1-C2-N2	-3.21	105.01	110.49
4	G	1	NAG	C1-C2-N2	-3.21	105.01	110.49
3	F	1	NAG	C1-C2-N2	-3.21	105.01	110.49
4	G	2	NAG	C1-C2-N2	-3.20	105.02	110.49
3	F	2	NAG	C1-C2-N2	-3.20	105.02	110.49

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	3	MAN	O5-C5-C6-O6
6	I	1	NAG	C4-C5-C6-O6
2	E	3	MAN	C4-C5-C6-O6
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
6	I	1	NAG	O5-C5-C6-O6
6	I	3	MAN	O5-C5-C6-O6
6	I	3	MAN	C4-C5-C6-O6
2	E	1	BMA	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
2	E	1	BMA	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
5	H	2	MAN	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6

There are no ring outliers.

15 monomers are involved in 52 short contacts:

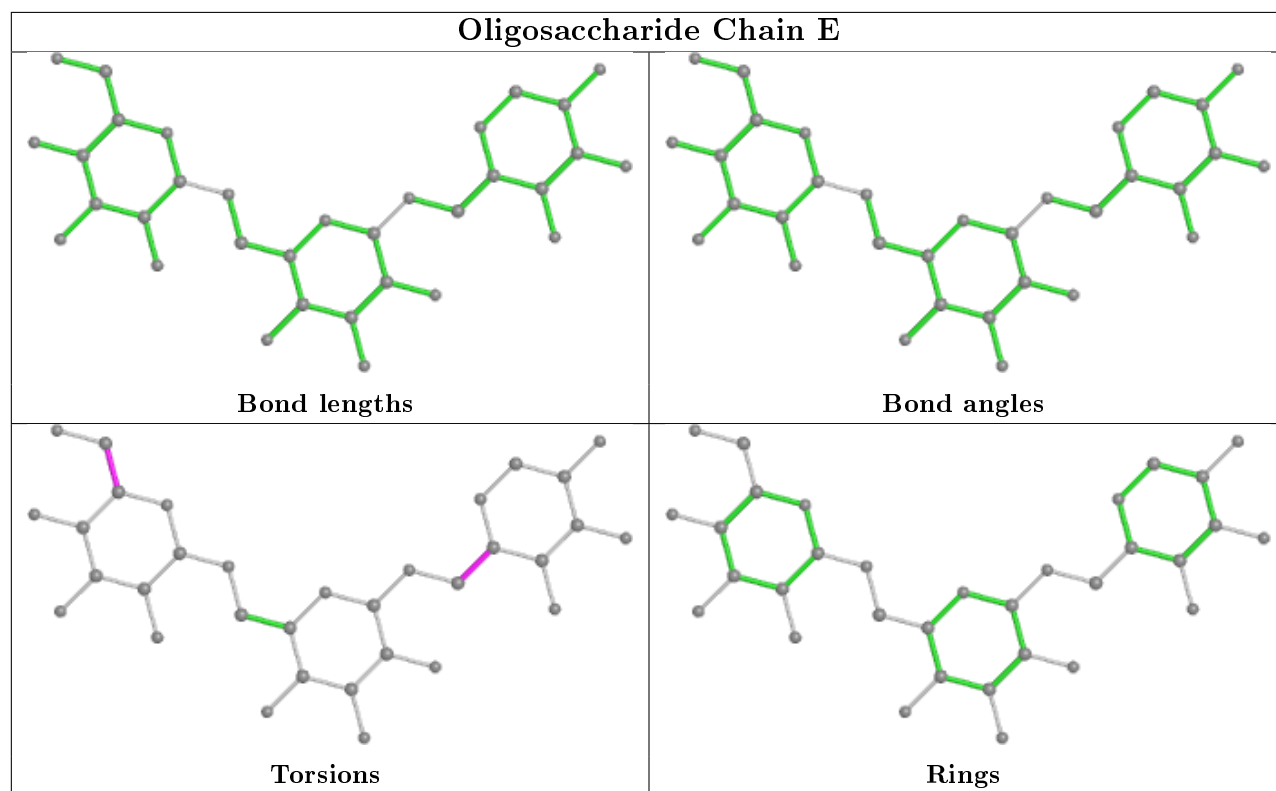
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	2	NAG	4	0
6	I	3	MAN	6	0
4	G	1	NAG	6	0
2	E	2	MAN	4	0
3	F	1	NAG	7	0
5	H	2	MAN	2	0
3	F	2	NAG	4	0
2	E	1	BMA	5	0
6	I	2	BMA	8	0

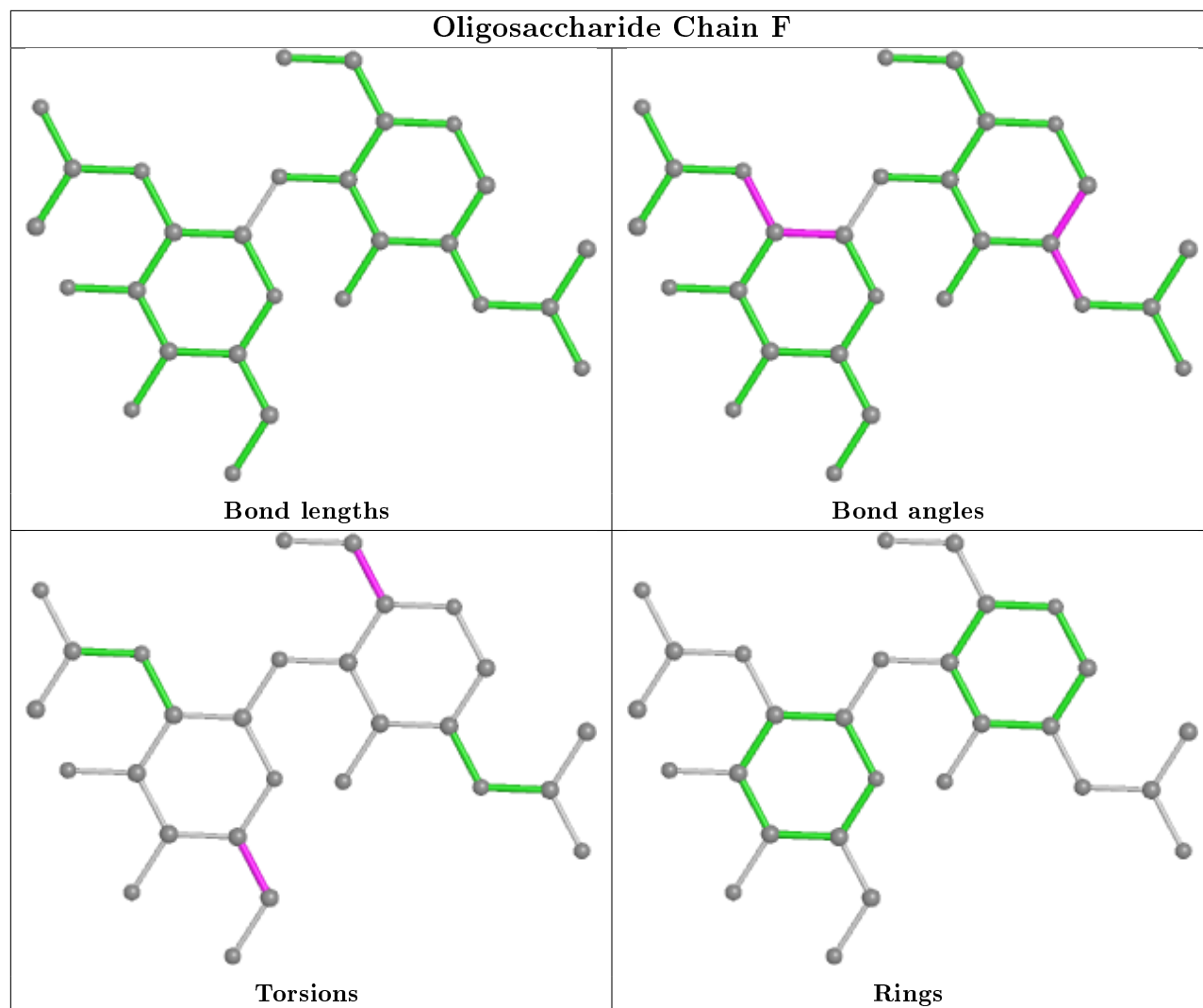
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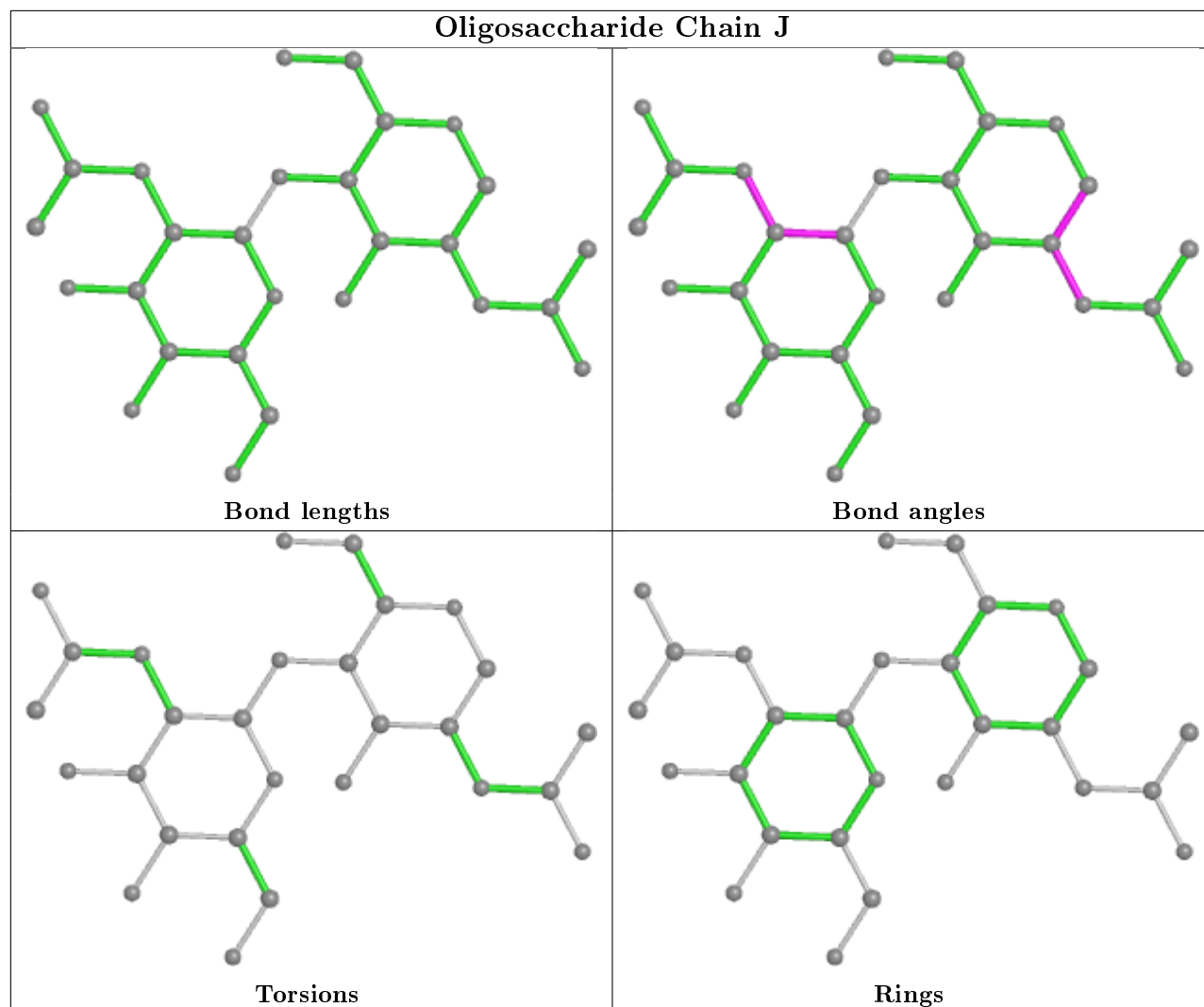
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	2	NAG	8	0
6	I	1	NAG	2	0
3	J	1	NAG	7	0
2	E	3	MAN	1	0
5	H	1	MAN	5	0
4	G	3	BMA	5	0

