



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:14 PM UTC

PDB ID : 8AEV / pdb\_00008aev  
Title : Human acetylcholinesterase in complex with N,N,N-trimethyl-2-oxo-2-(2-(pyridin-2-ylmethylene)hydrazineyl)ethan-1-aminium  
Authors : Nachon, F.; Dias, J.; Brazzolotto, X.  
Deposited on : 2022-07-13  
Resolution : 2.89 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

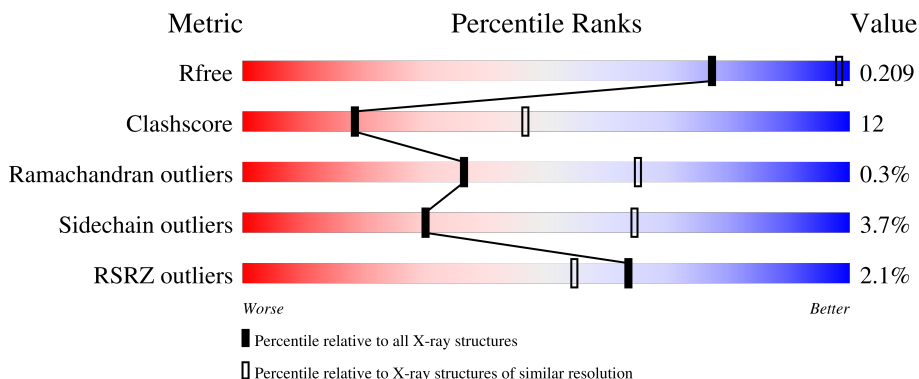
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.89 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))
$R_{free}$	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	543	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 72%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 24%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">72% 24% ..</p>
1	B	543	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 72%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 25%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">72% 25% ..</p>
2	C	3	<div style="width: 100%; height: 10px; background-color: yellow;"></div> <p style="text-align: center;">100%</p>
2	F	3	<div style="width: 100%; height: 10px; background-color: yellow;"></div> <p style="text-align: center;">100%</p>
3	D	2	<div style="display: flex; align-items: center;"> <div style="width: 50%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 50%; height: 10px; background-color: orange;"></div> </div> <p style="text-align: center;">50% 50%</p>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
4	E	2	 50% 50%

## 2 Entry composition [i](#)

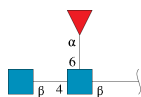
There are 10 unique types of molecules in this entry. The entry contains 8809 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acetylcholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	533	Total 4161	C 2671	N 727	O 750	S 13	0	1	0
1	B	535	Total 4172	C 2678	N 729	O 752	S 13	0	1	0

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



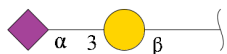
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	3	Total 38	C 22	N 2	O 14	0	0	0
2	F	3	Total 38	C 22	N 2	O 14	0	0	0

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



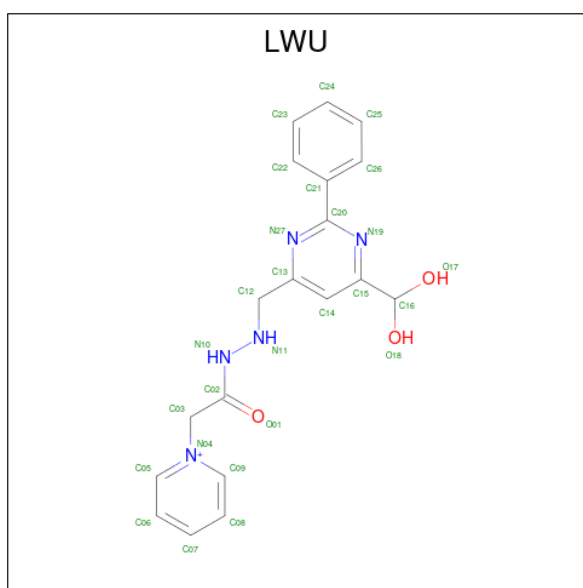
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	E	2	32	17	1	14	0	0	0

- Molecule 5 is 1-(2-(2-((6-(dihydroxymethyl)-2-phenylpyrimidin-4-yl)methylene)hydrazineyl)-2-oxoethyl)pyridin-1-ium (CCD ID: LWU) (formula: C<sub>19</sub>H<sub>20</sub>N<sub>5</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	27	19	5	3	0	0

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	14	Total Cl 14 14	0	0
7	B	17	Total Cl 17 17	0	0

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	2	Total Zn 2 2	0	0
8	B	3	Total Zn 3 3	0	0

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	8	Total Mg 8 8	0	0
9	B	6	Total Mg 6 6	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	108	Total O 108 108	0	0
10	B	75	Total O 75 75	0	0





- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 100%

MAG1  
MAG2  
FUC3

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 100%

MAG1  
MAG2  
FUC3

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

Chain D: 50% 50%

MAG1  
MAG2

- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain E: 50% 50%

GAL1  
SIA2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.83Å 211.83Å 116.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.64 – 2.89 46.64 – 2.89	Depositor EDS
% Data completeness (in resolution range)	94.5 (46.64-2.89) 83.7 (46.64-2.89)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.86 (at 2.91Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.184 , 0.207 0.185 , 0.209	Depositor DCC
$R_{free}$ test set	3198 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.5	Xtrriage
Anisotropy	0.372	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 76.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8809	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.94% 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: SIA, NAG, FUC, LWU, ZN, GAL, SO4, TIS, MG, CL

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	0.45	0/4281	0.67	2/5850 (0.0%)
1	B	0.43	0/4293	0.62	0/5867
All	All	0.44	0/8574	0.64	2/11717 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	VAL	CA-C-N	5.62	128.66	120.51
1	A	288	VAL	C-N-CA	5.62	128.66	120.51

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	4161	0	4042	102	0
1	B	4172	0	4053	104	0
2	C	38	0	34	0	0
2	F	38	0	34	0	0
3	D	28	0	25	1	0
4	E	32	0	28	1	0
5	A	27	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	45	0	0	0	0
6	B	35	0	0	1	0
7	A	14	0	0	0	0
7	B	17	0	0	3	0
8	A	2	0	0	0	0
8	B	3	0	0	0	0
9	A	8	0	0	0	0
9	B	6	0	0	0	0
10	A	108	0	0	4	0
10	B	75	0	0	0	0
All	All	8809	0	8216	202	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 12.

