



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2021 – 11:38 AM JST

PDB ID : 7BRJ  
Title : Atrial Natriuretic Peptide Receptor complexed with deletion mutant of human Atrial Natriuretic Peptide[7-28]  
Authors : Ogawa, H.  
Deposited on : 2020-03-29  
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.

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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 : 2.18  
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) : 2.18

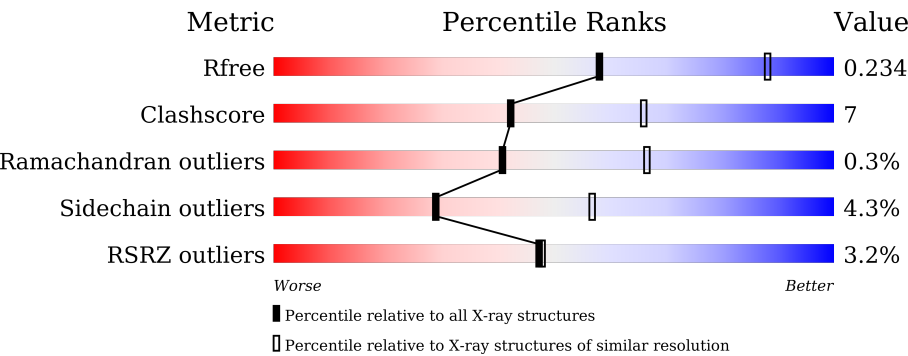
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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.



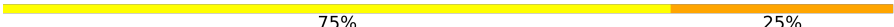
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	435	<div><div>4%</div><div><div></div><div>78%</div><div>20%</div><div></div></div><div></div></div>
1	B	435	<div><div>2%</div><div><div></div><div>78%</div><div>20%</div><div></div></div><div></div></div>
2	L	22	<div><div>5%</div><div><div></div><div>68%</div><div>27%</div><div>5%</div></div><div></div></div>
3	C	3	<div><div></div><div><div></div><div>67%</div><div>33%</div><div></div></div><div></div></div>
3	E	3	<div><div></div><div><div></div><div>67%</div><div>33%</div><div></div></div><div></div></div>
4	D	4	<div><div></div><div><div></div><div>25%</div><div>50%</div><div>25%</div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
4	F	4	 75% 25%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7286 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 Atrial natriuretic peptide receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	3	0
			3383	2167	590	615	11			
1	B	426	Total	C	N	O	S	0	3	0
			3383	2167	590	615	11			

- Molecule 2 is a protein called Urodilatin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	22	Total	C	N	O	S	0	6	0
			196	119	37	36	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	?	-	SER	deletion	UNP P01160
L	?	-	LEU	deletion	UNP P01160
L	?	-	ARG	deletion	UNP P01160
L	?	-	ARG	deletion	UNP P01160
L	?	-	SER	deletion	UNP P01160
L	?	-	SER	deletion	UNP P01160

- Molecule 3 is an oligosaccharide called alpha-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
3	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	F	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		
5	B	1	Total	Cl	0	0
			1	1		

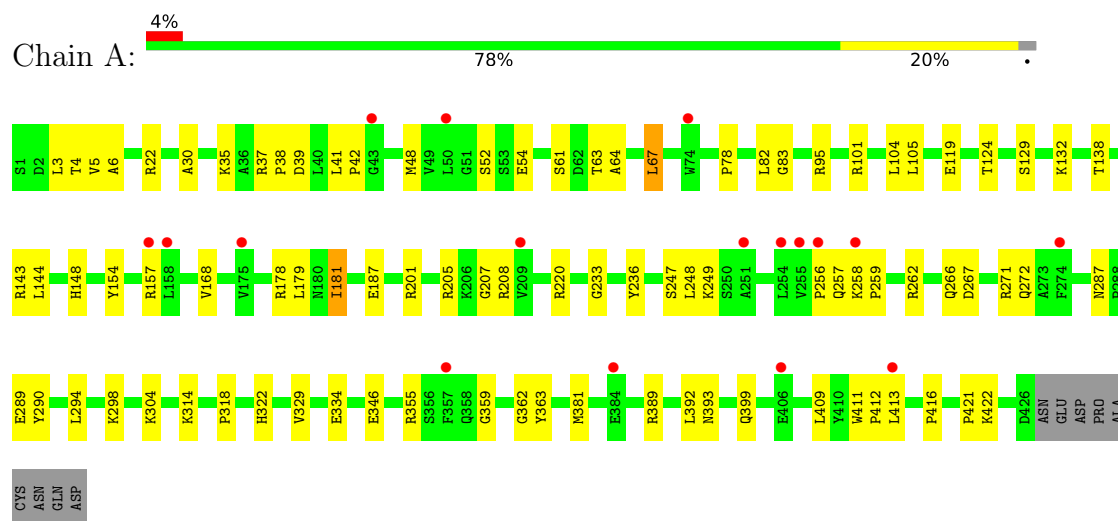
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	66	Total	O	0	0
			66	66		
6	B	64	Total	O	0	0
			64	64		
6	L	14	Total	O	0	0
			14	14		