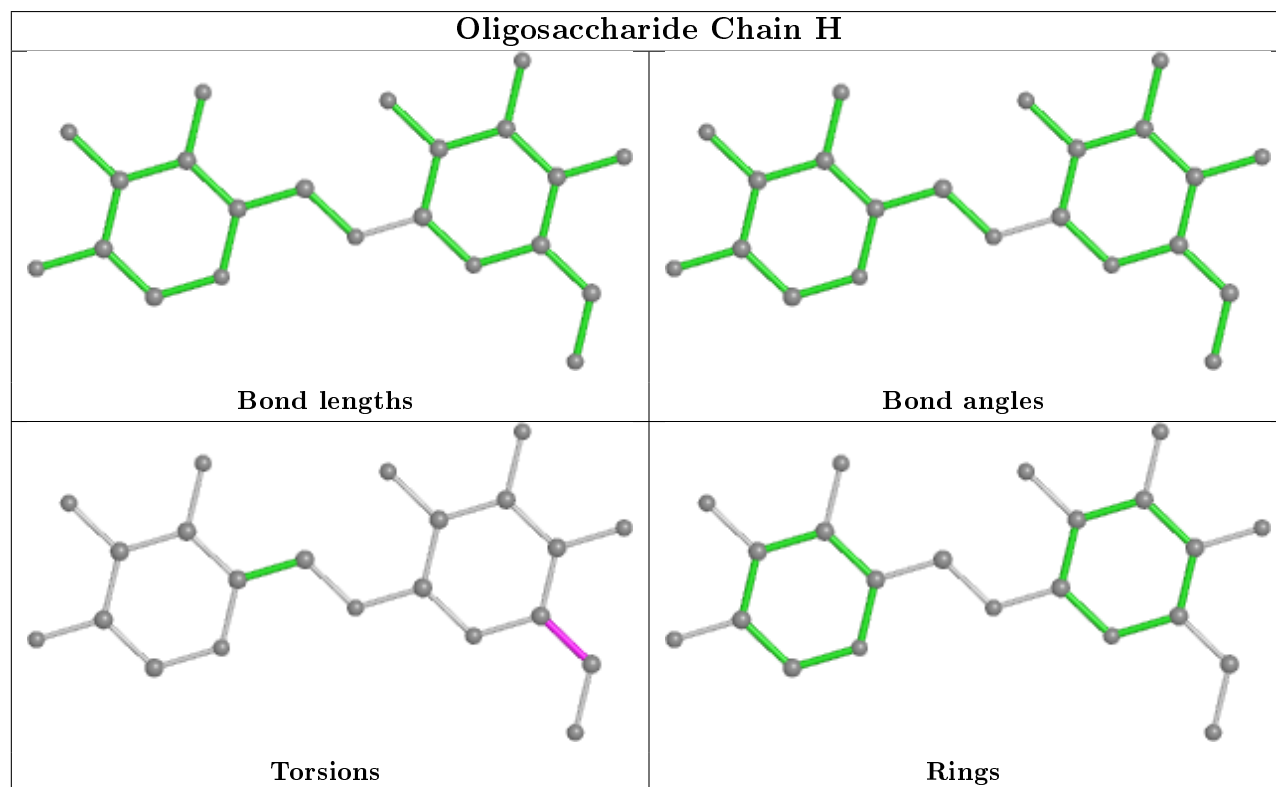
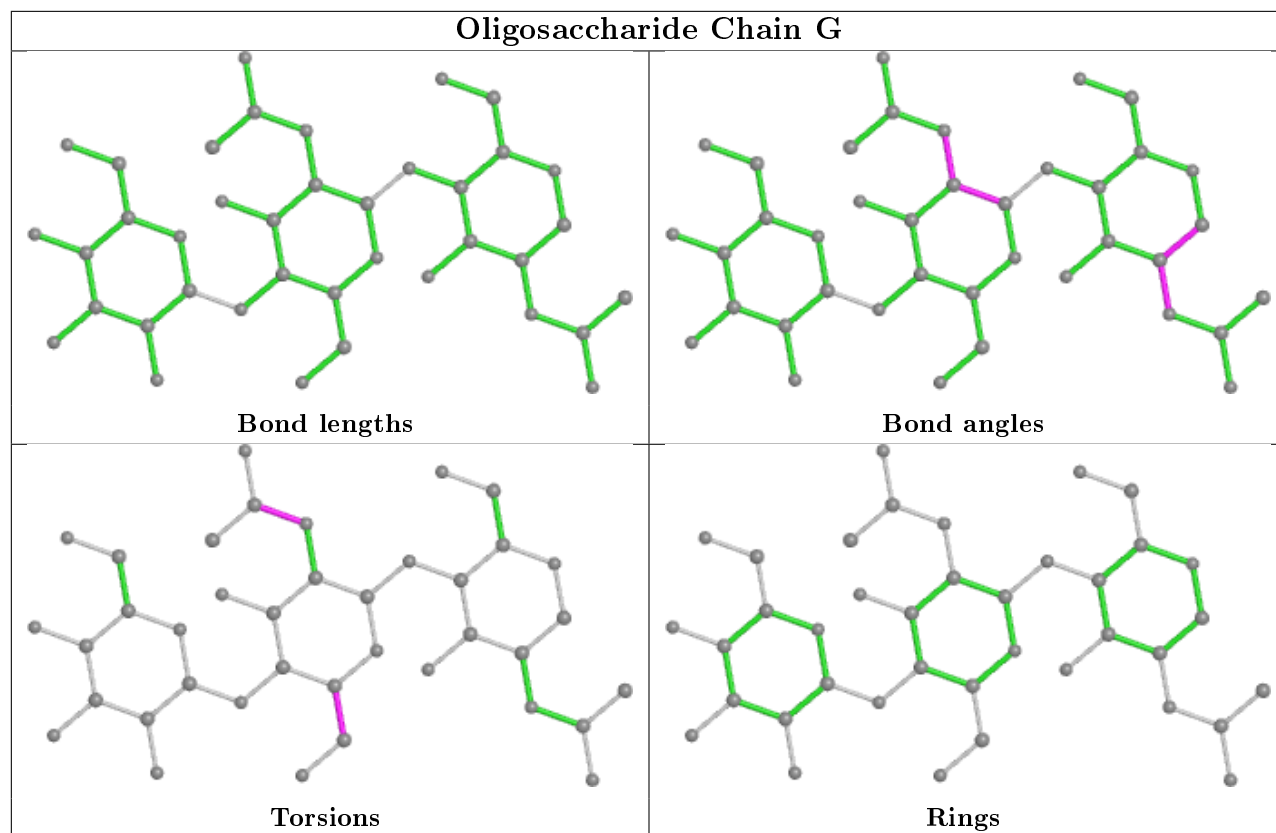
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

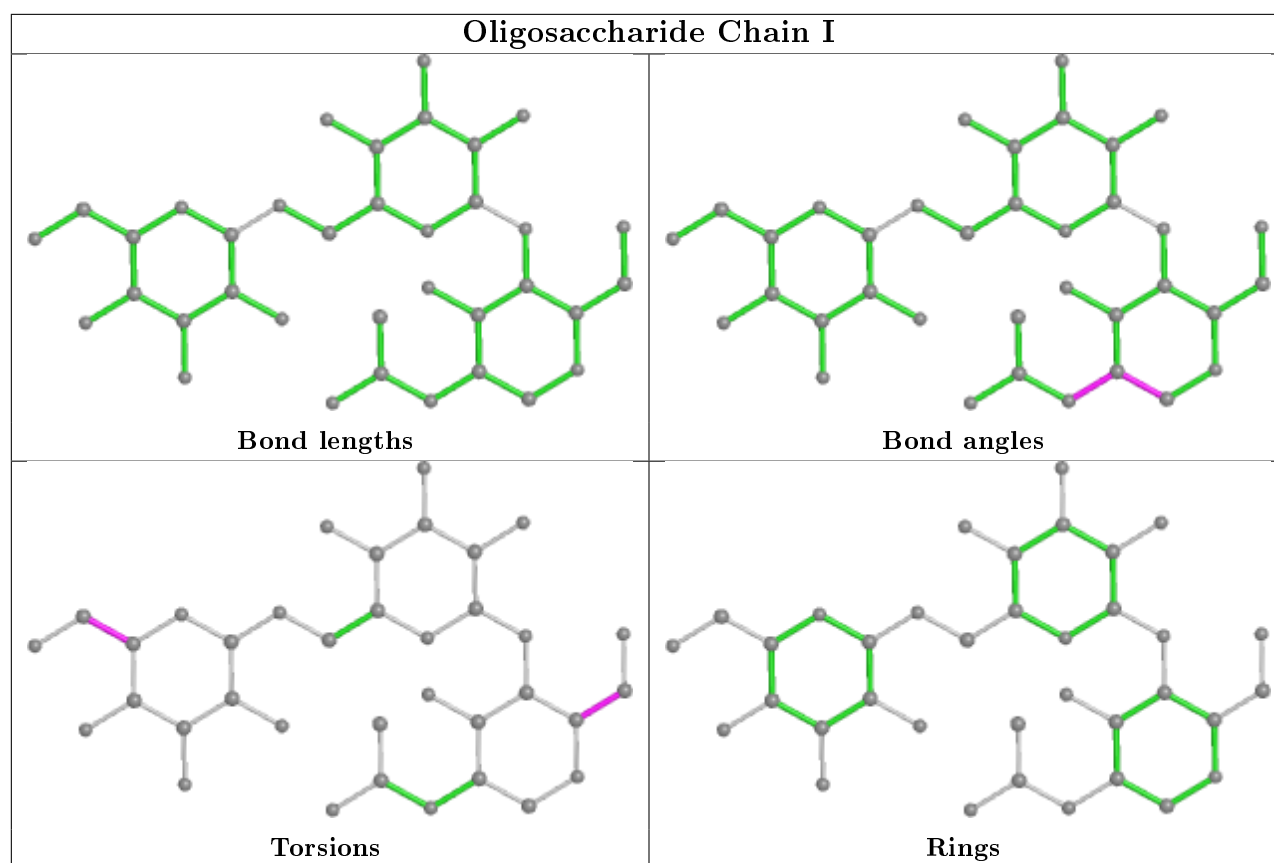












## 5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 4 are monoatomic - leaving 24 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	$\# Z  > 2$
10	NAG	B	2484	1	14,14,15	0.27	0	17,19,21	1.01	1 (5%)
12	PEG	C	3476	-	6,6,6	0.86	0	5,5,5	0.91	0
7	SIA	B	2478	-	18,21,21	0.74	1 (5%)	21,31,31	0.77	1 (4%)
7	SIA	C	3477	-	18,21,21	0.74	1 (5%)	21,31,31	0.79	1 (4%)
7	SIA	B	2477	-	18,21,21	0.74	1 (5%)	21,31,31	0.76	0
9	MAN	B	2483	-	11,11,12	0.27	0	15,15,17	0.63	0
11	GOL	B	2486	-	5,5,5	2.39	2 (40%)	5,5,5	2.44	2 (40%)
10	NAG	D	4482	1	14,14,15	0.26	0	17,19,21	1.02	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	NAG	A	1485	1	14,14,15	0.27	0	17,19,21	1.01	1 (5%)
7	SIA	A	1477	-	18,21,21	0.75	1 (5%)	21,31,31	0.77	1 (4%)
7	SIA	A	1478	-	18,21,21	0.75	1 (5%)	21,31,31	0.77	1 (4%)
9	MAN	A	1483	-	11,11,12	0.27	0	15,15,17	0.63	0
10	NAG	C	3486	-	14,14,15	0.28	0	17,19,21	1.02	1 (5%)
9	MAN	C	3483	-	11,11,12	0.26	0	15,15,17	0.63	0
11	GOL	A	1487	-	5,5,5	1.73	2 (40%)	5,5,5	2.21	2 (40%)
7	SIA	C	3478	-	18,21,21	0.74	1 (5%)	21,31,31	0.77	1 (4%)
7	SIA	D	4477	-	18,21,21	0.75	1 (5%)	21,31,31	0.79	1 (4%)
11	GOL	D	4483	-	5,5,5	2.03	3 (60%)	5,5,5	2.39	2 (40%)
11	GOL	C	3488	-	5,5,5	1.88	3 (60%)	5,5,5	2.05	1 (20%)
9	MAN	C	3481	-	11,11,12	0.26	0	15,15,17	0.63	0
13	BMA	D	4480	-	11,11,12	0.27	0	15,15,17	0.63	0
9	MAN	C	3484	-	11,11,12	0.27	0	15,15,17	0.64	0
10	NAG	A	1484	1	14,14,15	0.26	0	17,19,21	1.01	1 (5%)
7	SIA	D	4478	-	18,21,21	0.74	1 (5%)	21,31,31	0.77	1 (4%)