All (202) 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:D:1:NAG:H62	3:D:2:NAG:H2	1.56	0.88
1:B:467:ALA:HA	1:B:470:LYS:HD2	1.56	0.87
1:A:197:VAL:H	1:A:223:HIS:HD2	1.26	0.84
1:A:224:ARG:NH1	1:A:484:ALA:O	2.12	0.82
1:B:46:ARG:O	1:B:274:ARG:NH1	2.15	0.79
1:A:138:LEU:HA	1:A:477:MET:HE3	1.64	0.77
1:A:197:VAL:H	1:A:223:HIS:CD2	2.01	0.77
1:B:80:PHE:HD2	1:B:83:THR:HG23	1.51	0.75
1:A:118:ILE:HG12	1:A:149:MET:HE1	1.69	0.75
1:B:143:ARG:NH2	7:B:622:CL:CL	2.56	0.74
1:B:518:LEU:HD12	1:B:518:LEU:H	1.51	0.74
1:A:68:VAL:HG23	1:A:90:ARG:HB2	1.72	0.71
1:B:197:VAL:H	1:B:223:HIS:HD2	1.39	0.71
1:B:203:TIS:O1T	1:B:447:HIS:NE2	2.25	0.69
1:B:177:ARG:NH1	4:E:2:SIA:O1B	2.27	0.67
1:B:312:PRO:O	1:B:316:ILE:HG13	1.95	0.66
1:A:440:PRO:HG2	1:A:443:MET:HG3	1.77	0.65
1:B:479:TYR:OH	1:B:518:LEU:HD11	1.97	0.65
1:B:466:THR:HG22	1:B:468:GLU:H	1.61	0.64
1:B:376:GLU:O	1:B:380:LEU:HG	1.97	0.64
1:A:466:THR:HB	1:A:469:GLU:HB2	1.79	0.64
1:A:424:ARG:NH2	10:A:702:HOH:O	2.31	0.63
1:B:36:PRO:HB2	1:B:53:LYS:HD3	1.81	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:GLU:HG2	10:A:714:HOH:O	1.98	0.62
1:A:525:ARG:NH1	10:A:703:HOH:O	2.32	0.62
1:A:376:GLU:O	1:A:380:LEU:HD12	2.01	0.60
1:B:68:VAL:HG13	1:B:127:ALA:HB2	1.83	0.60
1:B:142:GLU:OE1	1:B:485:ARG:NH2	2.33	0.60
1:A:226:VAL:HG22	1:A:327:LEU:HB3	1.83	0.60
1:A:432:HIS:CE1	1:A:515:LEU:HD11	2.37	0.60
1:B:328:VAL:O	1:B:427:ALA:HA	2.02	0.60
1:B:277:PRO:O	1:B:280:VAL:HG12	2.02	0.59
1:B:313:GLU:HB2	7:B:618:CL:CL	2.40	0.59
1:A:270:VAL:HG12	1:A:274:ARG:HE	1.67	0.59
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.39	0.58
1:B:364:ARG:HE	1:B:375:ALA:HB1	1.69	0.57
1:A:496:LYS:C	1:A:496:LYS:HD2	2.29	0.57
1:B:246:ARG:HH11	1:B:246:ARG:HG2	1.70	0.57
1:B:496:LYS:HZ3	1:B:497:ALA:H	1.53	0.57
1:A:294:VAL:HG12	1:A:366:GLY:HA2	1.86	0.57
1:B:333:ASP:OD2	1:B:444:GLY:HA3	2.05	0.57
1:A:44:PRO:O	1:A:274:ARG:NH1	2.37	0.56
1:B:353:LEU:HB3	1:B:391:PRO:HB2	1.87	0.56
1:A:376:GLU:OE2	1:A:380:LEU:HD11	2.05	0.56
1:B:498:PRO:HB2	1:B:518:LEU:HD13	1.86	0.56
1:A:312:PRO:O	1:A:316:ILE:HG13	2.05	0.56
1:B:80:PHE:CE1	1:B:348:LYS:HE3	2.41	0.56
1:B:213:LEU:HD22	1:B:324:LEU:HD21	1.87	0.56
1:A:376:GLU:O	1:A:379:VAL:HG12	2.05	0.55
1:A:381[B]:HIS:NE2	1:B:381[B]:HIS:CE1	2.73	0.55
1:B:104:PRO:HB3	1:B:143:ARG:HG2	1.87	0.55
1:B:482:ASN:OD1	1:B:485:ARG:NH1	2.39	0.55
1:B:496:LYS:NZ	1:B:497:ALA:H	2.04	0.55
1:A:373:LEU:HD23	1:A:543:THR:HG21	1.89	0.55
1:A:245:ARG:NH2	1:A:266:ASP:OD2	2.40	0.55
1:B:322:HIS:HA	1:B:422:GLY:O	2.08	0.54
1:B:77:TYR:HB2	1:B:83:THR:HG21	1.90	0.54
1:A:66:GLN:HG2	1:A:98:TYR:CD2	2.42	0.54
1:A:122:GLY:N	1:A:203:TIS:O2T	2.35	0.53
1:A:105:TYR:HB3	1:A:106:PRO:HD3	1.90	0.53
1:A:364:ARG:NH2	1:A:372:ASP:OD1	2.41	0.53
1:B:13:ARG:HD2	1:B:185:GLU:OE1	2.08	0.53
1:A:162:PRO:HD2	1:A:245:ARG:NH1	2.23	0.53
1:A:254:LEU:HD12	1:A:284:HIS:HD2	1.74	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:VAL:HG11	1:B:525:ARG:HG3	1.91	0.53
1:A:16:ARG:HB2	1:A:59:VAL:HG12	1.90	0.52
1:B:491:GLU:HB3	1:B:494:ASP:OD1	2.10	0.52
1:A:66:GLN:HG2	1:A:98:TYR:CE2	2.44	0.52
1:A:322:HIS:HA	1:A:422:GLY:O	2.08	0.52
1:B:66:GLN:HG3	1:B:98:TYR:CD2	2.45	0.52
1:A:515:LEU:HD12	10:A:785:HOH:O	2.09	0.52
1:A:494:ASP:OD2	1:A:497:ALA:HB2	2.10	0.52
1:A:328:VAL:O	1:A:427:ALA:HA	2.09	0.52
1:B:77:TYR:CZ	1:B:348:LYS:HG2	2.45	0.52
1:A:510:TYR:CZ	1:A:521:ARG:HB2	2.45	0.51
1:A:42:MET:HE3	1:A:94:GLU:HB2	1.93	0.51
1:B:466:THR:HG22	1:B:468:GLU:N	2.26	0.51
1:A:543:THR:HG22	1:B:543:THR:HG22	1.92	0.50
1:B:329:GLY:HA3	1:B:428:TYR:CE2	2.46	0.50
1:A:91:GLU:OE2	1:A:91:GLU:HA	2.12	0.50
1:B:330:VAL:HG23	1:B:429:VAL:HG13	1.93	0.50
1:A:22:LEU:N	1:A:22:LEU:HD22	2.26	0.50
1:A:115:LEU:HD23	1:A:198:THR:HB	1.92	0.50
1:A:32:PHE:HB3	1:A:35:ILE:HD11	1.94	0.49
1:A:122:GLY:H	1:A:203:TIS:H10	1.55	0.49
1:A:329:GLY:HA3	1:A:428:TYR:CZ	2.48	0.49
1:A:466:THR:HB	1:A:469:GLU:H	1.77	0.49
1:A:466:THR:HG22	1:A:468:GLU:H	1.77	0.49
1:A:198:THR:HG23	1:A:224:ARG:HB2	1.94	0.49
1:B:252:ALA:CB	1:B:269:LEU:HD21	2.42	0.49
1:A:66:GLN:HG3	1:A:67:SER:H	1.78	0.48
1:A:381[B]:HIS:NE2	1:B:381[B]:HIS:HE1	2.11	0.48
1:B:276:ARG:HB3	1:B:280:VAL:HG11	1.95	0.48
1:A:466:THR:HG22	1:A:468:GLU:N	2.28	0.48
1:B:433:ARG:NH2	1:B:441:LEU:HA	2.28	0.48
1:A:36:PRO:HB2	1:A:53:LYS:HD3	1.96	0.48
1:A:458:PRO:HA	1:A:465:TYR:CD1	2.49	0.48
1:B:36:PRO:HB3	1:B:98:TYR:CE2	2.49	0.48
1:B:46:ARG:HD3	1:B:94:GLU:OE1	2.14	0.48
1:B:510:TYR:CZ	1:B:521:ARG:HB2	2.49	0.48
1:A:107:ARG:HG3	1:A:108:PRO:HD2	1.96	0.48
1:B:246:ARG:HG2	1:B:246:ARG:NH1	2.29	0.48
1:A:197:VAL:N	1:A:223:HIS:HD2	2.03	0.47
1:A:56:TRP:NE1	1:A:60:VAL:HG23	2.29	0.47
1:A:181:GLN:O	1:A:185:GLU:HG3	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:PHE:CZ	1:B:348:LYS:HE3	2.50	0.47
1:A:413:GLN:O	1:A:417:ARG:HG2	2.14	0.47
1:B:536:LEU:O	1:B:540:LEU:HD13	2.14	0.47
1:B:197:VAL:H	1:B:223:HIS:CD2	2.25	0.47
1:A:42:MET:HE2	1:A:42:MET:HB3	1.81	0.47
1:A:310:ASP:OD1	1:A:311:THR:N	2.44	0.47
1:A:66:GLN:HG2	1:A:98:TYR:CG	2.51	0.46
1:B:254:LEU:HD21	1:B:287:HIS:HB2	1.97	0.46
1:A:496:LYS:HD2	1:A:496:LYS:O	2.15	0.46
1:B:351:GLU:HB3	1:B:353:LEU:HG	1.96	0.46
1:B:433:ARG:CZ	1:B:437:LEU:HD23	2.45	0.46
1:B:475:ARG:NH1	1:B:479:TYR:OH	2.49	0.46
1:B:203:TIS:O1T	1:B:447:HIS:CD2	2.68	0.46
1:A:130:LEU:HD12	1:A:133:TYR:CE2	2.50	0.46
1:B:265:ASN:HD22	1:B:265:ASN:N	2.14	0.46
1:B:534:ARG:HG3	1:B:534:ARG:NH1	2.31	0.46
1:B:351:GLU:O	1:B:395:ARG:NH1	2.43	0.46
1:A:303:VAL:O	1:A:303:VAL:HG23	2.16	0.46
1:B:344:PRO:HB2	1:B:358:GLU:HG2	1.97	0.45
1:A:162:PRO:CB	1:A:241:MET:HG2	2.47	0.45
1:A:223:HIS:C	1:A:224:ARG:HG2	2.41	0.45
1:B:58:GLY:N	6:B:605:SO4:O4	2.35	0.45
1:B:390:ASP:OD2	1:B:393:ARG:HG3	2.16	0.45
1:B:45:ARG:NH2	1:B:51:GLU:OE2	2.50	0.45
1:B:172:GLY:O	1:B:175:ASP:HB2	2.17	0.45
1:A:216:PRO:HB2	1:A:217:PRO:HD3	1.98	0.45
1:A:498:PRO:HB2	1:A:518:LEU:HB2	1.99	0.45
1:B:76:LEU:HD22	1:B:341:TYR:CE1	2.52	0.45
1:A:211:MET:HG2	1:A:308:LEU:HD11	1.99	0.45
1:A:239:VAL:HG13	1:A:300:VAL:CG2	2.47	0.45
1:A:80:PHE:O	1:A:84:GLU:HG2	2.17	0.44
1:B:173:LEU:HD23	1:B:173:LEU:HA	1.85	0.44
1:B:329:GLY:HA3	1:B:428:TYR:CZ	2.52	0.44
1:B:488:ASP:OD1	1:B:490:ASN:HB2	2.17	0.44
1:B:470:LYS:O	1:B:474:GLN:HG3	2.17	0.44
1:B:70:TYR:OH	1:B:279:GLN:HG2	2.17	0.44
1:B:136:ARG:HG2	1:B:137:PHE:CD2	2.53	0.44
1:B:48:LEU:HD23	1:B:48:LEU:HA	1.76	0.44
1:B:203:TIS:HBA	1:B:447:HIS:NE2	2.32	0.44
1:A:101:VAL:HG22	1:A:147:VAL:HG22	2.00	0.44
1:B:24:THR:HG22	1:B:136:ARG:HD3	1.99	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:GLY:C	1:B:266:ASP:H	2.26	0.43
1:B:317:ASN:OD1	1:B:417:ARG:NH1	2.51	0.43
1:B:207:ALA:O	1:B:211:MET:HG3	2.18	0.43
1:A:226:VAL:HA	1:A:327:LEU:O	2.19	0.43
1:A:367:VAL:HG22	1:A:367:VAL:O	2.18	0.43
1:B:319:GLY:HA3	1:B:321:PHE:CE2	2.53	0.43
1:A:441:LEU:HD22	1:A:441:LEU:HA	1.83	0.43
1:B:429:VAL:HG23	1:B:510:TYR:CD2	2.54	0.43
1:A:24:THR:HB	1:A:140:GLN:HG3	2.01	0.43
1:B:197:VAL:N	1:B:223:HIS:HD2	2.12	0.43
1:B:200:PHE:CB	1:B:226:VAL:HB	2.48	0.43
1:A:138:LEU:HA	1:A:138:LEU:HD13	1.80	0.43
1:A:331:VAL:HB	1:A:445:VAL:HG12	2.01	0.43
1:A:381[A]:HIS:HE1	1:B:381[A]:HIS:NE2	2.17	0.43
1:B:331:VAL:HG22	1:B:334:GLU:CD	2.44	0.43
1:A:97:LEU:HD23	1:A:97:LEU:HA	1.71	0.42
1:B:356:ARG:HD3	1:B:388:PRO:O	2.19	0.42
1:B:384:ASP:O	1:B:386:LEU:N	2.52	0.42
1:B:219:ARG:HD2	1:B:219:ARG:HA	1.70	0.42
1:B:236:TRP:CD1	1:B:236:TRP:H	2.37	0.42
1:A:439:TRP:HB3	1:A:440:PRO:HD2	2.01	0.42
1:A:117:TRP:HA	1:A:200:PHE:O	2.19	0.42
1:A:149:MET:HE2	1:A:176:GLN:HG2	2.01	0.42
1:A:356:ARG:O	1:A:360:LEU:HD12	2.19	0.42
1:B:339:LEU:HD21	1:B:402:VAL:HG21	2.02	0.42
1:A:23:LYS:H	1:A:23:LYS:HD2	1.85	0.42
1:B:377:ALA:O	1:B:381[A]:HIS:HB2	2.19	0.42
1:A:210:GLY:HA3	1:A:232:PRO:HD3	2.01	0.42
1:B:33:LEU:HD13	1:B:100:ASN:HB3	2.02	0.42
1:A:114:VAL:HB	1:A:197:VAL:HG22	2.02	0.41
1:A:441:LEU:O	1:A:441:LEU:HD13	2.20	0.41
1:B:468:GLU:HA	1:B:468:GLU:OE1	2.20	0.41
1:B:44:PRO:HA	1:B:274:ARG:HD3	2.03	0.41
1:A:79:GLY:N	1:A:84:GLU:OE2	2.44	0.41
1:A:170:ASN:OD1	1:A:301:PRO:HA	2.20	0.41
1:B:337:TYR:CZ	1:B:341:TYR:HE2	2.38	0.41
1:A:381[A]:HIS:CE1	1:B:381[A]:HIS:NE2	2.88	0.41
1:B:37:PHE:CD1	1:B:99:LEU:HD23	2.56	0.41
1:A:66:GLN:HG2	1:A:98:TYR:CZ	2.56	0.41
1:A:306:ASP:OD1	1:A:306:ASP:C	2.63	0.41
1:A:81:GLU:O	1:A:85:MET:HG2	2.21	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:LEU:HD21	1:A:199:LEU:HD21	2.03	0.41
1:B:170:ASN:OD1	1:B:301:PRO:HA	2.21	0.41
1:A:376:GLU:O	1:A:379:VAL:N	2.51	0.41
1:B:164:SER:O	1:B:165:ARG:HB3	2.21	0.41
1:B:253:HIS:CD2	1:B:253:HIS:C	2.99	0.41
1:A:224:ARG:HE	1:A:325:GLN:NE2	2.18	0.41
1:A:453:PHE:HB3	1:A:476:LEU:HD12	2.03	0.40
1:B:496:LYS:HD2	1:B:496:LYS:HA	1.59	0.40
1:B:264:GLY:HA3	7:B:615:CL:CL	2.58	0.40
1:A:98:TYR:CD1	1:A:98:TYR:N	2.89	0.40
1:A:29:VAL:HG11	1:A:139:VAL:CG2	2.51	0.40
1:A:380:LEU:HD12	1:A:380:LEU:H	1.87	0.40
1:A:329:GLY:HA3	1:A:428:TYR:CE1	2.56	0.40
1:B:118:ILE:HG22	1:B:205:GLY:HA2	2.03	0.40
1:B:534:ARG:HG3	1:B:534:ARG:HH11	1.85	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	529/543 (97%)	495 (94%)	33 (6%)	1 (0%)	43	72
1	B	531/543 (98%)	484 (91%)	45 (8%)	2 (0%)	30	59
All	All	1060/1086 (98%)	979 (92%)	78 (7%)	3 (0%)	36	65