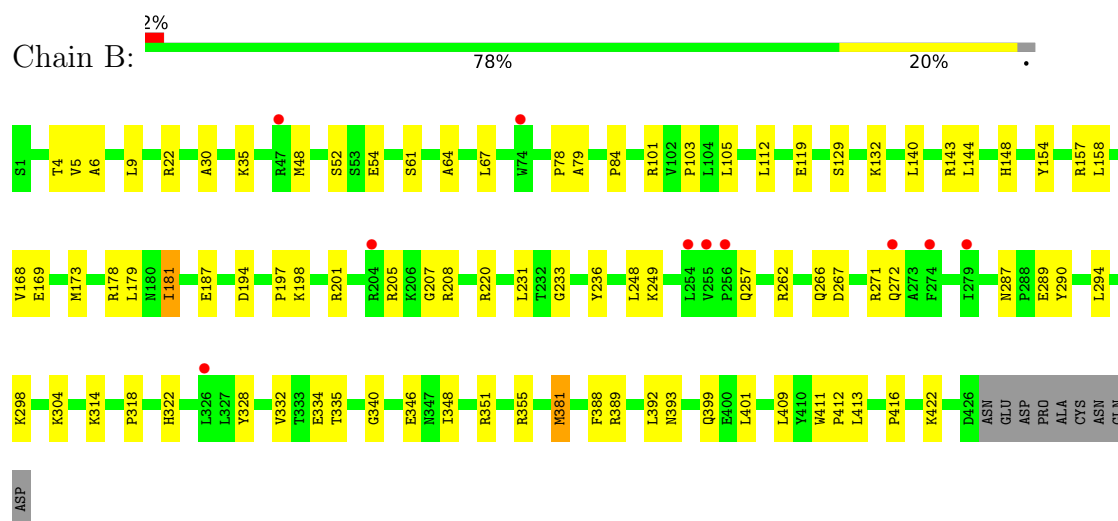
### 3 Residue-property plots [i](#)

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: Atrial natriuretic peptide receptor 1

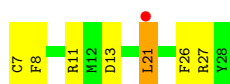


#### • Molecule 1: Atrial natriuretic peptide receptor 1



#### • Molecule 2: Urodilatin





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

Chain C: 67% 33%



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

Chain E: 67% 33%



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

Chain D: 25% 50% 25%



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

Chain F: 75% 25%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.79Å 99.79Å 260.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.26 – 2.70 43.26 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (43.26-2.70) 99.5 (43.26-2.70)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.86 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.193 , 0.234 0.194 , 0.234	Depositor DCC
$R_{free}$ test set	1219 reflections (3.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.7	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 64.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.489 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7286	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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: NAG, CL, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.35	0/3475	0.51	0/4734
1	B	0.35	0/3475	0.50	0/4734
2	L	0.32	0/218	0.66	0/284
All	All	0.35	0/7168	0.51	0/9752