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
10	NAG	B	2484	1	-	2/6/23/26	0/1/1/1
12	PEG	C	3476	-	-	4/4/4/4	-
7	SIA	B	2478	-	-	0/14/38/38	0/1/1/1
7	SIA	C	3477	-	-	0/14/38/38	0/1/1/1
7	SIA	B	2477	-	-	4/14/38/38	0/1/1/1
9	MAN	B	2483	-	-	2/2/19/22	0/1/1/1
11	GOL	B	2486	-	-	1/4/4/4	-
10	NAG	D	4482	1	-	0/6/23/26	0/1/1/1
10	NAG	A	1485	1	-	1/6/23/26	0/1/1/1
7	SIA	A	1477	-	-	2/14/38/38	0/1/1/1
7	SIA	A	1478	-	-	0/14/38/38	0/1/1/1
9	MAN	A	1483	-	-	1/2/19/22	0/1/1/1
10	NAG	C	3486	-	-	2/6/23/26	0/1/1/1
9	MAN	C	3483	-	-	2/2/19/22	0/1/1/1
11	GOL	A	1487	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SIA	C	3478	-	-	1/14/38/38	0/1/1/1
7	SIA	D	4477	-	-	0/14/38/38	0/1/1/1
11	GOL	D	4483	-	-	1/4/4/4	-
11	GOL	C	3488	-	-	2/4/4/4	-
9	MAN	C	3481	-	-	2/2/19/22	0/1/1/1
13	BMA	D	4480	-	-	0/2/19/22	0/1/1/1
9	MAN	C	3484	-	-	2/2/19/22	0/1/1/1
10	NAG	A	1484	1	-	0/6/23/26	0/1/1/1
7	SIA	D	4478	-	-	0/14/38/38	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	2486	GOL	O3-C3	3.56	1.57	1.42
7	A	1477	SIA	O2-C2	2.87	1.43	1.39
7	A	1478	SIA	O2-C2	2.87	1.43	1.39
11	C	3488	GOL	O3-C3	2.86	1.54	1.42
7	D	4477	SIA	O2-C2	2.85	1.43	1.39
7	B	2477	SIA	O2-C2	2.85	1.43	1.39
7	B	2478	SIA	O2-C2	2.85	1.43	1.39
7	C	3478	SIA	O2-C2	2.84	1.43	1.39
7	D	4478	SIA	O2-C2	2.84	1.43	1.39
11	B	2486	GOL	C3-C2	2.83	1.63	1.51
7	C	3477	SIA	O2-C2	2.82	1.43	1.39
11	A	1487	GOL	C3-C2	2.59	1.62	1.51
11	D	4483	GOL	O3-C3	2.57	1.53	1.42
11	D	4483	GOL	O2-C2	2.42	1.50	1.43
11	A	1487	GOL	O3-C3	2.41	1.52	1.42
11	D	4483	GOL	C3-C2	2.36	1.61	1.51
11	C	3488	GOL	O2-C2	2.23	1.50	1.43
11	C	3488	GOL	C3-C2	2.06	1.60	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	2486	GOL	O3-C3-C2	4.48	131.67	110.20
11	D	4483	GOL	O3-C3-C2	4.16	130.14	110.20
11	A	1487	GOL	O3-C3-C2	4.04	129.55	110.20
11	C	3488	GOL	O3-C3-C2	3.56	127.27	110.20
10	C	3486	NAG	C1-C2-N2	-3.22	104.99	110.49
10	A	1485	NAG	C1-C2-N2	-3.22	104.99	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	4482	NAG	C1-C2-N2	-3.21	105.00	110.49
10	B	2484	NAG	C1-C2-N2	-3.20	105.03	110.49
10	A	1484	NAG	C1-C2-N2	-3.20	105.03	110.49
11	D	4483	GOL	O1-C1-C2	2.81	123.70	110.20
11	A	1487	GOL	O2-C2-C3	2.45	119.89	109.12
11	B	2486	GOL	O1-C1-C2	2.07	120.14	110.20
7	C	3477	SIA	C6-C5-N5	-2.07	107.47	110.91
7	D	4478	SIA	C6-C5-N5	-2.07	107.48	110.91
7	B	2478	SIA	C6-C5-N5	-2.06	107.50	110.91
7	A	1478	SIA	C6-C5-N5	-2.05	107.50	110.91
7	D	4477	SIA	C6-C5-N5	-2.05	107.51	110.91
7	A	1477	SIA	C6-C5-N5	-2.05	107.52	110.91
7	C	3478	SIA	C6-C5-N5	-2.04	107.52	110.91

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	2477	SIA	O6-C6-C7-C8
7	B	2477	SIA	O6-C6-C7-O7
7	A	1477	SIA	O6-C6-C7-O7
9	C	3481	MAN	O5-C5-C6-O6
9	C	3481	MAN	C4-C5-C6-O6
9	C	3483	MAN	C4-C5-C6-O6
10	B	2484	NAG	O5-C5-C6-O6
12	C	3476	PEG	O2-C3-C4-O4
10	B	2484	NAG	C4-C5-C6-O6
9	C	3483	MAN	O5-C5-C6-O6
11	C	3488	GOL	O1-C1-C2-O2
9	B	2483	MAN	C4-C5-C6-O6
11	A	1487	GOL	O1-C1-C2-C3
11	C	3488	GOL	O1-C1-C2-C3
7	C	3478	SIA	O8-C8-C9-O9
12	C	3476	PEG	O1-C1-C2-O2
9	B	2483	MAN	O5-C5-C6-O6
10	C	3486	NAG	C4-C5-C6-O6
10	C	3486	NAG	O5-C5-C6-O6
9	C	3484	MAN	C4-C5-C6-O6
11	D	4483	GOL	O1-C1-C2-O2
12	C	3476	PEG	C4-C3-O2-C2
7	B	2477	SIA	C5-C6-C7-C8
7	B	2477	SIA	C5-C6-C7-O7

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Mol	Chain	Res	Type	Atoms
7	A	1477	SIA	O6-C6-C7-C8
11	B	2486	GOL	O1-C1-C2-O2
9	C	3484	MAN	O5-C5-C6-O6
9	A	1483	MAN	C4-C5-C6-O6
10	A	1485	NAG	C4-C5-C6-O6
12	C	3476	PEG	C1-C2-O2-C3

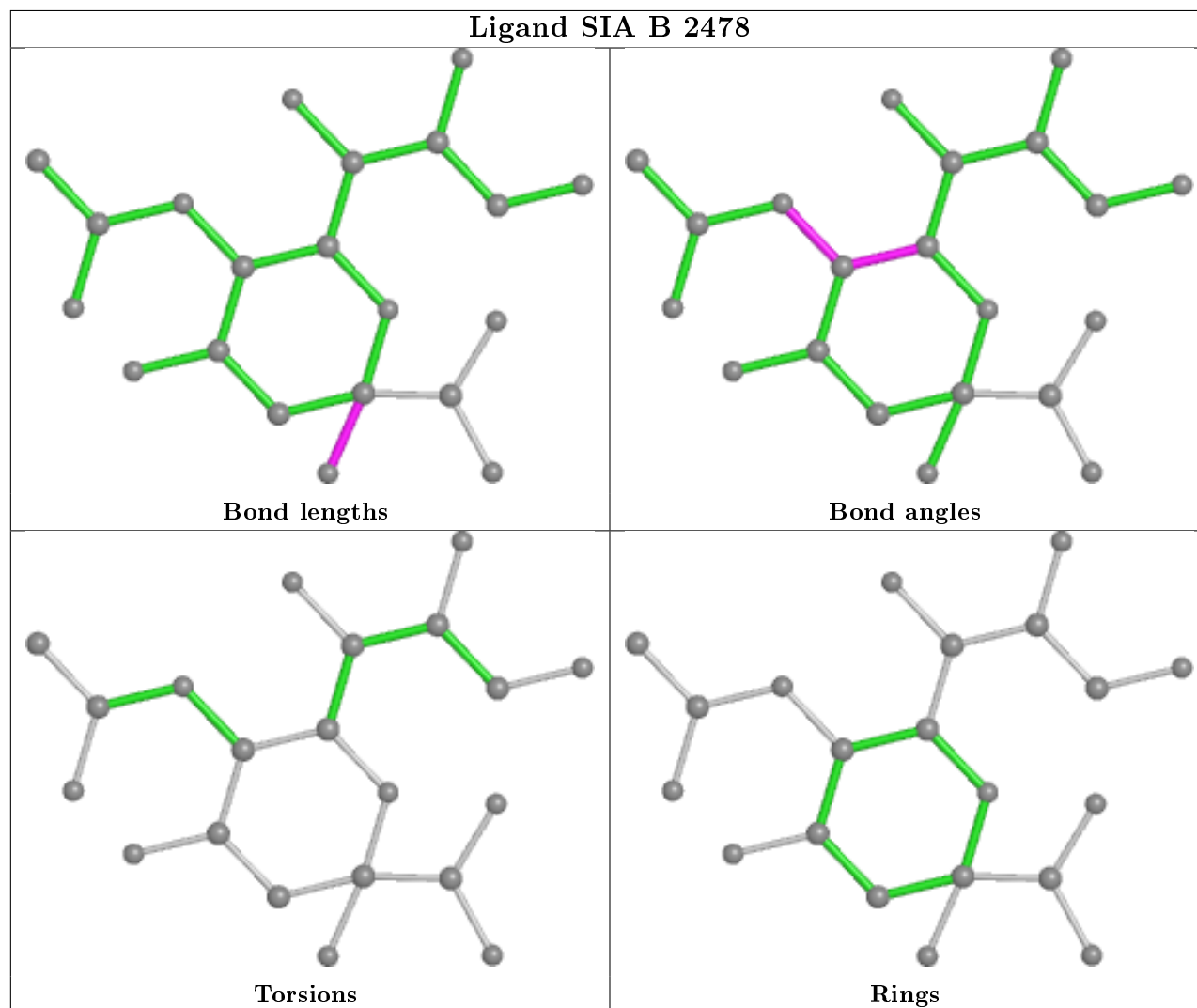
There are no ring outliers.

23 monomers are involved in 53 short contacts:

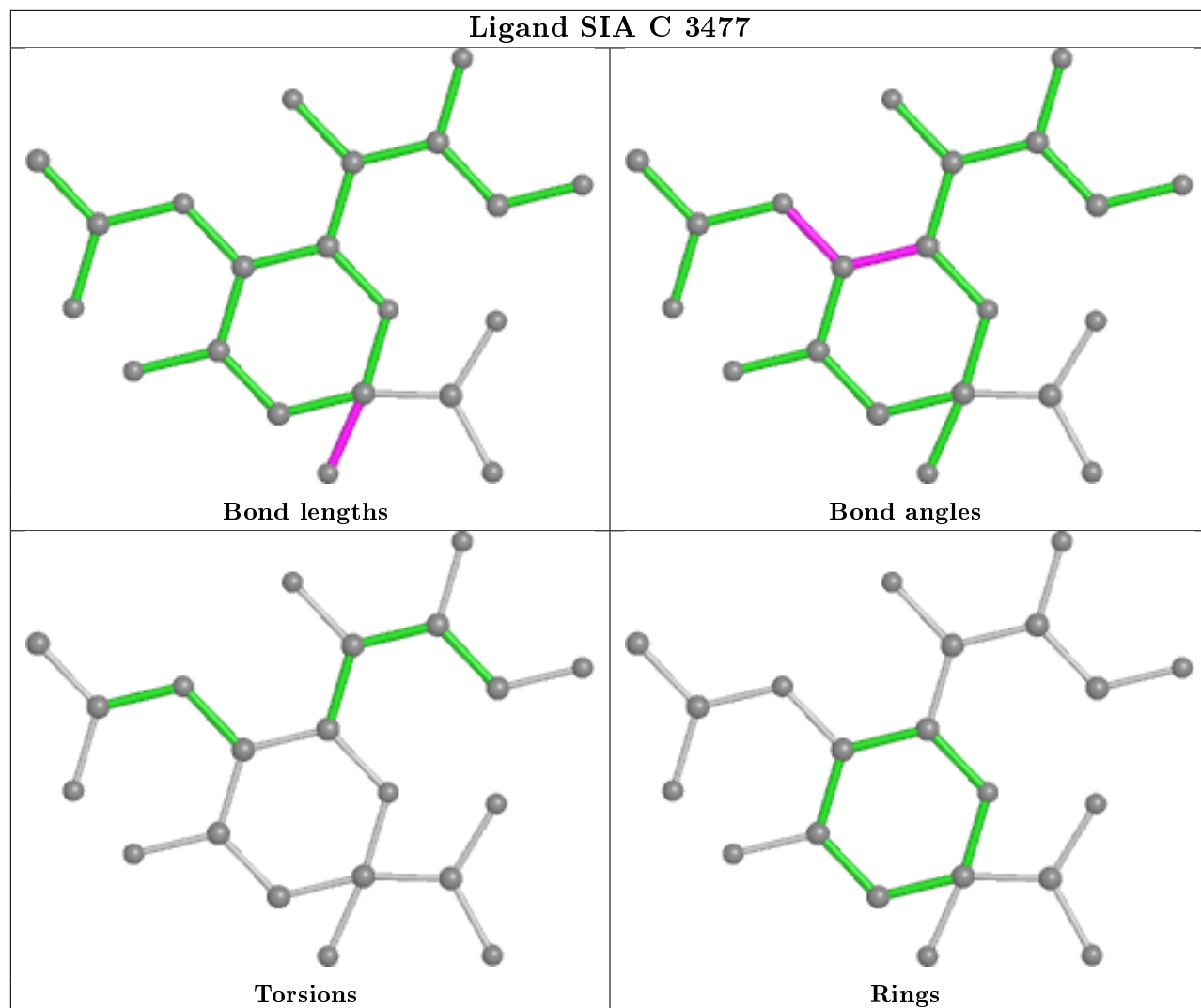
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	2484	NAG	2	0
12	C	3476	PEG	8	0
7	C	3477	SIA	2	0
7	B	2477	SIA	2	0
9	B	2483	MAN	2	0
11	B	2486	GOL	2	0
10	D	4482	NAG	1	0
10	A	1485	NAG	2	0
7	A	1477	SIA	3	0
7	A	1478	SIA	1	0
9	A	1483	MAN	2	0
10	C	3486	NAG	2	0
9	C	3483	MAN	2	0
11	A	1487	GOL	2	0
7	C	3478	SIA	3	0
7	D	4477	SIA	2	0
11	D	4483	GOL	2	0
11	C	3488	GOL	1	0
9	C	3481	MAN	4	0
13	D	4480	BMA	2	0
9	C	3484	MAN	3	0
10	A	1484	NAG	2	0
7	D	4478	SIA	1	0