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	265	ASN
1	B	290	PRO
1	A	121	GLY

### 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	433/437 (99%)	413 (95%)	20 (5%)	24	57
1	B	434/437 (99%)	420 (97%)	14 (3%)	34	68
All	All	867/874 (99%)	833 (96%)	34 (4%)	30	63

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	THR
1	A	110	SER
1	A	112	THR
1	A	138	LEU
1	A	145	VAL
1	A	200	PHE
1	A	267	THR
1	A	288	VAL
1	A	311	THR
1	A	328	VAL
1	A	347	SER
1	A	367	VAL
1	A	381[A]	HIS
1	A	381[B]	HIS
1	A	402	VAL
1	A	452	GLU
1	A	493	ARG
1	A	515	LEU
1	A	536	LEU
1	A	539	LEU
1	B	24	THR
1	B	129	SER
1	B	238	THR
1	B	239	VAL
1	B	328	VAL
1	B	367	VAL
1	B	381[A]	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	381[B]	HIS
1	B	452	GLU
1	B	462	SER
1	B	476	LEU
1	B	490	ASN
1	B	491	GLU
1	B	494	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	HIS
1	A	228	GLN
1	A	279	GLN
1	A	283	ASN
1	A	287	HIS
1	A	291	GLN
1	A	325	GLN
1	A	369	GLN
1	A	387	HIS
1	A	464	ASN
1	B	181	GLN
1	B	223	HIS
1	B	253	HIS
1	B	265	ASN
1	B	279	GLN
1	B	291	GLN
1	B	387	HIS
1	B	432	HIS
1	B	490	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	TIS	A	203	1	5,9,10	3.34	3 (60%)	3,12,14	1.43	0
1	TIS	B	203	1	5,9,10	3.42	4 (80%)	3,12,14	1.35	1 (33%)

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
1	TIS	A	203	1	-	0/3/8/10	-
1	TIS	B	203	1	-	1/3/8/10	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	TIS	C2T-C1T	6.09	1.61	1.50
1	A	203	TIS	C2T-C1T	5.84	1.60	1.50
1	A	203	TIS	CB-CA	3.34	1.61	1.52
1	B	203	TIS	CB-CA	3.31	1.61	1.52
1	A	203	TIS	CA-N	3.00	1.56	1.48
1	B	203	TIS	CA-N	2.34	1.54	1.48
1	B	203	TIS	OG-CB	-2.10	1.37	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	TIS	O1T-C1T-C2T	2.30	115.98	108.32

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	203	TIS	CA-CB-OG-C1T

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	203	TIS	2	0
1	B	203	TIS	3	0

