



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2023 – 02:07 PM EDT

PDB ID : 7U9F  
Title : Integrin  $\alpha$ IIB $\beta$ 3 complex with BMS compound 4 in Mn<sup>2+</sup>  
Authors : Lin, F.-Y.; Zhu, J.; Zhu, J.; Springer, T.A.  
Deposited on : 2022-03-10  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

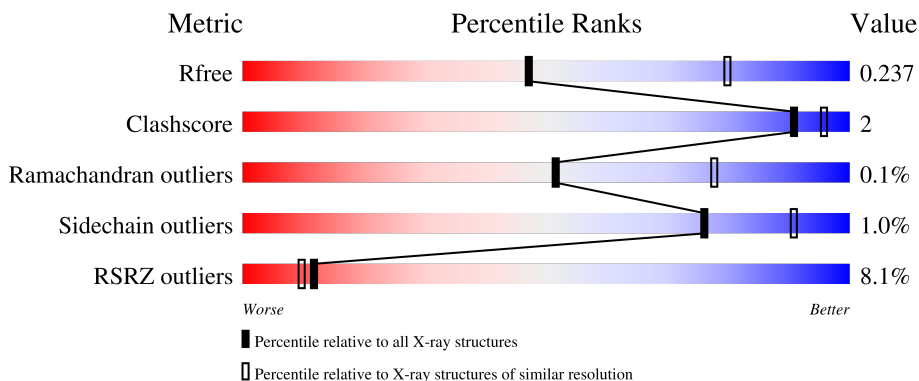
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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.



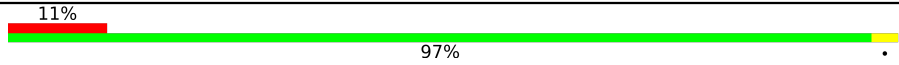
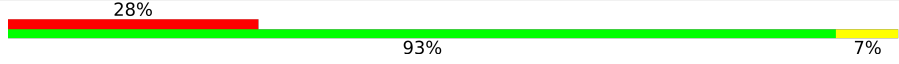
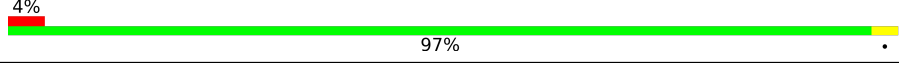
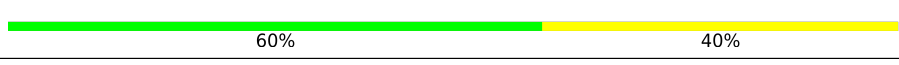
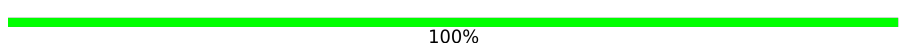

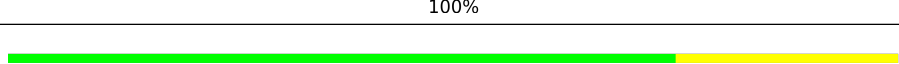
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	454	 95% 5%
1	C	454	 93% 7%
2	B	471	 93% 6% 5%
2	D	471	 94% 6% 7%
3	E	216	 94% 5% 29%

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Mol	Chain	Length	Quality of chain
3	H	216	 <p>11% 97% 7%</p>
4	F	214	 <p>28% 93% 7%</p>
4	L	214	 <p>4% 97% 7%</p>
5	G	5	 <p>60% 40%</p>
6	I	2	 <p>100%</p>
6	K	2	 <p>100%</p>
7	J	4	 <p>75% 25%</p>

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 22211 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	454	Total	C	N	O	S	0	4	0
			3499	2226	601	664	8			
1	C	453	Total	C	N	O	S	0	4	0
			3502	2224	604	666	8			

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	466	Total	C	N	O	S	4	4	0
			3618	2252	617	715	34			
2	D	471	Total	C	N	O	S	3	0	0
			3623	2255	619	715	34			

- Molecule 3 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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 alpha-D-mannopyranose-(1-3)-[alpha-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
			Total	C	N	O			
5	G	5	61	34	2	25	0	0	0

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

- Molecule 7 is an oligosaccharide called alpha-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
			Total	C	N	O			
7	J	4	50	28	2	20	0	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

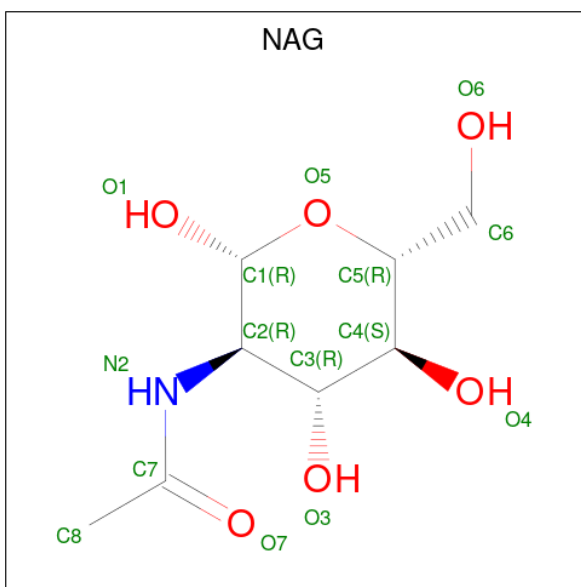
- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	4	Total	Ca	0	0
			4	4		
9	C	4	Total	Ca	0	0
			4	4		

- Molecule 10 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

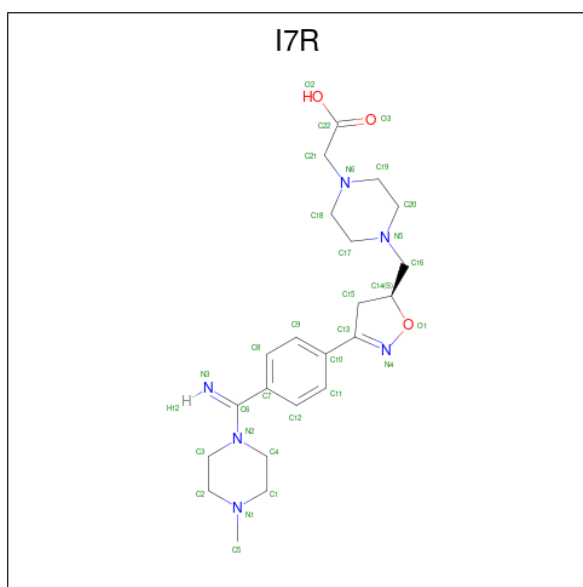
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	3	Total	Mn	0	0
			3	3		
10	D	3	Total	Mn	0	0
			3	3		

- 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 (4-{(5S)-3-{4-[(E)-imino(4-methylpiperazin-1-yl)methyl]phenyl}-4,5-dihydro-1,2-oxazol-5-yl)methyl}piperazin-1-yl)acetic acid (three-letter code: I7R) (formula: C<sub>22</sub>H<sub>32</sub>N<sub>6</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
12	B	1	Total	C	N	O	0	0
			31	22	6	3		
12	D	1	Total	C	N	O	0	0
			31	22	6	3		

- 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		
13	D	1	Total	Cl	0	0
			1	1		

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	408	Total	O	0	0
			408	408		
14	B	226	Total	O	0	0
			226	226		
14	C	185	Total	O	0	0
			185	185		
14	D	152	Total	O	0	0
			152	152		
14	E	19	Total	O	0	0
			19	19		

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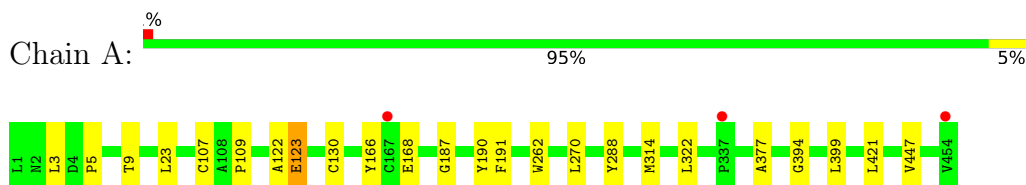
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
14	F	18	Total O 18 18	0	0
14	H	34	Total O 34 34	0	0
14	L	62	Total O 62 62	0	0

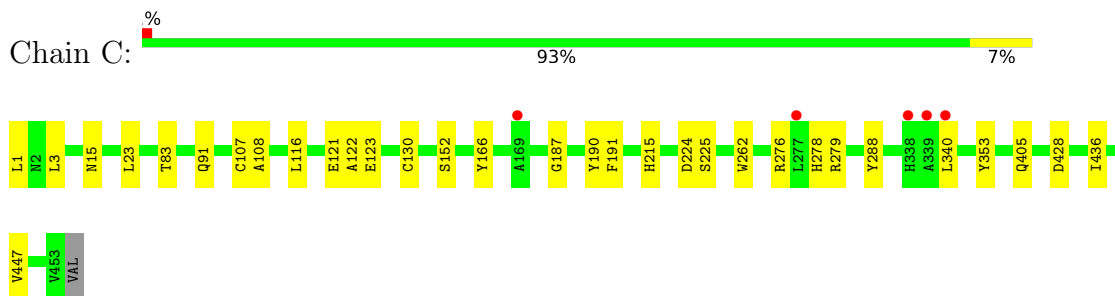
### 3 Residue-property plots [i](#)

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.

