



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:14 PM UTC

PDB ID : 4DBM / pdb\_00004dbm  
Title : Aplysia californica-AChBP in complex with triazole 18  
Authors : Nemezc, A.; Yamauchi, J.G.; Kim, C.  
Deposited on : 2012-01-16  
Resolution : 2.30 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

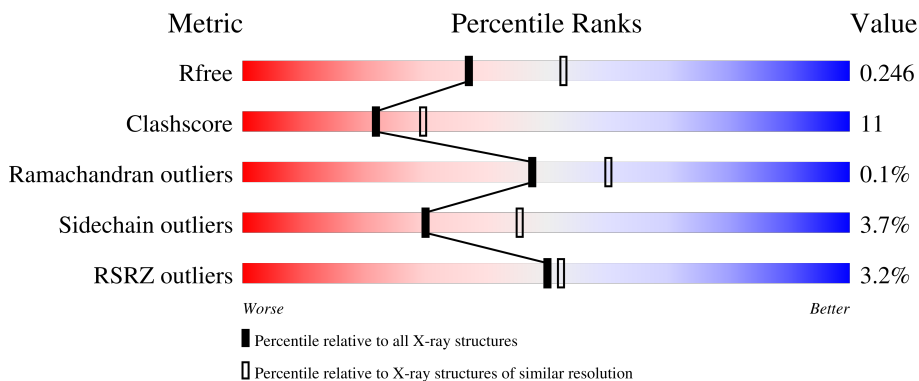
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	230	 3% 72% 17% • 8%
1	B	230	 % 73% 17% • 9%
1	C	230	 5% 67% 21% • 10%
1	D	230	 3% 71% 19% • 7%
1	E	230	 3% 71% 19% • 9%

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	F	5	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	OJ0	A	302	-	X	-	-
4	OJ0	B	300	-	X	-	-
4	OJ0	D	300	-	-	X	-

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 9095 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 Soluble acetylcholine receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	211	Total 1692	C 1067	N 279	O 337	S 9	0	1	0
1	B	209	Total 1675	C 1059	N 276	O 331	S 9	0	1	0
1	C	206	Total 1658	C 1049	N 272	O 329	S 8	0	2	0
1	D	213	Total 1718	C 1083	N 279	O 347	S 9	0	2	0
1	E	209	Total 1674	C 1057	N 276	O 332	S 9	0	1	0

There are 55 discrepancies between the modelled and reference sequences:

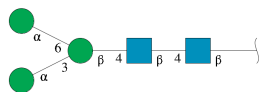
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ASP	-	expression tag	UNP Q8WSF8
A	-7	TYR	-	expression tag	UNP Q8WSF8
A	-6	LYS	-	expression tag	UNP Q8WSF8
A	-5	ASP	-	expression tag	UNP Q8WSF8
A	-4	ASP	-	expression tag	UNP Q8WSF8
A	-3	ASP	-	expression tag	UNP Q8WSF8
A	-2	ASP	-	expression tag	UNP Q8WSF8
A	-1	LYS	-	expression tag	UNP Q8WSF8
A	0	LEU	-	expression tag	UNP Q8WSF8
A	220	SER	-	expression tag	UNP Q8WSF8
A	221	ARG	-	expression tag	UNP Q8WSF8
B	-8	ASP	-	expression tag	UNP Q8WSF8
B	-7	TYR	-	expression tag	UNP Q8WSF8
B	-6	LYS	-	expression tag	UNP Q8WSF8
B	-5	ASP	-	expression tag	UNP Q8WSF8
B	-4	ASP	-	expression tag	UNP Q8WSF8
B	-3	ASP	-	expression tag	UNP Q8WSF8
B	-2	ASP	-	expression tag	UNP Q8WSF8
B	-1	LYS	-	expression tag	UNP Q8WSF8