## 5.5 Carbohydrates [i](#)

10 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	C	1	1,2	14,14,15	0.60	0	17,19,21	1.07	3 (17%)
2	NAG	C	2	2	14,14,15	0.70	1 (7%)	17,19,21	0.47	0
2	FUC	C	3	2	10,10,11	1.56	2 (20%)	14,14,16	1.45	2 (14%)
3	NAG	D	1	1,3	14,14,15	0.87	2 (14%)	17,19,21	0.78	0
3	NAG	D	2	3	14,14,15	0.34	0	17,19,21	0.62	0
4	GAL	E	1	4	12,12,12	1.52	2 (16%)	17,17,17	1.15	2 (11%)
4	SIA	E	2	4	20,20,21	1.86	5 (25%)	21,28,31	1.93	6 (28%)
2	NAG	F	1	1,2	14,14,15	0.61	0	17,19,21	1.01	1 (5%)
2	NAG	F	2	2	14,14,15	0.81	1 (7%)	17,19,21	0.51	0
2	FUC	F	3	2	10,10,11	1.84	4 (40%)	14,14,16	1.12	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
2	FUC	C	3	2	-	-	0/1/1/1
3	NAG	D	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GAL	E	1	4	-	1/2/22/22	0/1/1/1
4	SIA	E	2	4	-	8/18/34/38	0/1/1/1
2	NAG	F	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	F	2	2	-	4/6/23/26	0/1/1/1
2	FUC	F	3	2	-	-	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	2	SIA	C2-C1	4.69	1.58	1.52
4	E	2	SIA	C7-C6	3.68	1.57	1.52
4	E	1	GAL	O3-C3	3.49	1.51	1.43
2	C	3	FUC	C4-C5	3.43	1.60	1.52
2	F	3	FUC	C4-C5	3.32	1.60	1.52
4	E	2	SIA	O6-C2	2.66	1.48	1.43
2	F	2	NAG	O5-C1	2.60	1.48	1.43
4	E	1	GAL	C3-C2	2.44	1.58	1.52
4	E	2	SIA	C6-C5	2.42	1.56	1.53
2	F	3	FUC	O5-C5	2.42	1.48	1.43
4	E	2	SIA	C8-C7	2.35	1.57	1.53
2	C	2	NAG	O5-C1	2.34	1.47	1.43
2	F	3	FUC	C4-C3	2.31	1.58	1.52
2	F	3	FUC	C1-C2	2.30	1.57	1.52
3	D	1	NAG	O5-C1	-2.24	1.39	1.43
2	C	3	FUC	O5-C5	2.20	1.47	1.43
3	D	1	NAG	C1-C2	2.02	1.55	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	2	SIA	O1A-C1-C2	-5.48	111.00	122.85
2	C	3	FUC	O5-C5-C4	3.15	115.23	109.55
4	E	1	GAL	O3-C3-C2	3.09	117.67	110.38
4	E	2	SIA	O1B-C1-O1A	3.05	131.00	124.08
2	F	1	NAG	C1-O5-C5	2.93	116.12	112.19
4	E	2	SIA	C8-C7-C6	2.79	118.29	113.05
2	F	3	FUC	O5-C5-C4	2.56	114.17	109.55
2	C	1	NAG	C1-O5-C5	2.26	115.22	112.19
2	C	1	NAG	C2-N2-C7	2.20	125.85	122.90
2	C	1	NAG	C1-C2-N2	2.20	113.90	110.43
4	E	2	SIA	C9-C8-C7	2.20	116.66	112.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1	GAL	O5-C5-C4	2.13	113.54	109.70
2	C	3	FUC	C3-C4-C5	2.09	112.98	109.81
4	E	2	SIA	O1B-C1-C2	2.03	118.00	112.71
4	E	2	SIA	O6-C2-C3	-2.01	107.85	110.56

There are no chirality outliers.

All (24) torsion outliers are listed below:

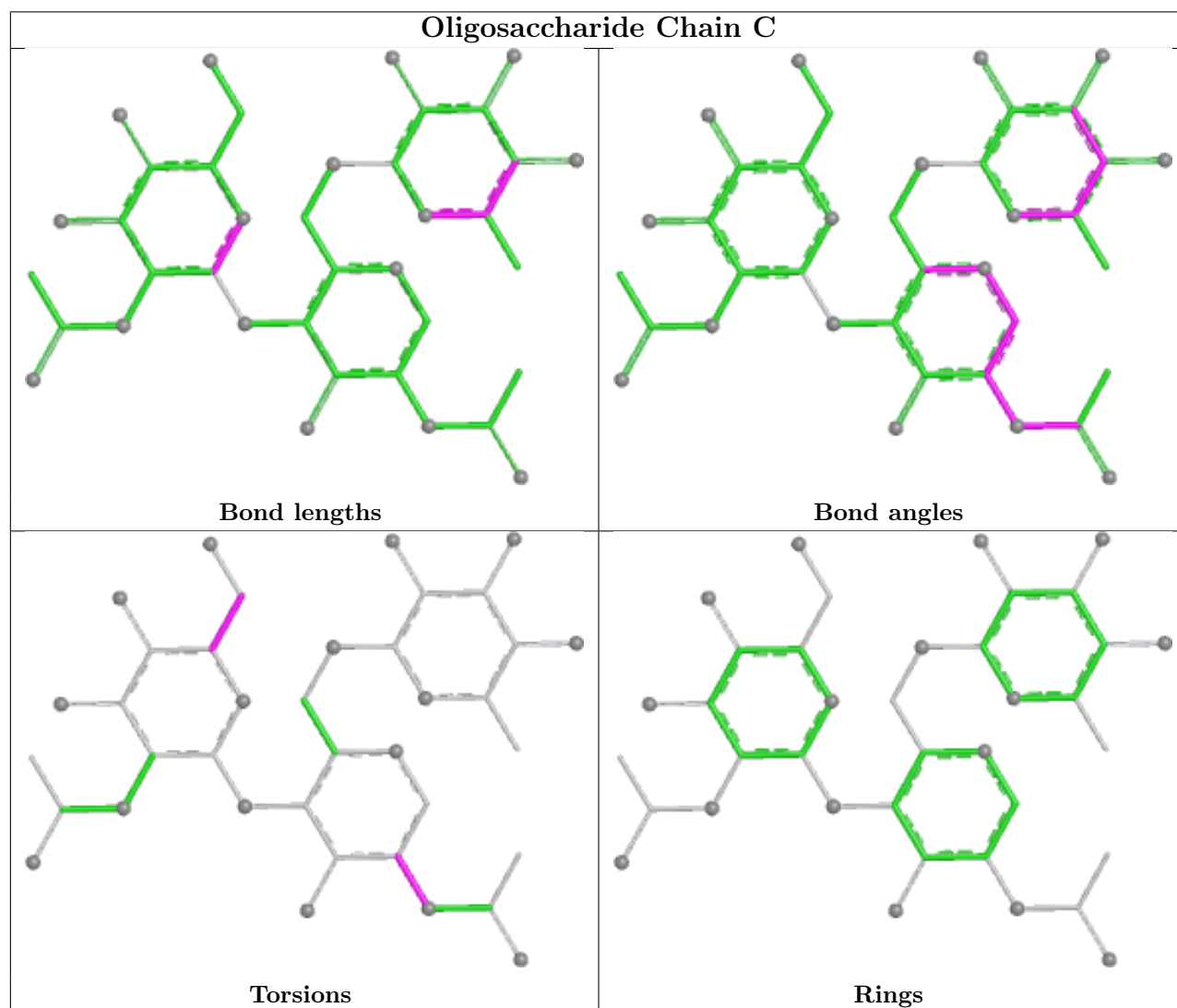
Mol	Chain	Res	Type	Atoms
4	E	2	SIA	O7-C7-C8-C9
2	F	2	NAG	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
4	E	2	SIA	C6-C7-C8-C9
2	F	1	NAG	C4-C5-C6-O6
4	E	2	SIA	O7-C7-C8-O8
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
4	E	2	SIA	C11-C10-N5-C5
4	E	2	SIA	O10-C10-N5-C5
2	F	1	NAG	O5-C5-C6-O6
4	E	1	GAL	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
4	E	2	SIA	O8-C8-C9-O9
2	C	1	NAG	C1-C2-N2-C7
2	C	1	NAG	C3-C2-N2-C7
4	E	2	SIA	O1A-C1-C2-O6
4	E	2	SIA	C6-C7-C8-O8

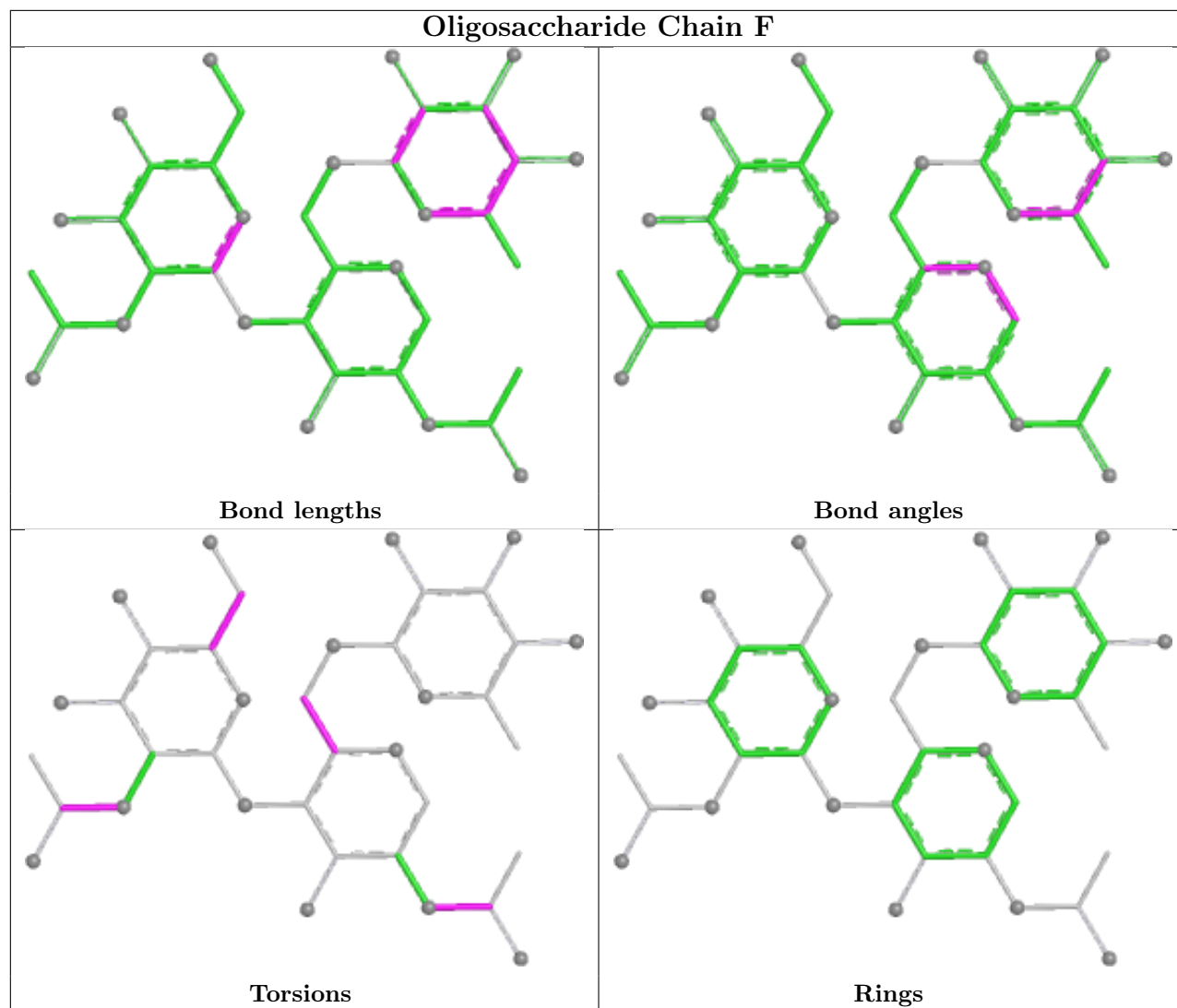
There are no ring outliers.