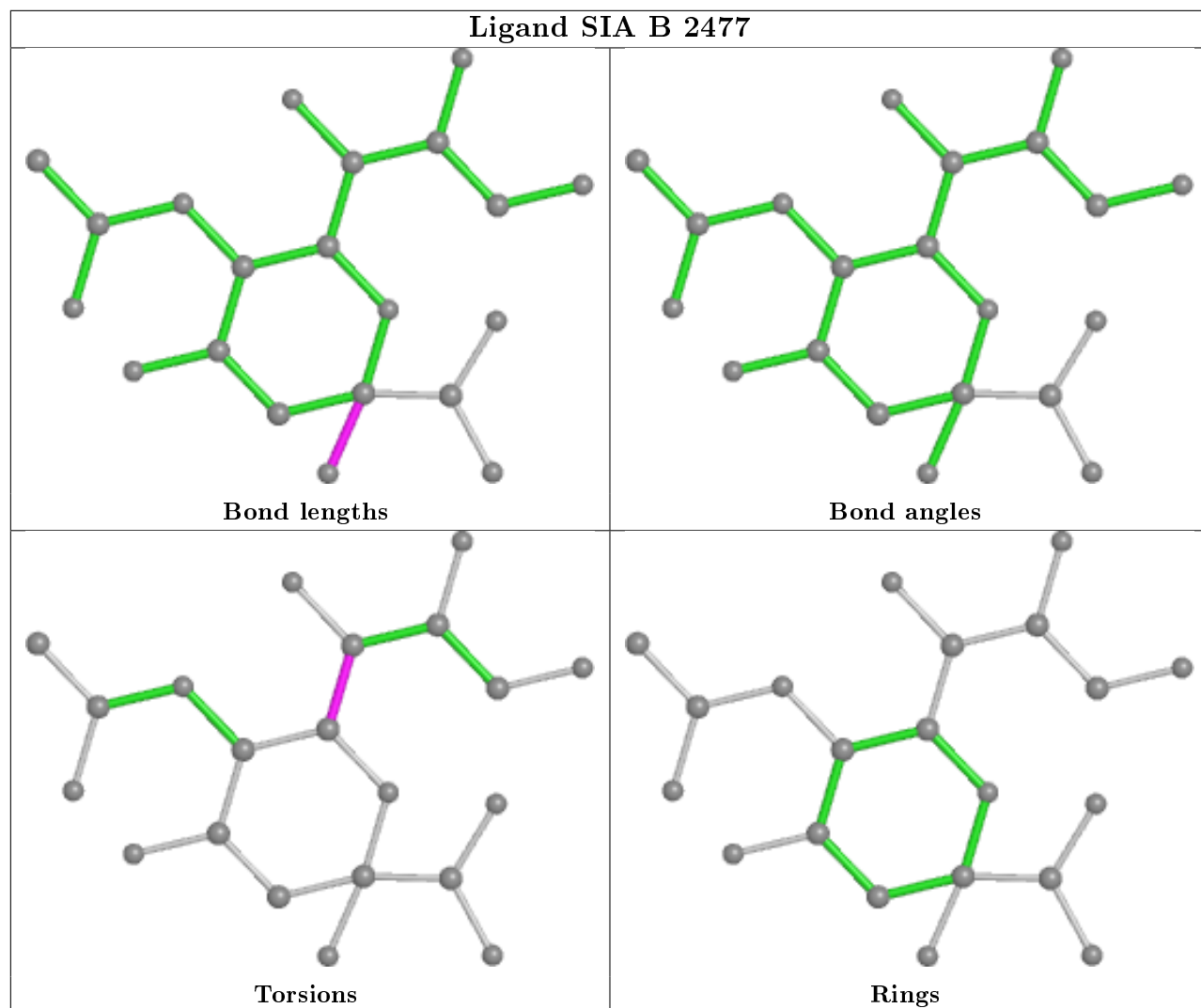
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

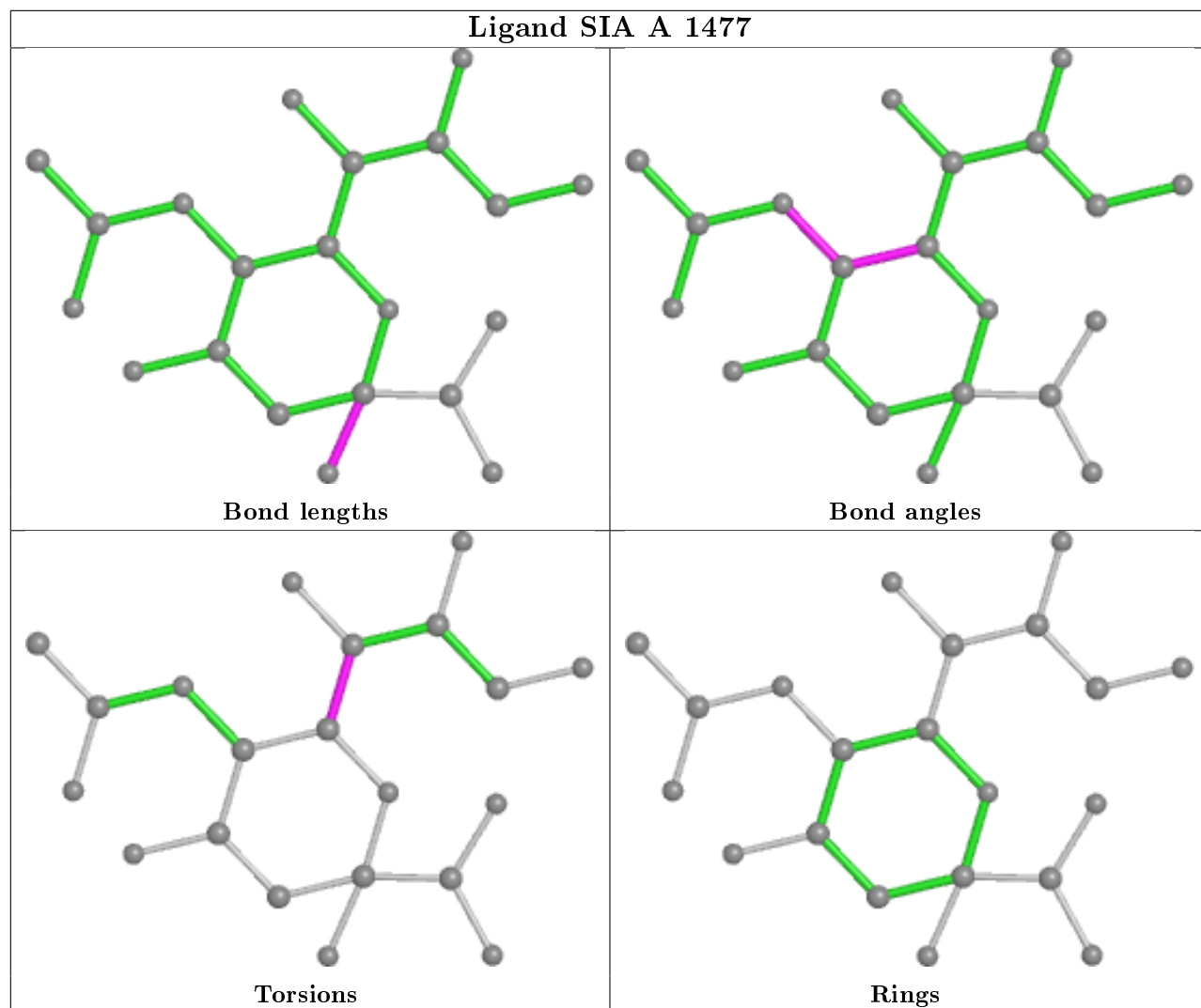
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