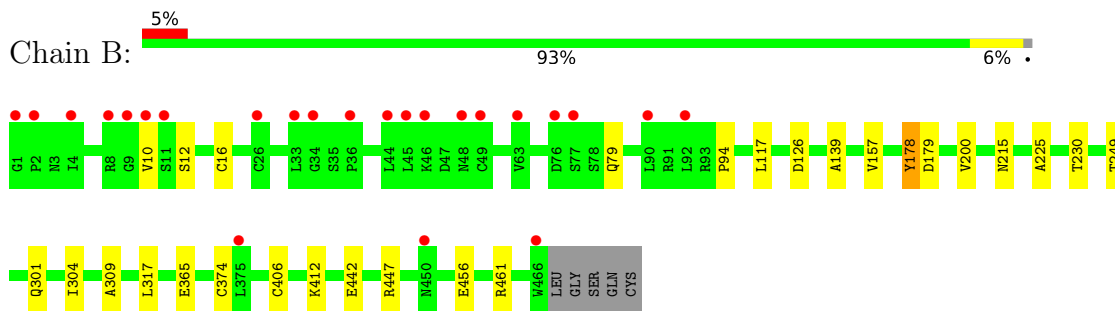
- Molecule 1: Integrin alpha-IIb



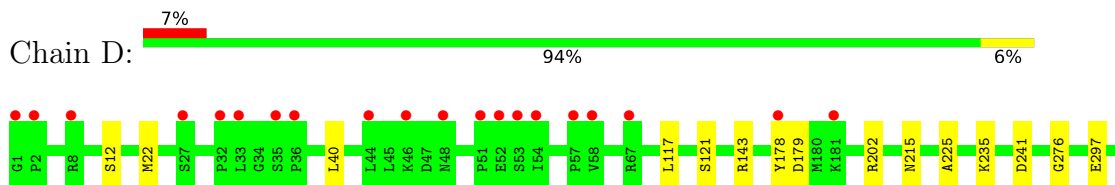
- Molecule 1: Integrin alpha-IIb

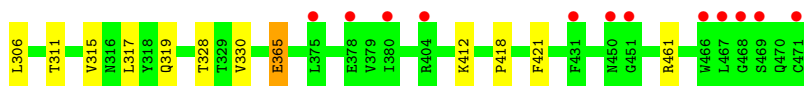


- Molecule 2: Integrin beta-3

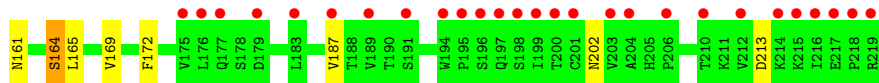
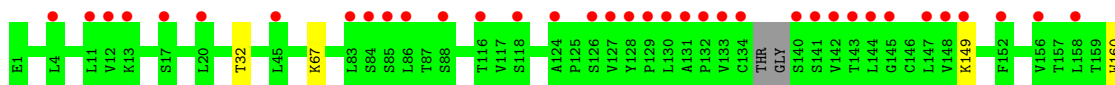
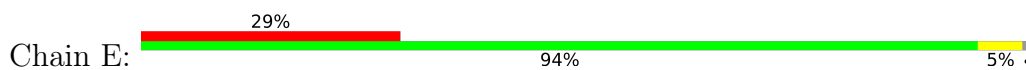


- Molecule 2: Integrin beta-3

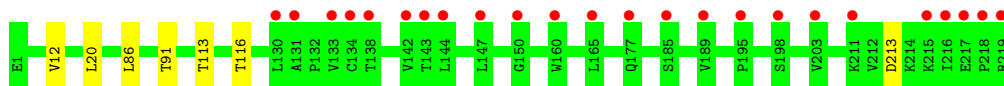




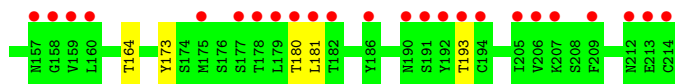
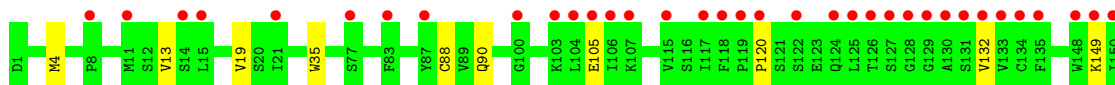
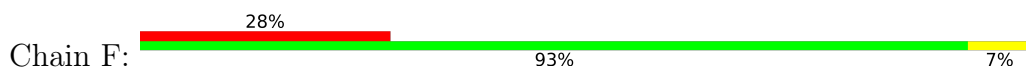
- Molecule 3: Fab heavy chain



- Molecule 3: Fab heavy chain



- Molecule 4: Fab light chain



- Molecule 4: Fab light chain



- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-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



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

Chain I:  100%

NAG1  
NAG2

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

Chain K:  100%

NAG1  
NAG2

- Molecule 7: alpha-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:  75% 25%

NAG1  
NAG2  
BMA3  
MAN4

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	259.40Å 144.29Å 104.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.09 – 2.70 46.09 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.7 (46.09-2.70) 89.5 (46.09-2.70)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.16 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.217 , 0.237 0.217 , 0.237	Depositor DCC
$R_{free}$ test set	1998 reflections (1.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.9	Xtrriage
Anisotropy	0.366	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 42.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	22211	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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: MN, MAN, NAG, CL, SO4, CA, BMA, I7R

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	0.25	0/3608	0.46	0/4918
1	C	0.26	0/3605	0.45	0/4912
2	B	0.24	0/3688	0.44	0/5000
2	D	0.24	0/3690	0.42	0/5003
3	E	0.24	0/1673	0.45	0/2290
3	H	0.24	0/1684	0.45	0/2305
4	F	0.24	0/1673	0.43	0/2269
4	L	0.24	0/1673	0.45	0/2269
All	All	0.24	0/21294	0.44	0/28966

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	3499	0	3345	10	0
1	C	3502	0	3334	16	0
2	B	3618	0	3533	14	0
2	D	3623	0	3540	13	0
3	E	1631	0	1590	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1642	0	1600	4	0
4	F	1637	0	1553	8	0
4	L	1637	0	1553	4	0
5	G	61	0	52	0	0
6	I	28	0	25	0	0
6	K	28	0	25	0	0
7	J	50	0	43	0	0
8	A	20	0	0	0	0
8	C	20	0	0	0	0
8	L	5	0	0	0	0
9	A	4	0	0	0	0
9	C	4	0	0	0	0
10	B	3	0	0	0	0
10	D	3	0	0	0	0
11	B	14	0	13	0	0
11	D	14	0	13	0	0
12	B	31	0	0	0	0
12	D	31	0	0	1	0
13	C	1	0	0	0	0
13	D	1	0	0	0	0
14	A	408	0	0	0	1
14	B	226	0	0	1	0
14	C	185	0	0	1	1
14	D	152	0	0	0	0
14	E	19	0	0	0	0
14	F	18	0	0	0	0
14	H	34	0	0	0	0
14	L	62	0	0	1	0
All	All	22211	0	20219	71	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (71) 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)
3:E:161:ASN:HB2	3:E:164:SER:HB3	1.67	0.75
3:E:165:LEU:HD21	3:E:187:VAL:HG21	1.82	0.60
2:D:12:SER:HB3	2:D:461:ARG:HD3	1.82	0.60
2:B:139:ALA:HB2	2:B:200:VAL:HG11	1.87	0.56
1:C:121:GLU:HG3	1:C:123:GLU:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:306:LEU:HB3	2:D:328:THR:HG22	1.89	0.55
2:D:121:SER:HB2	12:D:2006:I7R:O2	2.07	0.53
2:B:230:THR:HG23	2:B:304:ILE:HG13	1.91	0.52
1:C:83:THR:HB	1:C:116:LEU:HB2	1.91	0.52
3:E:160:TRP:HE1	3:E:169:VAL:HG11	1.75	0.51
1:A:262:TRP:HB3	2:B:317:LEU:HD13	1.91	0.51
2:B:10:VAL:HG21	2:B:16:CYS:HB2	1.92	0.50
1:A:9:THR:HB	1:A:447:VAL:HB	1.92	0.50
2:D:117:LEU:HD11	2:D:225:ALA:HB1	1.94	0.50
2:D:365:GLU:OE2	2:D:412:LYS:NZ	2.44	0.49
2:B:126[A]:ASP:OD1	2:B:126[A]:ASP:N	2.44	0.49
3:H:20:LEU:HD22	3:H:113:THR:HG21	1.94	0.49
1:A:394:GLY:HA2	1:A:399:LEU:HD23	1.95	0.49
1:C:262:TRP:HB3	2:D:317:LEU:HD13	1.94	0.48
1:A:377:ALA:HB2	1:A:421:LEU:HD11	1.96	0.48
1:A:187:GLY:HA2	1:A:191:PHE:HA	1.96	0.48
2:B:117:LEU:HD11	2:B:225:ALA:HB1	1.95	0.48
4:L:193:THR:HG23	4:L:208:SER:HB3	1.96	0.47
2:B:365:GLU:OE2	2:B:412:LYS:NZ	2.39	0.47
1:A:314:MET:HB3	1:A:322:LEU:HB3	1.97	0.47
2:D:319:GLN:HA	2:D:330:VAL:HG21	1.97	0.46
4:L:4:MET:HE2	4:L:90:GLN:HB3	1.97	0.46
1:C:353:TYR:OH	2:D:297:GLU:OE1	2.27	0.45
4:F:13:VAL:HG11	4:F:19:VAL:HG11	1.99	0.45
3:H:12:VAL:HG21	3:H:86:LEU:HD13	1.97	0.45
4:F:120:PRO:HD3	4:F:132:VAL:HG22	1.99	0.45
3:H:91:THR:HG23	3:H:116:THR:HA	1.99	0.45
3:E:149:LYS:NZ	4:F:180:THR:HG21	2.31	0.45
1:C:224:ASP:OD1	1:C:225:SER:N	2.43	0.45
1:C:107:CYS:HA	1:C:130:CYS:HA	1.98	0.45
1:C:276:ARG:HD2	1:C:279:ARG:HB2	1.99	0.45
4:L:161:ASN:ND2	14:L:404:HOH:O	2.49	0.45
1:A:107:CYS:HA	1:A:130:CYS:HA	1.97	0.44
3:E:172:PHE:CD2	4:F:164:THR:HG23	2.52	0.44
1:A:3:LEU:O	1:A:5:PRO:HD3	2.18	0.44
1:C:278[A]:HIS:NE2	1:C:340:LEU:O	2.50	0.44
3:E:202:ASN:HA	3:E:213:ASP:HB3	1.99	0.44
1:C:187:GLY:HA2	1:C:191:PHE:HA	2.00	0.44
2:B:442:GLU:OE1	2:B:447:ARG:NH1	2.51	0.43
1:C:215:HIS:CE1	3:E:32:THR:HG22	2.53	0.43
2:D:22:MET:HG2	2:D:40:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:178:TYR:CG	2:D:179:ASP:N	2.86	0.43
3:H:213:ASP:OD1	3:H:213:ASP:N	2.52	0.43
2:B:456:GLU:OE2	2:B:461:ARG:NH1	2.52	0.43
1:A:122:ALA:O	1:A:123:GLU:HB2	2.19	0.42
3:E:67:LYS:HE3	3:E:67:LYS:HB2	1.90	0.42
2:B:301:GLN:NE2	14:B:2107:HOH:O	2.43	0.42
1:C:123:GLU:HG3	1:C:152:SER:HB2	2.02	0.42
4:F:35:TRP:CZ3	4:F:88:CYS:HB3	2.55	0.42
1:C:122:ALA:O	1:C:123:GLU:HB2	2.18	0.42
2:D:311:THR:O	2:D:315:VAL:HG23	2.21	0.41
2:D:418:PRO:HB2	2:D:421:PHE:CD1	2.55	0.41
2:B:178:TYR:CG	2:B:179:ASP:N	2.88	0.41
2:B:249:THR:HA	2:B:309:ALA:O	2.19	0.41
1:C:3:LEU:O	1:C:405:GLN:NE2	2.47	0.41
1:C:428:ASP:CG	14:C:602:HOH:O	2.59	0.41
4:F:105:GLU:OE1	4:F:173:TYR:OH	2.27	0.41
4:F:149:LYS:HB2	4:F:193:THR:HB	2.03	0.41
2:B:94:PRO:HG3	2:B:406:CYS:HB2	2.03	0.41
1:A:109:PRO:O	1:A:168:GLU:HA	2.21	0.41
2:B:12:SER:HB3	2:B:461:ARG:HD3	2.03	0.41
1:C:436:ILE:HG22	1:C:447:VAL:HG22	2.03	0.41
2:D:235:LYS:HE3	2:D:276:GLY:O	2.21	0.41
4:F:4:MET:HE2	4:F:90:GLN:HB3	2.02	0.41
4:L:66:GLY:HA3	4:L:71:TYR:HA	2.03	0.41
1:C:91:GLN:HB2	1:C:108:ALA:HB1	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:902:HOH:O	14:C:761:HOH:O[1_554]	2.19	0.01

