



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2022 – 02:11 PM EDT

PDB ID : 7TCT  
Title : Integrin  $\alpha$ IIb $\beta$ 3 complex with UR2922  
Authors : Zhu, J.; Lin, F.-Y.; Zhu, J.; Springer, T.A.  
Deposited on : 2021-12-28  
Resolution : 2.50 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>.

---

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 : 2.29  
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) : 2.29

**i**

## X-RAY DIFFRACTION

A.

the following graphic. The table shows the number of entries on which the scores are based.



Whole archive  
(#Entries)

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.

### Quality of chain

Category	Red (%)	Green (%)	Yellow (%)	Grey (%)
1	1	94	5	0
2	1	91	8	0
3	13	93	6	0
4	9	92	8	0
5	28	88	9	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	H	221	
4	F	214	
4	L	214	
5	G	5	
6	I	2	
6	K	2	
7	J	4	

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
7	BMA	J	3	-	-	-	X

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 22118 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 Integrin alpha-IIb heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	5	0
			3503	2227	604	664	8			
1	C	453	Total	C	N	O	S	1	3	0
			3493	2219	602	664	8			

- Molecule 2 is a protein called Isoform Beta-3C of Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	466	Total	C	N	O	S	4	4	0
			3620	2256	618	712	34			
2	D	471	Total	C	N	O	S	1	1	0
			3631	2260	620	716	35			

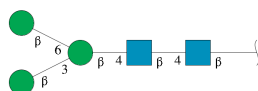
- Molecule 3 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	214	Total	C	N	O	S	0	0	0
			1631	1035	264	326	6			
3	H	216	Total	C	N	O	S	0	0	0
			1642	1041	266	329	6			

- Molecule 4 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	214	Total	C	N	O	S	0	0	0
			1637	1019	268	341	9			
4	L	214	Total	C	N	O	S	0	0	0
			1637	1019	268	341	9			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 6 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
6	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-3)-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
7	J	4	Total	C	N	O	0	0	0
			50	28	2	20			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	4	Total	Ca	0	0
			4	4		
8	B	2	Total	Ca	0	0
			2	2		
8	C	4	Total	Ca	0	0
			4	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total	Ca	0	0
			2	2		

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

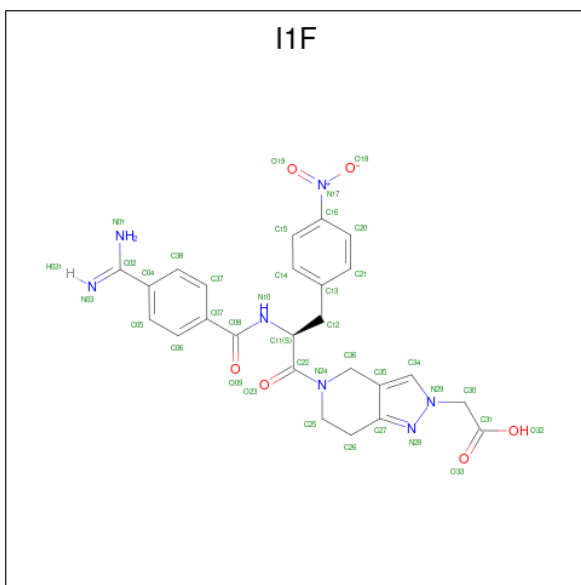
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	Mg	0	0
			1	1		
10	D	1	Total	Mg	0	0
			1	1		

- Molecule 11 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>).



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

- Molecule 12 is {5-[N-(4-carbamimidoylbenzoyl)-4-nitro-L-phenylalanyl]-4,5,6,7-tetrahydro-2H-pyrazolo[4,3-c]pyridin-2-yl}acetic acid (three-letter code: I1F) (formula: C<sub>25</sub>H<sub>25</sub>N<sub>7</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	C	N	O	0	0
			38	25	7	6		
12	D	1	Total	C	N	O	0	0
			38	25	7	6		

- Molecule 13 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	C	1	Total	Cl	0	0
			1	1		

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	334	Total	O	0	0
			334	334		
14	B	145	Total	O	0	0
			145	145		
14	C	231	Total	O	0	0
			231	231		
14	D	166	Total	O	0	0
			166	166		
14	E	18	Total	O	0	0
			18	18		
14	F	17	Total	O	0	0
			17	17		

*Continued on next page...*



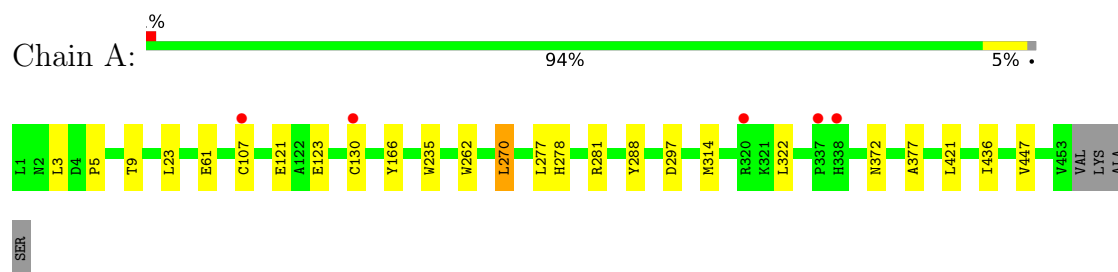
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	H	44	Total 44	O 44	0	0
14	L	43	Total 43	O 43	0	0

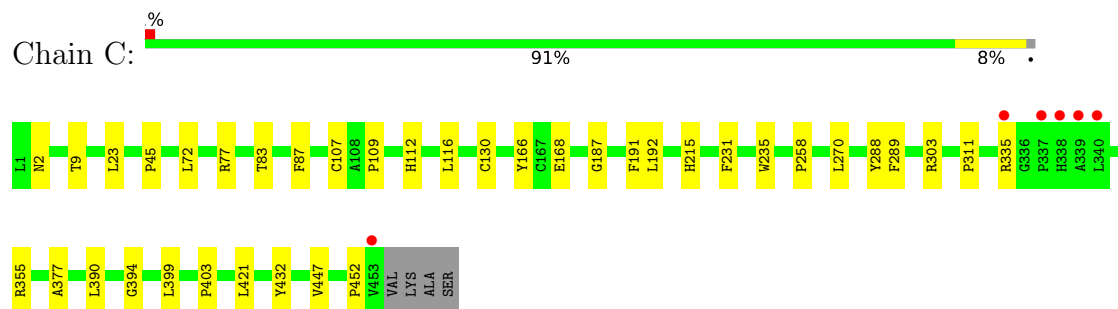
### 3 Residue-property plots [i](#)

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.

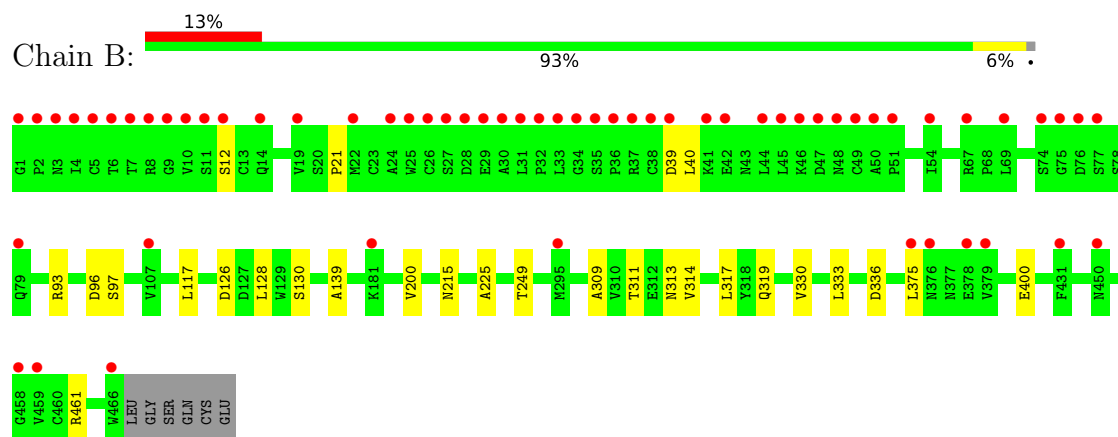
- Molecule 1: Integrin alpha-IIb heavy chain



- Molecule 1: Integrin alpha-IIb heavy chain

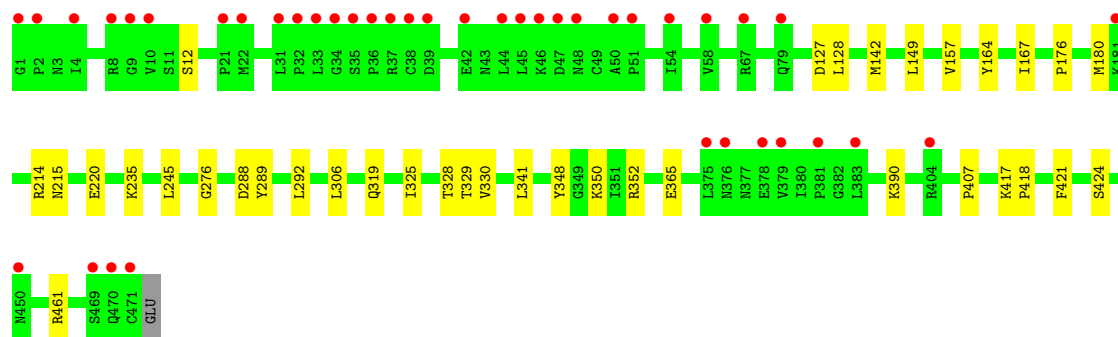


- Molecule 2: Isoform Beta-3C of Integrin beta-3

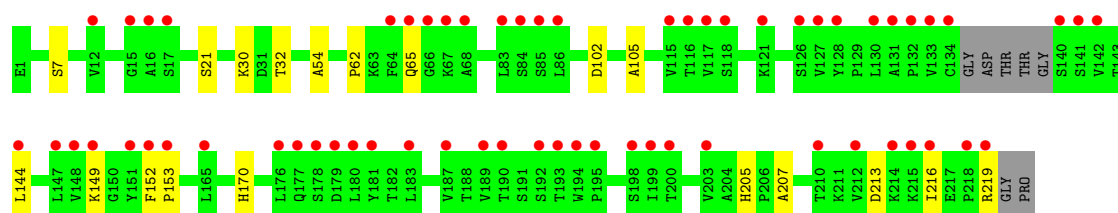
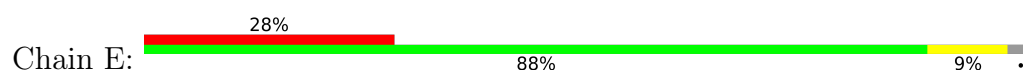