*Continued on next page...*

*Continued from previous page...*

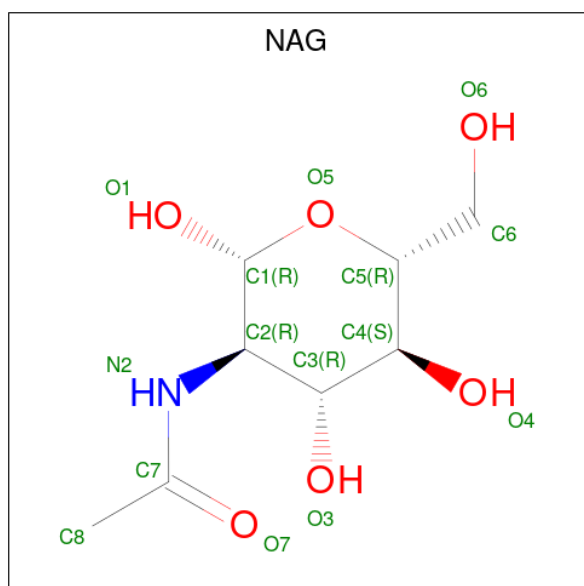
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	LEU	-	expression tag	UNP Q8WSF8
B	220	SER	-	expression tag	UNP Q8WSF8
B	221	ARG	-	expression tag	UNP Q8WSF8
C	-8	ASP	-	expression tag	UNP Q8WSF8
C	-7	TYR	-	expression tag	UNP Q8WSF8
C	-6	LYS	-	expression tag	UNP Q8WSF8
C	-5	ASP	-	expression tag	UNP Q8WSF8
C	-4	ASP	-	expression tag	UNP Q8WSF8
C	-3	ASP	-	expression tag	UNP Q8WSF8
C	-2	ASP	-	expression tag	UNP Q8WSF8
C	-1	LYS	-	expression tag	UNP Q8WSF8
C	0	LEU	-	expression tag	UNP Q8WSF8
C	220	SER	-	expression tag	UNP Q8WSF8
C	221	ARG	-	expression tag	UNP Q8WSF8
D	-8	ASP	-	expression tag	UNP Q8WSF8
D	-7	TYR	-	expression tag	UNP Q8WSF8
D	-6	LYS	-	expression tag	UNP Q8WSF8
D	-5	ASP	-	expression tag	UNP Q8WSF8
D	-4	ASP	-	expression tag	UNP Q8WSF8
D	-3	ASP	-	expression tag	UNP Q8WSF8
D	-2	ASP	-	expression tag	UNP Q8WSF8
D	-1	LYS	-	expression tag	UNP Q8WSF8
D	0	LEU	-	expression tag	UNP Q8WSF8
D	220	SER	-	expression tag	UNP Q8WSF8
D	221	ARG	-	expression tag	UNP Q8WSF8
E	-8	ASP	-	expression tag	UNP Q8WSF8
E	-7	TYR	-	expression tag	UNP Q8WSF8
E	-6	LYS	-	expression tag	UNP Q8WSF8
E	-5	ASP	-	expression tag	UNP Q8WSF8
E	-4	ASP	-	expression tag	UNP Q8WSF8
E	-3	ASP	-	expression tag	UNP Q8WSF8
E	-2	ASP	-	expression tag	UNP Q8WSF8
E	-1	LYS	-	expression tag	UNP Q8WSF8
E	0	LEU	-	expression tag	UNP Q8WSF8
E	220	SER	-	expression tag	UNP Q8WSF8
E	221	ARG	-	expression tag	UNP Q8WSF8

- Molecule 2 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.



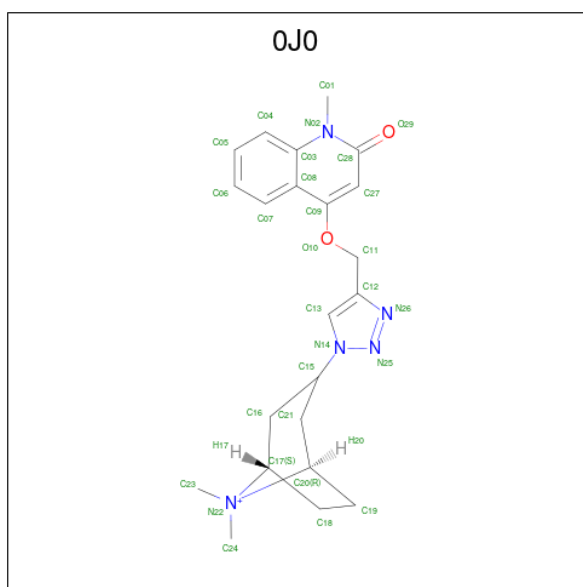
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	F	5	61	34	2	25	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 4 is (3-exo)-8,8-dimethyl-3-(4-[[[(1-methyl-2-oxo-1,2-dihydroquinolin-4-yl)oxy]methyl]-1H-1,2,3-triazol-1-yl])-8-azoniabicyclo[3.2.1]octane (CCD ID: 0J0) (formula:  $C_{22}H_{28}N_5O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	29	22	5	2	18	0
4	B	1	29	22	5	2	19	0
4	C	1	29	22	5	2	0	0
4	D	1	29	22	5	2	0	0
4	E	1	29	22	5	2	0	0