## 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	456/454 (100%)	440 (96%)	15 (3%)	1 (0%)	47	73
1	C	455/454 (100%)	438 (96%)	17 (4%)	0	100	100
2	B	468/471 (99%)	451 (96%)	16 (3%)	1 (0%)	47	73
2	D	469/471 (100%)	445 (95%)	24 (5%)	0	100	100
3	E	210/216 (97%)	194 (92%)	16 (8%)	0	100	100
3	H	212/216 (98%)	203 (96%)	9 (4%)	0	100	100
4	F	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
4	L	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
All	All	2694/2710 (99%)	2580 (96%)	112 (4%)	2 (0%)	51	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
2	B	157	VAL

### 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	366/362 (101%)	361 (99%)	5 (1%)	67	86
1	C	365/362 (101%)	359 (98%)	6 (2%)	62	85
2	B	416/416 (100%)	412 (99%)	4 (1%)	76	91
2	D	416/416 (100%)	411 (99%)	5 (1%)	71	88
3	E	186/187 (100%)	185 (100%)	1 (0%)	88	96
3	H	187/187 (100%)	187 (100%)	0	100	100
4	F	188/188 (100%)	187 (100%)	1 (0%)	88	96
4	L	188/188 (100%)	188 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2312/2306 (100%)	2290 (99%)	22 (1%)	76 91

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	166	TYR
1	A	190	TYR
1	A	270	LEU
1	A	288	TYR
2	B	79	GLN
2	B	178	TYR
2	B	215	ASN
2	B	374	CYS
1	C	1	LEU
1	C	15	ASN
1	C	23	LEU
1	C	166	TYR
1	C	190	TYR
1	C	288	TYR
2	D	143	ARG
2	D	202	ARG
2	D	215	ASN
2	D	241	ASP
2	D	365	GLU
3	E	164	SER
4	F	181	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	280	HIS
2	D	301	GLN
2	D	438	GLN

### 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](#)

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	2,5	14,14,15	0.33	0	17,19,21	0.48	0
5	NAG	G	2	5	14,14,15	0.15	0	17,19,21	0.45	0
5	BMA	G	3	5	11,11,12	0.96	0	15,15,17	0.94	0
5	MAN	G	4	5	11,11,12	0.71	0	15,15,17	1.07	2 (13%)
5	MAN	G	5	5	11,11,12	1.17	1 (9%)	15,15,17	2.15	2 (13%)
6	NAG	I	1	6,2	14,14,15	0.39	0	17,19,21	0.41	0
6	NAG	I	2	6	14,14,15	0.18	0	17,19,21	0.38	0
7	NAG	J	1	2,7	14,14,15	0.30	0	17,19,21	0.52	0
7	NAG	J	2	7	14,14,15	0.32	0	17,19,21	0.39	0
7	BMA	J	3	7	11,11,12	0.84	0	15,15,17	0.91	0
7	MAN	J	4	7	11,11,12	0.76	0	15,15,17	1.08	2 (13%)
6	NAG	K	1	6,2	14,14,15	0.30	0	17,19,21	0.42	0
6	NAG	K	2	6	14,14,15	0.18	0	17,19,21	0.45	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	2,5	-	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	MAN	G	4	5	-	0/2/19/22	0/1/1/1
5	MAN	G	5	5	-	1/2/19/22	0/1/1/1
6	NAG	I	1	6,2	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	I	2	6	-	3/6/23/26	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	-	2/2/19/22	0/1/1/1
7	MAN	J	4	7	-	2/2/19/22	0/1/1/1
6	NAG	K	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	5	MAN	O5-C5	3.30	1.50	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	5	MAN	C1-O5-C5	6.96	121.62	112.19
5	G	4	MAN	C1-O5-C5	2.93	116.16	112.19
7	J	4	MAN	C1-O5-C5	2.86	116.07	112.19
5	G	5	MAN	O5-C1-C2	2.50	114.62	110.77
7	J	4	MAN	O2-C2-C3	-2.20	105.72	110.14
5	G	4	MAN	O2-C2-C3	-2.19	105.76	110.14

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	3	BMA	O5-C5-C6-O6
5	G	3	BMA	C4-C5-C6-O6
7	J	3	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
7	J	3	BMA	C4-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
7	J	4	MAN	O5-C5-C6-O6