- Molecule 2: Isoform Beta-3C of Integrin beta-3

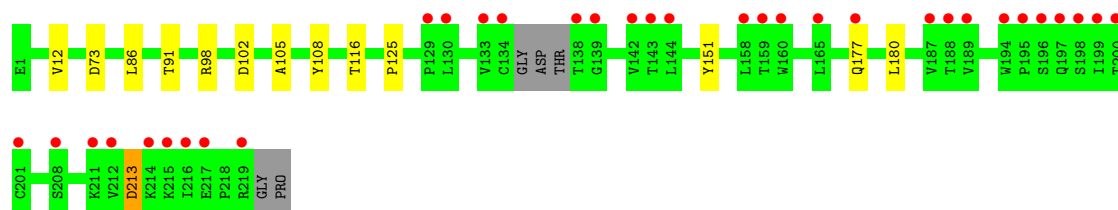
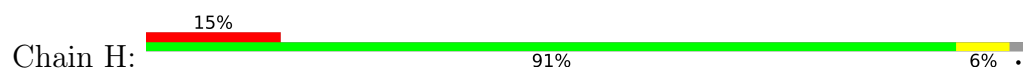




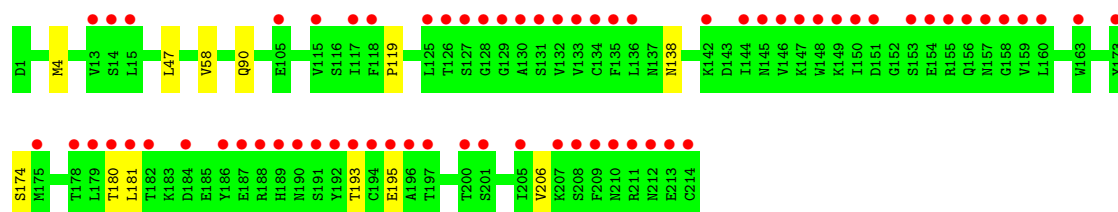
• Molecule 3: Fab heavy chain



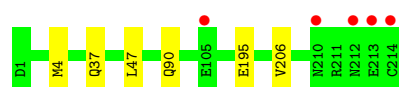
• Molecule 3: Fab heavy chain



• Molecule 4: Fab light chain

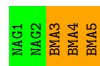


• Molecule 4: Fab light chain



- Molecule 5: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  40% 60%



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

Chain I:  50% 50%



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

Chain K:  100%



- Molecule 7: beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 50%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	259.16Å 143.84Å 104.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.28 – 2.50 49.28 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.28-2.50) 99.4 (49.28-2.50)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.195 , 0.227 0.195 , 0.227	Depositor DCC
$R_{free}$ test set	2000 reflections (1.48%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 52.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	22118	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, CA, NAG, IIF, CL, SO4, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.26	0/3612	0.47	0/4922
1	C	0.25	0/3596	0.46	0/4900
2	B	0.24	0/3690	0.43	0/5002
2	D	0.25	0/3698	0.44	0/5013
3	E	0.25	0/1673	0.45	0/2290
3	H	0.25	0/1684	0.46	0/2305
4	F	0.25	0/1673	0.44	0/2269
4	L	0.25	0/1673	0.45	0/2269
All	All	0.25	0/21299	0.45	0/28970

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 [i](#)

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	3503	0	3348	12	0
1	C	3493	0	3327	20	0
2	B	3620	0	3546	15	0
2	D	3631	0	3548	20	0
3	E	1631	0	1590	13	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1642	0	1600	8	0
4	F	1637	0	1553	7	0
4	L	1637	0	1553	3	0
5	G	61	0	52	2	0
6	I	28	0	25	1	0
6	K	28	0	25	0	0
7	J	50	0	43	0	0
8	A	4	0	0	0	0
8	B	2	0	0	0	0
8	C	4	0	0	0	0
8	D	2	0	0	0	0
9	A	25	0	0	0	0
9	C	15	0	0	0	0
10	B	1	0	0	0	0
10	D	1	0	0	0	0
11	B	14	0	13	0	0
11	D	14	0	13	0	0
12	B	38	0	0	0	0
12	D	38	0	0	0	0
13	C	1	0	0	0	0
14	A	334	0	0	0	0
14	B	145	0	0	0	0
14	C	231	0	0	0	0
14	D	166	0	0	2	0
14	E	18	0	0	0	0
14	F	17	0	0	0	0
14	H	44	0	0	0	0
14	L	43	0	0	0	0
All	All	22118	0	20236	91	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 2.

All (91) 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)
2:D:417:LYS:HG3	2:D:424:SER:HB3	1.74	0.67
2:D:365:GLU:N	2:D:365:GLU:OE1	2.26	0.66
2:D:292:LEU:HD22	2:D:325:ILE:HD11	1.83	0.59
3:E:62:PRO:HA	3:E:65:GLN:HG2	1.85	0.59
3:H:12:VAL:HG21	3:H:86:LEU:HD13	1.88	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:CYS:HA	1:A:130:CYS:HA	1.88	0.55
2:D:306:LEU:HB3	2:D:328:THR:HG22	1.87	0.55
2:D:176:PRO:O	2:D:214:ARG:NH1	2.40	0.53
2:B:39:ASP:OD1	2:B:40:LEU:N	2.36	0.53
4:F:193:THR:HG23	4:F:206:VAL:HG13	1.89	0.53
3:E:30:LYS:HG3	3:E:54:ALA:HA	1.90	0.53
1:A:281:ARG:HD2	5:G:4:BMA:H62	1.90	0.52
1:C:83:THR:HB	1:C:116:LEU:HB2	1.92	0.52
1:C:107:CYS:HA	1:C:130:CYS:HA	1.92	0.51
3:H:125:PRO:HB3	3:H:151:TYR:HB3	1.93	0.50
4:L:37:GLN:HB2	4:L:47:LEU:HD11	1.94	0.50
3:H:91:THR:HG23	3:H:116:THR:HA	1.94	0.50
3:H:177:GLN:N	3:H:180:LEU:O	2.44	0.50
2:B:126:ASP:OD1	2:B:126:ASP:N	2.43	0.50
3:E:102:ASP:HB3	3:E:105:ALA:HB2	1.94	0.50
1:A:262:TRP:HB3	2:B:317:LEU:HD13	1.94	0.49
1:A:436:ILE:HG22	1:A:447:VAL:HG22	1.94	0.49
2:D:319:GLN:HA	2:D:330:VAL:HG21	1.95	0.49
3:E:149:LYS:NZ	4:F:180:THR:HG21	2.28	0.49
1:A:9:THR:HB	1:A:447:VAL:HB	1.94	0.48
2:D:12:SER:HB3	2:D:461:ARG:HD3	1.95	0.48
3:E:144:LEU:HD13	3:E:216:ILE:HG21	1.95	0.48
2:D:418:PRO:HB2	2:D:421:PHE:CD1	2.49	0.47
4:F:195:GLU:HG2	4:F:206:VAL:HG22	1.95	0.47
1:C:235:TRP:CZ2	1:C:270:LEU:HD11	2.48	0.47
1:C:394:GLY:HA2	1:C:399:LEU:HD23	1.96	0.47
2:B:12:SER:HB3	2:B:461:ARG:HD3	1.96	0.47
2:D:390:LYS:NZ	3:H:73:ASP:OD1	2.47	0.47
2:B:21:PRO:O	2:B:93:ARG:NH1	2.48	0.46
2:B:319[A]:GLN:HA	2:B:330:VAL:HG21	1.97	0.46
1:A:377:ALA:HB2	1:A:421:LEU:HD11	1.97	0.46
3:H:102:ASP:HB3	3:H:105:ALA:HB2	1.97	0.46
2:D:235:LYS:HE3	2:D:276:GLY:O	2.15	0.46
2:B:319[B]:GLN:HA	2:B:330:VAL:HG21	1.98	0.46
1:C:187:GLY:HA2	1:C:191:PHE:HA	1.97	0.46
2:B:130:SER:OG	2:B:336:ASP:O	2.34	0.45
2:D:329:THR:O	14:D:2101:HOH:O	2.21	0.45
3:H:98:ARG:HG3	3:H:108:TYR:HB2	1.97	0.45
4:L:4:MET:HE1	4:L:90:GLN:HB3	1.99	0.45
5:G:3:BMA:H62	5:G:5:BMA:H2	1.58	0.44
2:B:139:ALA:HB2	2:B:200:VAL:HG11	1.98	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:213:ASP:OD1	3:H:213:ASP:N	2.47	0.44
1:C:390:LEU:HD23	1:C:403:PRO:HG3	1.99	0.44
1:C:9:THR:HB	1:C:447:VAL:HB	2.00	0.44
2:D:164:TYR:O	2:D:215:ASN:HB2	2.18	0.44
1:A:277:LEU:O	1:A:278[B]:HIS:ND1	2.50	0.44
2:B:313:ASN:ND2	2:B:314:VAL:HG13	2.33	0.43
2:D:329:THR:HG23	2:D:350:LYS:HD2	1.99	0.43
3:E:7:SER:HB3	3:E:21:SER:HB3	2.00	0.43
3:E:219:ARG:CZ	4:F:119:PRO:HG2	2.48	0.43
2:B:311:THR:HA	2:B:333:LEU:O	2.18	0.43
4:L:195:GLU:HG2	4:L:206:VAL:HG22	1.99	0.43
1:C:87:PHE:HB2	1:C:112:HIS:HB2	2.01	0.43
1:C:377:ALA:HB2	1:C:421:LEU:HD11	2.00	0.43
2:D:288:ASP:OD1	2:D:289:TYR:N	2.50	0.43
1:C:303:ARG:HH22	1:C:335:ARG:HE	1.67	0.43
3:E:152:PHE:HA	3:E:153:PRO:HA	1.74	0.43
2:B:96:ASP:OD1	2:B:97:SER:N	2.44	0.42
4:F:4:MET:HE1	4:F:90:GLN:HB3	2.01	0.42
2:B:117:LEU:HD11	2:B:225:ALA:HB1	2.01	0.42
2:B:249:THR:HA	2:B:309:ALA:O	2.19	0.42
2:B:400:GLU:HB2	6:I:1:NAG:H83	2.02	0.42
2:D:365:GLU:OE2	2:D:407:PRO:HB3	2.19	0.42
1:A:3:LEU:O	1:A:5:PRO:HD3	2.19	0.42
1:C:45:PRO:HD3	1:C:72:LEU:HD12	2.02	0.42
2:D:157:VAL:O	2:D:220:GLU:HB3	2.20	0.42
2:D:142:MET:HB2	2:D:149:LEU:HD22	2.02	0.42
1:C:215:HIS:CE1	3:E:32:THR:HG22	2.55	0.41
1:C:77:ARG:NH2	3:E:102:ASP:OD2	2.45	0.41
1:A:314:MET:HB3	1:A:322:LEU:HB3	2.02	0.41
1:C:2:ASN:N	1:C:2:ASN:OD1	2.54	0.41
1:C:311:PRO:O	1:C:355:ARG:HA	2.20	0.41
1:C:432:TYR:CZ	1:C:452:PRO:HA	2.55	0.41
2:D:352:ARG:NH1	14:D:2113:HOH:O	2.51	0.41
3:E:213:ASP:OD1	3:E:213:ASP:N	2.53	0.41
1:C:109:PRO:O	1:C:168:GLU:HA	2.20	0.41
2:D:245:LEU:HD11	2:D:348:TYR:HD1	1.86	0.41
3:E:205:HIS:CE1	3:E:207:ALA:HB3	2.56	0.41
1:A:297:ASP:O	1:A:372:ASN:HB2	2.21	0.41
1:C:112:HIS:CD2	2:D:167:ILE:HD11	2.56	0.41
4:F:47:LEU:HA	4:F:58:VAL:HG21	2.02	0.41
1:A:121:GLU:HG3	1:A:123:GLU:H	1.85	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:TRP:CZ2	1:A:270:LEU:HD11	2.55	0.40
1:C:258:PRO:HA	1:C:289:PHE:O	2.21	0.40
1:C:192:LEU:HD11	1:C:231:PHE:CD1	2.57	0.40
3:E:170:HIS:CE1	4:F:174:SER:HG	2.39	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	456/457 (100%)	444 (97%)	12 (3%)	0	100	100
1	C	454/457 (99%)	438 (96%)	16 (4%)	0	100	100
2	B	468/472 (99%)	446 (95%)	21 (4%)	1 (0%)	47	68
2	D	470/472 (100%)	452 (96%)	18 (4%)	0	100	100
3	E	210/221 (95%)	197 (94%)	13 (6%)	0	100	100
3	H	212/221 (96%)	203 (96%)	9 (4%)	0	100	100
4	F	212/214 (99%)	201 (95%)	10 (5%)	1 (0%)	29	48
4	L	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
All	All	2694/2728 (99%)	2587 (96%)	105 (4%)	2 (0%)	51	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	375	LEU
4	F	138	ASN