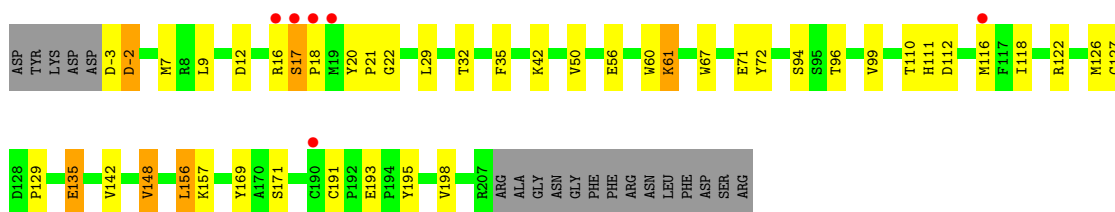
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	100	100	100	0	0
5	B	92	92	92	0	0
5	C	85	85	85	0	0
5	D	83	83	83	0	0
5	E	98	98	98	0	0

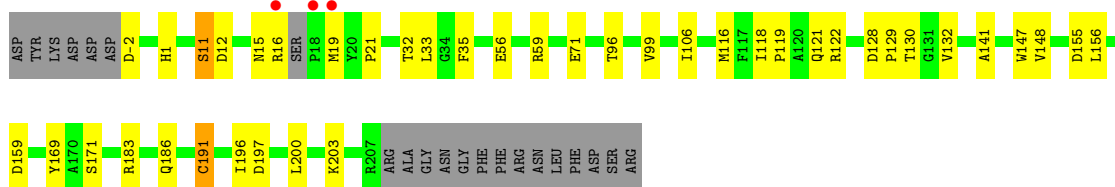
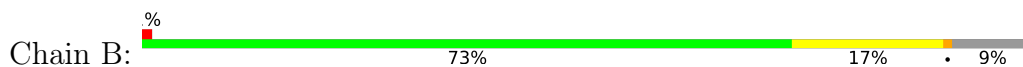
### 3 Residue-property plots [i](#)

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.

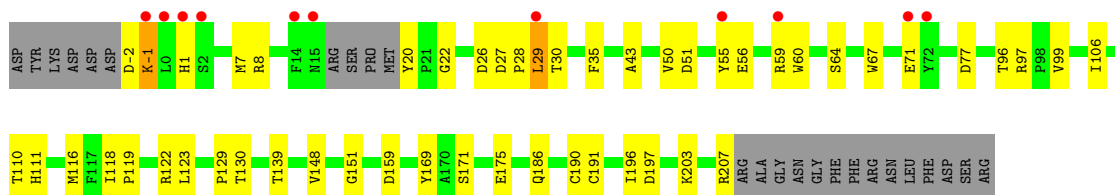
- Molecule 1: Soluble acetylcholine receptor