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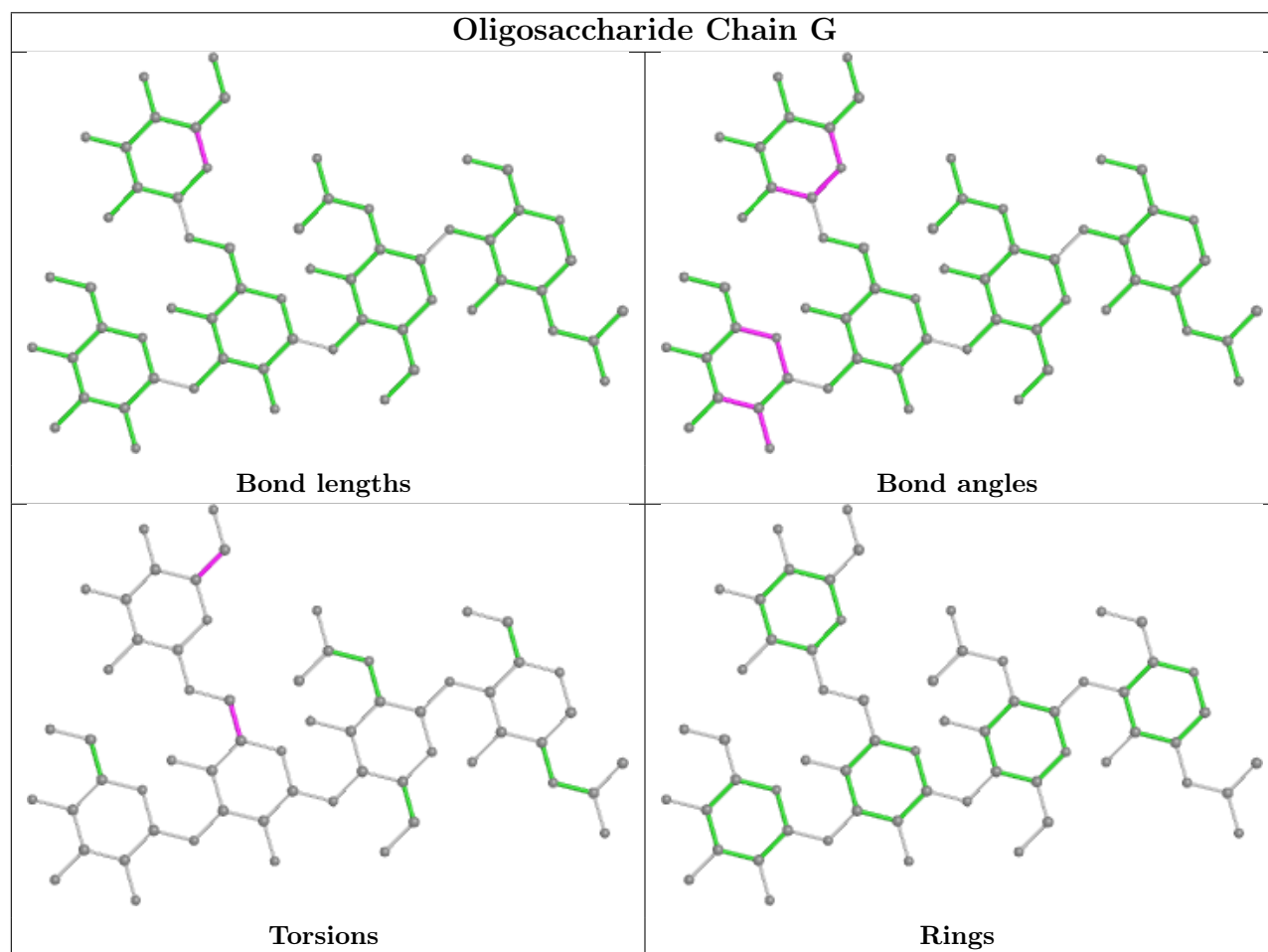
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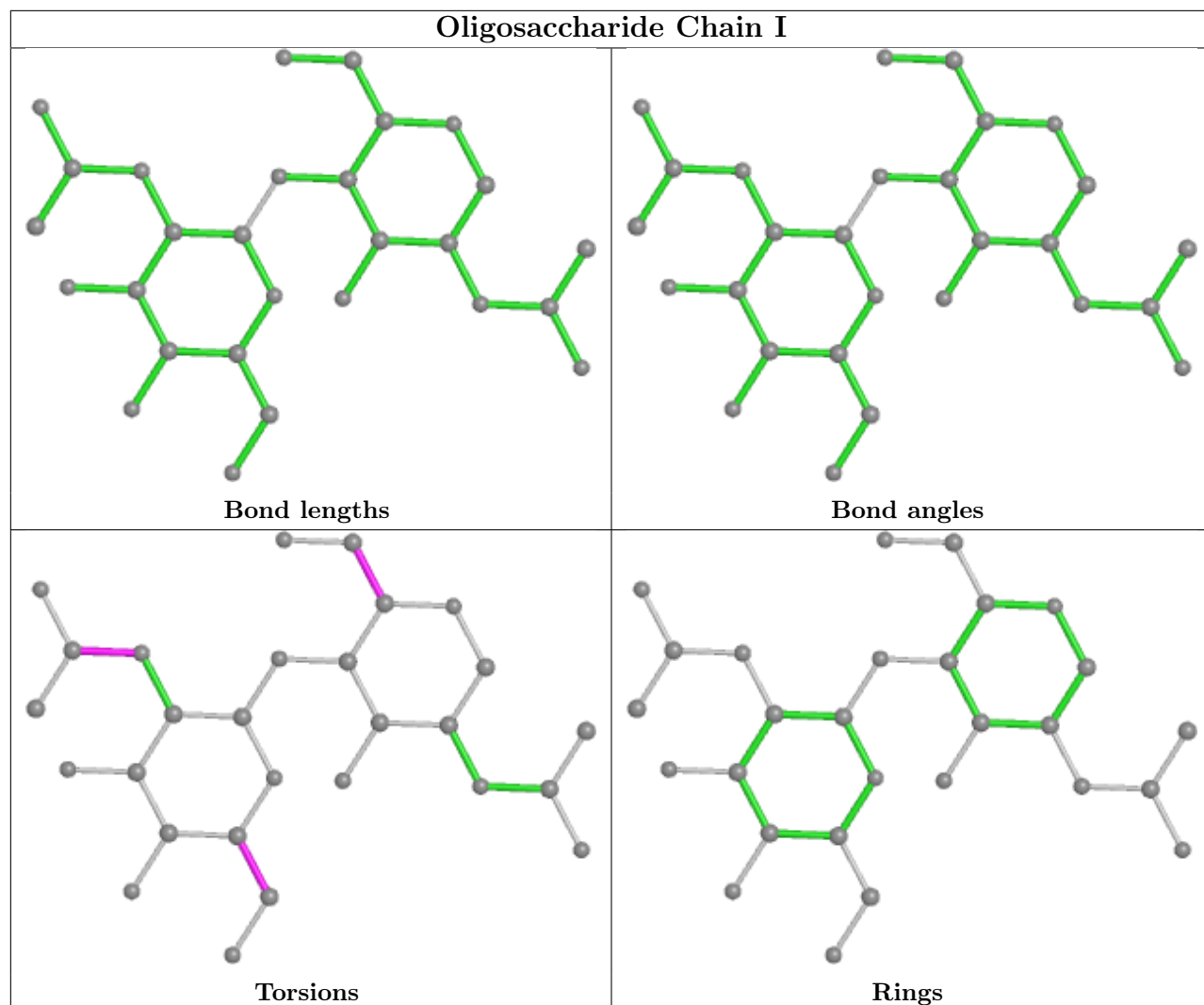
Mol	Chain	Res	Type	Atoms
5	G	5	MAN	C4-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
7	J	4	MAN	C4-C5-C6-O6
6	I	1	NAG	C4-C5-C6-O6

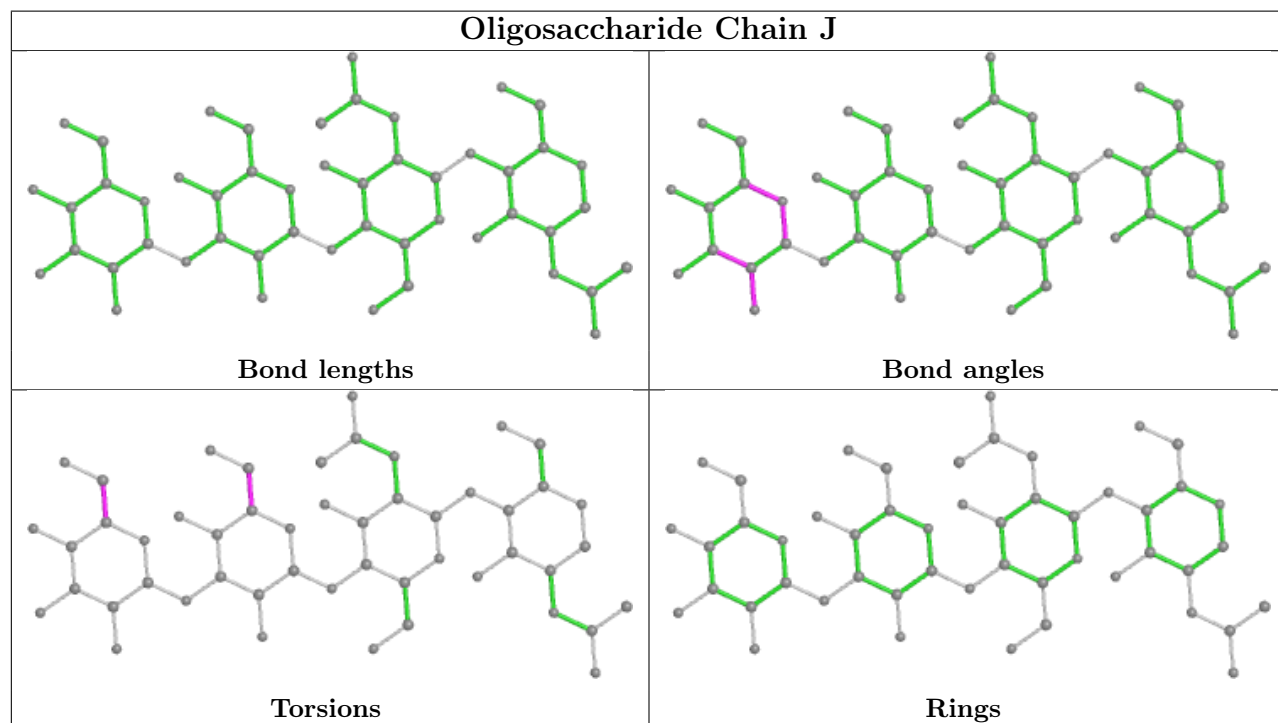
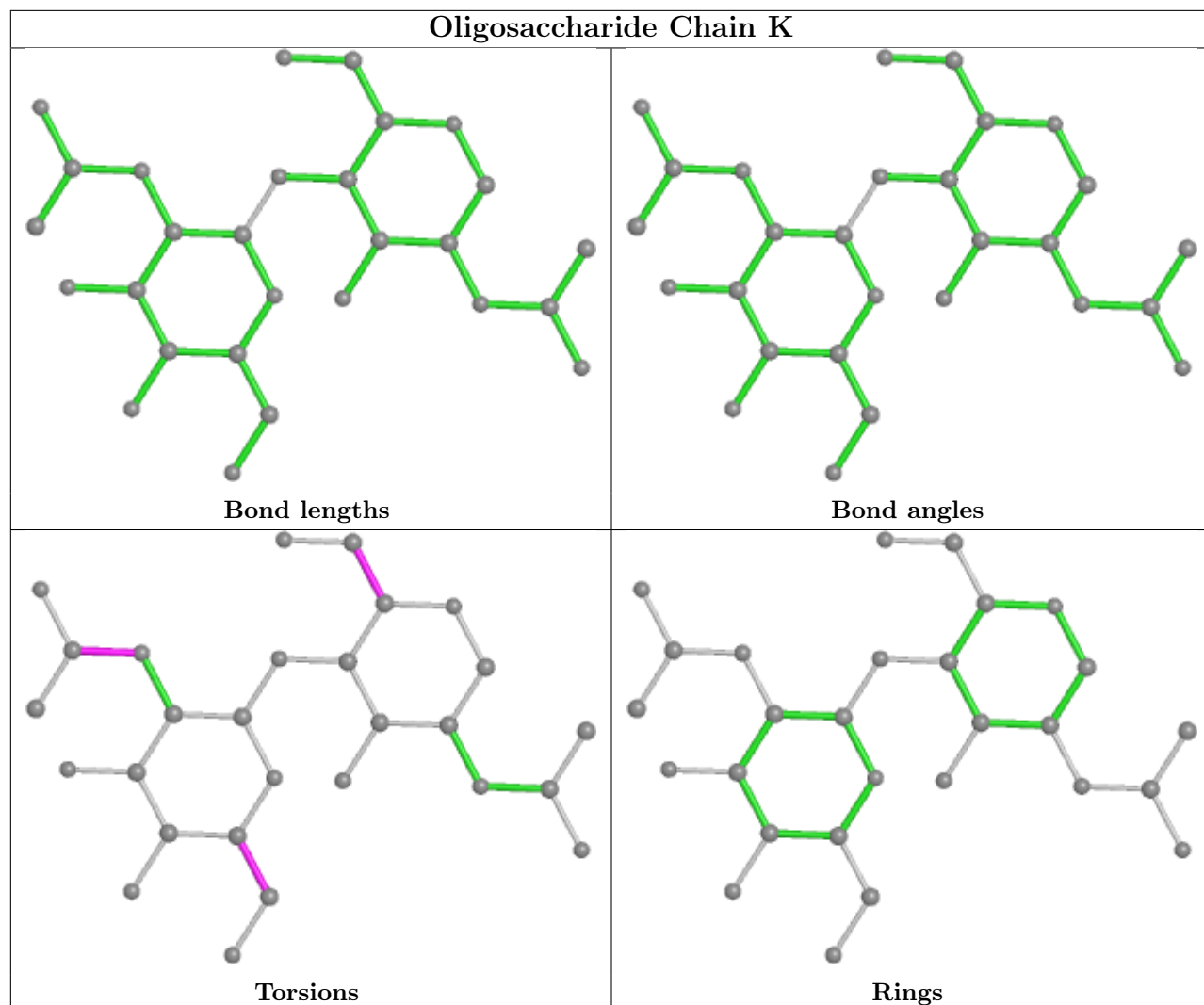
There are no ring outliers.