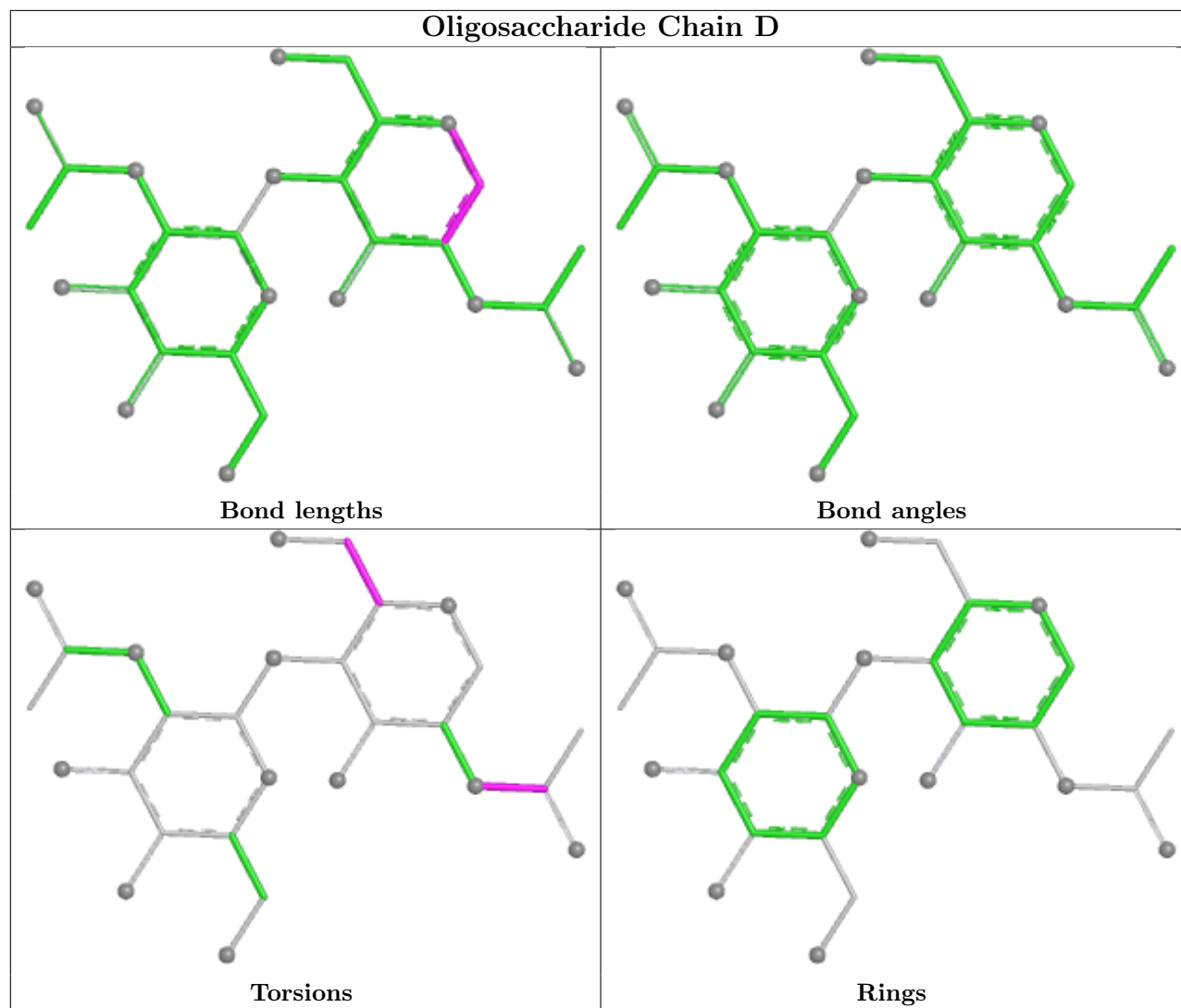
3 monomers are involved in 2 short contacts:

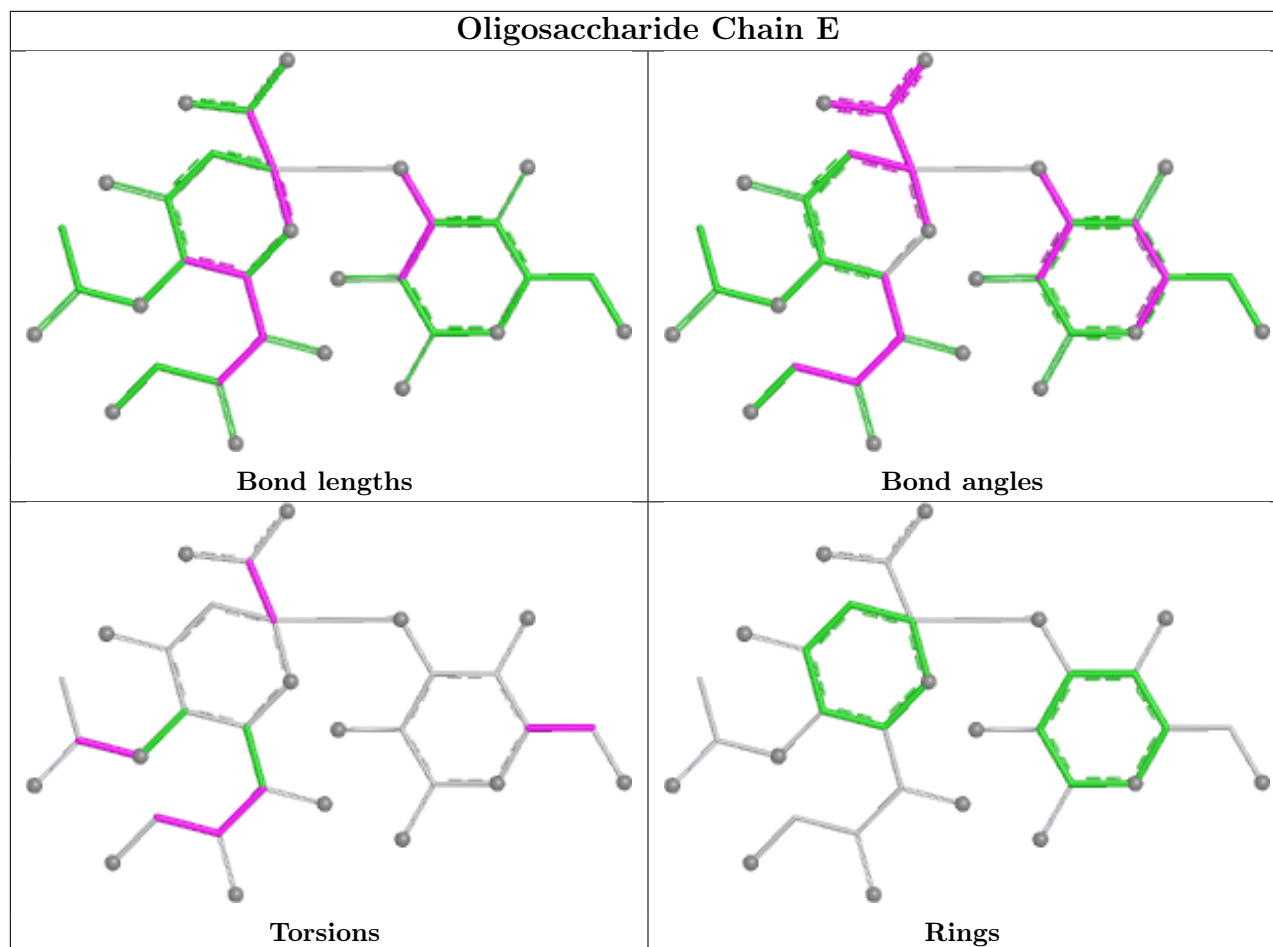
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	2	SIA	1	0
3	D	2	NAG	1	0
3	D	1	NAG	1	0