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	366/364 (100%)	361 (99%)	5 (1%)	67	86
1	C	364/364 (100%)	361 (99%)	3 (1%)	81	93
2	B	416/417 (100%)	414 (100%)	2 (0%)	88	96
2	D	417/417 (100%)	413 (99%)	4 (1%)	76	90
3	E	186/190 (98%)	186 (100%)	0	100	100
3	H	187/190 (98%)	186 (100%)	1 (0%)	88	96
4	F	188/188 (100%)	187 (100%)	1 (0%)	88	96
4	L	188/188 (100%)	188 (100%)	0	100	100
All	All	2312/2318 (100%)	2296 (99%)	16 (1%)	84	94

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	61	GLU
1	A	166	TYR
1	A	270	LEU
1	A	288	TYR
2	B	128	LEU
2	B	215	ASN
1	C	23	LEU
1	C	166	TYR
1	C	288	TYR
2	D	127	ASP
2	D	128	LEU
2	D	180	MET
2	D	341	LEU
4	F	181	LEU
3	H	213	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	GLN
2	B	301	GLN
1	C	197	GLN
1	C	219	GLN
2	D	301	GLN
2	D	408	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

13 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	$\# Z  > 2$
5	NAG	G	1	5,2	14,14,15	0.32	0	17,19,21	0.48	0
5	NAG	G	2	5	14,14,15	0.20	0	17,19,21	0.52	0
5	BMA	G	3	5	11,11,12	1.46	3 (27%)	15,15,17	1.94	3 (20%)
5	BMA	G	4	5	11,11,12	1.01	1 (9%)	15,15,17	1.27	2 (13%)
5	BMA	G	5	5	11,11,12	0.98	1 (9%)	15,15,17	1.41	2 (13%)
6	NAG	I	1	2,6	14,14,15	0.24	0	17,19,21	0.44	0
6	NAG	I	2	6	14,14,15	0.26	0	17,19,21	0.40	0
7	NAG	J	1	2,7	14,14,15	0.29	0	17,19,21	0.47	0
7	NAG	J	2	7	14,14,15	0.21	0	17,19,21	0.56	0
7	BMA	J	3	7	11,11,12	0.99	0	15,15,17	1.45	2 (13%)
7	BMA	J	4	7	11,11,12	0.83	0	15,15,17	1.24	2 (13%)
6	NAG	K	1	2,6	14,14,15	0.31	0	17,19,21	0.46	0
6	NAG	K	2	6	14,14,15	0.24	0	17,19,21	0.42	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
5	NAG	G	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	2/2/19/22	0/1/1/1
5	BMA	G	4	5	-	0/2/19/22	0/1/1/1
5	BMA	G	5	5	-	2/2/19/22	0/1/1/1
6	NAG	I	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	4/6/23/26	0/1/1/1
7	NAG	J	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	J	2	7	-	0/6/23/26	0/1/1/1
7	BMA	J	3	7	-	1/2/19/22	0/1/1/1
7	BMA	J	4	7	-	0/2/19/22	0/1/1/1
6	NAG	K	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	3	BMA	O5-C5	3.01	1.49	1.43
5	G	3	BMA	C2-C3	2.40	1.56	1.52
5	G	5	BMA	C4-C5	2.31	1.57	1.53
5	G	3	BMA	O3-C3	2.05	1.47	1.43
5	G	4	BMA	C4-C3	2.03	1.57	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	3	BMA	O5-C5-C6	4.58	114.38	107.20
5	G	3	BMA	O3-C3-C2	4.52	118.64	109.99
7	J	3	BMA	O3-C3-C2	4.33	118.28	109.99
5	G	5	BMA	C1-C2-C3	-3.63	105.20	109.67
7	J	4	BMA	O5-C1-C2	-2.89	106.31	110.77
5	G	4	BMA	O5-C1-C2	-2.59	106.78	110.77
5	G	5	BMA	O5-C1-C2	-2.54	106.85	110.77
7	J	3	BMA	C1-C2-C3	-2.36	106.77	109.67
5	G	4	BMA	C1-C2-C3	-2.26	106.88	109.67
5	G	3	BMA	C1-C2-C3	-2.14	107.04	109.67
7	J	4	BMA	C1-C2-C3	-2.04	107.16	109.67

There are no chirality outliers.

All (13) torsion outliers are listed below:

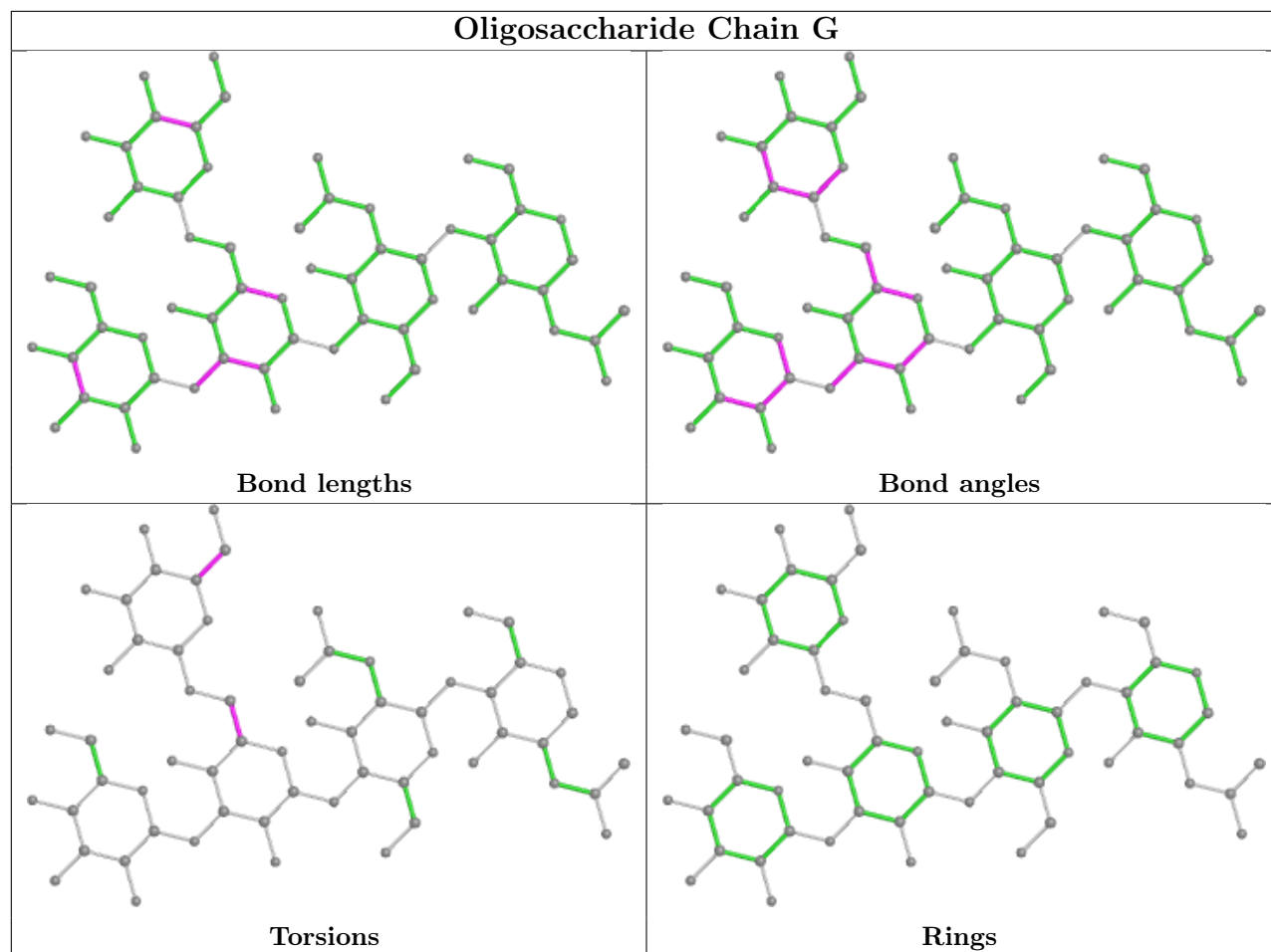
Mol	Chain	Res	Type	Atoms
5	G	3	BMA	O5-C5-C6-O6
5	G	5	BMA	C4-C5-C6-O6
5	G	3	BMA	C4-C5-C6-O6
5	G	5	BMA	O5-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6
6	I	2	NAG	C8-C7-N2-C2
6	I	2	NAG	O7-C7-N2-C2
6	K	2	NAG	C8-C7-N2-C2
6	K	2	NAG	O7-C7-N2-C2
6	K	1	NAG	C4-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
7	J	3	BMA	O5-C5-C6-O6
6	I	2	NAG	C4-C5-C6-O6