No monomer is involved in short contacts.

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









## 5.6 Ligand geometry

Of 29 ligands modelled in this entry, 16 are monoatomic - leaving 13 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
8	SO4	A	501	-	4,4,4	0.15	0	6,6,6	0.06	0
8	SO4	A	507	-	4,4,4	0.14	0	6,6,6	0.07	0
11	NAG	B	2004	2	14,14,15	0.31	0	17,19,21	0.68	1 (5%)
8	SO4	C	509	-	4,4,4	0.18	0	6,6,6	0.10	0
8	SO4	C	501	-	4,4,4	0.13	0	6,6,6	0.06	0
8	SO4	L	301	-	4,4,4	0.14	0	6,6,6	0.06	0
11	NAG	D	2004	2	14,14,15	0.33	0	17,19,21	0.58	0
12	I7R	D	2006	10	34,34,34	1.08	2 (5%)	44,47,47	0.96	1 (2%)
8	SO4	A	502	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	C	503	-	4,4,4	0.14	0	6,6,6	0.06	0
8	SO4	C	502	-	4,4,4	0.14	0	6,6,6	0.06	0
8	SO4	A	508	-	4,4,4	0.14	0	6,6,6	0.05	0
12	I7R	B	2005	10	34,34,34	1.09	2 (5%)	44,47,47	1.07	2 (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
12	I7R	B	2005	10	-	5/18/49/49	0/4/4/4
11	NAG	B	2004	2	-	2/6/23/26	0/1/1/1
11	NAG	D	2004	2	-	2/6/23/26	0/1/1/1
12	I7R	D	2006	10	-	4/18/49/49	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	2005	I7R	C6-N3	2.92	1.34	1.27
12	D	2006	I7R	C6-N3	2.92	1.34	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	2006	I7R	O1-C14	-2.60	1.43	1.46
12	B	2005	I7R	O1-C14	-2.54	1.43	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	2005	I7R	C4-C1-N1	-2.60	107.87	110.80
11	B	2004	NAG	C1-O5-C5	2.42	115.47	112.19
12	D	2006	I7R	C14-C15-C13	2.14	102.81	100.85
12	B	2005	I7R	C10-C13-N4	2.04	125.55	120.74

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	B	2005	I7R	C15-C14-C16-N5
12	B	2005	I7R	O1-C14-C16-N5
12	D	2006	I7R	O1-C14-C16-N5
11	B	2004	NAG	O5-C5-C6-O6
11	B	2004	NAG	C4-C5-C6-O6
11	D	2004	NAG	O5-C5-C6-O6
12	B	2005	I7R	C7-C6-N2-C3
12	D	2006	I7R	C7-C6-N2-C3
11	D	2004	NAG	C4-C5-C6-O6
12	B	2005	I7R	N3-C6-C7-C12
12	B	2005	I7R	N3-C6-C7-C8
12	D	2006	I7R	N3-C6-C7-C12
12	D	2006	I7R	N3-C6-C7-C8

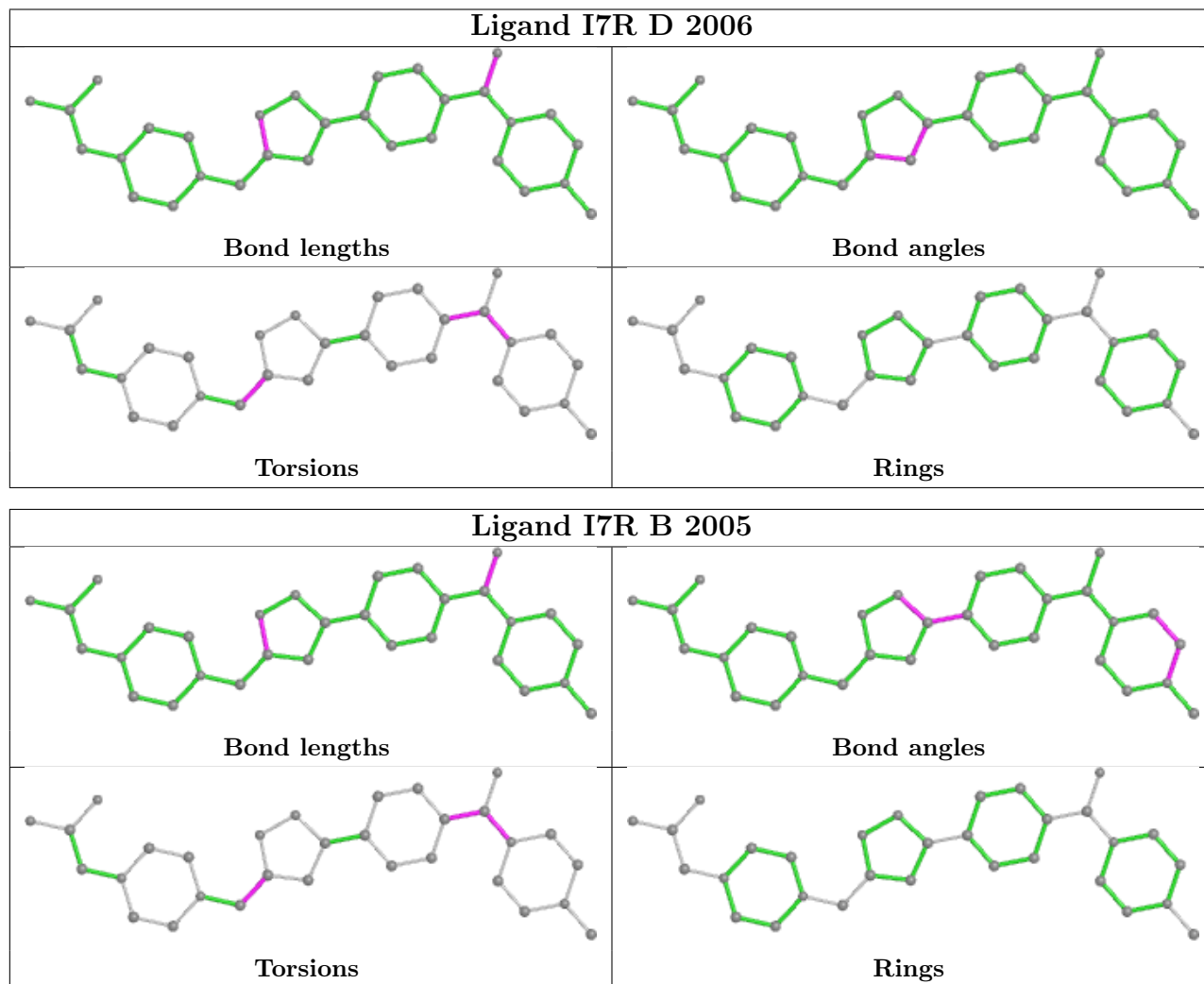
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	2006	I7R	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.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	134:CYS	C	138:THR	N	6.94