- Molecule 1: Soluble acetylcholine receptor

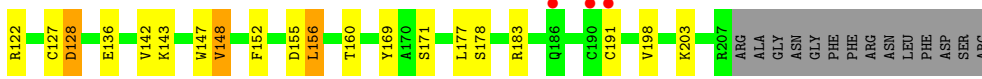


- Molecule 1: Soluble acetylcholine receptor



- Molecule 1: Soluble acetylcholine receptor





- Molecule 1: Soluble acetylcholine receptor



- Molecule 2: 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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.34Å 115.10Å 131.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.29 – 2.30 43.29 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.0 (43.29-2.30) 94.4 (43.29-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.12 (at 2.29Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.194 , 0.252 0.195 , 0.246	Depositor DCC
$R_{free}$ test set	2000 reflections (3.32%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.1	Xtrriage
Anisotropy	0.415	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 30.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9095	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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, BMA, OJ0, 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	0.48	0/1733	0.84	1/2363 (0.0%)
1	B	0.44	0/1718	0.87	4/2340 (0.2%)
1	C	0.46	0/1700	0.80	0/2316
1	D	0.49	0/1761	0.87	6/2399 (0.3%)
1	E	0.48	0/1716	0.88	6/2337 (0.3%)
All	All	0.47	0/8628	0.85	17/11755 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	148	VAL	N-CA-C	7.67	120.43	112.83
1	D	128	ASP	CA-C-N	-7.51	114.06	121.65
1	D	128	ASP	C-N-CA	-7.51	114.06	121.65
1	B	21	PRO	CB-CA-C	-7.33	100.37	111.44
1	B	191	CYS	CA-C-N	7.02	127.00	119.28
1	B	191	CYS	C-N-CA	7.02	127.00	119.28
1	E	128	ASP	CA-C-N	6.71	126.85	119.87
1	E	128	ASP	C-N-CA	6.71	126.85	119.87
1	D	20	TYR	CA-C-N	6.59	126.73	119.87
1	D	20	TYR	C-N-CA	6.59	126.73	119.87
1	E	148	VAL	N-CA-C	6.08	118.85	112.83
1	B	148	VAL	N-CA-C	5.90	118.67	112.83
1	D	47	THR	N-CA-C	5.51	120.11	113.17
1	E	94	SER	N-CA-C	5.46	119.63	112.92
1	A	148	VAL	N-CA-C	5.34	119.79	113.22
1	E	104	PRO	CA-C-N	-5.25	115.55	122.85
1	E	104	PRO	C-N-CA	-5.25	115.55	122.85

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1692	0	1620	36	0
1	B	1675	0	1612	26	0
1	C	1658	0	1595	53	0
1	D	1718	0	1635	44	0
1	E	1674	0	1608	31	0
2	F	61	0	52	0	0
3	A	14	0	13	1	0
4	A	29	0	28	0	0
4	B	29	0	28	1	0
4	C	29	0	28	8	0
4	D	29	0	28	12	0
4	E	29	0	28	7	0
5	A	100	0	0	3	0
5	B	92	0	0	2	0
5	C	85	0	0	4	0
5	D	83	0	0	5	0
5	E	98	0	0	3	0
All	All	9095	0	8275	180	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 11.

All (180) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:PRO:HB2	1:E:7:MET:SD	1.68	1.32
1:B:12:ASP:O	1:B:16:ARG:HG2	1.47	1.12
1:D:116:MET:HB3	4:E:306:OJ0:C06	1.99	0.91
1:C:-1:LYS:HE2	1:D:27:ASP:OD1	1.72	0.88
1:A:18:PRO:CB	1:E:7:MET:SD	2.59	0.86
1:B:12:ASP:O	1:B:16:ARG:CG	2.24	0.86
1:D:116:MET:HE2	5:D:412:HOH:O	1.80	0.80