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	3383	0	3325	48	0
1	B	3383	0	3325	46	0
2	L	196	0	187	6	0
3	C	39	0	34	0	0
3	E	39	0	34	0	0
4	D	50	0	43	1	0
4	F	50	0	43	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	66	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	64	0	0	3	0
6	L	14	0	0	2	0
All	All	7286	0	6991	97	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (97) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:GLU:HG3	2:L:8:PHE:HB3	1.67	0.76
1:B:119[B]:GLU:OE2	6:B:601:HOH:O	2.08	0.71
1:A:129:SER:HB2	1:A:132:LYS:HG2	1.73	0.71
1:B:248:LEU:HD22	1:B:257:GLN:HG3	1.73	0.69
1:B:22:ARG:NH1	6:B:604:HOH:O	2.26	0.68
1:A:119[B]:GLU:OE2	6:A:601:HOH:O	2.11	0.67
1:A:22:ARG:NH1	6:A:602:HOH:O	2.27	0.67
1:B:129:SER:HB2	1:B:132:LYS:HG2	1.77	0.67
1:A:168:VAL:HG12	2:L:21:LEU:HD11	1.76	0.66
1:A:248:LEU:HD22	1:A:257:GLN:HG3	1.77	0.65
1:B:249:LYS:HB2	1:B:257:GLN:HE22	1.62	0.63
1:B:220:ARG:HD2	1:B:262:ARG:HH21	1.63	0.62
1:B:154:TYR:HB3	1:B:168:VAL:HG21	1.82	0.59
1:B:101:ARG:NH1	1:B:346:GLU:OE1	2.35	0.59
1:A:220:ARG:HD2	1:A:262:ARG:HH21	1.67	0.59
1:B:201:ARG:HE	1:B:205:ARG:NH1	2.01	0.58
1:A:201:ARG:HE	1:A:205:ARG:NH1	2.01	0.58
1:B:178:ARG:HH12	1:B:399:GLN:HE22	1.53	0.56
1:A:178:ARG:HH12	1:A:399:GLN:HE22	1.54	0.55
2:L:7:CYS:O	6:L:101:HOH:O	2.18	0.55
1:B:154:TYR:CZ	1:B:187:GLU:HB2	2.43	0.54
1:A:154:TYR:HB3	1:A:168:VAL:HG21	1.88	0.54
1:B:334:GLU:OE1	1:B:355:ARG:NH2	2.41	0.54
1:A:154:TYR:CZ	1:A:187:GLU:HB2	2.43	0.54
1:A:52:SER:OG	1:A:54:GLU:HG2	2.09	0.53
1:A:262:ARG:N	1:A:267:ASP:OD1	2.38	0.52
1:B:262:ARG:N	1:B:267:ASP:OD1	2.38	0.52
1:B:287:ASN:HD22	1:B:289:GLU:HB2	1.74	0.52
1:A:334:GLU:OE1	1:A:355:ARG:NH2	2.43	0.52
1:B:52:SER:OG	1:B:54:GLU:HG2	2.11	0.51
1:A:233:GLY:HA3	1:A:412:PRO:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95[B]:ARG:NH2	2:L:13[B]:ASP:OD1	2.33	0.51
1:B:287:ASN:HB2	1:B:289:GLU:OE2	2.12	0.50
1:A:249:LYS:HB2	1:A:257:GLN:HE22	1.77	0.49
1:B:233:GLY:HA3	1:B:412:PRO:HG2	1.93	0.49
1:A:83:GLY:O	1:A:104:LEU:HD11	2.13	0.49
1:B:5:VAL:HB	1:B:48:MET:HG2	1.95	0.49
1:B:411:TRP:CZ2	1:B:416:PRO:HB3	2.47	0.49
1:B:143:ARG:HD3	1:B:401:LEU:HD12	1.94	0.48
1:A:6:ALA:HB2	1:A:78:PRO:HG3	1.94	0.48
1:A:287:ASN:HD22	1:A:289:GLU:HB2	1.79	0.48
1:A:208:ARG:HD3	1:A:421:PRO:HD3	1.94	0.48
1:B:332:VAL:HG22	1:B:348:ILE:HD13	1.96	0.48
1:B:158:LEU:HB2	2:L:27:ARG:HH22	1.79	0.47
1:B:22:ARG:HG2	1:B:318:PRO:HG3	1.97	0.47
1:A:287:ASN:HB2	1:A:289:GLU:OE2	2.15	0.47
1:B:179:LEU:HB3	1:B:181:ILE:HG23	1.96	0.46
1:B:143:ARG:O	1:B:144:LEU:HD12	2.16	0.46
1:A:30:ALA:HB2	1:A:322:HIS:CD2	2.52	0.45
1:B:105:LEU:HD11	1:B:328:TYR:HB2	1.97	0.45
1:B:381:MET:HB3	1:B:388:PHE:CE1	2.50	0.45
1:B:198:LYS:HB3	2:L:26:PHE:CZ	2.52	0.45
1:B:6:ALA:HB2	1:B:78:PRO:HG3	1.98	0.44
1:A:143:ARG:O	1:A:144:LEU:HD12	2.18	0.44
1:A:290:TYR:CE2	1:A:294:LEU:HD11	2.53	0.44
1:B:290:TYR:CE2	1:B:294:LEU:HD11	2.53	0.44
1:B:9:LEU:HD23	1:B:84:PRO:HA	2.00	0.44
1:A:61:SER:HB3	1:A:64:ALA:HB3	2.00	0.43
1:B:194:ASP:O	1:B:197:PRO:HD2	2.18	0.43
1:A:38:PRO:O	1:A:42:PRO:HG3	2.19	0.43
1:B:351:ARG:O	1:B:355:ARG:HD2	2.18	0.43
1:A:207:GLY:C	1:A:208:ARG:HD2	2.39	0.43
1:B:112:LEU:HD22	1:B:173:MET:HG3	2.00	0.43
1:A:179:LEU:HB3	1:A:181:ILE:HG23	2.00	0.43
1:A:314:LYS:HG3	6:A:647:HOH:O	2.18	0.43
1:A:41:LEU:HG	1:A:329:VAL:HG13	2.01	0.42
1:B:79:ALA:O	1:B:103:PRO:HD2	2.19	0.42
1:A:22:ARG:HG2	1:A:318:PRO:HG3	2.01	0.42
1:A:247:SER:O	1:A:259:PRO:HB3	2.18	0.42
1:A:208:ARG:NH2	1:A:236:TYR:OH	2.52	0.42
1:A:82:LEU:HD12	1:A:82:LEU:HA	1.91	0.42
1:A:148:HIS:O	1:A:181:ILE:HB	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:GLY:O	1:A:362:GLY:N	2.50	0.42
1:A:411:TRP:CZ2	1:A:416:PRO:HB3	2.55	0.42
1:A:5:VAL:HB	1:A:48:MET:HG2	2.01	0.42
1:A:105:LEU:HD23	1:A:124:THR:HB	2.02	0.41
1:A:294:LEU:O	1:A:298:LYS:HG3	2.19	0.41
1:A:256:PRO:HG2	1:A:258:LYS:HE3	2.02	0.41
1:B:140:LEU:HD12	1:B:140:LEU:HA	1.90	0.41
1:B:294:LEU:O	1:B:298:LYS:HG3	2.20	0.41
1:B:178:ARG:HH22	1:B:399:GLN:NE2	2.18	0.41
1:A:138:THR:HG23	1:A:179:LEU:HD21	2.01	0.41
1:B:314:LYS:HG3	6:B:636:HOH:O	2.20	0.41
1:A:37:ARG:HB3	1:A:39:ASP:OD1	2.21	0.41
1:A:101:ARG:NH1	1:A:346:GLU:OE1	2.54	0.41
1:B:231:LEU:HD22	1:B:236:TYR:CE1	2.56	0.40
1:A:363:TYR:CD2	4:D:1:NAG:H3	2.56	0.40
1:B:30:ALA:HB2	1:B:322:HIS:CD2	2.56	0.40
1:B:148:HIS:O	1:B:181:ILE:HB	2.21	0.40
1:A:63:THR:HG22	1:A:67:LEU:HD22	2.04	0.40
1:A:178:ARG:HH22	1:A:399:GLN:NE2	2.19	0.40
4:F:1:NAG:H61	4:F:2:NAG:C7	2.51	0.40
1:B:61:SER:HB3	1:B:64:ALA:HB3	2.02	0.40
1:B:207:GLY:O	1:B:208:ARG:HD2	2.22	0.40
1:A:3:LEU:HD12	1:A:3:LEU:HA	1.95	0.40
1:B:335:THR:HG22	1:B:340:GLY:HA3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	427/435 (98%)	411 (96%)	15 (4%)	1 (0%)	47 73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	427/435 (98%)	408 (96%)	18 (4%)	1 (0%)	47	73
2	L	26/22 (118%)	17 (65%)	7 (27%)	2 (8%)	1	1
All	All	880/892 (99%)	836 (95%)	40 (4%)	4 (0%)	41	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	422	LYS
1	B	422	LYS
2	L	11[A]	ARG
2	L	11[B]	ARG

### 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	356/361 (99%)	341 (96%)	15 (4%)	30	58
1	B	356/361 (99%)	341 (96%)	15 (4%)	30	58
2	L	21/16 (131%)	20 (95%)	1 (5%)	25	53
All	All	733/738 (99%)	702 (96%)	31 (4%)	29	58

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	35	LYS
1	A	67	LEU
1	A	157	ARG
1	A	181	ILE
1	A	266	GLN
1	A	271	ARG
1	A	272	GLN
1	A	304	LYS
1	A	381	MET