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









## 5.6 Ligand geometry [i](#)

Of 67 ligands modelled in this entry, 50 are monoatomic - leaving 17 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
6	SO4	A	609	-	4,4,4	0.38	0	6,6,6	0.17	0
5	LWU	A	601	-	26,29,29	<b>2.25</b>	<b>6 (23%)</b>	31,38,38	<b>2.22</b>	<b>3 (9%)</b>
6	SO4	B	603	9	4,4,4	0.29	0	6,6,6	0.22	0
6	SO4	B	605	-	4,4,4	0.38	0	6,6,6	0.26	0
6	SO4	B	604	-	4,4,4	0.30	0	6,6,6	0.19	0
6	SO4	B	601	-	4,4,4	0.41	0	6,6,6	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SO4	B	607	-	4,4,4	0.26	0	6,6,6	0.24	0
6	SO4	A	602	9	4,4,4	0.33	0	6,6,6	0.11	0
6	SO4	A	604	-	4,4,4	0.42	0	6,6,6	0.36	0
6	SO4	A	608	-	4,4,4	0.33	0	6,6,6	0.24	0
6	SO4	A	607	-	4,4,4	0.30	0	6,6,6	0.15	0
6	SO4	A	610	-	4,4,4	0.29	0	6,6,6	0.61	0
6	SO4	B	606	-	4,4,4	0.28	0	6,6,6	0.34	0
6	SO4	A	605	-	4,4,4	0.39	0	6,6,6	0.39	0
6	SO4	B	602	-	4,4,4	0.30	0	6,6,6	0.62	0
6	SO4	A	606	-	4,4,4	0.36	0	6,6,6	0.64	0
6	SO4	A	603	-	4,4,4	0.36	0	6,6,6	0.59	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	LWU	A	601	-	-	0/18/18/18	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	LWU	O01-C02	7.59	1.38	1.23
5	A	601	LWU	N10-N11	4.35	1.44	1.41
5	A	601	LWU	C02-N10	-3.59	1.29	1.34
5	A	601	LWU	C13-N27	2.74	1.39	1.34
5	A	601	LWU	C05-N04	2.23	1.40	1.34
5	A	601	LWU	O18-C16	2.01	1.44	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	LWU	C03-C02-N10	8.89	125.36	115.15
5	A	601	LWU	C13-C12-N11	5.42	126.94	113.05
5	A	601	LWU	O01-C02-C03	-4.68	111.98	120.26

There are no chirality outliers.

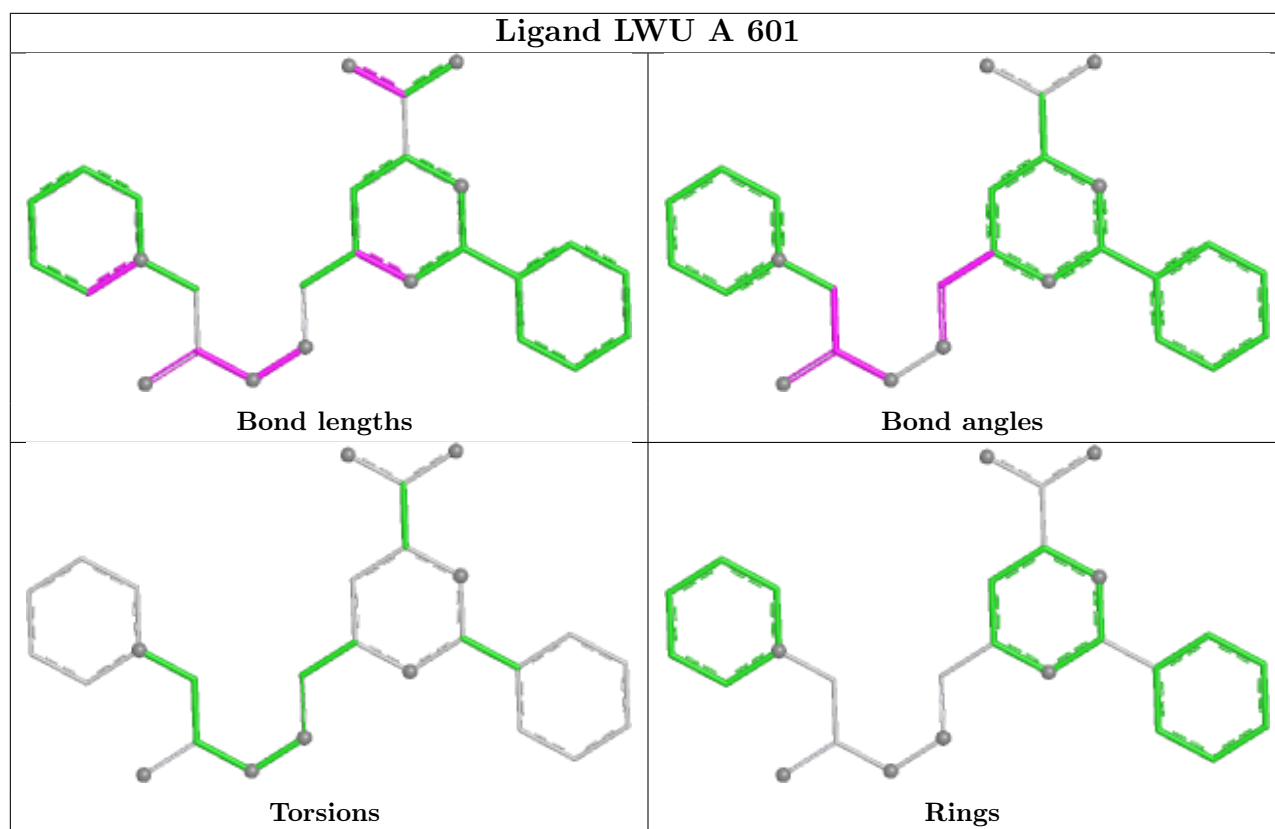
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	605	SO4	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](#)

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	532/543 (97%)	-0.26	8 (1%) 72 64	47, 78, 110, 173	1 (0%)
1	B	534/543 (98%)	-0.05	14 (2%) 57 48	49, 89, 129, 202	1 (0%)
All	All	1066/1086 (98%)	-0.16	22 (2%) 63 54	47, 83, 123, 202	2 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	259	PRO	5.8
1	A	258	PRO	5.4
1	B	105	TYR	4.9
1	B	258	PRO	4.7
1	B	6	ALA	3.9
1	A	495	PRO	3.8
1	A	496	LYS	3.7
1	B	492	PRO	3.1
1	B	497	ALA	2.6
1	B	493	ARG	2.4
1	A	105	TYR	2.4
1	A	493	ARG	2.4
1	B	30	SER	2.3
1	A	491	GLU	2.3
1	A	542	ALA	2.3
1	B	498	PRO	2.3
1	A	498	PRO	2.2
1	B	70	TYR	2.2
1	B	5	ASP	2.1
1	B	291	GLN	2.1
1	B	542	ALA	2.1
1	B	292	GLU	2.1

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

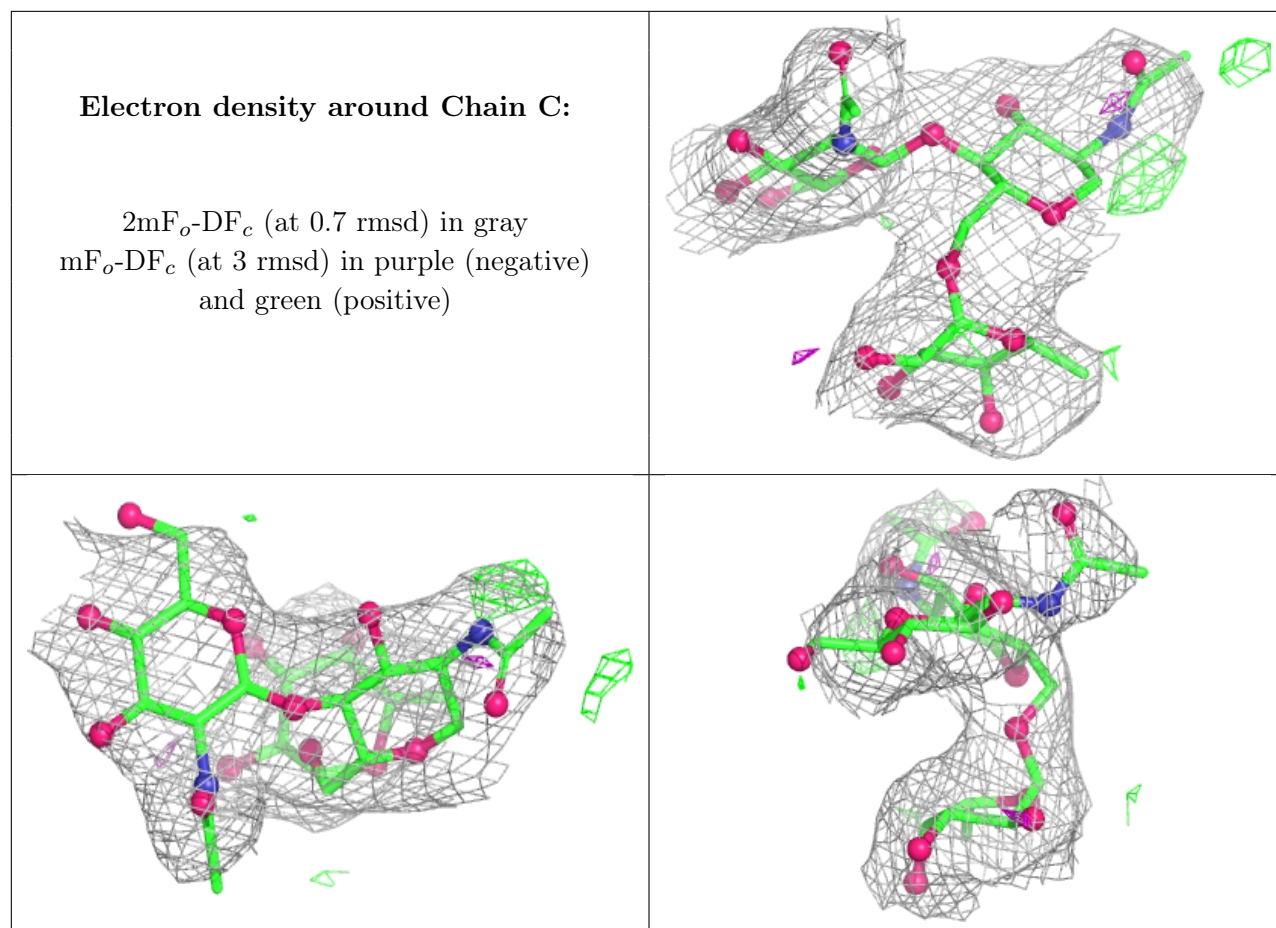
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	TIS	A	203	10/11	0.98	0.07	60,64,69,72	2
1	TIS	B	203	10/11	0.98	0.06	64,70,79,82	0