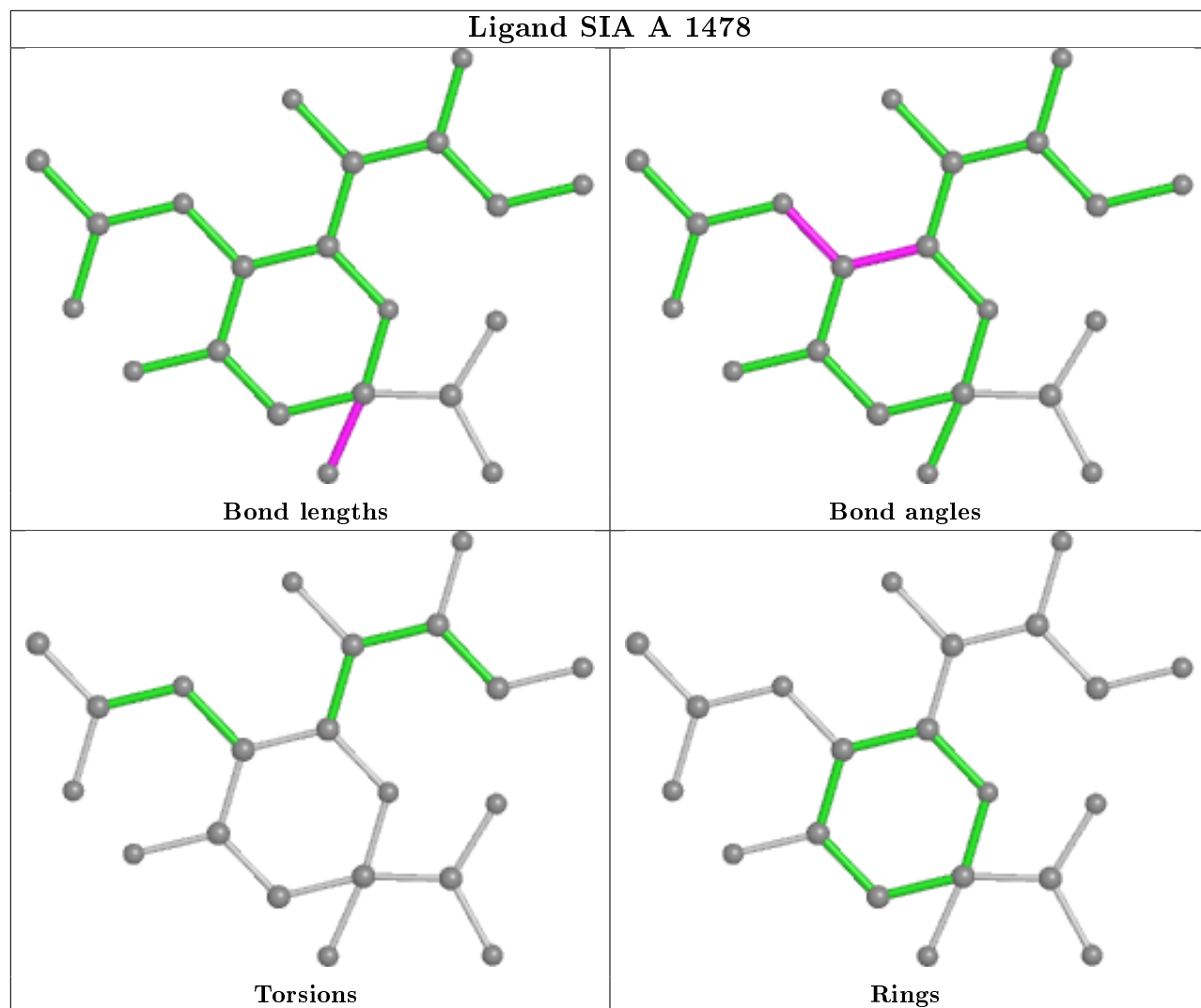




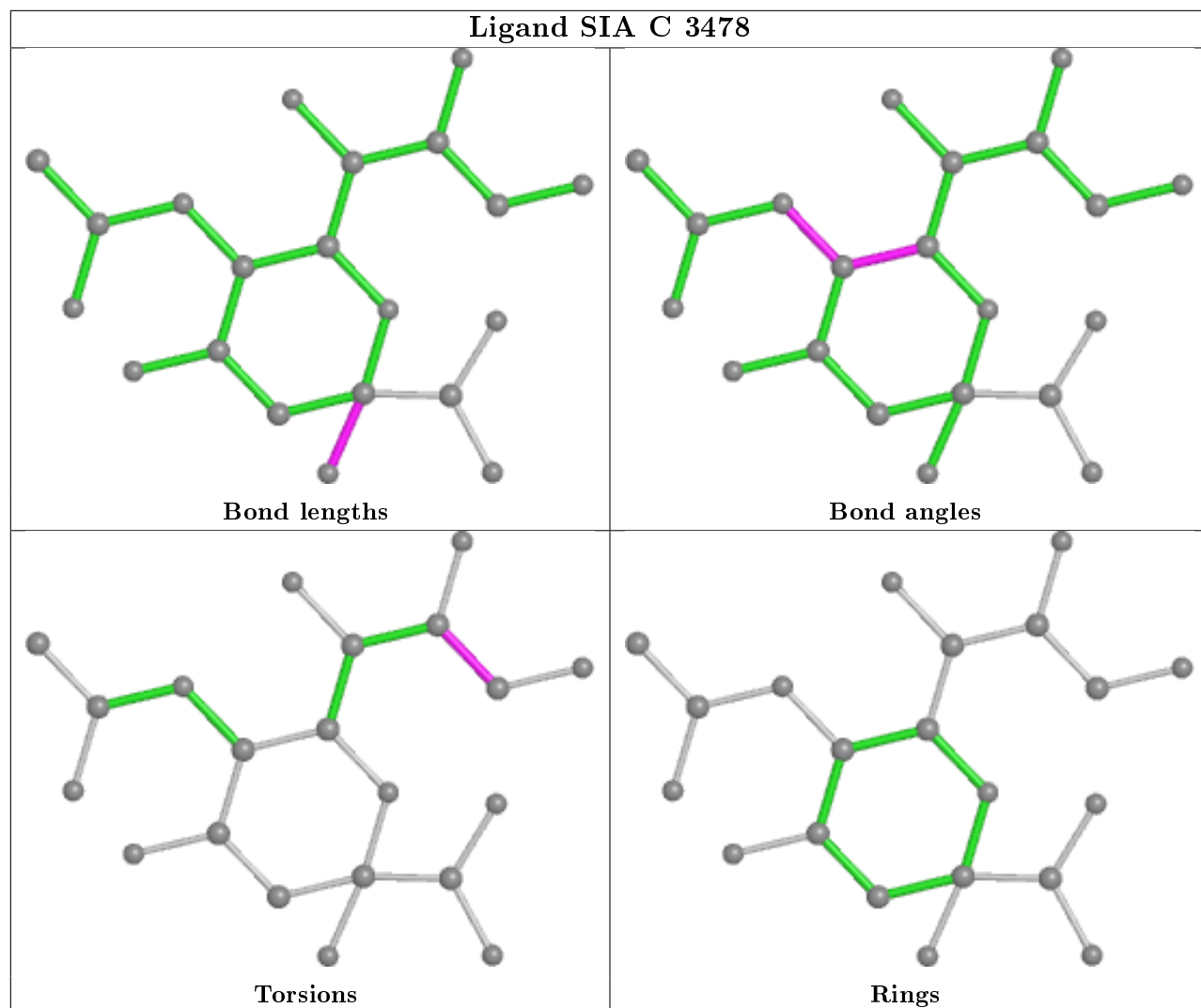


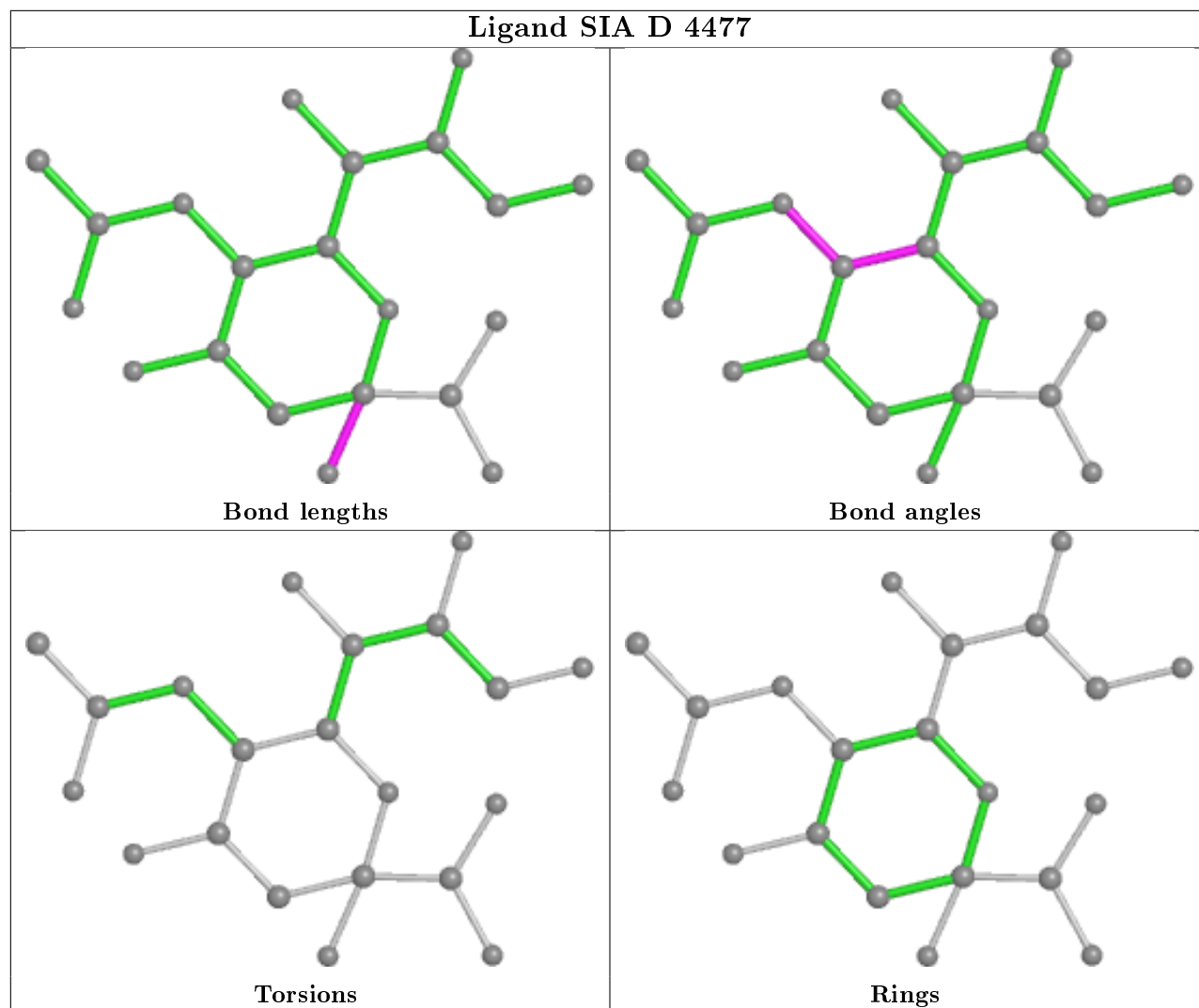


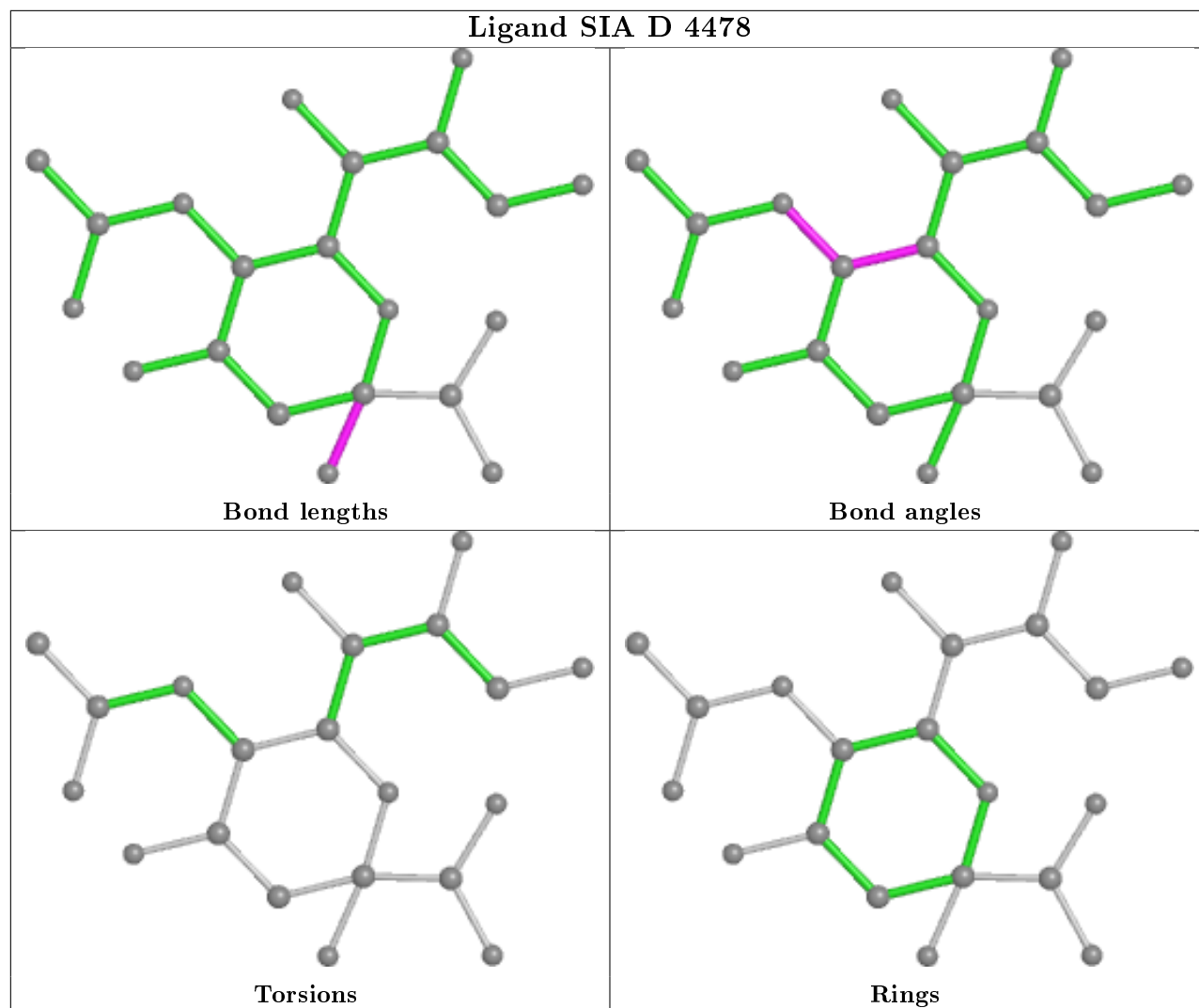




## Ligand SIA C 3478







## 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	389/389 (100%)	-0.41	0 100 100	11, 18, 26, 39	0
1	B	389/389 (100%)	-0.30	2 (0%) 91 90	12, 18, 27, 47	0
1	C	389/389 (100%)	-0.37	1 (0%) 94 93	12, 19, 28, 43	0
1	D	389/389 (100%)	-0.33	1 (0%) 94 93	11, 19, 27, 41	0
All	All	1556/1556 (100%)	-0.35	4 (0%) 94 93	11, 19, 27, 47	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1089	THR	3.1
1	B	1088	ARG	2.7
1	C	2088	ARG	2.6
1	D	3460	ARG	2.2