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Mol	Chain	Res	Type
1	A	389	ARG
1	A	392	LEU
1	A	393	ASN
1	A	409	LEU
1	A	413	LEU
1	B	4	THR
1	B	35	LYS
1	B	67	LEU
1	B	157	ARG
1	B	181	ILE
1	B	266	GLN
1	B	271	ARG
1	B	272	GLN
1	B	304	LYS
1	B	381	MET
1	B	389	ARG
1	B	392	LEU
1	B	393	ASN
1	B	409	LEU
1	B	413	LEU
2	L	21	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	HIS
1	A	246	GLN
1	A	252	GLN
1	A	266	GLN
1	A	322	HIS
1	A	358	GLN
1	A	399	GLN
1	B	180	ASN
1	B	246	GLN
1	B	252	GLN
1	B	266	GLN
1	B	322	HIS
1	B	330	GLN
1	B	358	GLN
1	B	399	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 ⓘ

14 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$
3	NAG	C	1	3,1	14,14,15	0.45	0	17,19,21	0.54	0
3	NAG	C	2	3	14,14,15	0.32	0	17,19,21	0.46	0
3	MAN	C	3	3	11,11,12	1.06	1 (9%)	15,15,17	1.68	1 (6%)
4	NAG	D	1	4,1	14,14,15	0.79	1 (7%)	17,19,21	0.68	0
4	NAG	D	2	4	14,14,15	0.35	0	17,19,21	0.40	0
4	MAN	D	3	4	11,11,12	0.96	0	15,15,17	1.42	2 (13%)
4	MAN	D	4	4	11,11,12	0.83	0	15,15,17	0.98	1 (6%)
3	NAG	E	1	3,1	14,14,15	0.43	0	17,19,21	0.51	0
3	NAG	E	2	3	14,14,15	0.41	0	17,19,21	0.38	0
3	MAN	E	3	3	11,11,12	1.00	1 (9%)	15,15,17	1.69	2 (13%)
4	NAG	F	1	4,1	14,14,15	0.77	1 (7%)	17,19,21	0.62	0
4	NAG	F	2	4	14,14,15	0.36	0	17,19,21	0.40	0
4	MAN	F	3	4	11,11,12	0.90	0	15,15,17	1.37	2 (13%)
4	MAN	F	4	4	11,11,12	0.84	0	15,15,17	1.00	1 (6%)

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
3	NAG	C	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	MAN	C	3	3	-	2/2/19/22	1/1/1/1
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	MAN	D	3	4	-	0/2/19/22	1/1/1/1
4	MAN	D	4	4	-	0/2/19/22	0/1/1/1
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	1/6/23/26	0/1/1/1
3	MAN	E	3	3	-	2/2/19/22	1/1/1/1
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	MAN	F	3	4	-	0/2/19/22	1/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	MAN	O5-C5	2.59	1.48	1.43
3	E	3	MAN	O5-C5	2.59	1.48	1.43
4	D	1	NAG	O5-C1	2.22	1.47	1.43
4	F	1	NAG	C1-C2	2.03	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	MAN	C1-O5-C5	5.40	119.52	112.19
3	E	3	MAN	C1-O5-C5	5.35	119.44	112.19
4	D	3	MAN	C1-O5-C5	4.33	118.06	112.19
4	F	3	MAN	C1-O5-C5	4.18	117.85	112.19
4	F	4	MAN	C1-O5-C5	2.44	115.50	112.19
4	F	3	MAN	O5-C1-C2	2.29	114.30	110.77
4	D	4	MAN	C1-O5-C5	2.19	115.16	112.19
4	D	3	MAN	O5-C1-C2	2.16	114.10	110.77
3	E	3	MAN	O5-C1-C2	2.04	113.91	110.77

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	3	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	E	1	NAG	O5-C5-C6-O6
3	C	3	MAN	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
3	E	3	MAN	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	C	3	MAN	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6

All (4) ring outliers are listed below:

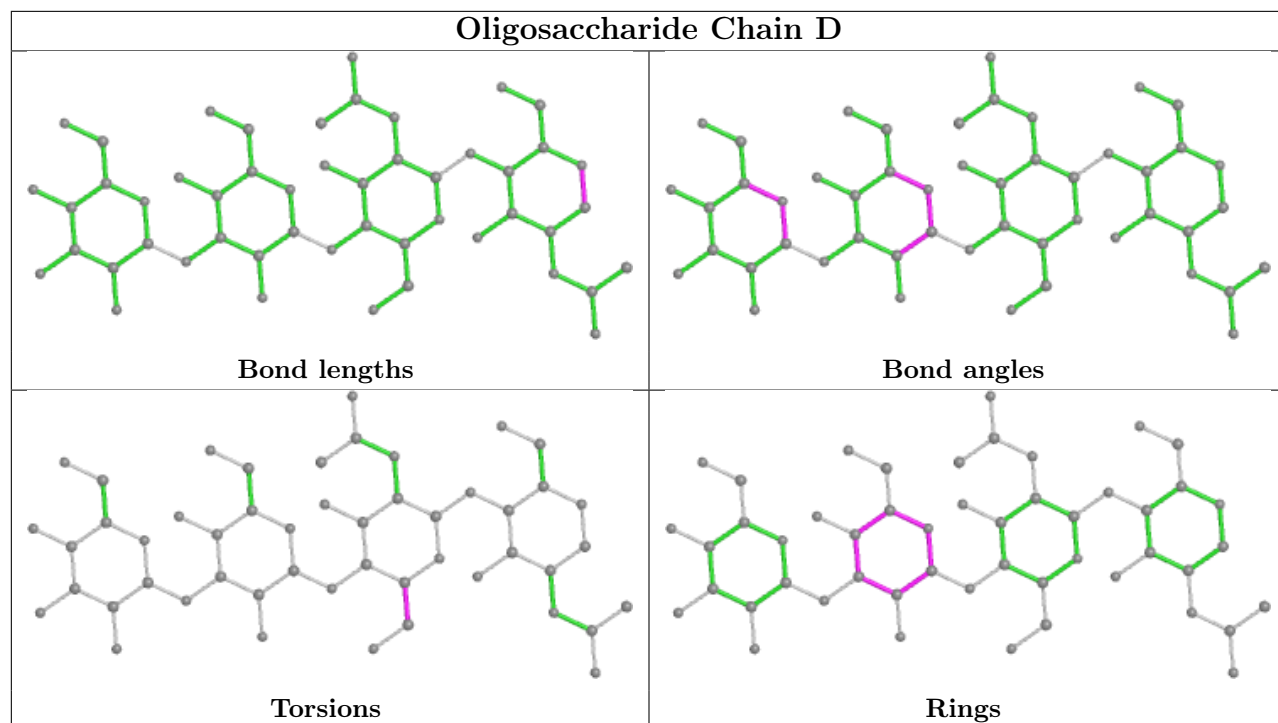
Mol	Chain	Res	Type	Atoms
3	E	3	MAN	C1-C2-C3-C4-C5-O5
3	C	3	MAN	C1-C2-C3-C4-C5-O5
4	D	3	MAN	C1-C2-C3-C4-C5-O5
4	F	3	MAN	C1-C2-C3-C4-C5-O5