## 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	454/454 (100%)	0.14	3 (0%) 87 89	32, 43, 61, 76	0
1	C	453/454 (99%)	0.23	5 (1%) 80 82	40, 64, 89, 111	0
2	B	466/471 (98%)	0.43	24 (5%) 27 25	33, 66, 142, 157	1 (0%)
2	D	471/471 (100%)	0.45	32 (6%) 17 15	46, 83, 117, 132	1 (0%)
3	E	214/216 (99%)	1.65	63 (29%) 0 0	82, 127, 191, 194	0
3	H	216/216 (100%)	0.52	24 (11%) 5 4	54, 90, 138, 144	0
4	F	214/214 (100%)	1.44	59 (27%) 0 0	85, 131, 189, 194	0
4	L	214/214 (100%)	0.33	8 (3%) 41 41	59, 91, 111, 130	0
All	All	2702/2710 (99%)	0.53	218 (8%) 12 10	32, 76, 163, 194	2 (0%)

All (218) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	144	LEU	10.4
3	E	147	LEU	9.6
3	E	134	CYS	9.3
3	E	129	PRO	9.3
4	F	125	LEU	8.5
3	E	145	GLY	8.2
4	F	193	THR	8.0
2	D	375	LEU	7.8
3	E	216	ILE	7.7
3	E	194	TRP	7.4
3	E	219	ARG	7.4
3	E	195	PRO	7.2
2	D	181	LYS	7.0
3	E	133	VAL	6.9
4	F	118	PHE	6.9
4	F	133	VAL	6.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	E	142	VAL	6.6
2	D	469	SER	6.6
3	E	212	VAL	6.5
3	E	130	LEU	6.4
3	E	132	PRO	6.4
4	F	181	LEU	6.4
3	E	148	VAL	6.3
2	B	10	VAL	6.3
3	E	199	ILE	6.2
4	F	214	CYS	6.2
4	F	179	LEU	6.2
4	F	132	VAL	6.1
3	E	201	CYS	5.9
2	B	33	LEU	5.9
3	E	198	SER	5.8
3	H	216	ILE	5.7
3	E	131	ALA	5.6
3	H	217	GLU	5.6
4	F	130	ALA	5.5
3	H	130	LEU	5.4
4	F	206	VAL	5.2
4	F	117	ILE	5.2
3	E	128	TYR	5.2
2	B	1	GLY	5.1
3	E	217	GLU	5.0
2	B	44	LEU	5.0
4	F	134	CYS	5.0
4	F	180	THR	5.0
3	E	84	SER	4.9
3	E	127	VAL	4.8
3	E	203	VAL	4.8
4	F	148	TRP	4.8
4	F	115	VAL	4.8
2	B	77	SER	4.8
4	F	182	THR	4.7
3	E	218	PRO	4.6
4	F	178	THR	4.5
2	B	466	TRP	4.5
4	F	150	ILE	4.4
3	H	198	SER	4.3
1	A	454	VAL	4.3
4	L	214	CYS	4.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	E	204	ALA	4.3
3	E	143	THR	4.2
4	F	129	GLY	4.2
4	F	160	LEU	4.2
2	D	33	LEU	4.1
3	E	149	LYS	4.1
2	B	2	PRO	4.1
2	D	451	GLY	4.1
2	B	375	LEU	4.0
2	D	450	ASN	4.0
3	E	215	LYS	4.0
4	F	83	PHE	3.9
4	F	149	LYS	3.9
2	B	8	ARG	3.8
4	F	126	THR	3.8
2	B	48	ASN	3.7
3	E	156	VAL	3.7
2	D	2	PRO	3.7
3	E	176	LEU	3.7
4	F	209	PHE	3.7
2	D	48	ASN	3.5
3	E	158	LEU	3.4
3	H	195	PRO	3.4
1	C	277	LEU	3.4
4	F	135	PHE	3.4
2	D	8	ARG	3.4
2	B	49	CYS	3.3
3	H	133	VAL	3.2
4	F	15	LEU	3.2
2	D	46	LYS	3.2
2	D	178	TYR	3.2
1	C	340	LEU	3.2
2	D	471	CYS	3.2
2	D	32	PRO	3.2
2	D	44	LEU	3.2
3	H	142	VAL	3.1
4	F	207	LYS	3.1
2	B	450	ASN	3.1
3	H	219	ARG	3.1
4	L	212	ASN	3.1
2	B	34	GLY	3.1
4	F	122	SER	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	4	ILE	3.1
2	D	53	SER	3.1
3	E	175	VAL	3.1
4	F	191	SER	3.1
4	F	205	ILE	3.1
3	E	20	LEU	3.0
2	D	52	GLU	3.0
2	D	431	PHE	3.0
4	F	212	ASN	3.0
4	F	158	GLY	3.0
3	E	196	SER	3.0
2	D	468	GLY	2.9
3	E	126	SER	2.9
3	E	200	THR	2.9
4	F	119	PRO	2.9
4	F	8	PRO	2.9
4	F	177	SER	2.9
4	F	87	TYR	2.9
2	D	1	GLY	2.8
2	D	35	SER	2.8
4	F	100	GLY	2.8
3	E	183	LEU	2.8
1	A	337	PRO	2.8
4	F	192	TYR	2.8
4	F	194	CYS	2.8
2	B	63	VAL	2.8
4	F	128	GLY	2.8
3	H	165	LEU	2.8
4	L	135	PHE	2.8
2	D	51	PRO	2.7
3	H	189	VAL	2.7
2	D	36	PRO	2.7
2	B	36	PRO	2.7
2	B	26	CYS	2.7
4	F	127	SER	2.7
2	B	92	LEU	2.7
3	E	86	LEU	2.7
3	E	187	VAL	2.7
4	F	21	ILE	2.7
4	F	11	MET	2.6
3	H	215	LYS	2.6
2	B	76	ASP	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	L	83	PHE	2.6
3	E	124	ALA	2.6
4	F	105	GLU	2.6
2	B	11	SER	2.6
3	H	160	TRP	2.6
3	E	17	SER	2.5
4	F	190	ASN	2.5
2	D	57	PRO	2.5
3	E	191	SER	2.5
4	F	157	ASN	2.5
3	E	177	GLN	2.5
3	H	138	THR	2.5
3	E	45	LEU	2.5
3	H	144	LEU	2.5
3	E	140	SER	2.5
4	F	159	VAL	2.5
3	E	116	THR	2.4
2	D	54	ILE	2.4
2	D	378	GLU	2.4
2	B	9	GLY	2.4
4	L	205	ILE	2.4
3	E	141	SER	2.4
4	F	186	TYR	2.4
3	H	134	CYS	2.4
3	H	143	THR	2.4
3	H	131	ALA	2.4
4	L	115	VAL	2.4
1	C	339	ALA	2.4
2	B	46	LYS	2.4
4	F	213	GLU	2.4
4	F	120	PRO	2.3
2	B	45	LEU	2.3
2	D	380	ILE	2.3
4	F	124	GLN	2.3
3	E	83	LEU	2.3
4	F	14	SER	2.2
4	F	131	SER	2.2
4	F	104	LEU	2.2
4	L	125	LEU	2.2
3	E	210	THR	2.2
3	E	12	VAL	2.2
3	E	189	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	467	LEU	2.2
3	E	197	GLN	2.2
3	E	179	ASP	2.2
2	D	58	VAL	2.2
3	E	88	SER	2.2
3	E	11	LEU	2.2
2	D	67	ARG	2.2
4	L	111	ALA	2.2
1	A	167	CYS	2.2
3	E	152	PHE	2.2
2	D	27	SER	2.1
3	E	13	LYS	2.1
3	H	147	LEU	2.1
4	F	77	SER	2.1
4	F	106	ILE	2.1
3	H	218	PRO	2.1
1	C	169	ALA	2.1
3	E	214	LYS	2.1
4	F	107	LYS	2.1
4	F	103	LYS	2.1
3	E	118	SER	2.1
3	H	150	GLY	2.1
3	E	4	LEU	2.1
2	D	466	TRP	2.1
3	H	185	SER	2.1
4	F	175	MET	2.1
3	E	85	SER	2.0
2	B	90	LEU	2.0
1	C	338	HIS	2.0
2	D	404	ARG	2.0
3	H	211	LYS	2.0
3	H	177	GLN	2.0
3	E	206	PRO	2.0
3	H	203	VAL	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