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:-2:ASP:N	1:C:1:HIS:HD2	1.81	0.79
1:B:116:MET:HB3	4:C:300:0J0:C05	2.13	0.78
1:C:116:MET:HB3	4:D:300:0J0:C05	2.17	0.74
1:B:11:SER:O	1:B:15:ASN:HB2	1.87	0.74
4:C:300:0J0:H07	4:C:300:0J0:H11	1.69	0.73
1:C:-1:LYS:CE	1:D:27:ASP:OD1	2.36	0.73
1:A:32:THR:OG1	1:A:157:LYS:HE3	1.89	0.72
1:D:94:SER:OG	1:D:142:VAL:HG23	1.91	0.71
4:C:300:0J0:H07	4:C:300:0J0:C11	2.22	0.70
1:D:136:GLU:O	1:D:203:LYS:HE3	1.92	0.69
1:C:151:GLY:HA2	1:C:196:ILE:HD12	1.74	0.69
1:B:35:PHE:CE1	1:B:56:GLU:HG3	2.26	0.69
1:C:29:LEU:HD21	1:C:60:TRP:HB2	1.75	0.69
1:C:139:THR:OG1	1:C:203[B]:LYS:HG2	1.92	0.69
1:A:193:GLU:HG2	1:A:195:TYR:CE1	2.28	0.68
1:B:116:MET:HE2	5:B:467:HOH:O	1.93	0.68
4:D:300:0J0:H07	4:D:300:0J0:C12	2.24	0.68
4:E:306:0J0:H11	4:E:306:0J0:H07	1.76	0.68
3:A:301:NAG:O7	3:A:301:NAG:H3	1.93	0.68
1:A:61:LYS:HD2	1:A:112:ASP:O	1.94	0.67
1:D:35:PHE:CE2	1:D:56:GLU:HG2	2.30	0.67
1:C:27:ASP:N	1:C:28:PRO:HD3	2.10	0.67
1:D:7:MET:SD	1:E:19:MET:N	2.68	0.67
1:A:12:ASP:O	1:A:16:ARG:HB2	1.96	0.66
1:E:116:MET:HG3	5:E:448:HOH:O	1.96	0.66
1:E:56:GLU:O	1:E:119:PRO:HD2	1.96	0.65
1:A:135:GLU:H	1:A:135:GLU:CD	2.01	0.65
1:C:118:ILE:HG13	4:D:300:0J0:H06	1.78	0.65
4:D:300:0J0:H07	4:D:300:0J0:C11	2.25	0.65
1:D:79:ARG:HG3	1:E:149:TYR:CE1	2.32	0.64
1:A:110:THR:HG23	5:A:499:HOH:O	1.97	0.64
4:D:300:0J0:H07	4:D:300:0J0:H11	1.80	0.63
1:A:116:MET:HG2	5:A:499:HOH:O	1.97	0.63
1:D:79:ARG:HD2	1:D:108:VAL:HG22	1.80	0.63
1:A:169:TYR:CZ	1:A:171:SER:HB2	2.35	0.62
1:E:35:PHE:CE1	1:E:56:GLU:HG3	2.34	0.62
1:C:35:PHE:CE2	1:C:56:GLU:HG3	2.34	0.62
1:A:193:GLU:HG2	1:A:195:TYR:HE1	1.64	0.62
1:E:20:TYR:CE2	1:E:22:GLY:HA2	2.35	0.61
1:A:191:CYS:HB3	1:A:193:GLU:CD	2.26	0.61
1:B:203:LYS:NZ	1:B:203:LYS:HB3	2.15	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:169:TYR:CZ	1:E:171:SER:HB2	2.35	0.61
1:D:116:MET:HB3	4:E:306:OJ0:C05	2.30	0.61
1:C:59:ARG:HG2	1:C:116:MET:HG2	1.83	0.60
1:D:4:ALA:HA	1:D:7:MET:HE2	1.83	0.60
4:C:300:OJ0:H07	4:C:300:OJ0:C12	2.32	0.59
1:E:116:MET:HE2	5:E:448:HOH:O	2.01	0.59
1:C:-2:ASP:H2	1:C:1:HIS:HD2	1.50	0.59
4:E:306:OJ0:H07	4:E:306:OJ0:C11	2.32	0.59
1:A:16:ARG:O	1:A:17:SER:HB2	2.02	0.59
1:D:169:TYR:CZ	1:D:171:SER:HB2	2.38	0.58
1:C:26:ASP:C	1:C:28:PRO:HD3	2.29	0.58
1:A:-2:ASP:OD1	1:A:-2:ASP:N	2.24	0.58
1:E:50:VAL:HG21	1:E:127:CYS:SG	2.44	0.57
1:C:29:LEU:HD23	1:C:30:THR:H	1.69	0.57
1:E:77:ASP:HB3	1:E:110:THR:HG22	1.86	0.57
1:D:106:ILE:HB	1:E:148:VAL:HG11	1.88	0.56
1:C:29:LEU:HD23	1:C:30:THR:N	2.21	0.56
1:B:106:ILE:HB	1:C:148:VAL:HG11	1.88	0.55
1:D:68:ASP:HB3	1:D:71:GLU:HG3	1.88	0.55