3 monomers are involved in 2 short contacts:

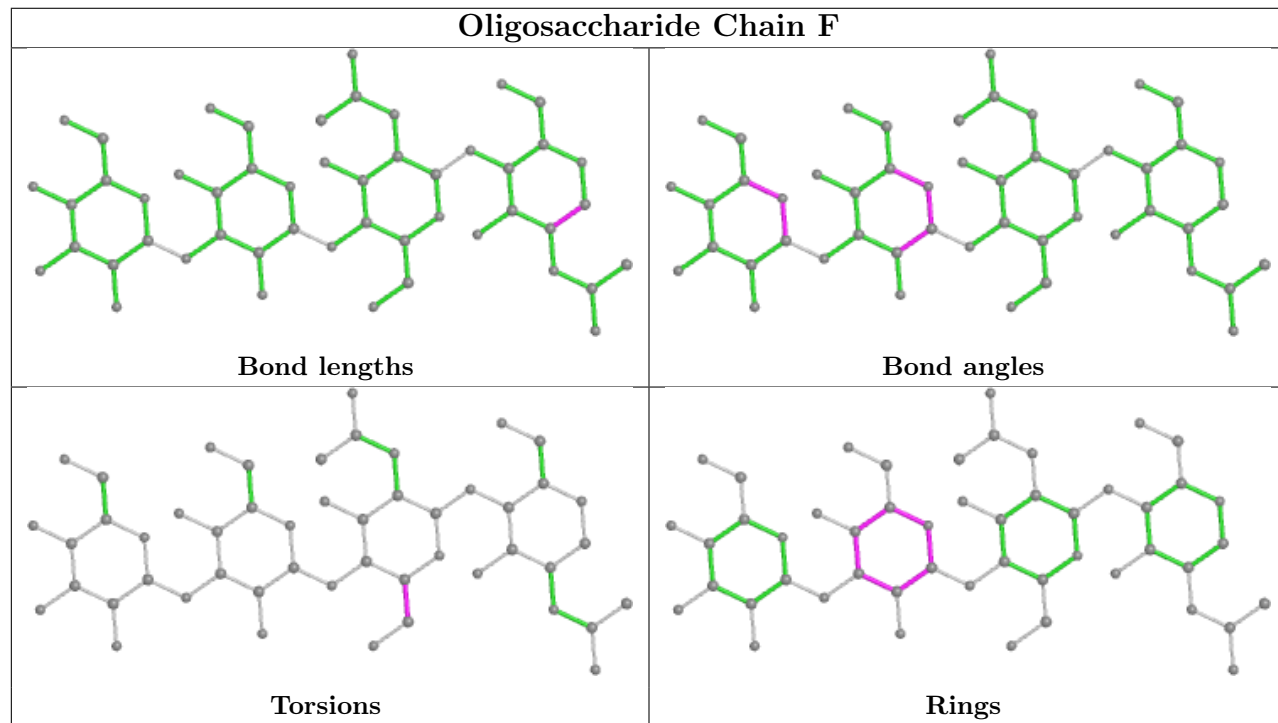
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1	NAG	1	0
4	F	2	NAG	1	0
4	D	1	NAG	1	0

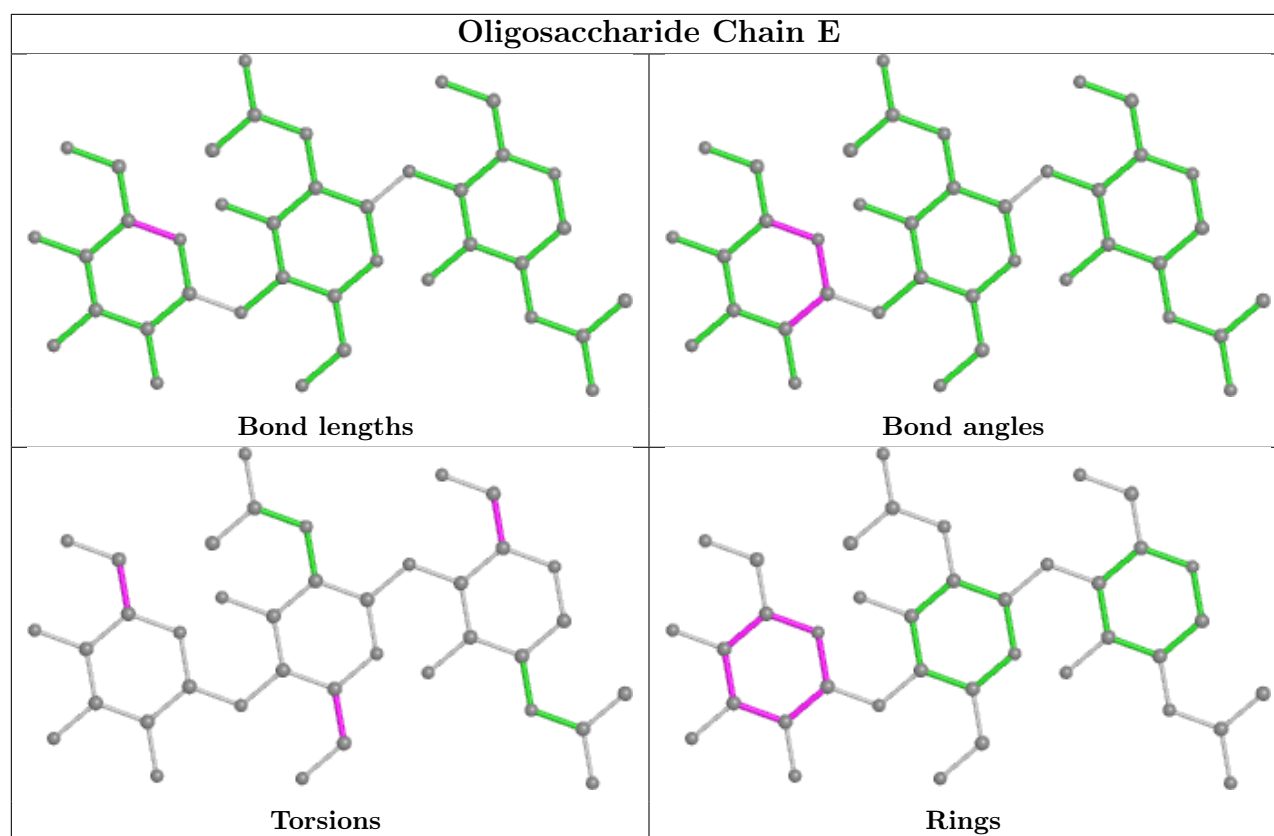
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