## 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.

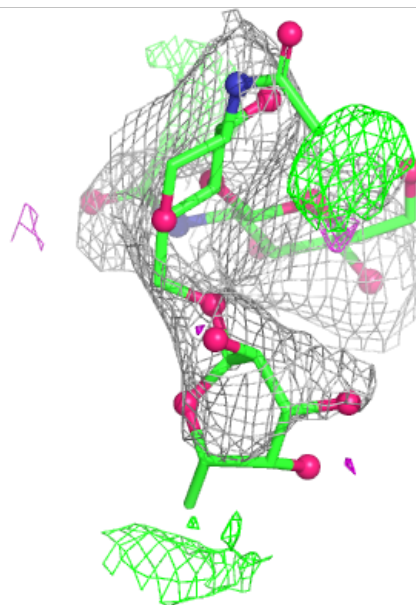
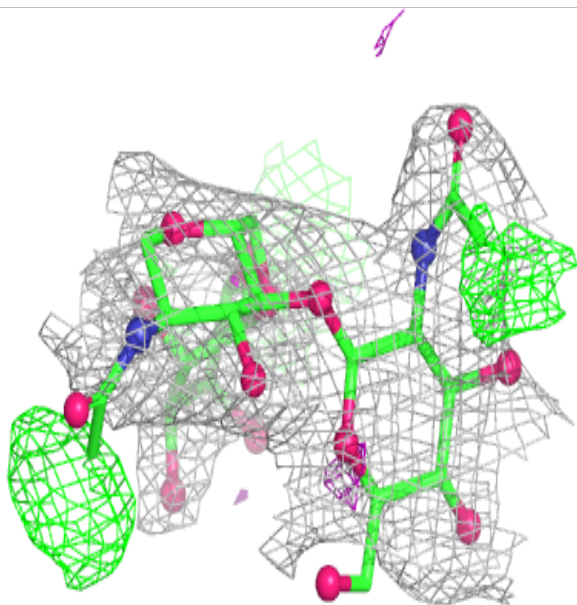
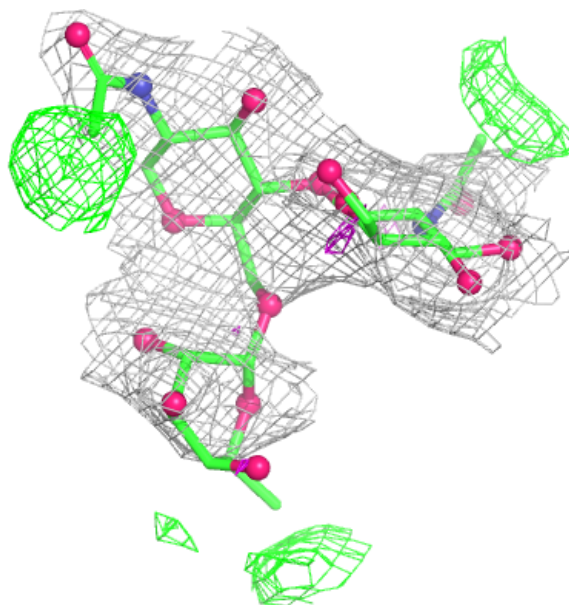
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	FUC	F	3	10/11	0.35	0.27	157,176,184,188	0
3	NAG	D	1	14/15	0.65	0.17	143,162,174,177	0
3	NAG	D	2	14/15	0.65	0.19	177,182,186,186	0
2	NAG	F	2	14/15	0.71	0.16	131,149,154,154	0
2	FUC	C	3	10/11	0.77	0.16	122,131,138,139	0
4	GAL	E	1	12/12	0.82	0.27	183,191,203,207	0
2	NAG	F	1	14/15	0.83	0.14	133,141,154,166	0
2	NAG	C	2	14/15	0.83	0.12	107,138,142,150	0
4	SIA	E	2	20/21	0.83	0.28	179,189,198,200	0
2	NAG	C	1	14/15	0.91	0.12	110,120,127,129	0

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



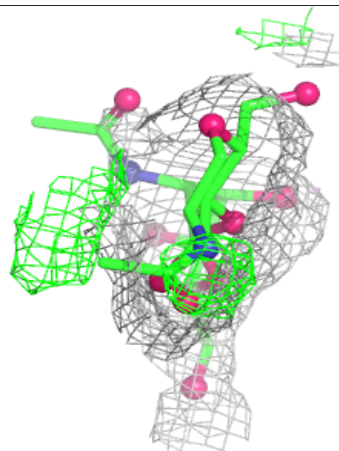
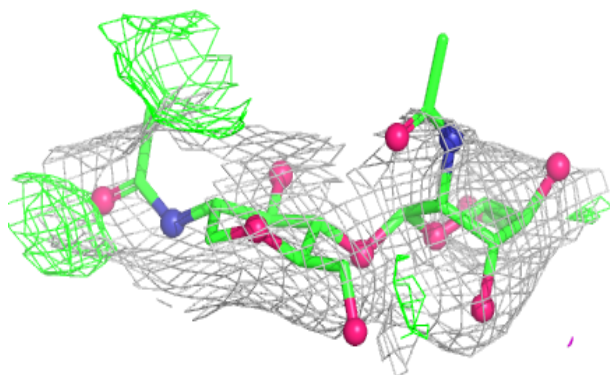
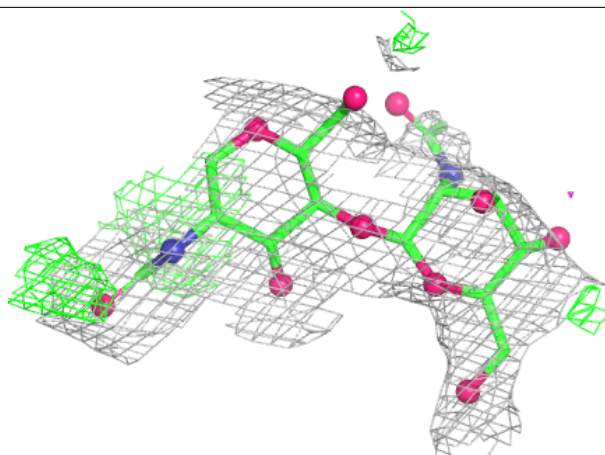
**Electron density around Chain F:**

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

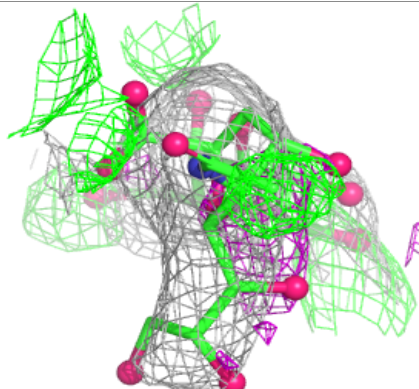
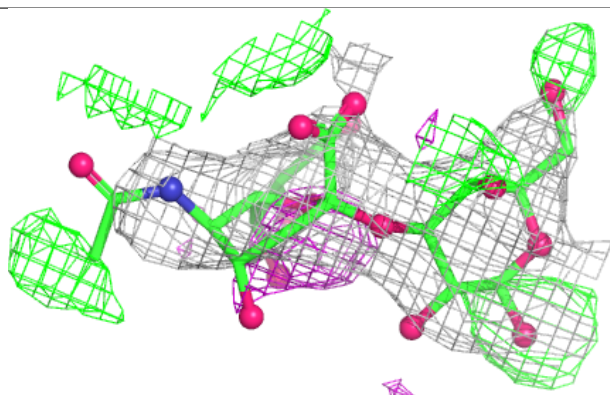
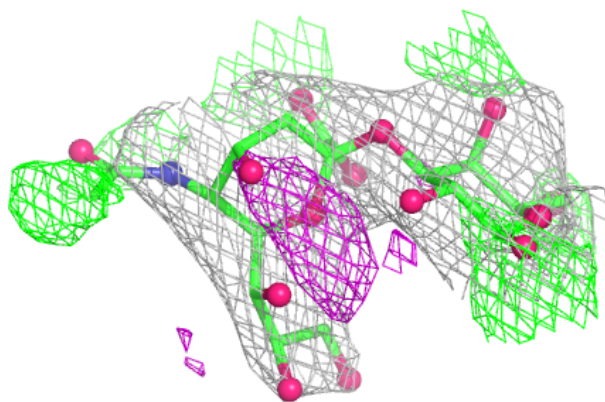