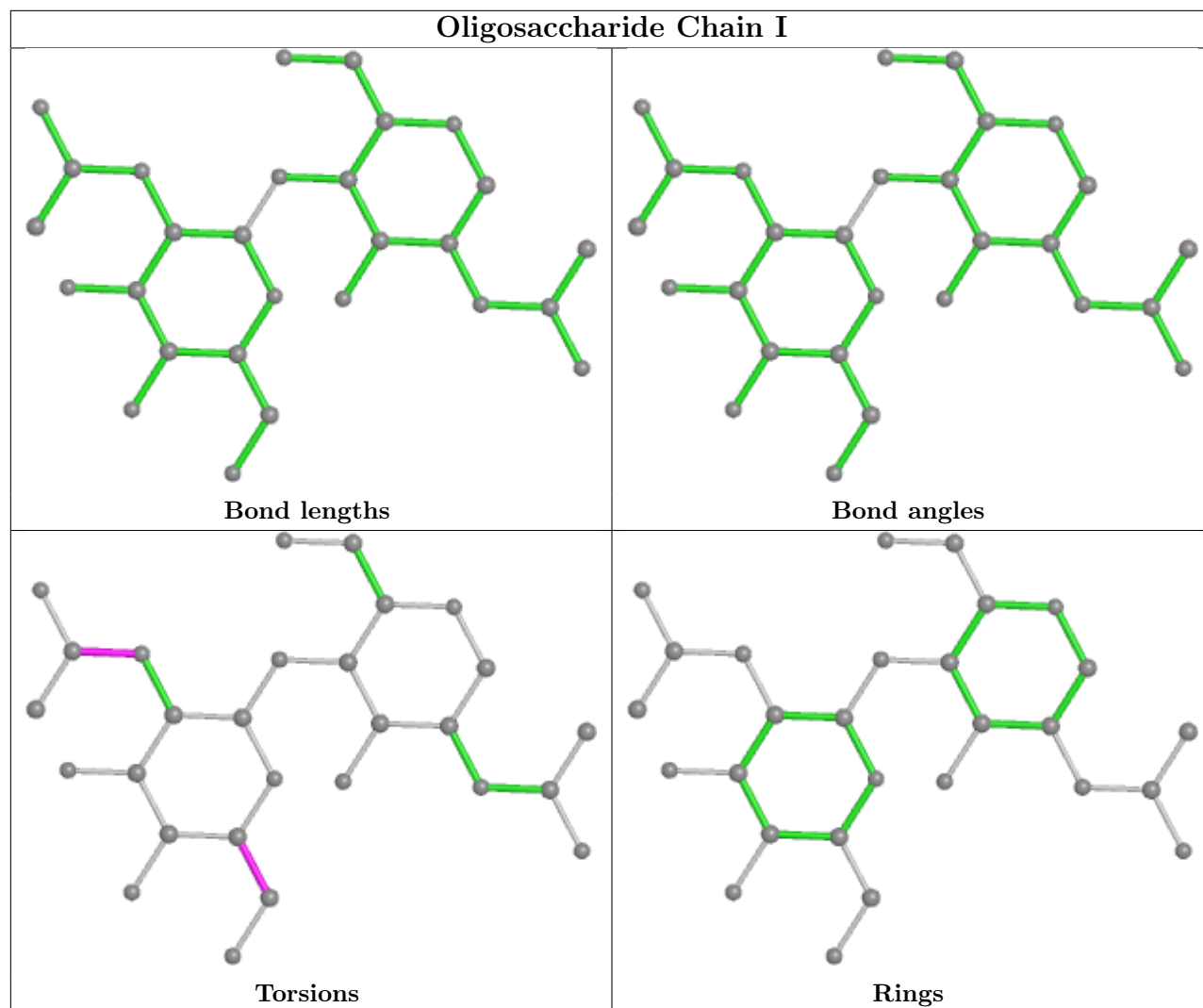
There are no ring outliers.

4 monomers are involved in 3 short contacts:

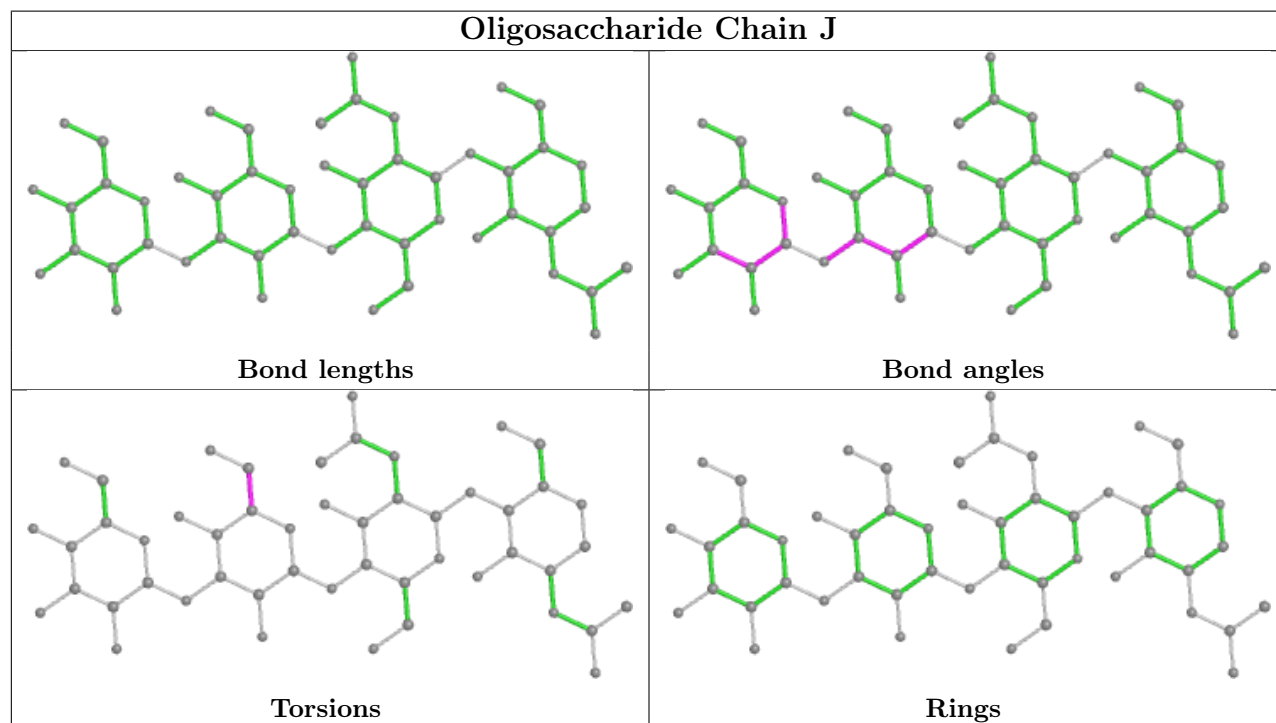
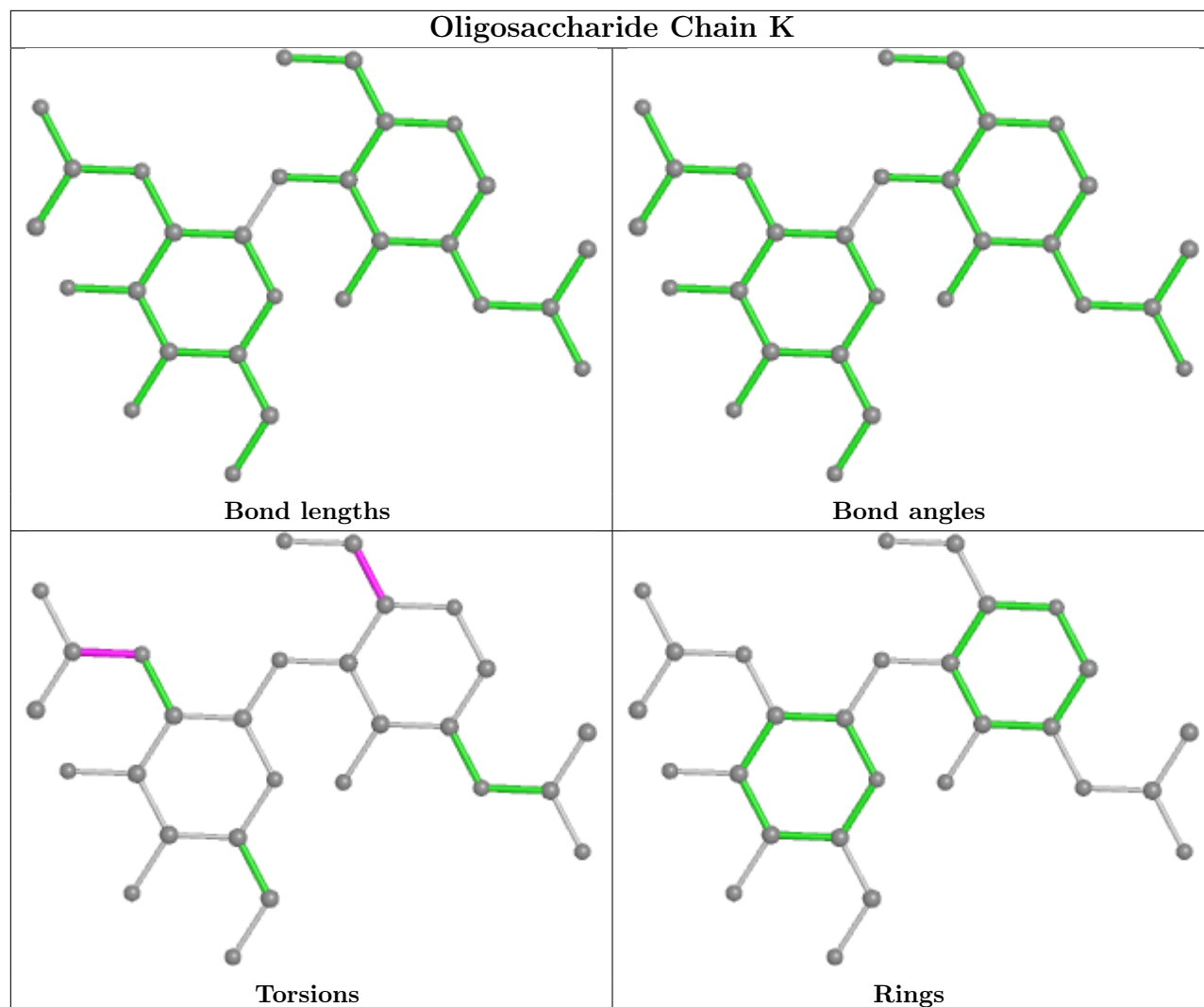
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	4	BMA	1	0
6	I	1	NAG	1	0
5	G	3	BMA	1	0
5	G	5	BMA	1	0