## Oligosaccharide Chain D



## Oligosaccharide Chain F





## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	426/435 (97%)	0.46	17 (3%) 38 37	42, 82, 138, 219	0
1	B	426/435 (97%)	0.42	10 (2%) 60 62	44, 81, 140, 214	0
2	L	22/22 (100%)	0.84	1 (4%) 33 31	77, 96, 129, 135	0
All	All	874/892 (97%)	0.45	28 (3%) 47 48	42, 82, 139, 219	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	256	PRO	8.8
1	A	255	VAL	8.5
1	A	254	LEU	7.1
1	B	256	PRO	6.3
1	B	255	VAL	6.3
1	B	74[A]	TRP	4.9
1	B	254	LEU	4.7
2	L	21	LEU	4.3
1	A	74[A]	TRP	3.8
1	A	43	GLY	2.9
1	A	413	LEU	2.8
1	A	384	GLU	2.8
1	B	272	GLN	2.7
1	A	157	ARG	2.7
1	A	251	ALA	2.5
1	A	274	PHE	2.5
1	B	279	ILE	2.4
1	B	47	ARG	2.4
1	A	158	LEU	2.4
1	A	357	PHE	2.3
1	B	326	LEU	2.3
1	B	274	PHE	2.2
1	A	209	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	406	GLU	2.1
1	A	258	LYS	2.1
1	B	204	ARG	2.1
1	A	50	LEU	2.0
1	A	175	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

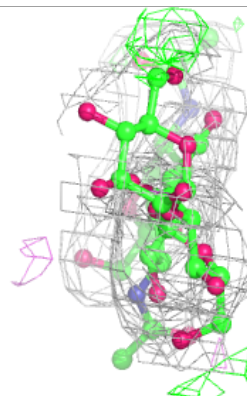
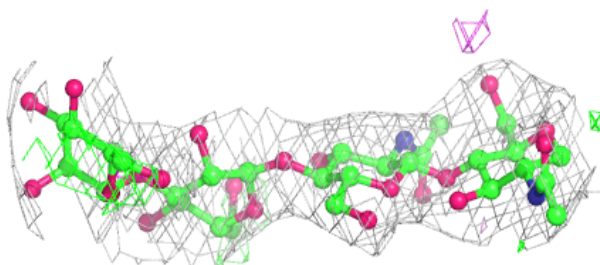
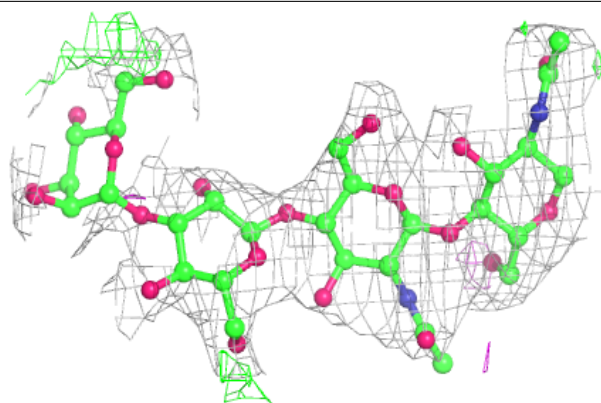
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MAN	C	3	11/12	0.33	0.30	152,158,165,165	0
3	MAN	E	3	11/12	0.49	0.30	151,159,169,170	0
4	MAN	F	4	11/12	0.55	0.17	141,161,170,173	0
4	MAN	F	3	11/12	0.61	0.19	148,162,170,177	0
4	MAN	D	4	11/12	0.65	0.14	143,159,167,172	0
4	MAN	D	3	11/12	0.71	0.16	157,169,173,177	0
3	NAG	E	2	14/15	0.88	0.24	98,116,128,143	0
3	NAG	C	2	14/15	0.88	0.23	98,113,124,139	0
4	NAG	D	2	14/15	0.92	0.15	115,124,133,151	0
4	NAG	F	2	14/15	0.93	0.15	118,121,134,148	0
4	NAG	F	1	14/15	0.94	0.13	62,77,95,104	0
4	NAG	D	1	14/15	0.95	0.13	52,72,95,95	0
3	NAG	C	1	14/15	0.97	0.16	48,70,93,94	0
3	NAG	E	1	14/15	0.97	0.16	49,71,98,102	0