### 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	F	1	14/15	0.74	0.26	54,62,63,64	0
4	NAG	G	1	14/15	0.78	0.25	35,39,40,41	0
6	MAN	I	3	11/12	0.79	0.21	35,42,45,47	0

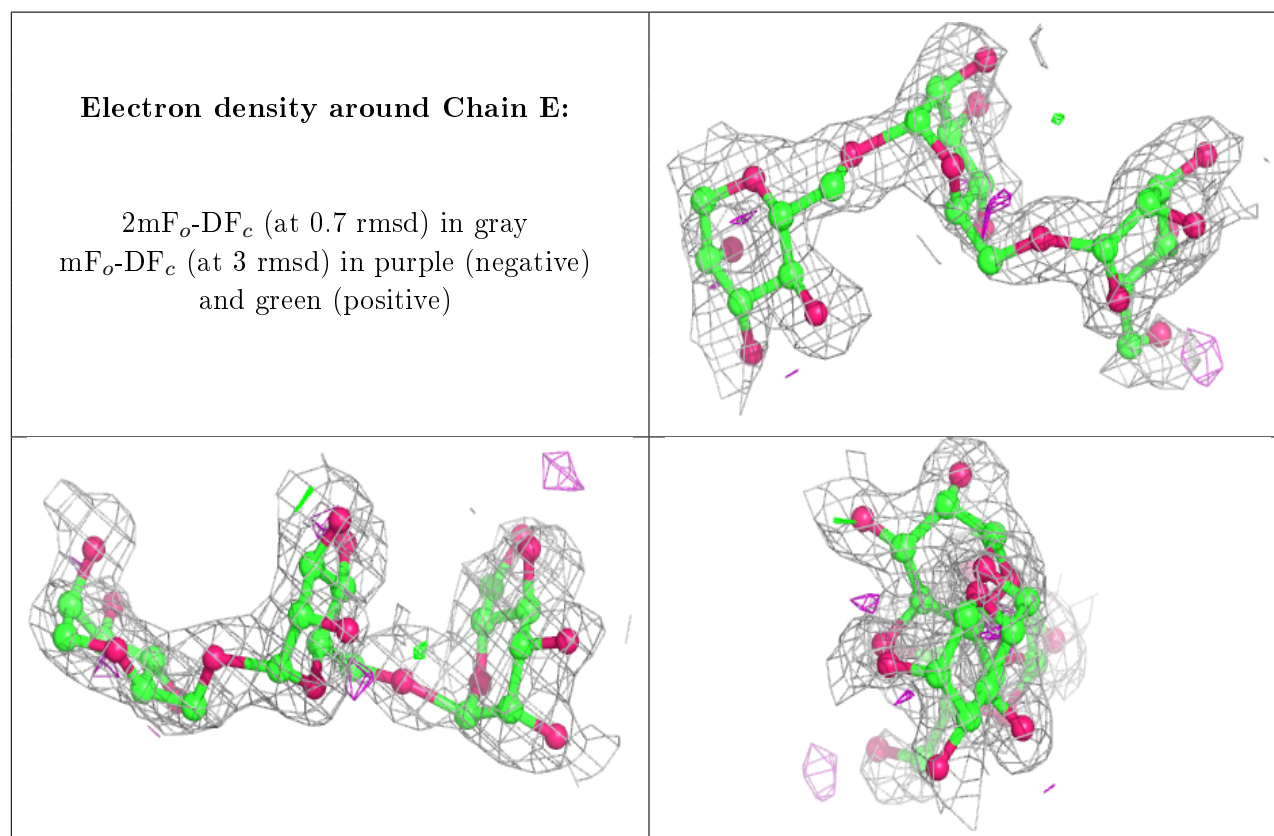
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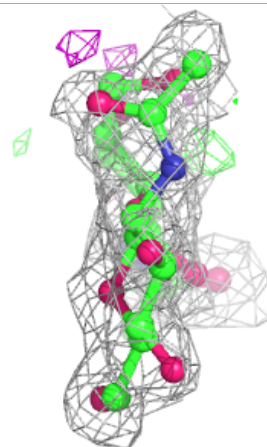
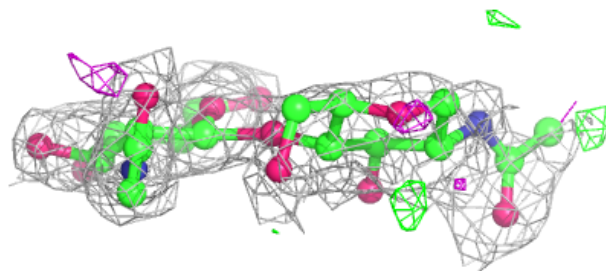
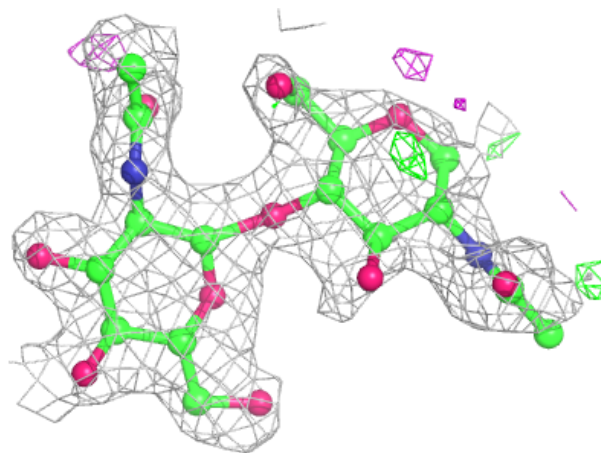
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BMA	E	1	11/12	0.79	0.25	35,43,48,49	0
4	BMA	G	3	11/12	0.79	0.30	49,54,59,59	0
5	MAN	H	2	11/12	0.81	0.29	45,49,53,53	0
3	NAG	J	1	14/15	0.81	0.28	41,43,45,46	0
3	NAG	F	2	14/15	0.81	0.21	40,44,47,47	0
6	NAG	I	1	14/15	0.82	0.20	35,40,42,43	0
6	BMA	I	2	11/12	0.82	0.24	38,42,44,48	0
4	NAG	G	2	14/15	0.82	0.24	29,40,42,43	0
5	MAN	H	1	11/12	0.83	0.23	45,48,50,50	0
2	MAN	E	2	11/12	0.84	0.20	37,41,44,46	0
2	MAN	E	3	11/12	0.86	0.16	42,46,52,53	0
3	NAG	J	2	14/15	0.88	0.23	33,38,43,47	0

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



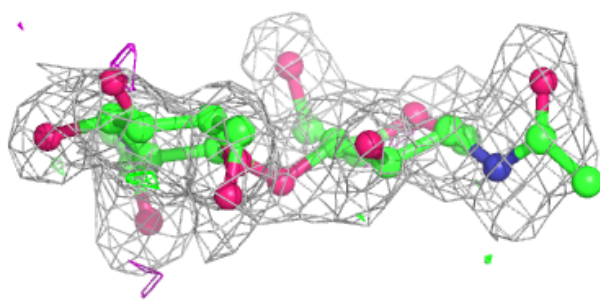
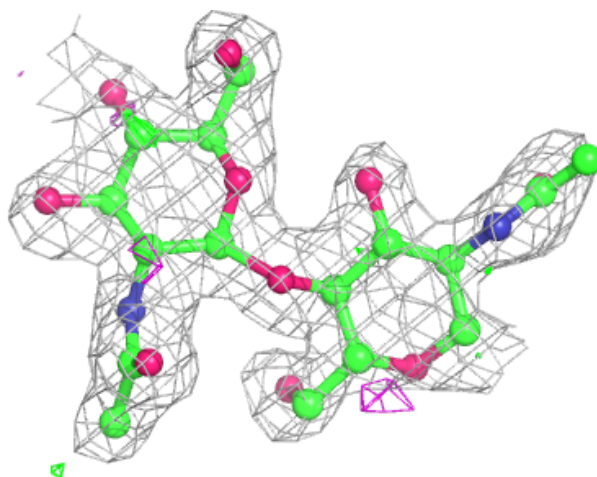
**Electron density around Chain F:**

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



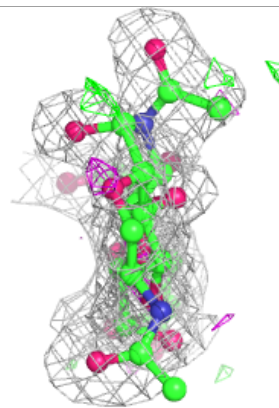
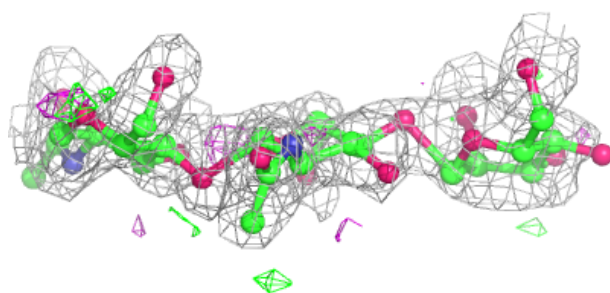
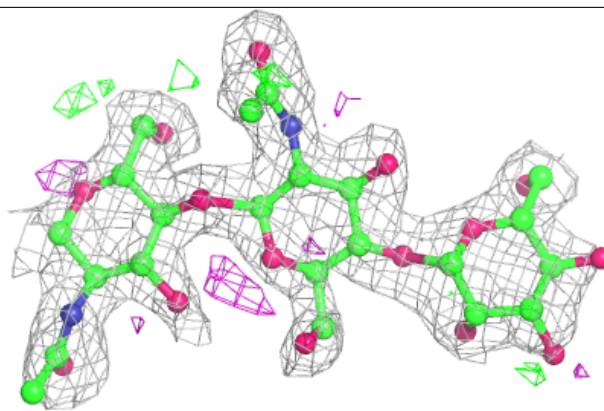
**Electron density around Chain J:**

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



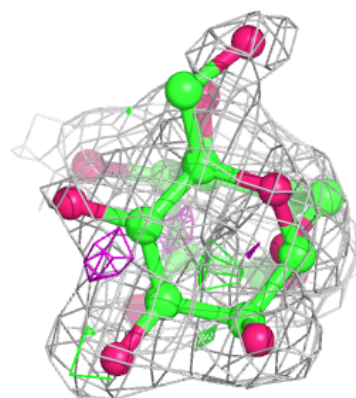
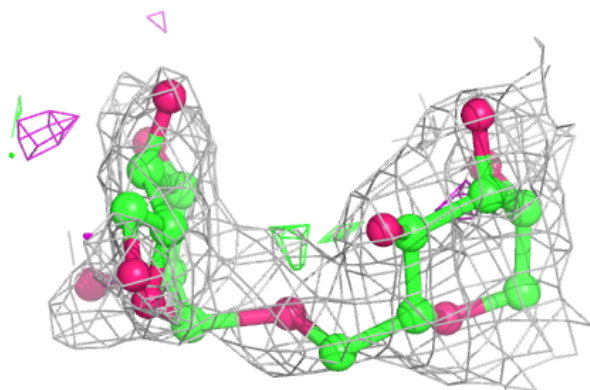
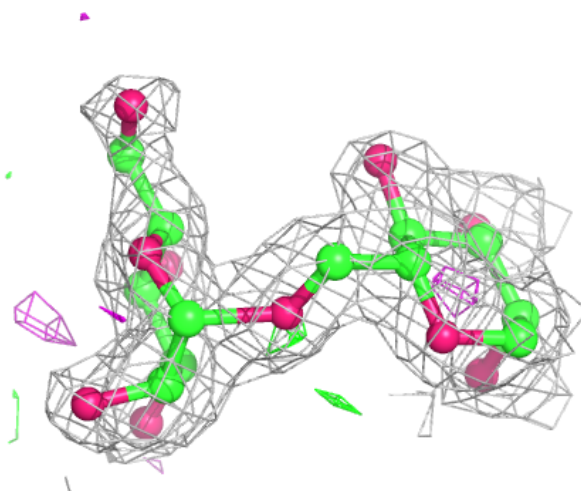
**Electron density around Chain G:**