1:E:19:MET:O	1:E:20:TYR:C	2.50	0.55
1:A:50:VAL:HG21	1:A:127:CYS:SG	2.47	0.55
1:C:77:ASP:HB3	1:C:110:THR:HG22	1.88	0.55
1:A:9:LEU:HA	1:A:72:TYR:CE1	2.43	0.54
1:B:186:GLN:HG3	1:B:197:ASP:OD2	2.08	0.53
1:D:156:LEU:HD23	1:D:198:VAL:HG23	1.91	0.53
1:A:96:THR:O	1:E:122:ARG:HD2	2.09	0.53
1:A:191:CYS:HB3	1:A:193:GLU:OE2	2.09	0.53
1:D:59:ARG:HG2	1:D:116:MET:HG2	1.90	0.53
1:D:116:MET:SD	4:E:306:OJ0:C04	2.97	0.53
1:C:122:ARG:HD2	1:D:96:THR:O	2.10	0.52
1:B:169:TYR:CZ	1:B:171:SER:HB2	2.45	0.52
1:E:0:LEU:H	1:E:0:LEU:HD12	1.72	0.52
1:C:67:TRP:CZ3	1:C:111:HIS:HA	2.44	0.52
1:E:12:ASP:OD2	1:E:72:TYR:OH	2.24	0.51
1:A:21:PRO:HB2	1:E:6:LEU:HD23	1.92	0.51
1:C:151:GLY:HA2	1:C:196:ILE:CD1	2.40	0.51
1:B:155:ASP:OD1	1:B:196:ILE:HD13	2.10	0.51
1:D:50:VAL:HG21	1:D:127:CYS:SG	2.51	0.51
1:A:94:SER:OG	1:A:142:VAL:HG23	2.12	0.50
1:C:116:MET:HE2	5:C:477:HOH:O	2.11	0.50
1:D:79:ARG:HD3	5:D:438:HOH:O	2.11	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:LYS:HE3	5:D:458:HOH:O	2.12	0.49
1:C:7:MET:HE2	1:D:21:PRO:HD3	1.95	0.49
1:B:32:THR:HG21	1:B:59:ARG:HH21	1.78	0.48
1:C:8:ARG:NH2	1:C:71:GLU:O	2.47	0.48
1:A:126:MET:HE1	1:E:38:GLN:HB3	1.94	0.48
1:C:175:GLU:HB3	1:C:207:ARG:HG3	1.95	0.48
1:C:67:TRP:CE3	1:C:111:HIS:HA	2.49	0.47
4:C:300:OJ0:H11	4:C:300:OJ0:C07	2.40	0.47
4:C:300:OJ0:C11	4:C:300:OJ0:C07	2.92	0.47
5:A:406:HOH:O	1:E:3:GLN:HG3	2.14	0.47
1:B:203:LYS:HB3	1:B:203:LYS:HZ2	1.78	0.47
1:D:191:CYS:SG	4:D:300:OJ0:C09	3.02	0.47
1:D:156:LEU:O	1:D:183:ARG:HD2	2.14	0.47
1:B:59:ARG:HG3	1:B:116:MET:HG2	1.96	0.47
1:D:191:CYS:SG	4:D:300:OJ0:C27	3.03	0.47
1:C:29:LEU:CD2	1:C:30:THR:N	2.77	0.47
1:C:55:TYR:HE2	5:C:474:HOH:O	1.97	0.47
1:D:57:GLN:HG2	5:D:480:HOH:O	2.14	0.47
1:E:25:LYS:HG2	1:E:152:PHE:HB3	1.96	0.47
1:E:33:LEU:CD2	1:E:58:GLN:HG2	2.45	0.46
1:A:156:LEU:HD23	1:A:198:VAL:HG23	1.97	0.46
1:C:186:GLN:HG3	1:C:197:ASP:OD2	2.16	0.46
1:E:66:MET:HG2	1:E:112:ASP:C	2.41	0.46
1:D:4:ALA:HA	1:D:7:MET:CE	2.45	0.46
1:D:122:ARG:HD2	1:E:96:THR:O	2.16	0.46
1:B:-2:ASP:HA	1:B:1:HIS:CD2	2.50	0.46
1:C:55:TYR:CE1	1:D:147:TRP:HH2	2.34	0.45
1:C:116:MET:HG3	5:C:477:HOH:O	2.16	0.45
1:A:67:TRP:CE3	1:A:111:HIS:HA	2.51	0.45
1:D:29:LEU:HD11	1:D:60:TRP:HB2	1.99	0.45
1:E:151:GLY:HA2	1:E:154:ILE:O	2.16	0.45
1:B:59:ARG:NH2	1:B:159:ASP:OD2	2.49	0.45
1:B:121:GLN:NE2	5:B:457:HOH:O	2.43	0.45
1:C:-2:ASP:CA	1:C:1:HIS:HD2	2.29	0.45
1:C:56:GLU:O	1:C:119:PRO:HD2	2.16	0.45
1:C:116:MET:SD	4:D:300:OJ0:C04	3.05	0.45
1:D:28:PRO:HB3	1:D:152:PHE:O	2.17	0.45
1:A:191:CYS:CB	1:A:193:GLU:OE2	2.65	0.45
1:B:118:ILE:HG13	4:C:300:OJ0:H06	1.98	0.44
1:D:10:LYS:NZ	5:D:436:HOH:O	2.49	0.44