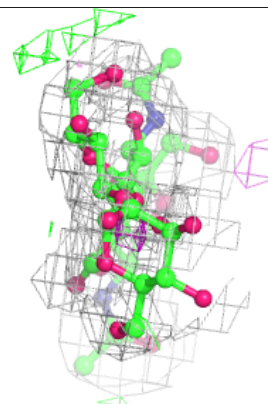
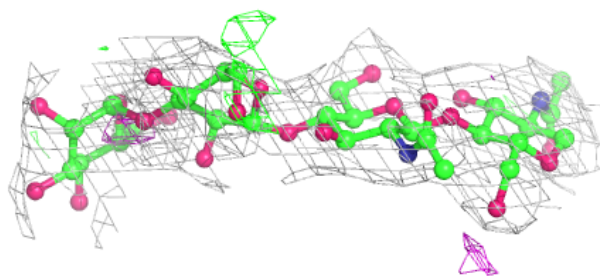
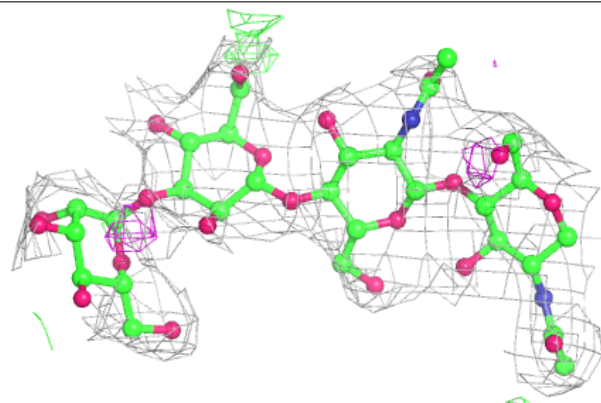
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