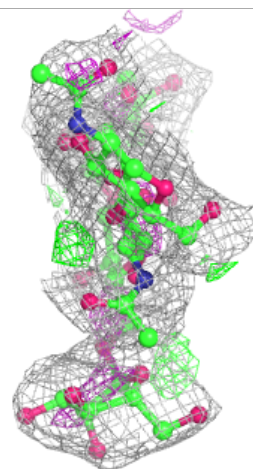
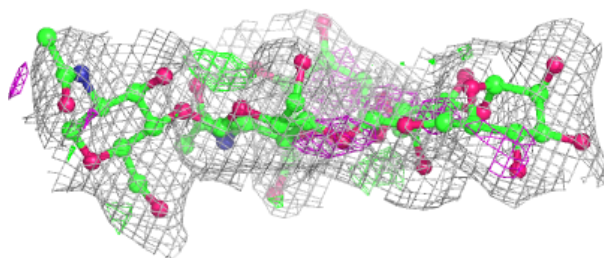
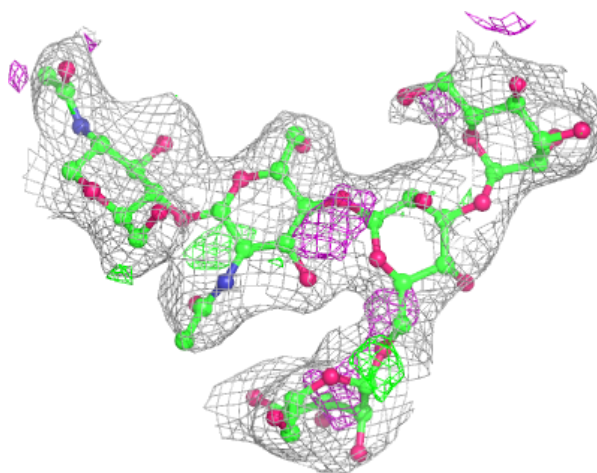
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
7	BMA	J	3	11/12	0.76	0.24	94,94,94,94	0
5	MAN	G	5	11/12	0.79	0.23	79,79,79,79	0
6	NAG	I	2	14/15	0.80	0.33	105,105,105,105	0
6	NAG	K	2	14/15	0.82	0.30	107,107,107,107	0
5	BMA	G	3	11/12	0.82	0.18	75,75,75,75	0
6	NAG	K	1	14/15	0.83	0.21	103,103,103,103	0
5	NAG	G	2	14/15	0.85	0.16	64,64,64,64	0
7	NAG	J	2	14/15	0.86	0.20	85,85,85,85	0
5	MAN	G	4	11/12	0.86	0.20	73,73,73,73	0
7	MAN	J	4	11/12	0.87	0.30	95,95,95,95	0
6	NAG	I	1	14/15	0.91	0.22	99,99,99,99	0
7	NAG	J	1	14/15	0.92	0.18	74,74,74,74	0
5	NAG	G	1	14/15	0.95	0.17	51,51,51,51	0

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

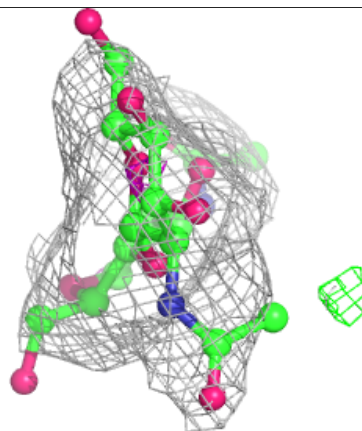
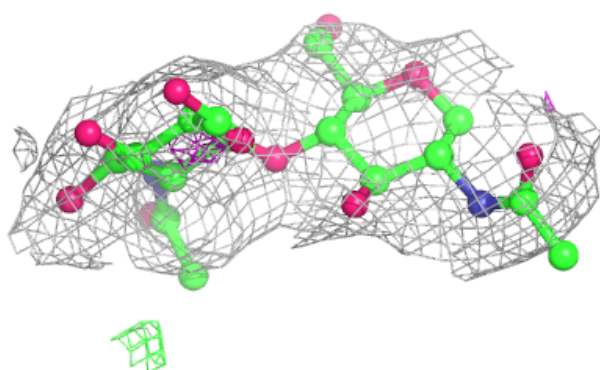
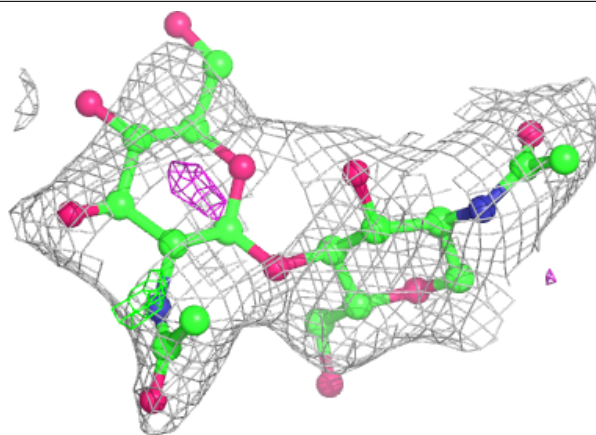
**Electron density around Chain G:**

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

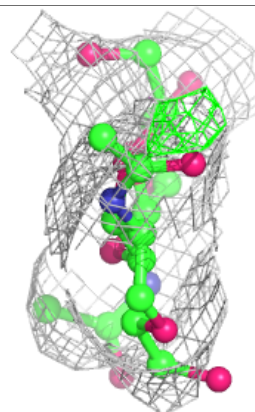
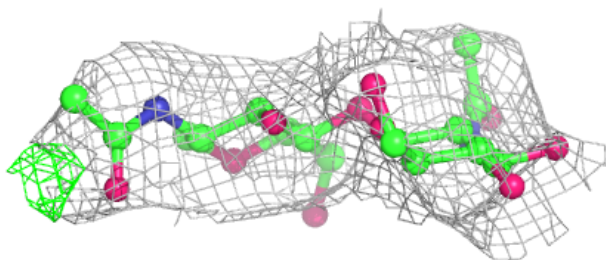
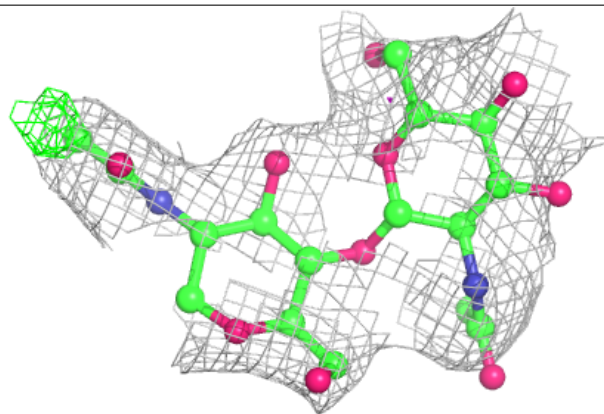