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









## 5.6 Ligand geometry

Of 27 ligands modelled in this entry, 15 are monoatomic - leaving 12 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
9	SO4	A	505	-	4,4,4	0.14	0	6,6,6	0.05	0
9	SO4	C	506	-	4,4,4	0.14	0	6,6,6	0.05	0
11	NAG	B	2004	2	14,14,15	0.40	0	17,19,21	0.52	0
9	SO4	C	507	-	4,4,4	0.14	0	6,6,6	0.05	0
12	I1F	B	2005	10	38,41,41	5.21	19 (50%)	45,58,58	2.44	8 (17%)
12	I1F	D	2005	10	38,41,41	5.22	19 (50%)	45,58,58	2.46	8 (17%)
9	SO4	C	508	-	4,4,4	0.14	0	6,6,6	0.06	0
9	SO4	A	507	-	4,4,4	0.14	0	6,6,6	0.05	0
11	NAG	D	2004	2	14,14,15	0.33	0	17,19,21	0.52	0
9	SO4	A	509	-	4,4,4	0.14	0	6,6,6	0.08	0
9	SO4	A	506	-	4,4,4	0.16	0	6,6,6	0.05	0
9	SO4	A	508	-	4,4,4	0.14	0	6,6,6	0.06	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
11	NAG	D	2004	2	-	2/6/23/26	0/1/1/1
11	NAG	B	2004	2	-	0/6/23/26	0/1/1/1
12	I1F	D	2005	10	-	2/30/41/41	0/4/4/4
12	I1F	B	2005	10	-	4/30/41/41	0/4/4/4

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	2005	I1F	C34-N29	-14.20	1.20	1.35
12	D	2005	I1F	C34-N29	-14.04	1.20	1.35
12	D	2005	I1F	C27-N28	12.88	1.51	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	2005	I1F	C27-N28	12.86	1.51	1.34
12	D	2005	I1F	C35-C27	10.91	1.57	1.41
12	B	2005	I1F	C35-C27	10.90	1.57	1.41
12	D	2005	I1F	O19-N17	8.76	1.37	1.22
12	B	2005	I1F	O19-N17	8.76	1.37	1.22
12	D	2005	I1F	C15-C14	7.79	1.52	1.38
12	B	2005	I1F	C15-C14	7.67	1.52	1.38
12	D	2005	I1F	C06-C05	7.52	1.52	1.38
12	D	2005	I1F	C38-C04	7.39	1.51	1.39
12	B	2005	I1F	C38-C04	7.35	1.51	1.39
12	B	2005	I1F	C06-C05	7.26	1.52	1.38
12	D	2005	I1F	C37-C07	7.25	1.51	1.39
12	B	2005	I1F	C37-C07	7.24	1.51	1.39
12	B	2005	I1F	C20-C16	7.13	1.52	1.38
12	D	2005	I1F	C20-C16	7.11	1.52	1.38
12	D	2005	I1F	C22-N24	6.76	1.44	1.34
12	B	2005	I1F	C22-N24	6.58	1.44	1.34
12	D	2005	I1F	C21-C13	6.21	1.52	1.38
12	B	2005	I1F	C21-C13	6.20	1.52	1.38
12	D	2005	I1F	C26-C27	-4.93	1.42	1.50
12	B	2005	I1F	C26-C27	-4.79	1.43	1.50
12	D	2005	I1F	C08-N10	4.23	1.43	1.34
12	B	2005	I1F	C08-N10	4.13	1.43	1.34
12	D	2005	I1F	C36-C35	3.81	1.59	1.51
12	B	2005	I1F	C36-C35	3.72	1.59	1.51
12	D	2005	I1F	C36-N24	3.12	1.51	1.46
12	D	2005	I1F	C04-C02	3.07	1.53	1.47
12	B	2005	I1F	C36-N24	3.06	1.51	1.46
12	B	2005	I1F	C04-C02	2.89	1.52	1.47
12	B	2005	I1F	C25-C26	-2.72	1.46	1.51
12	D	2005	I1F	C25-C26	-2.63	1.46	1.51
12	B	2005	I1F	C06-C07	-2.27	1.35	1.39
12	B	2005	I1F	C05-C04	-2.21	1.35	1.39
12	D	2005	I1F	C06-C07	-2.11	1.35	1.39
12	D	2005	I1F	C05-C04	-2.10	1.35	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	2005	I1F	C26-C25-N24	9.82	121.61	110.04
12	B	2005	I1F	C26-C25-N24	8.92	120.55	110.04
12	B	2005	I1F	C34-N29-N28	7.00	116.93	111.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	2005	I1F	C34-N29-N28	6.41	116.47	111.45
12	B	2005	I1F	C30-N29-C34	-6.25	121.22	129.19
12	D	2005	I1F	C30-N29-C34	-6.10	121.41	129.19
12	B	2005	I1F	C35-C36-N24	-5.97	102.51	111.35
12	D	2005	I1F	C35-C36-N24	-4.99	103.96	111.35
12	D	2005	I1F	C34-C35-C27	-4.35	99.89	104.71
12	B	2005	I1F	C34-C35-C27	-4.01	100.26	104.71
12	D	2005	I1F	C35-C34-N29	3.78	112.04	107.58
12	B	2005	I1F	C35-C34-N29	3.39	111.58	107.58
12	B	2005	I1F	C36-C35-C34	2.78	137.43	129.11
12	D	2005	I1F	C36-C35-C34	2.75	137.34	129.11
12	D	2005	I1F	O32-C31-C30	2.43	120.53	112.29
12	B	2005	I1F	O32-C31-C30	2.21	119.78	112.29

There are no chirality outliers.

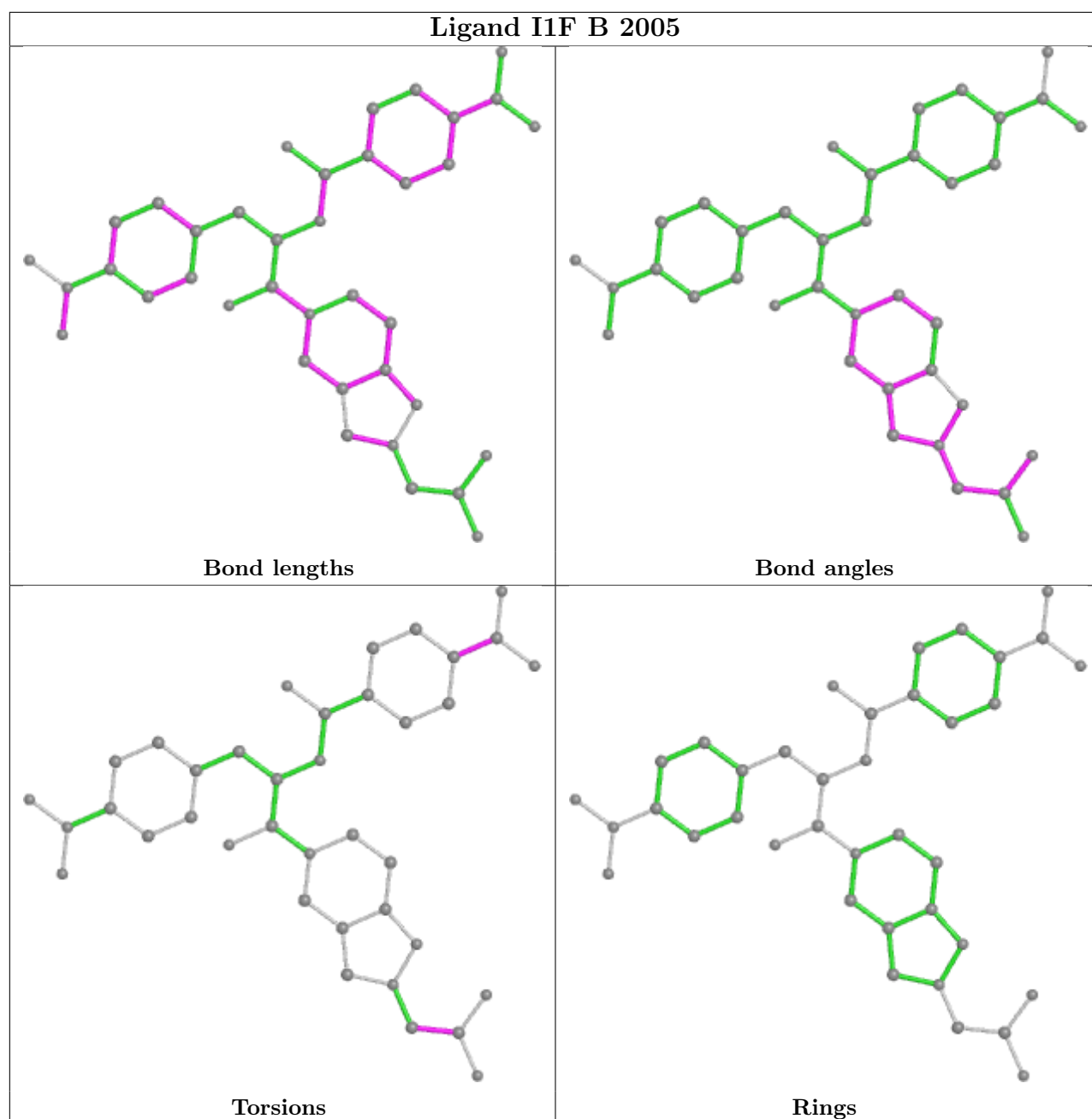
All (8) torsion outliers are listed below:

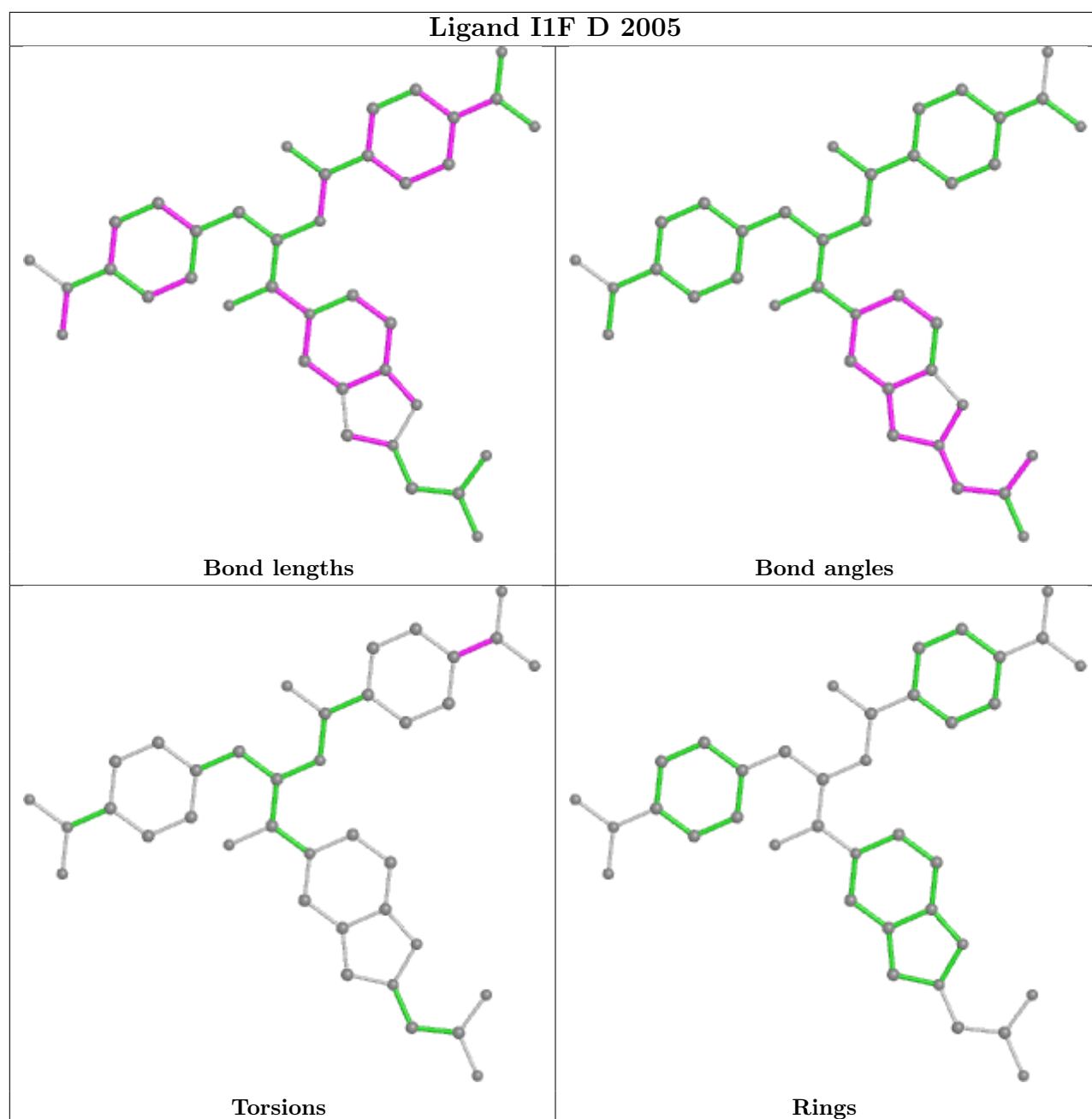
Mol	Chain	Res	Type	Atoms
12	B	2005	I1F	N01-C02-C04-C05
12	B	2005	I1F	N01-C02-C04-C38
12	D	2005	I1F	N01-C02-C04-C05
12	D	2005	I1F	N01-C02-C04-C38
11	D	2004	NAG	O5-C5-C6-O6
11	D	2004	NAG	C4-C5-C6-O6
12	B	2005	I1F	N29-C30-C31-O33
12	B	2005	I1F	N29-C30-C31-O32

There are no ring outliers.

No monomer is involved in short contacts.

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

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	453/457 (99%)	0.17	5 (1%) 80 82	22, 35, 57, 93	1 (0%)
1	C	453/457 (99%)	0.16	6 (1%) 77 79	27, 47, 75, 110	1 (0%)
2	B	466/472 (98%)	0.76	61 (13%) 3 3	25, 62, 128, 152	1 (0%)
2	D	471/472 (99%)	0.40	41 (8%) 10 10	31, 58, 107, 142	1 (0%)
3	E	214/221 (96%)	1.25	62 (28%) 0 0	52, 92, 121, 149	0
3	H	216/221 (97%)	0.59	33 (15%) 2 1	41, 72, 122, 131	0
4	F	214/214 (100%)	1.58	68 (31%) 0 0	59, 89, 160, 173	0
4	L	214/214 (100%)	0.12	5 (2%) 60 63	43, 64, 92, 140	0
All	All	2701/2728 (99%)	0.54	281 (10%) 6 6	22, 57, 121, 173	4 (0%)

All (281) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	193	THR	10.7
3	E	133	VAL	10.2
4	F	209	PHE	10.0
2	B	33	LEU	9.0
4	F	148	TRP	8.7
2	B	48	ASN	8.1
4	F	214	CYS	8.1
2	B	466	TRP	8.0
4	F	146	VAL	7.8
4	F	150	ILE	7.4
4	F	192	TYR	7.3
2	B	49	CYS	7.1
4	F	144	ILE	7.0
2	B	450	ASN	7.0
4	F	191	SER	6.9
3	E	132	PRO	6.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	D	44	LEU	6.8
3	E	212	VAL	6.7
2	B	36	PRO	6.5
2	B	44	LEU	6.5
2	B	31	LEU	6.5
4	F	186	TYR	6.5
3	E	127	VAL	6.5
4	F	212	ASN	6.4
4	F	130	ALA	6.4
2	B	2	PRO	6.3
2	B	6	THR	6.2
4	F	155	ARG	6.1
2	B	10	VAL	6.1
4	F	181	LEU	6.1
3	E	176	LEU	6.1
3	H	160	TRP	6.0
3	E	189	VAL	6.0
4	L	214	CYS	5.9
2	B	35	SER	5.9
3	H	216	ILE	5.8
2	D	376	ASN	5.7
3	E	134	CYS	5.6
2	B	4	ILE	5.6
3	H	165	LEU	5.5
3	E	85	SER	5.5
2	B	1	GLY	5.3
2	B	46	LYS	5.3
4	F	179	LEU	5.3
2	D	36	PRO	5.3
2	B	28	ASP	5.3
3	E	128	TYR	5.2
4	F	182	THR	5.2
4	F	127	SER	5.1
4	F	194	CYS	5.1
2	B	34	GLY	5.1
2	D	45	LEU	5.0
2	B	181	LYS	4.9
2	B	32	PRO	4.9
2	B	25	TRP	4.9
4	F	180	THR	4.8
4	F	133	VAL	4.8
2	B	26	CYS	4.8

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	8	ARG	4.8
2	B	30	ALA	4.8
2	B	7	THR	4.7
4	F	132	VAL	4.7
2	D	375	LEU	4.7
2	D	33	LEU	4.6
4	F	160	LEU	4.6
4	F	157	ASN	4.5
3	H	212	VAL	4.5
4	F	131	SER	4.5
3	E	183	LEU	4.5
3	E	131	ALA	4.5
2	B	54	ILE	4.4
2	B	50	ALA	4.4
4	F	147	LYS	4.4
4	F	196	ALA	4.3
2	D	46	LYS	4.3
3	E	84	SER	4.3
4	F	178	THR	4.3
2	B	375	LEU	4.3
2	B	24	ALA	4.3
2	D	35	SER	4.2
4	L	212	ASN	4.2
3	E	144	LEU	4.2
2	B	47	ASP	4.1
2	B	38	CYS	4.1
1	C	453	VAL	4.1
2	B	37	ARG	4.1
2	D	471	CYS	4.1
2	B	27	SER	4.0
2	D	383	LEU	4.0
4	F	205	ILE	4.0
3	E	194	TRP	4.0
2	B	9	GLY	4.0
2	D	48	ASN	4.0
4	F	149	LYS	4.0
3	H	144	LEU	3.9
3	H	200	THR	3.9
4	F	126	THR	3.9
2	B	376	ASN	3.8
4	F	118	PHE	3.8
3	E	153	PRO	3.8

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	F	188	ARG	3.8
4	F	128	GLY	3.8
1	C	335	ARG	3.8
3	H	198	SER	3.8
3	E	149	LYS	3.8
4	F	210	ASN	3.8
3	H	199	ILE	3.8
4	F	208	SER	3.8
3	E	86	LEU	3.8
3	H	187	VAL	3.7
3	E	219	ARG	3.7
3	H	133	VAL	3.7
2	B	51	PRO	3.7
2	B	378	GLU	3.7
3	E	118	SER	3.7
2	D	10	VAL	3.7
2	B	22	MET	3.7
3	E	141	SER	3.6
2	B	379	VAL	3.6
3	E	214	LYS	3.6
4	F	190	ASN	3.6
2	B	45	LEU	3.6
2	B	39	ASP	3.6
4	F	184	ASP	3.5
3	E	17	SER	3.5
3	E	148	VAL	3.5
3	E	177	GLN	3.5
3	H	197	GLN	3.5
2	D	378	GLU	3.5
1	C	339	ALA	3.5
2	D	22	MET	3.5
3	E	216	ILE	3.4
2	B	74	SER	3.4
4	F	135	PHE	3.4
2	D	470	GLN	3.4
4	F	115	VAL	3.4
4	F	207	LYS	3.4
2	D	1	GLY	3.3
4	F	129	GLY	3.3
3	H	134	CYS	3.3
2	B	458	GLY	3.3
3	E	12	VAL	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	H	201	CYS	3.3
3	E	142	VAL	3.3
3	H	195	PRO	3.3
3	E	121	LYS	3.3
2	D	8	ARG	3.2
2	D	54	ILE	3.2
2	D	469	SER	3.2
2	B	79	GLN	3.2
3	E	193	THR	3.2
3	H	142	VAL	3.2
3	E	83	LEU	3.1
4	F	213	GLU	3.1
2	B	41	LYS	3.1
4	F	159	VAL	3.1
3	H	188	THR	3.1
3	H	129	PRO	3.0
4	F	175	MET	3.0
4	F	158	GLY	3.0
2	D	181	LYS	3.0
3	H	189	VAL	3.0
1	A	337	PRO	3.0
3	E	181	TYR	3.0
2	B	11	SER	3.0
3	H	194	TRP	3.0
2	B	5	CYS	3.0
2	D	58	VAL	2.9
2	D	79	GLN	2.9
4	F	145	ASN	2.9
3	H	177	GLN	2.9
3	E	199	ILE	2.9
3	E	215	LYS	2.9
3	E	15	GLY	2.8
2	D	51	PRO	2.8
4	F	117	ILE	2.8
2	B	19	VAL	2.8
2	D	4	ILE	2.8
2	D	39	ASP	2.8
4	F	105	GLU	2.7
3	E	147	LEU	2.7
3	E	180	LEU	2.7
2	D	21	PRO	2.7
4	L	105	GLU	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	E	16	ALA	2.7
4	F	211	ARG	2.7
4	F	197	THR	2.7
3	E	130	LEU	2.7
4	F	195	GLU	2.6
2	D	2	PRO	2.6
3	E	195	PRO	2.6
2	B	29	GLU	2.6
2	D	38	CYS	2.6
3	E	68	ALA	2.6
3	E	117	VAL	2.6
4	F	163	TRP	2.6
1	C	338	HIS	2.6
3	E	151	TYR	2.6
3	H	208	SER	2.6
4	L	213	GLU	2.6
4	F	156	GLN	2.5
2	D	9	GLY	2.5
4	F	187	GLU	2.5
3	H	138	THR	2.5
3	E	203	VAL	2.5
2	B	431	PHE	2.5
3	H	217	GLU	2.5
3	E	192	SER	2.5
3	H	219	ARG	2.5
4	F	200	THR	2.5
3	H	158	LEU	2.5
3	H	215	LYS	2.5
2	B	42	GLU	2.5
3	E	218	PRO	2.5
3	E	126	SER	2.5
3	E	152	PHE	2.5
3	H	196	SER	2.5
4	F	201	SER	2.5
3	E	165	LEU	2.5
4	F	154	GLU	2.5
2	B	295	MET	2.4
2	B	14	GLN	2.4
2	D	31	LEU	2.4
3	E	200	THR	2.4
4	F	173	TYR	2.4
3	H	211	LYS	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	F	134	CYS	2.4
2	D	37	ARG	2.4
4	F	189	HIS	2.4
3	E	179	ASP	2.4
2	D	379	VAL	2.4
2	D	50	ALA	2.4
3	E	116	THR	2.4
3	H	130	LEU	2.4
2	B	12	SER	2.3
3	E	140	SER	2.3
2	B	75	GLY	2.3
2	B	76	ASP	2.3
2	D	32	PRO	2.3
3	E	210	THR	2.3
1	A	338	HIS	2.3
1	C	337	PRO	2.3
4	F	14	SER	2.3
1	A	130	CYS	2.3
2	D	404	ARG	2.3
2	B	77	SER	2.3
4	F	136	LEU	2.3
2	D	67	ARG	2.2
4	F	142	LYS	2.2
1	A	107	CYS	2.2
4	F	125	LEU	2.2
4	F	151	ASP	2.2
2	D	42	GLU	2.2
3	E	67	LYS	2.2
2	D	47	ASP	2.2
2	B	69	LEU	2.2
4	L	210	ASN	2.2
1	A	320	ARG	2.2
2	B	67	ARG	2.2
2	D	381	PRO	2.1
3	E	198	SER	2.1
3	E	66	GLY	2.1
3	H	139	GLY	2.1
3	E	187	VAL	2.1
3	E	190	THR	2.1
3	E	178	SER	2.1
3	H	143	THR	2.1
1	C	340	LEU	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	F	15	LEU	2.1
4	F	153	SER	2.1
3	H	214	LYS	2.1
2	B	107	VAL	2.1
2	D	450	ASN	2.1
3	E	115	VAL	2.0
4	F	13	VAL	2.0
2	B	459	VAL	2.0
3	E	65	GLN	2.0
3	H	159	THR	2.0
2	B	3	ASN	2.0
2	D	34	GLY	2.0
3	E	64	PHE	2.0