1:C:129:PRO:O	1:C:130:THR:C	2.61	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:LEU:O	1:B:183:ARG:HD2	2.17	0.44
1:C:27:ASP:N	1:C:28:PRO:CD	2.80	0.44
1:E:-2:ASP:O	1:E:-2:ASP:OD1	2.35	0.44
1:A:193:GLU:CG	1:A:195:TYR:CE1	2.99	0.44
4:E:306:OJ0:H07	4:E:306:OJ0:C12	2.47	0.44
1:A:122:ARG:HD2	1:B:96:THR:O	2.16	0.44
1:B:141:ALA:HA	1:B:200:LEU:O	2.17	0.44
1:A:21:PRO:HB2	1:E:6:LEU:CD2	2.47	0.44
1:E:99:VAL:HG13	5:E:404:HOH:O	2.16	0.44
1:D:147:TRP:CH2	4:D:300:OJ0:H20	2.53	0.44
1:A:148:VAL:HG11	1:E:106:ILE:HB	2.00	0.43
1:C:7:MET:CE	1:D:21:PRO:HD3	2.47	0.43
1:D:20:TYR:CD1	1:D:21:PRO:HD2	2.54	0.43
4:E:306:OJ0:H11	4:E:306:OJ0:C07	2.46	0.43
1:A:127:CYS:O	1:A:129:PRO:HD3	2.18	0.43
1:A:71:GLU:HB3	1:A:72:TYR:CD2	2.53	0.43
4:D:300:OJ0:C11	4:D:300:OJ0:C07	2.95	0.43
1:A:35:PHE:CE2	1:A:56:GLU:HG2	2.54	0.43
1:C:169:TYR:CZ	1:C:171:SER:HB2	2.53	0.43
1:A:29:LEU:HD11	1:A:60:TRP:HB2	1.99	0.43
1:C:106:ILE:HB	1:D:148:VAL:HG11	2.00	0.43
1:C:116:MET:HB3	4:D:300:OJ0:C06	2.48	0.43
1:C:-2:ASP:N	1:C:1:HIS:CD2	2.73	0.43
1:A:67:TRP:CZ3	1:A:111:HIS:HA	2.54	0.42
1:B:122:ARG:HD2	1:C:96:THR:O	2.18	0.42
1:C:99:VAL:HG12	5:C:446:HOH:O	2.19	0.42
1:C:43:ALA:HA	1:C:50:VAL:HG22	2.00	0.42
1:C:171:SER:HB3	1:D:128:ASP:HB2	2.02	0.42
1:B:56:GLU:O	1:B:119:PRO:HD2	2.20	0.42
1:C:59:ARG:NH2	1:C:159:ASP:OD2	2.46	0.42
1:C:106:ILE:HG21	1:D:148:VAL:HG21	2.01	0.42
1:C:190:CYS:SG	4:C:300:OJ0:H16A	2.59	0.42
1:C:77:ASP:CB	1:C:110:THR:HG22	2.49	0.42
1:E:110:THR:OG1	1:E:114:SER:HB2	2.20	0.42
1:B:129:PRO:O	1:B:132:VAL:HB	2.20	0.42
1:A:20:TYR:CE2	1:A:22:GLY:HA2	2.55	0.41
1:A:191:CYS:HB3	1:A:193:GLU:OE1	2.19	0.41
1:C:29:LEU:CD2	1:C:60:TRP:HB2	2.48	0.41
1:A:171:SER:HB3	1:B:128:ASP:HB2	2.03	0.41
1:D:52:LEU:O	1:D:122:ARG:HA	2.20	0.41
1:B:147:TRP:CE2	4:B:300:OJ0:H21	2.56	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:TYR:CE2	1:C:22:GLY:HA2	2.55	0.41
1:D:108:VAL:HB	1:D:116:MET:HE3	2.02	0.41
1:E:160:THR:HG23	1:E:162:GLN:O	2.20	0.41
1:C:-2:ASP:O	1:C:1:HIS:HB2	2.20	0.41
1:C:-1:LYS:O	1:C:-1:LYS:HG2	2.21	0.41
1:C:51:ASP:HA	1:C:123:LEU:O	2.21	0.41
1:D:30:THR:HA	1:D:155:ASP:O	2.21	0.40
1:D:177:LEU:O	1:D:178:SER:HB3	2.21	0.40
1:D:147:TRP:O	4:D:300:OJ0:H23A	2.21	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	210/230 (91%)	209 (100%)	0	1 (0%)	24	31
1	B	206/230 (90%)	203 (98%)	3 (2%)	0	100	100
1	C	204/230 (89%)	201 (98%)	3 (2%)	0	100	100
1	D	211/230 (92%)	208 (99%)	3 (1%)	0	100	100
1	E	206/230 (90%)	205 (100%)	1 (0%)	0	100	100
All	All	1037/1150 (90%)	1026 (99%)	10 (1%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	SER