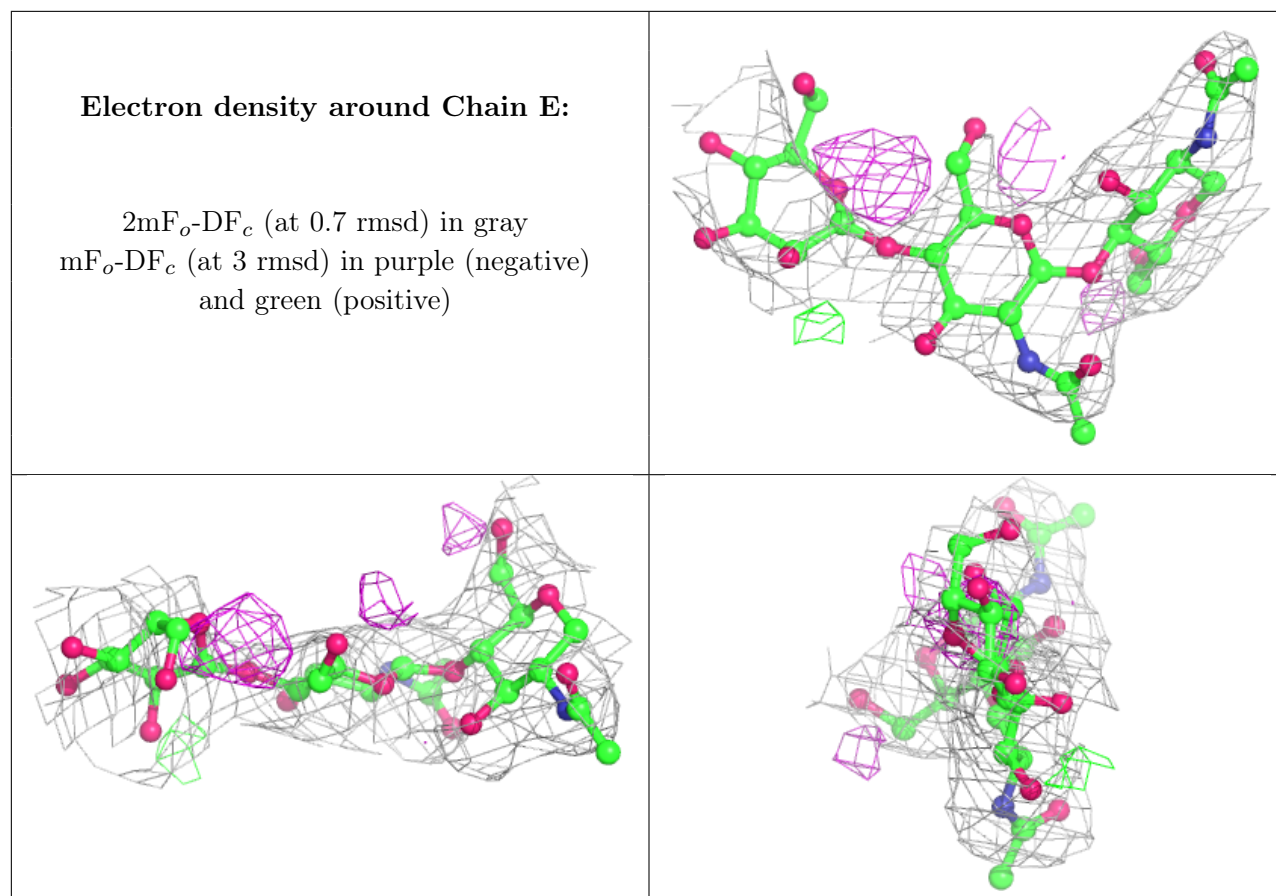
**Electron density around Chain D:**

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

**Electron density around Chain F:**

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





## 6.4 Ligands [i](#)

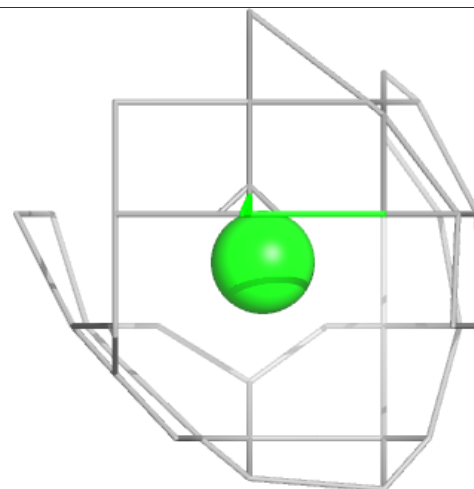
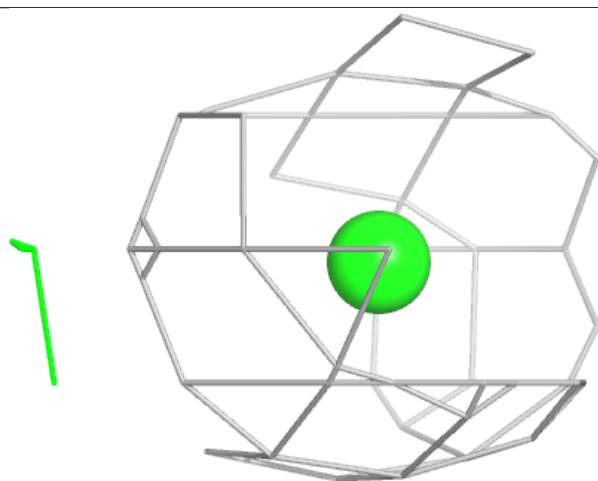
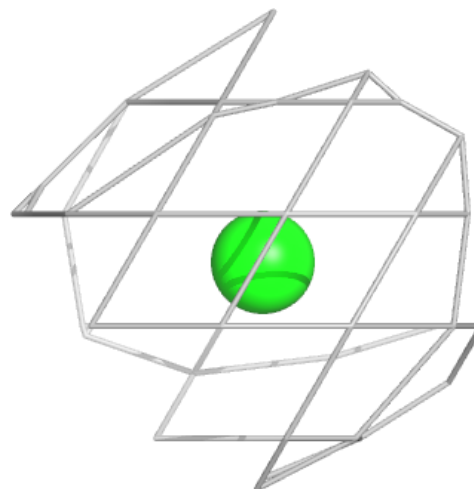
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 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
5	CL	A	501	1/1	0.97	0.10	61,61,61,61	0
5	CL	B	501	1/1	0.98	0.13	57,57,57,57	0

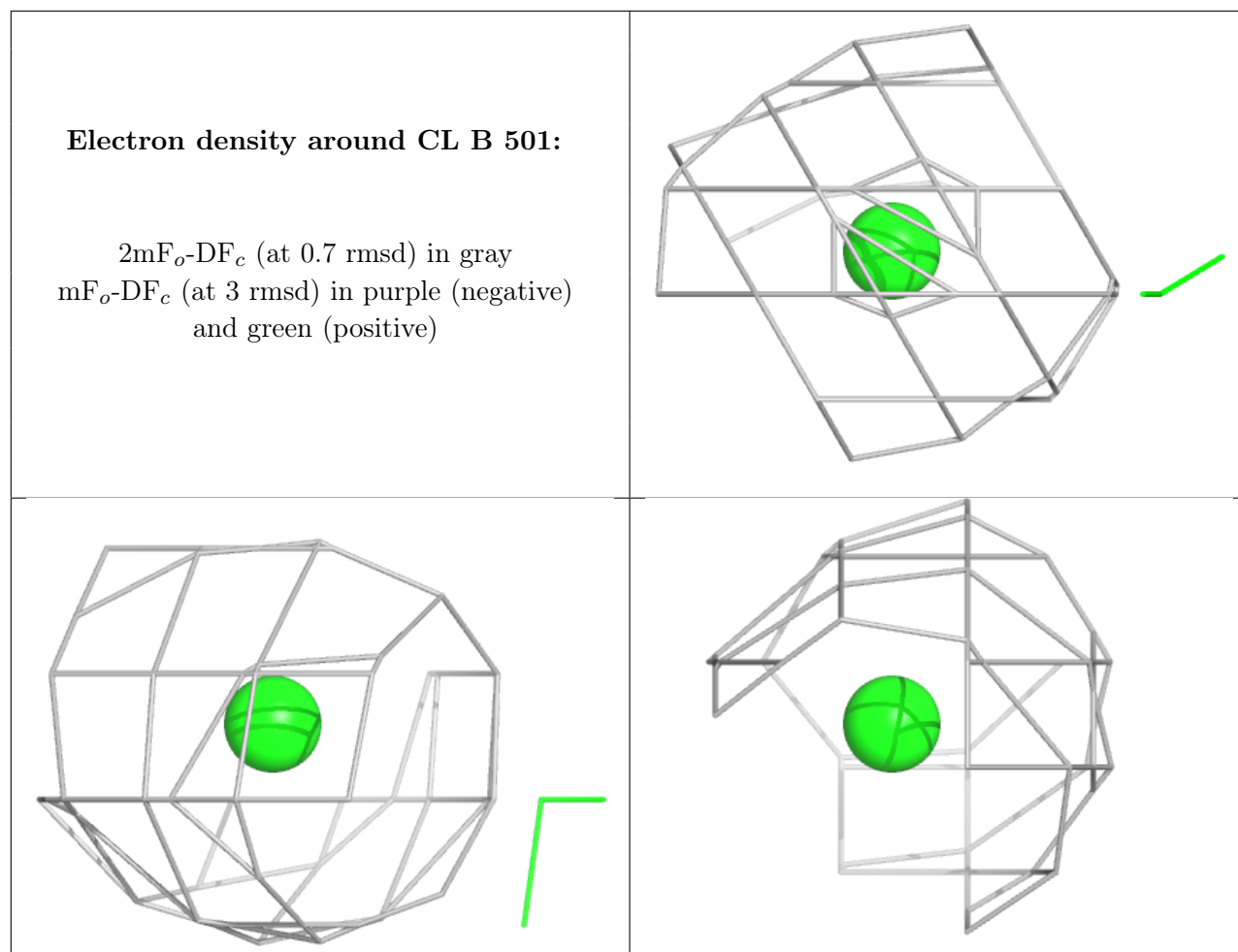
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around CL A 501:**

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







## 6.5 Other polymers [i](#)

There are no such residues in this entry.