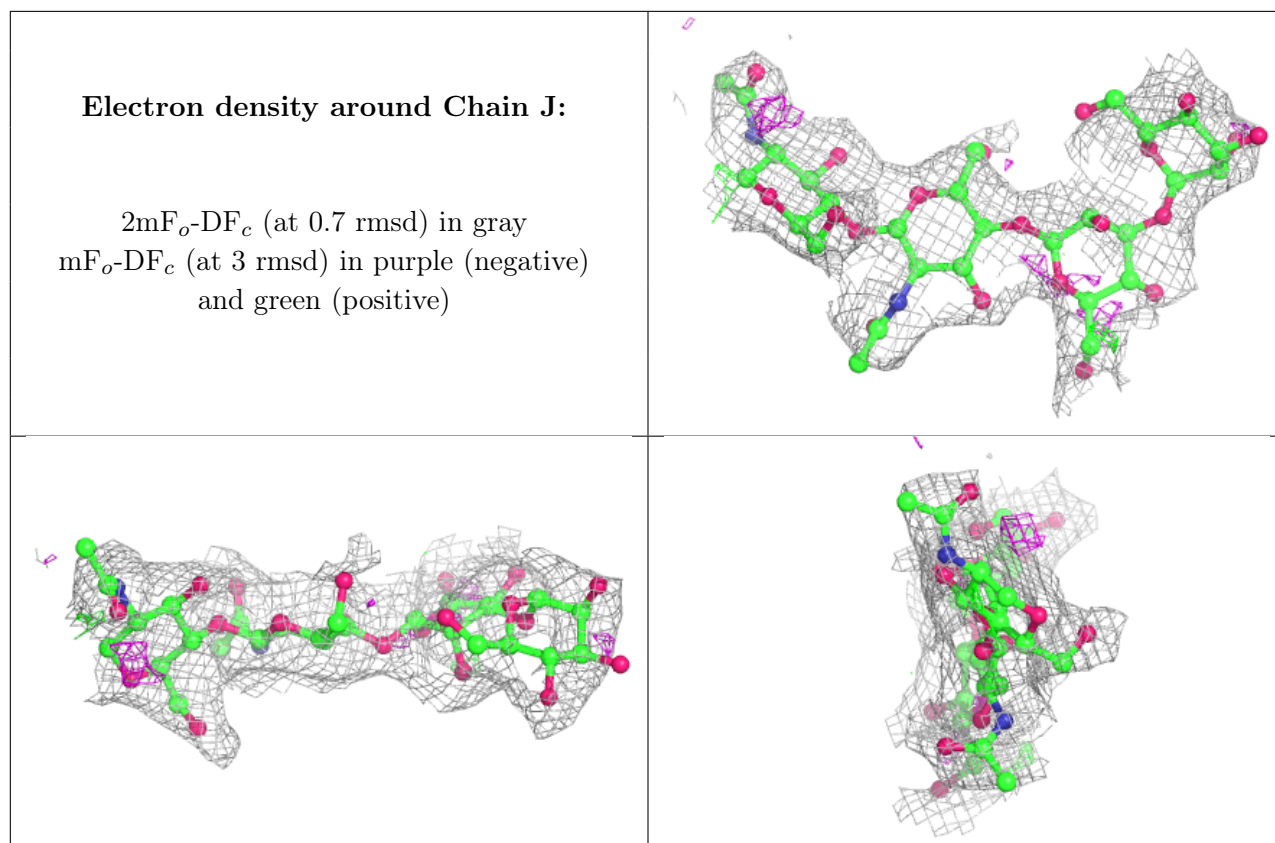
**Electron density around Chain I:**

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

**Electron density around Chain 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.

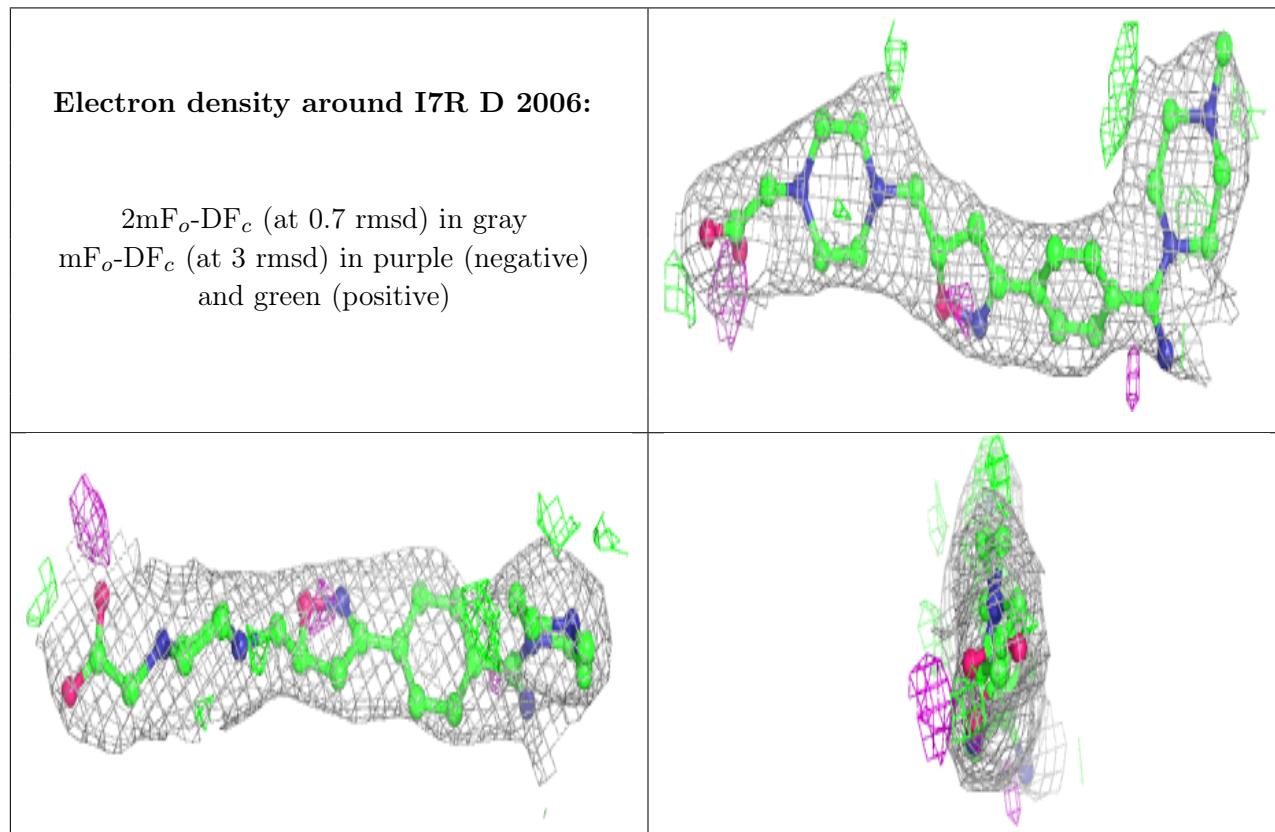
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
11	NAG	D	2004	14/15	0.72	0.33	96,96,96,96	0
9	CA	C	506	1/1	0.75	0.09	75,75,75,75	0
8	SO4	C	502	5/5	0.77	0.21	84,84,84,84	0
13	CL	D	2005	1/1	0.80	0.15	89,89,89,89	0
11	NAG	B	2004	14/15	0.84	0.39	102,102,102,102	0
9	CA	A	503	1/1	0.85	0.09	48,48,48,48	0
9	CA	C	507	1/1	0.86	0.14	66,66,66,66	0
9	CA	C	505	1/1	0.87	0.10	94,94,94,94	0
9	CA	A	504	1/1	0.89	0.10	40,40,40,40	0
8	SO4	A	507	5/5	0.90	0.34	70,70,70,70	0
8	SO4	C	501	5/5	0.90	0.20	76,76,76,76	0
10	MN	D	2003	1/1	0.90	0.07	62,62,62,62	0
12	I7R	D	2006	31/31	0.91	0.19	69,69,69,69	0
12	I7R	B	2005	31/31	0.92	0.21	46,46,46,46	0

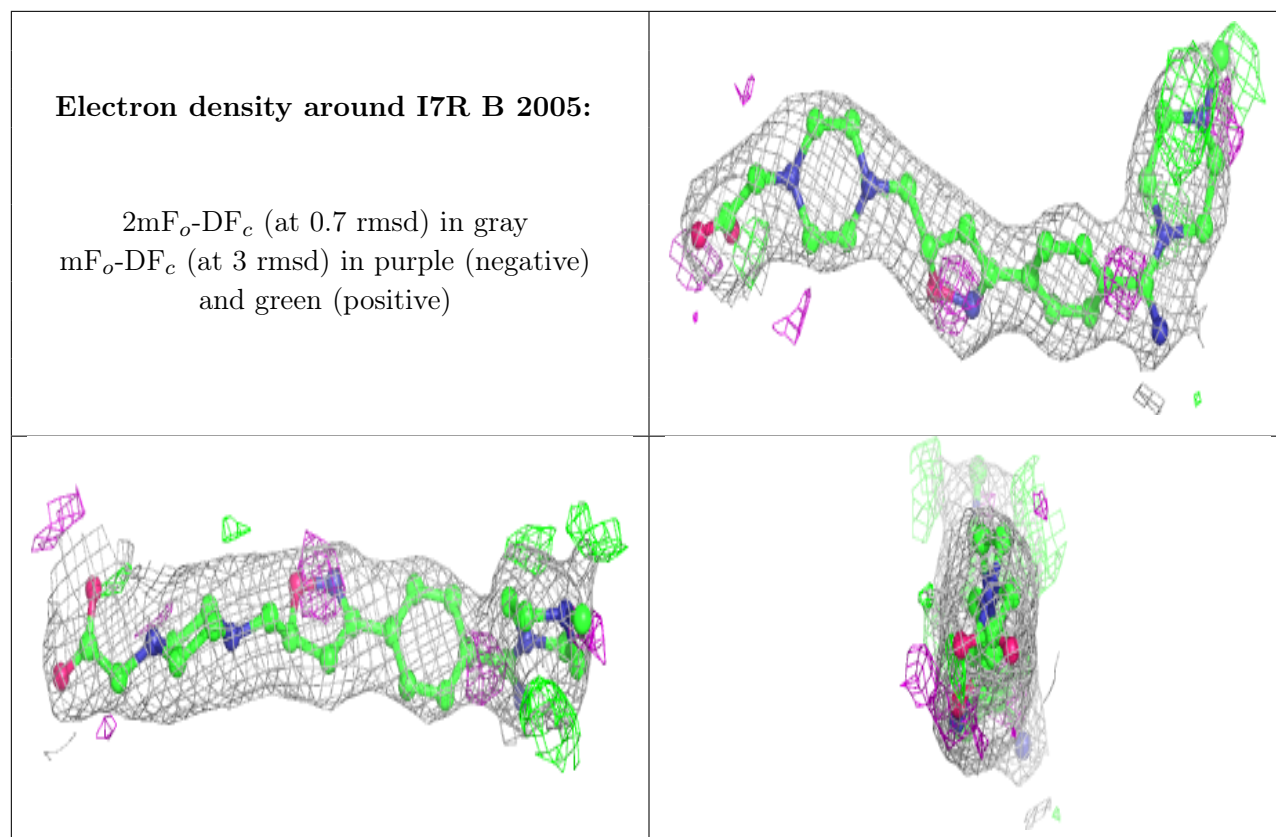
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	SO4	A	508	5/5	0.92	0.20	68,68,68,68	0
8	SO4	C	509	5/5	0.92	0.20	92,92,92,92	0
8	SO4	C	503	5/5	0.93	0.24	94,94,94,94	0
8	SO4	A	501	5/5	0.94	0.25	56,56,56,56	0
13	CL	C	504	1/1	0.94	0.17	68,68,68,68	0
10	MN	D	2002	1/1	0.94	0.08	73,73,73,73	0
9	CA	A	505	1/1	0.95	0.20	38,38,38,38	0
9	CA	C	508	1/1	0.95	0.12	59,59,59,59	0
10	MN	D	2001	1/1	0.96	0.08	64,64,64,64	0
8	SO4	L	301	5/5	0.96	0.18	77,77,77,77	0
8	SO4	A	502	5/5	0.96	0.12	56,56,56,56	0
10	MN	B	2001	1/1	0.97	0.16	35,35,35,35	0
10	MN	B	2002	1/1	0.97	0.12	64,64,64,64	0
10	MN	B	2003	1/1	0.97	0.10	42,42,42,42	0
9	CA	A	506	1/1	0.99	0.13	38,38,38,38	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.