**Electron density around Chain D:**

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

**Electron density around Chain E:**

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



## 6.4 Ligands i

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

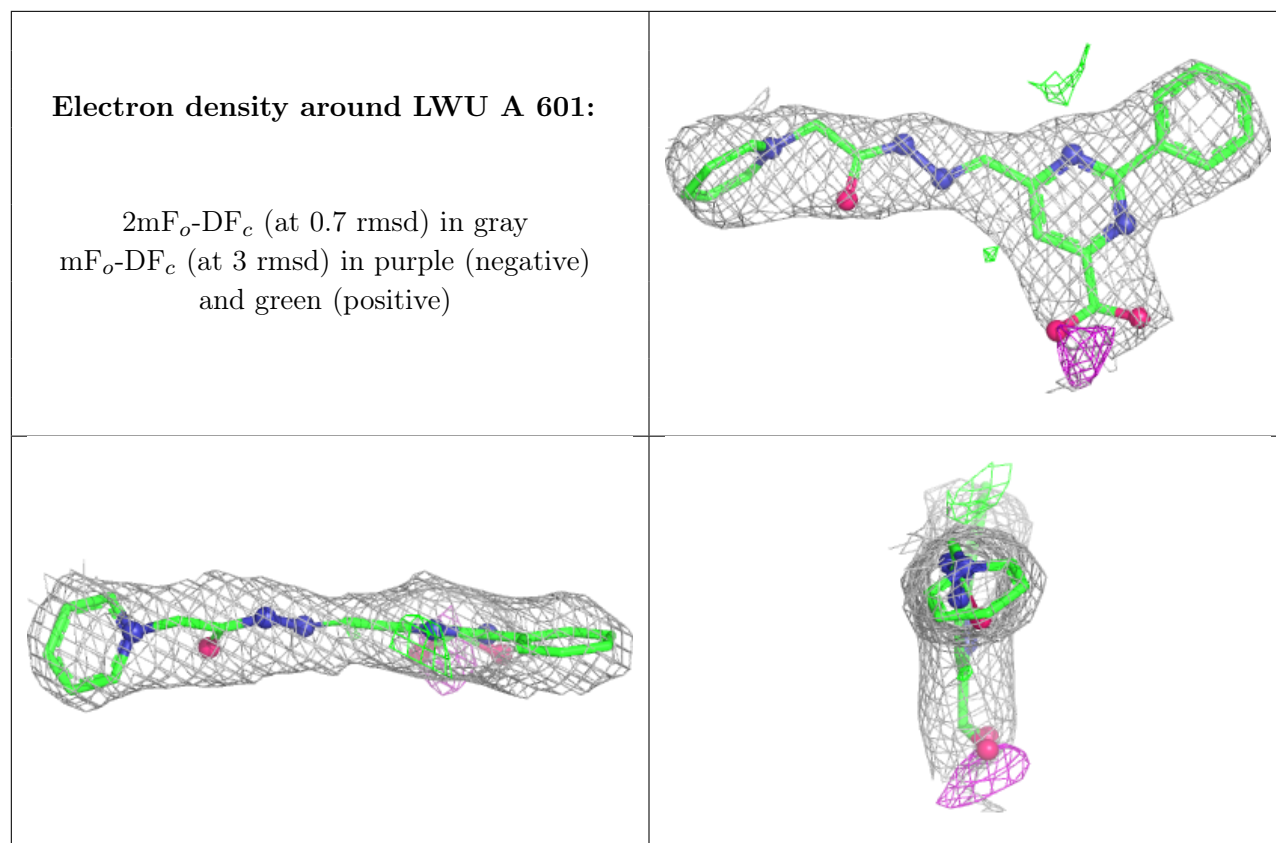
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	SO4	B	606	5/5	0.47	0.15	142,150,162,166	0
9	MG	B	631	1/1	0.54	0.16	118,118,118,118	0
6	SO4	B	607	5/5	0.59	0.13	146,146,157,164	0
6	SO4	B	605	5/5	0.61	0.13	149,150,152,165	0
6	SO4	B	604	5/5	0.66	0.09	155,158,167,172	0
7	CL	B	619	1/1	0.71	0.14	127,127,127,127	0
6	SO4	A	605	5/5	0.73	0.13	134,137,141,155	0
6	SO4	A	610	5/5	0.75	0.24	130,132,159,185	0
6	SO4	A	606	5/5	0.78	0.15	100,104,136,140	0
6	SO4	A	603	5/5	0.79	0.18	94,97,105,110	5
6	SO4	A	608	5/5	0.80	0.18	99,100,103,107	5
7	CL	A	616	1/1	0.80	0.22	117,117,117,117	0
9	MG	B	632	1/1	0.80	0.27	93,93,93,93	0
7	CL	B	615	1/1	0.81	0.10	134,134,134,134	0
7	CL	B	624	1/1	0.81	0.13	117,117,117,117	0
7	CL	A	622	1/1	0.82	0.13	109,109,109,109	0
7	CL	B	609	1/1	0.84	0.10	120,120,120,120	0
6	SO4	A	609	5/5	0.85	0.13	102,103,115,116	5
6	SO4	A	607	5/5	0.85	0.16	89,95,109,111	5
7	CL	A	613	1/1	0.87	0.14	106,106,106,106	0
9	MG	A	628	1/1	0.87	0.13	88,88,88,88	0
7	CL	A	612	1/1	0.88	0.16	126,126,126,126	0
9	MG	A	633	1/1	0.88	0.15	95,95,95,95	0
7	CL	B	616	1/1	0.88	0.12	108,108,108,108	0
9	MG	A	627	1/1	0.88	0.14	97,97,97,97	0
7	CL	B	608	1/1	0.89	0.12	95,95,95,95	0
8	ZN	A	625	1/1	0.89	0.14	94,94,94,94	1
9	MG	A	630	1/1	0.89	0.17	81,81,81,81	0
7	CL	A	614	1/1	0.90	0.08	110,110,110,110	0
7	CL	B	620	1/1	0.90	0.19	112,112,112,112	0
9	MG	A	632	1/1	0.90	0.19	78,78,78,78	0
7	CL	A	623	1/1	0.90	0.13	102,102,102,102	0
9	MG	B	630	1/1	0.90	0.20	93,93,93,93	0
7	CL	A	611	1/1	0.90	0.09	127,127,127,127	0
7	CL	B	618	1/1	0.90	0.20	98,98,98,98	0
7	CL	A	624	1/1	0.91	0.12	117,117,117,117	0
7	CL	B	611	1/1	0.91	0.13	112,112,112,112	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	CL	B	614	1/1	0.91	0.14	117,117,117,117	0
9	MG	B	633	1/1	0.91	0.20	102,102,102,102	0
7	CL	A	619	1/1	0.92	0.13	100,100,100,100	0
6	SO4	B	603	5/5	0.92	0.12	106,107,114,115	5
8	ZN	B	626	1/1	0.92	0.13	123,123,123,123	1
7	CL	A	615	1/1	0.92	0.24	95,95,95,95	0
7	CL	B	613	1/1	0.92	0.32	107,107,107,107	0
6	SO4	A	602	5/5	0.92	0.12	96,97,114,115	5
7	CL	A	618	1/1	0.93	0.11	94,94,94,94	0
8	ZN	B	625	1/1	0.93	0.13	93,93,93,93	1
7	CL	B	617	1/1	0.93	0.11	112,112,112,112	0
6	SO4	A	604	5/5	0.94	0.15	89,97,100,107	0
7	CL	B	621	1/1	0.94	0.09	93,93,93,93	0
8	ZN	B	627	1/1	0.94	0.11	136,136,136,136	0
7	CL	B	622	1/1	0.94	0.07	126,126,126,126	0
7	CL	B	612	1/1	0.94	0.20	96,96,96,96	0
6	SO4	B	602	5/5	0.94	0.14	84,88,99,101	0
6	SO4	B	601	5/5	0.95	0.16	102,103,115,120	0
7	CL	B	610	1/1	0.95	0.10	94,94,94,94	0
7	CL	A	620	1/1	0.95	0.07	84,84,84,84	0
9	MG	B	628	1/1	0.95	0.16	81,81,81,81	0
7	CL	B	623	1/1	0.96	0.09	81,81,81,81	0
7	CL	A	617	1/1	0.96	0.10	90,90,90,90	0
9	MG	A	631	1/1	0.96	0.11	82,82,82,82	0
5	LWU	A	601	27/27	0.96	0.13	77,90,95,100	0
8	ZN	A	626	1/1	0.96	0.08	101,101,101,101	1
9	MG	A	629	1/1	0.97	0.09	102,102,102,102	0
9	MG	A	634	1/1	0.97	0.14	76,76,76,76	0
7	CL	A	621	1/1	0.97	0.08	98,98,98,98	0
9	MG	B	629	1/1	0.97	0.06	74,74,74,74	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.