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

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

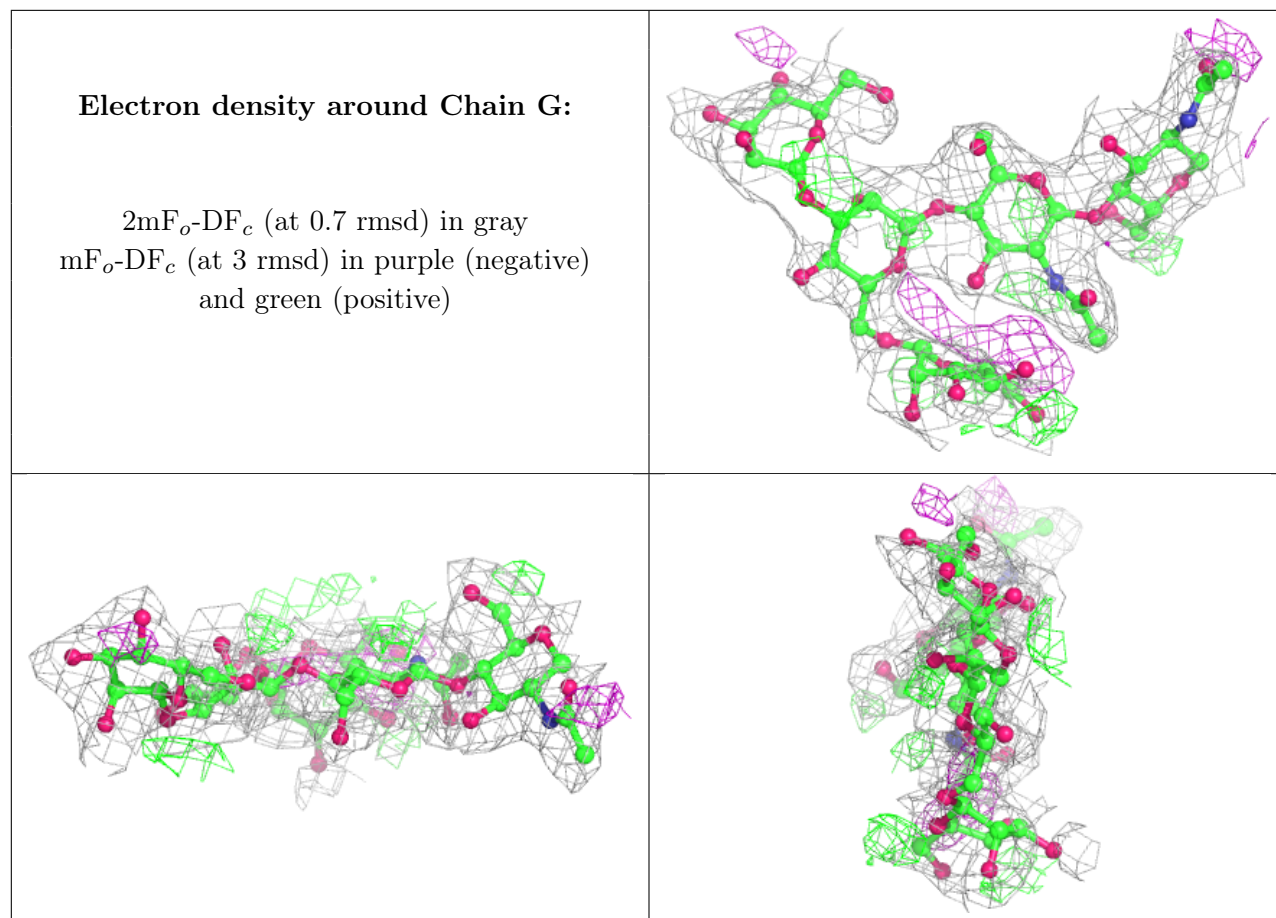
## 6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	BMA	G	5	11/12	0.51	0.33	107,113,120,122	0
7	BMA	J	3	11/12	0.57	0.43	101,113,119,124	0
5	BMA	G	3	11/12	0.71	0.19	93,102,109,113	0
6	NAG	K	2	14/15	0.74	0.37	106,120,129,130	0
5	BMA	G	4	11/12	0.78	0.23	83,91,97,101	0
6	NAG	I	2	14/15	0.83	0.32	118,129,131,132	0
7	BMA	J	4	11/12	0.84	0.31	94,100,112,119	0
6	NAG	K	1	14/15	0.85	0.27	85,101,112,120	0
7	NAG	J	2	14/15	0.86	0.25	66,81,92,104	0
6	NAG	I	1	14/15	0.87	0.25	91,107,114,123	0
5	NAG	G	2	14/15	0.89	0.14	52,78,89,99	0
7	NAG	J	1	14/15	0.90	0.16	44,56,69,74	0
5	NAG	G	1	14/15	0.94	0.13	33,49,63,70	0

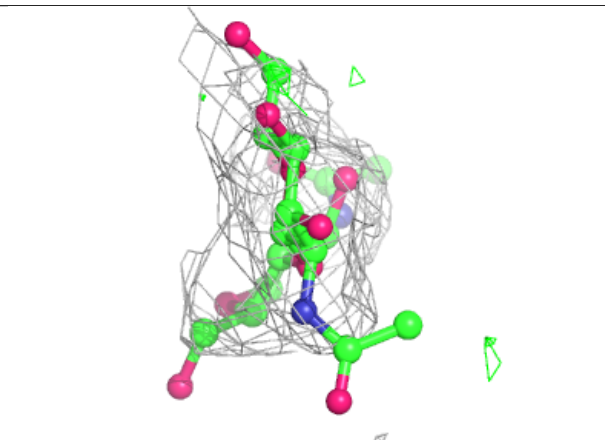
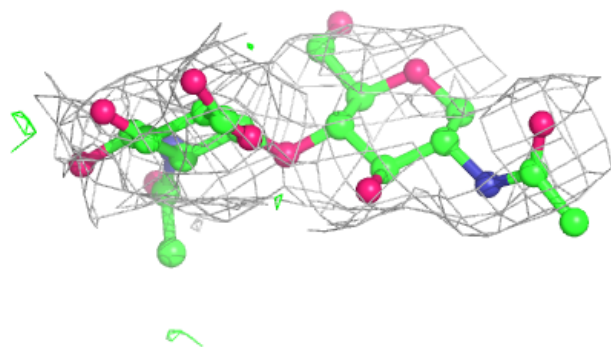
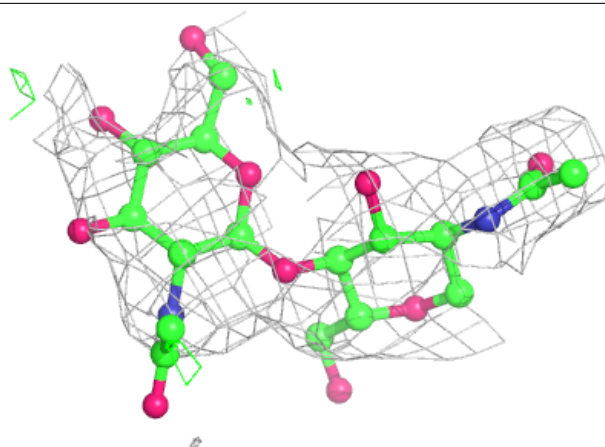
The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