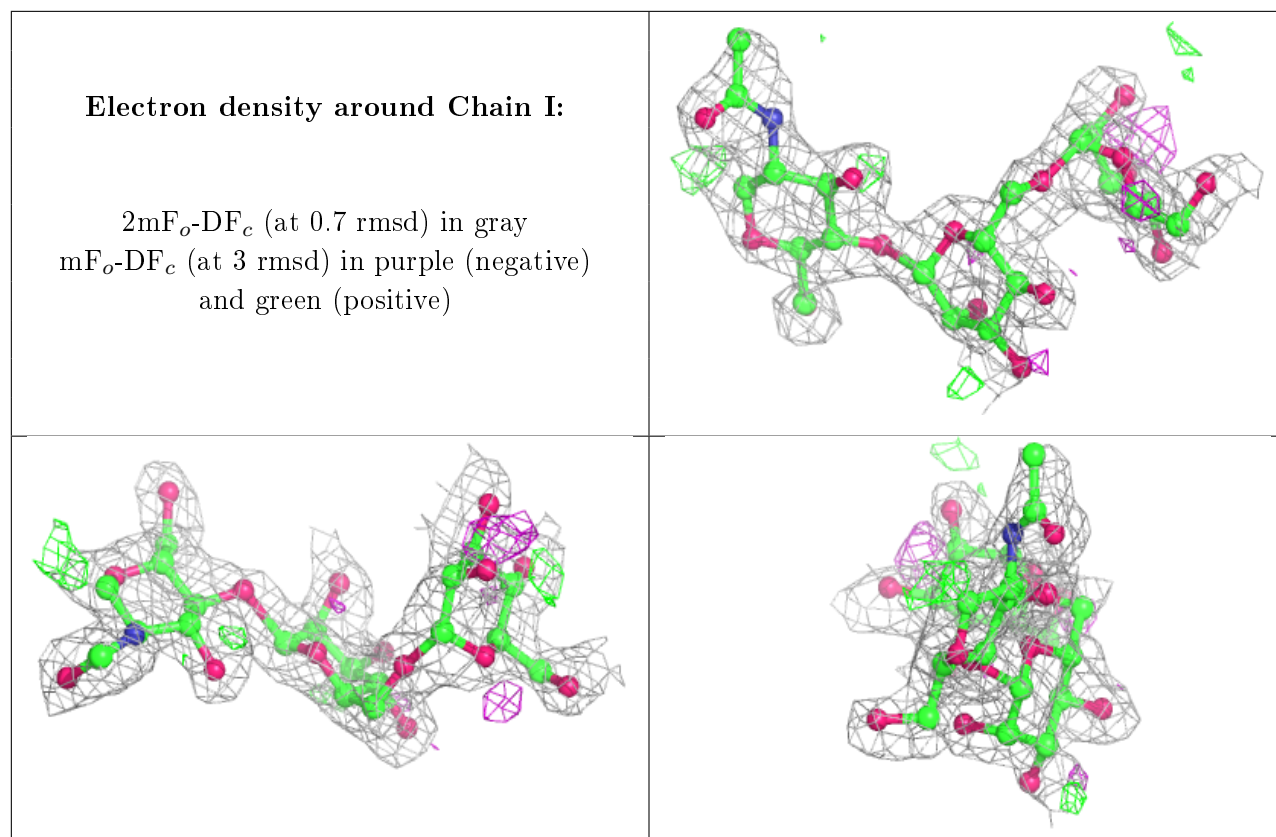
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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)





## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
7	SIA	A	1478	21/21	0.59	0.54	29,36,40,45	21
7	SIA	C	3478	21/21	0.60	0.74	26,35,38,39	21
7	SIA	D	4478	21/21	0.66	0.30	30,40,43,47	21
7	SIA	B	2477	21/21	0.73	0.24	23,26,28,32	0
11	GOL	B	2486	6/6	0.74	0.21	22,30,33,33	0
13	BMA	D	4480	11/12	0.76	0.28	41,43,47,51	0
11	GOL	D	4483	6/6	0.76	0.21	22,31,33,35	0
7	SIA	B	2478	21/21	0.78	0.20	29,37,41,41	21
9	MAN	B	2483	11/12	0.80	0.26	48,51,53,54	0
11	GOL	A	1487	6/6	0.80	0.20	27,30,34,35	0
7	SIA	A	1477	21/21	0.80	0.21	23,26,29,33	0
9	MAN	C	3484	11/12	0.81	0.21	41,43,45,46	0
10	NAG	A	1484	14/15	0.82	0.19	36,42,44,45	0
9	MAN	C	3481	11/12	0.82	0.22	38,42,44,46	0

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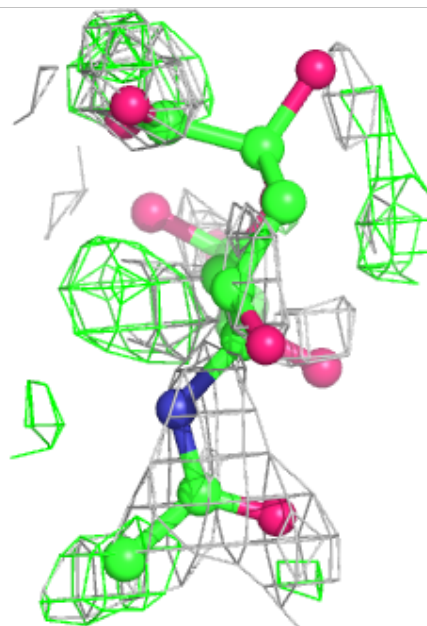
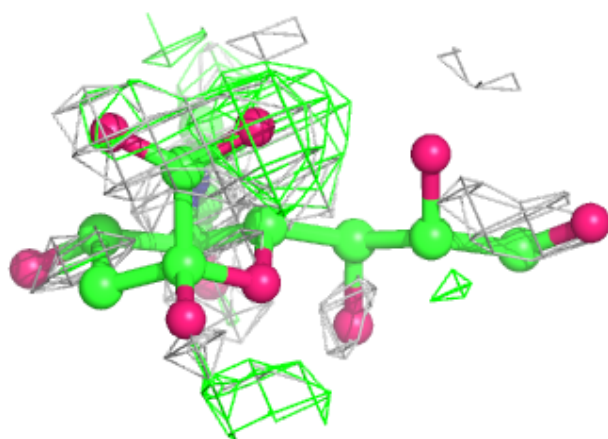
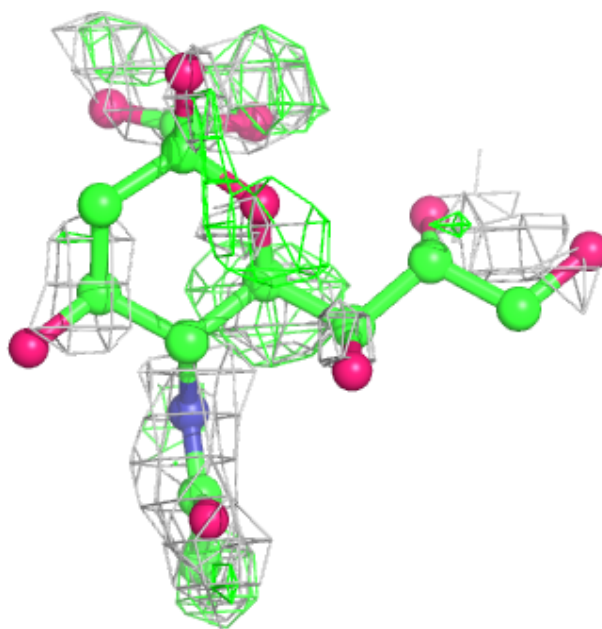
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	SIA	C	3477	21/21	0.83	0.19	21,25,28,35	0
10	NAG	C	3486	14/15	0.85	0.17	27,30,34,37	0
7	SIA	D	4477	21/21	0.85	0.16	21,25,28,31	0
12	PEG	C	3476	7/7	0.86	0.21	28,38,46,49	0
11	GOL	C	3488	6/6	0.87	0.16	17,28,30,31	0
10	NAG	B	2484	14/15	0.87	0.15	21,33,39,43	0
9	MAN	A	1483	11/12	0.88	0.16	28,36,40,42	0
10	NAG	D	4482	14/15	0.89	0.16	25,33,37,38	0
10	NAG	A	1485	14/15	0.91	0.14	24,32,38,42	0
9	MAN	C	3483	11/12	0.91	0.16	41,46,48,50	0
8	CA	C	3479	1/1	0.94	0.38	16,16,16,16	0
8	CA	D	4479	1/1	0.96	0.35	11,11,11,11	0
8	CA	A	1479	1/1	0.97	0.43	6,6,6,6	0
8	CA	B	2479	1/1	0.97	0.41	14,14,14,14	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 SIA A 1478:**

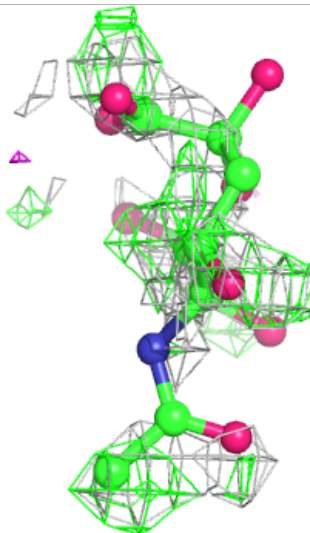
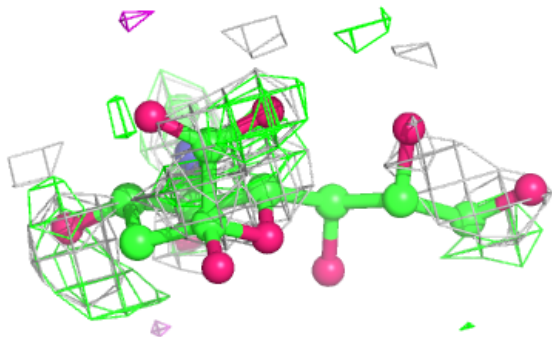
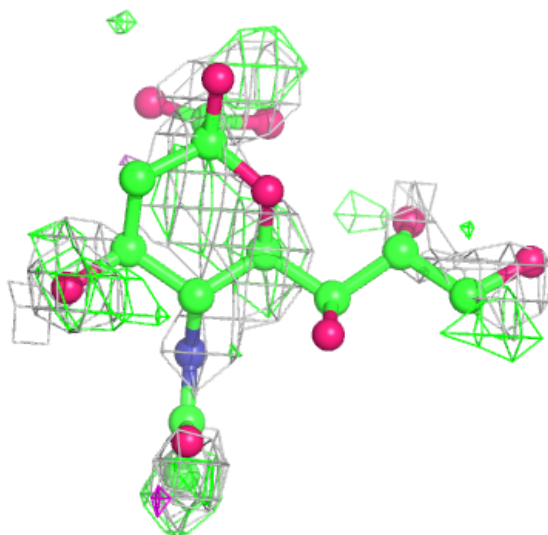
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





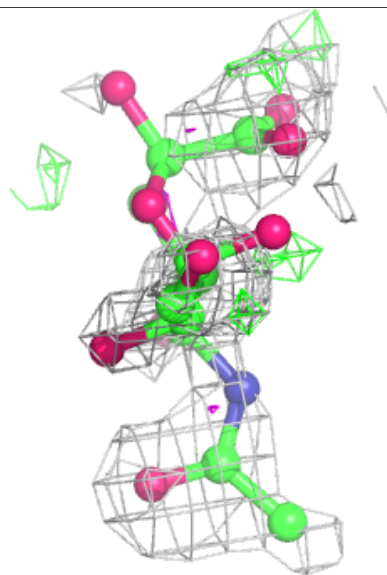
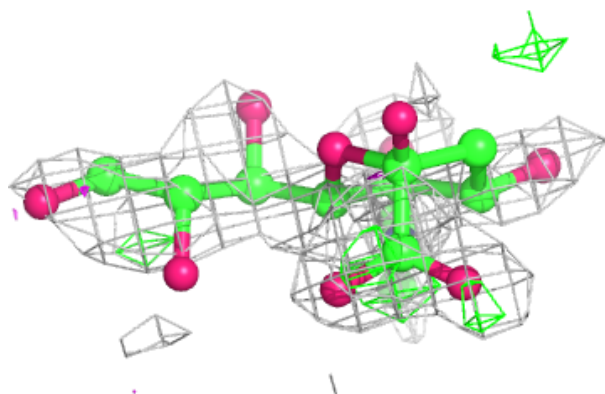
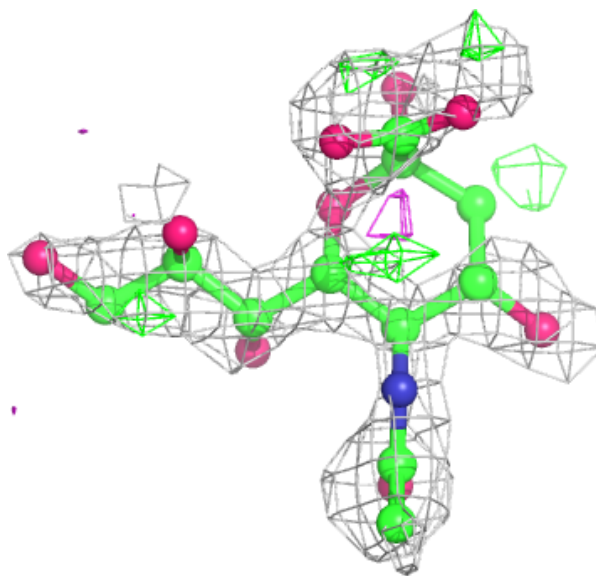
**Electron density around SIA C 3478:**

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



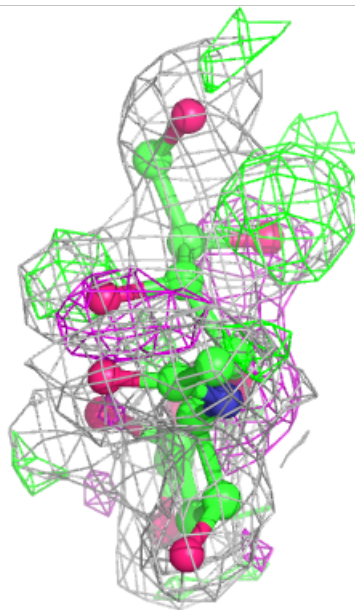
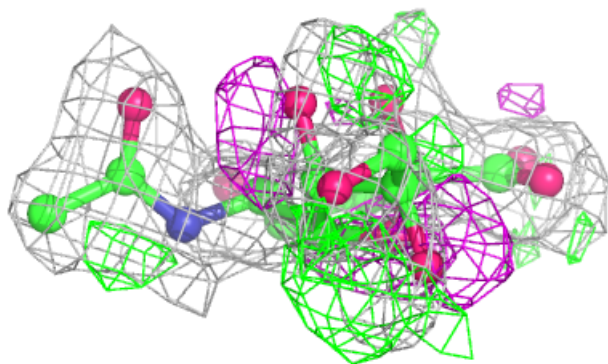
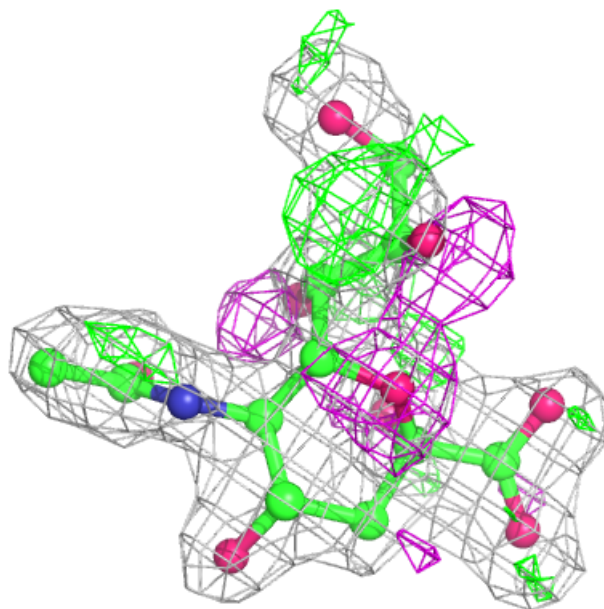
**Electron density around SIA D 4478:**

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



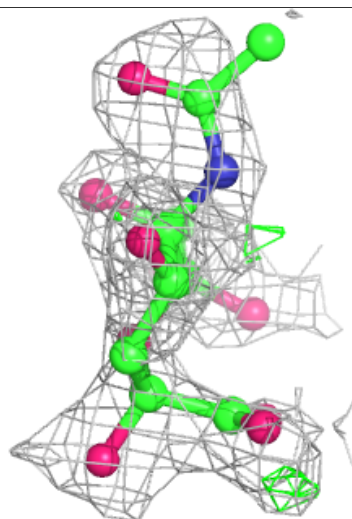
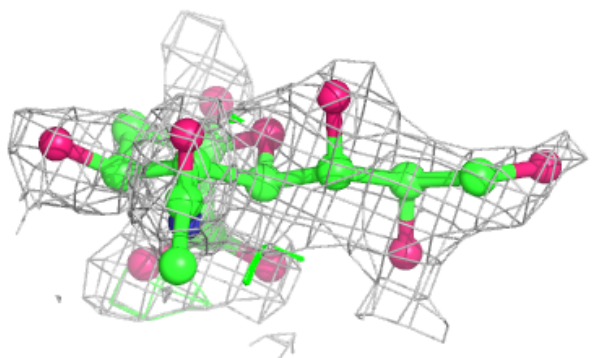
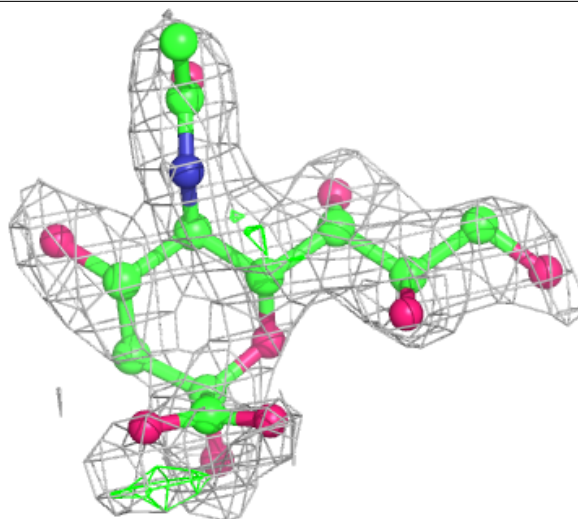
**Electron density around SIA B 2477:**

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



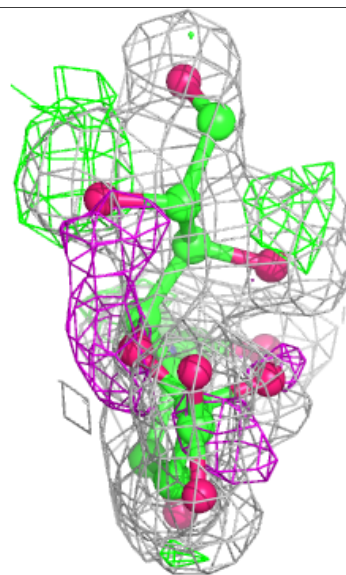
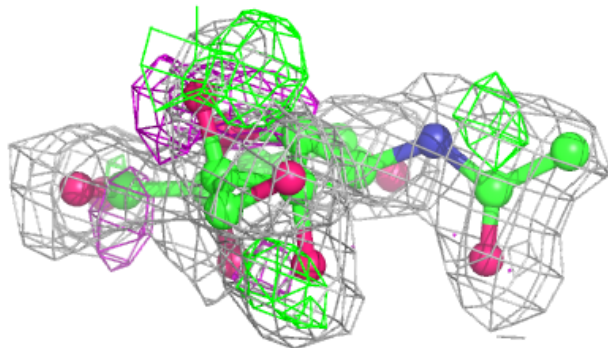
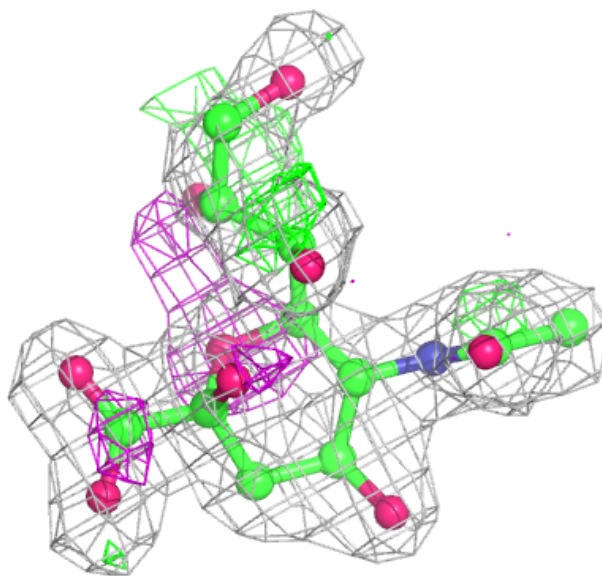
**Electron density around SIA B 2478:**

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



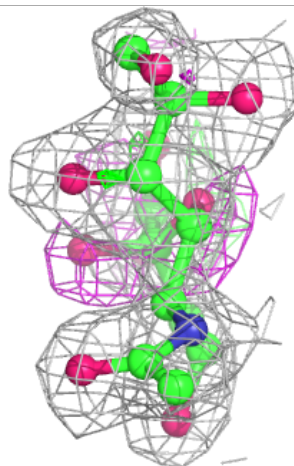
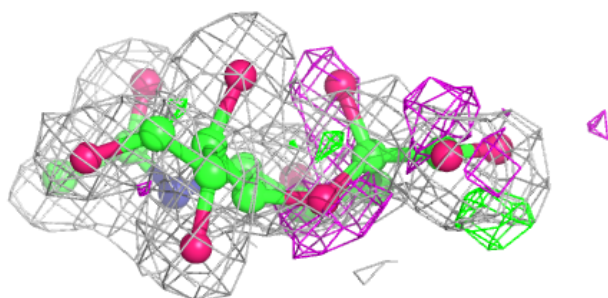
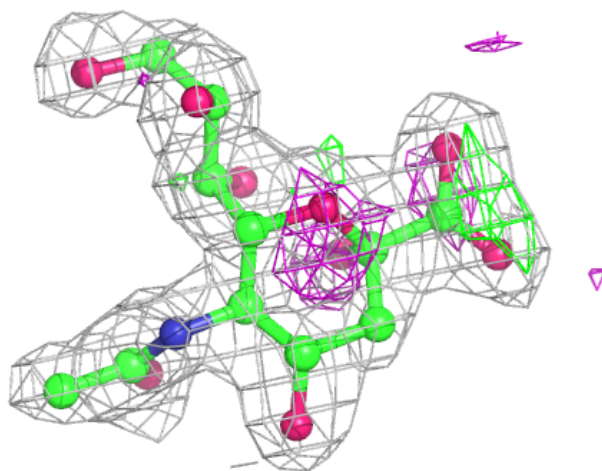
**Electron density around SIA A 1477:**

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



**Electron density around SIA C 3477:**

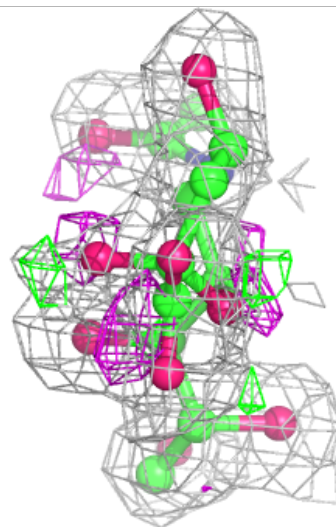
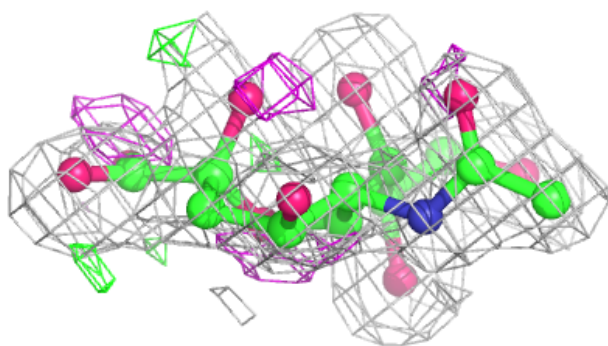
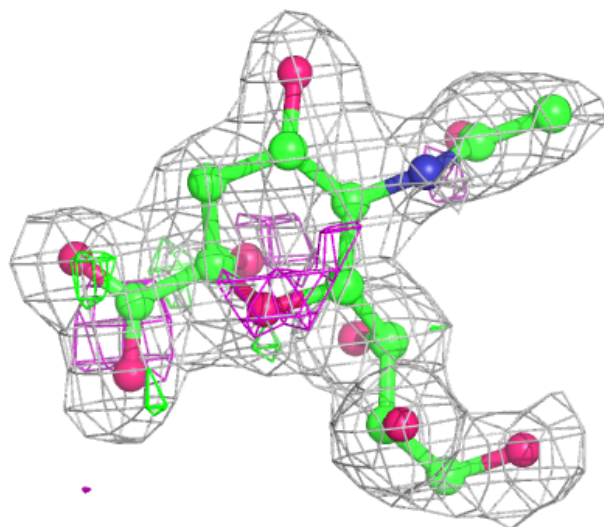
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around SIA D 4477:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.