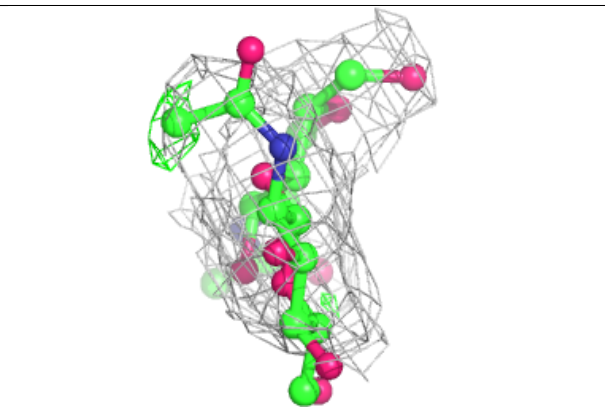
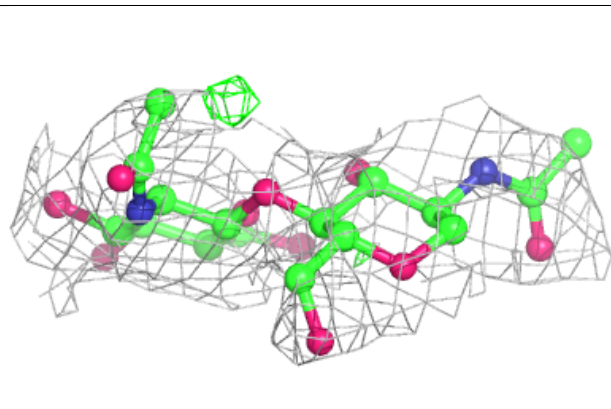
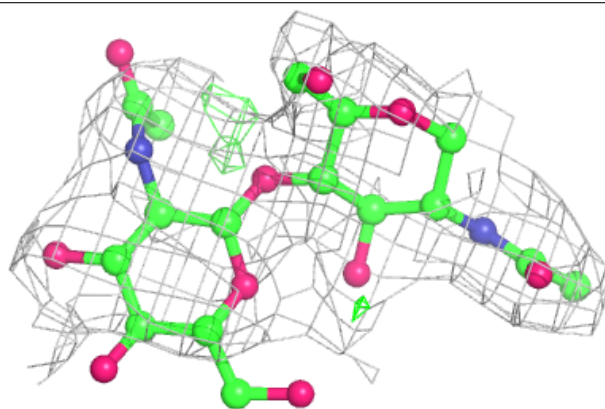


**Electron density around Chain I:**

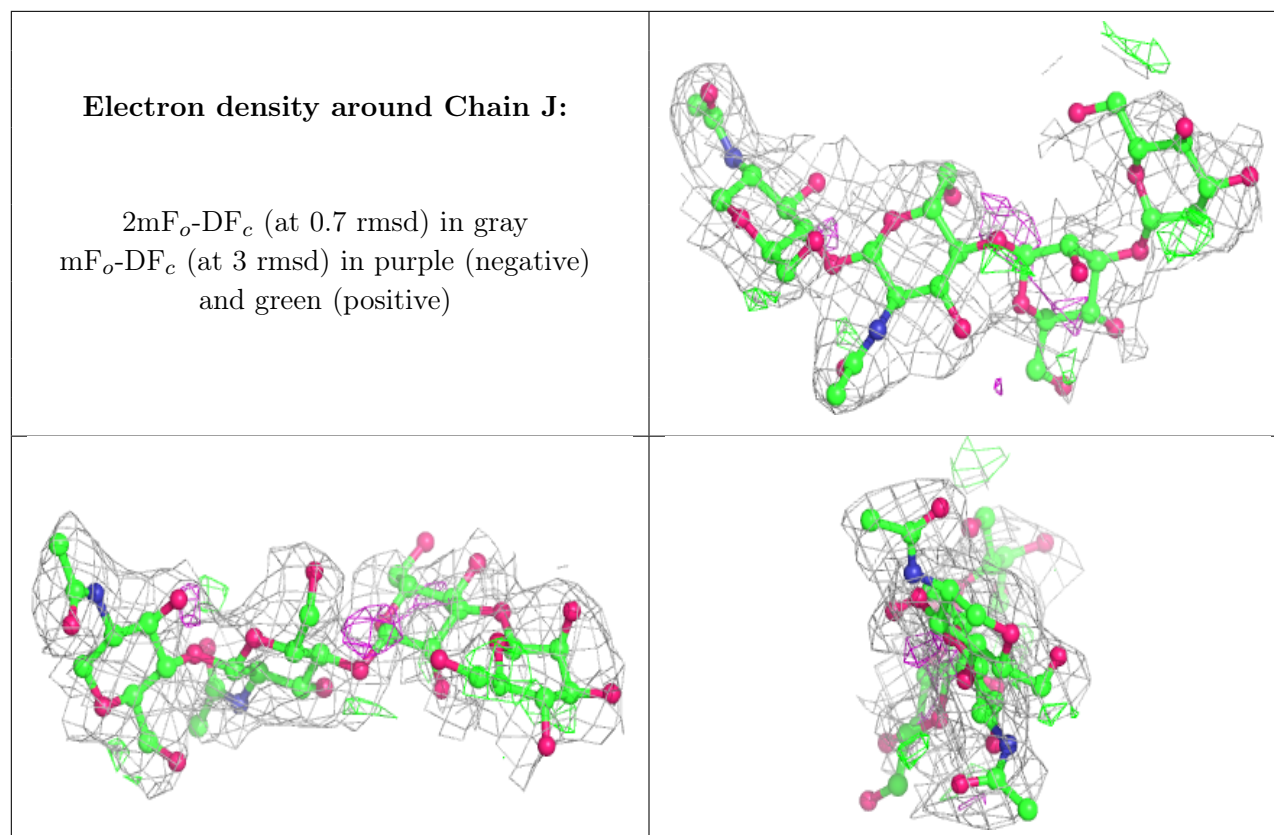
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around Chain K:**

$2mF_o-DF_c$  (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( $\text{\AA}^2$ )	Q<0.9
13	CL	C	501	1/1	0.67	0.37	92,92,92,92	0
10	MG	B	2001	1/1	0.85	0.18	21,21,21,21	0
9	SO4	C	506	5/5	0.86	0.14	76,85,90,93	0
11	NAG	B	2004	14/15	0.86	0.28	90,105,118,120	0
11	NAG	D	2004	14/15	0.86	0.29	84,103,109,115	0
9	SO4	C	507	5/5	0.86	0.13	88,98,100,104	0
8	CA	C	502	1/1	0.90	0.09	60,60,60,60	0
8	CA	C	503	1/1	0.92	0.06	58,58,58,58	0
9	SO4	A	505	5/5	0.93	0.11	68,72,77,83	0
9	SO4	C	508	5/5	0.94	0.10	66,68,74,83	5
9	SO4	A	506	5/5	0.94	0.11	69,70,73,80	0
9	SO4	A	508	5/5	0.94	0.14	80,84,88,94	0
8	CA	C	504	1/1	0.94	0.08	56,56,56,56	0
12	IIF	D	2005	38/38	0.94	0.19	28,42,71,74	0

*Continued on next page...*

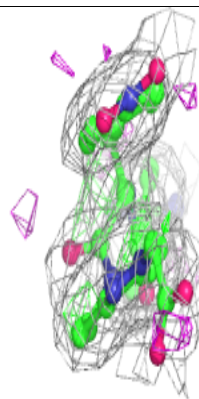
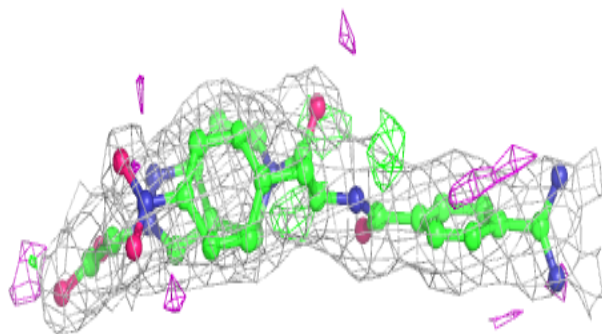
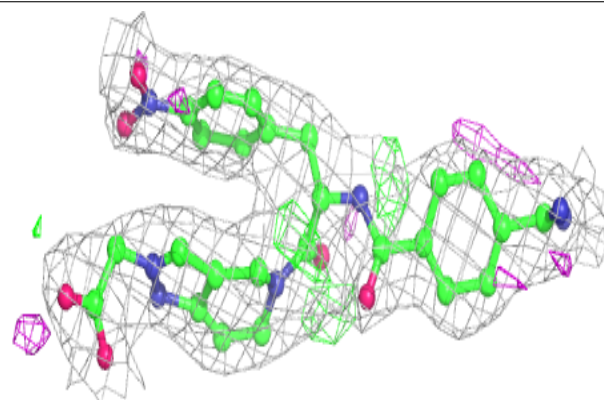
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	CA	A	503	1/1	0.94	0.12	28,28,28,28	0
8	CA	B	2002	1/1	0.95	0.15	43,43,43,43	0
8	CA	A	501	1/1	0.95	0.09	41,41,41,41	0
12	I1F	B	2005	38/38	0.95	0.17	21,37,53,68	0
9	SO4	A	507	5/5	0.95	0.12	62,80,86,88	0
8	CA	D	2002	1/1	0.95	0.17	40,40,40,40	0
10	MG	D	2001	1/1	0.96	0.15	23,23,23,23	0
9	SO4	A	509	5/5	0.96	0.16	50,58,63,67	0
8	CA	C	505	1/1	0.97	0.09	52,52,52,52	0
8	CA	D	2003	1/1	0.98	0.10	34,34,34,34	0
8	CA	A	502	1/1	0.98	0.10	31,31,31,31	0
8	CA	B	2003	1/1	0.99	0.20	32,32,32,32	0
8	CA	A	504	1/1	0.99	0.16	31,31,31,31	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.

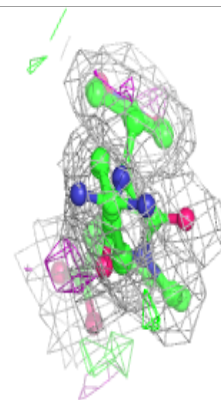
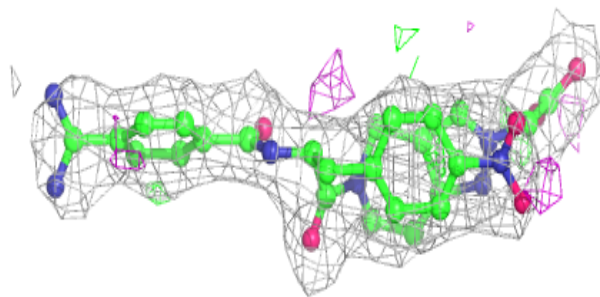
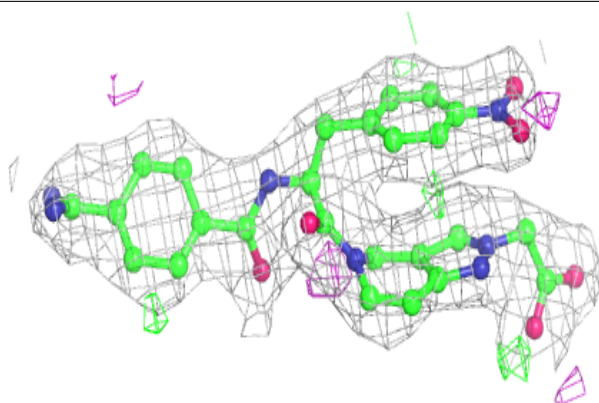
**Electron density around I1F D 2005:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around I1F B 2005:**

$2mF_o - DF_c$  (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.