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	193/208 (93%)	184 (95%)	9 (5%)	23	35
1	B	191/208 (92%)	184 (96%)	7 (4%)	30	45
1	C	189/208 (91%)	183 (97%)	6 (3%)	34	51
1	D	196/208 (94%)	189 (96%)	7 (4%)	31	47
1	E	191/208 (92%)	184 (96%)	7 (4%)	30	45
All	All	960/1040 (92%)	924 (96%)	36 (4%)	30	44

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	ASP
1	A	-2	ASP
1	A	7	MET
1	A	42	LYS
1	A	61	LYS
1	A	99	VAL
1	A	118	ILE
1	A	135	GLU
1	A	156	LEU
1	B	11	SER
1	B	19	MET
1	B	33	LEU
1	B	71	GLU
1	B	99	VAL
1	B	130	THR
1	B	191	CYS
1	C	-1	LYS
1	C	29	LEU
1	C	64	SER
1	C	97[A]	ARG
1	C	97[B]	ARG
1	C	191	CYS
1	D	-6	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	0	LEU
1	D	25	LYS
1	D	63	ASN
1	D	79	ARG
1	D	156	LEU
1	D	160	THR
1	E	3	GLN
1	E	52	LEU
1	E	71	GLU
1	E	99	VAL
1	E	105	GLN
1	E	130	THR
1	E	142	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	GLN
1	B	1	HIS
1	B	105	GLN
1	B	121	GLN
1	C	1	HIS
1	C	100	GLN
1	C	105	GLN
1	C	121	GLN
1	C	184	GLN
1	D	38	GLN
1	D	57	GLN
1	D	187	HIS
1	E	162	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

5 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	F	1	2,1	14,14,15	0.50	0	17,19,21	0.89	0
2	NAG	F	2	2	14,14,15	0.56	0	17,19,21	0.93	0
2	BMA	F	3	2	11,11,12	0.39	0	15,15,17	0.96	1 (6%)
2	MAN	F	4	2	11,11,12	0.50	0	15,15,17	0.99	1 (6%)
2	MAN	F	5	2	11,11,12	0.60	0	15,15,17	0.66	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
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1
2	MAN	F	4	2	-	0/2/19/22	0/1/1/1
2	MAN	F	5	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	4	MAN	C1-O5-C5	2.30	115.26	112.19
2	F	3	BMA	C1-C2-C3	2.15	112.77	109.64

There are no chirality outliers.

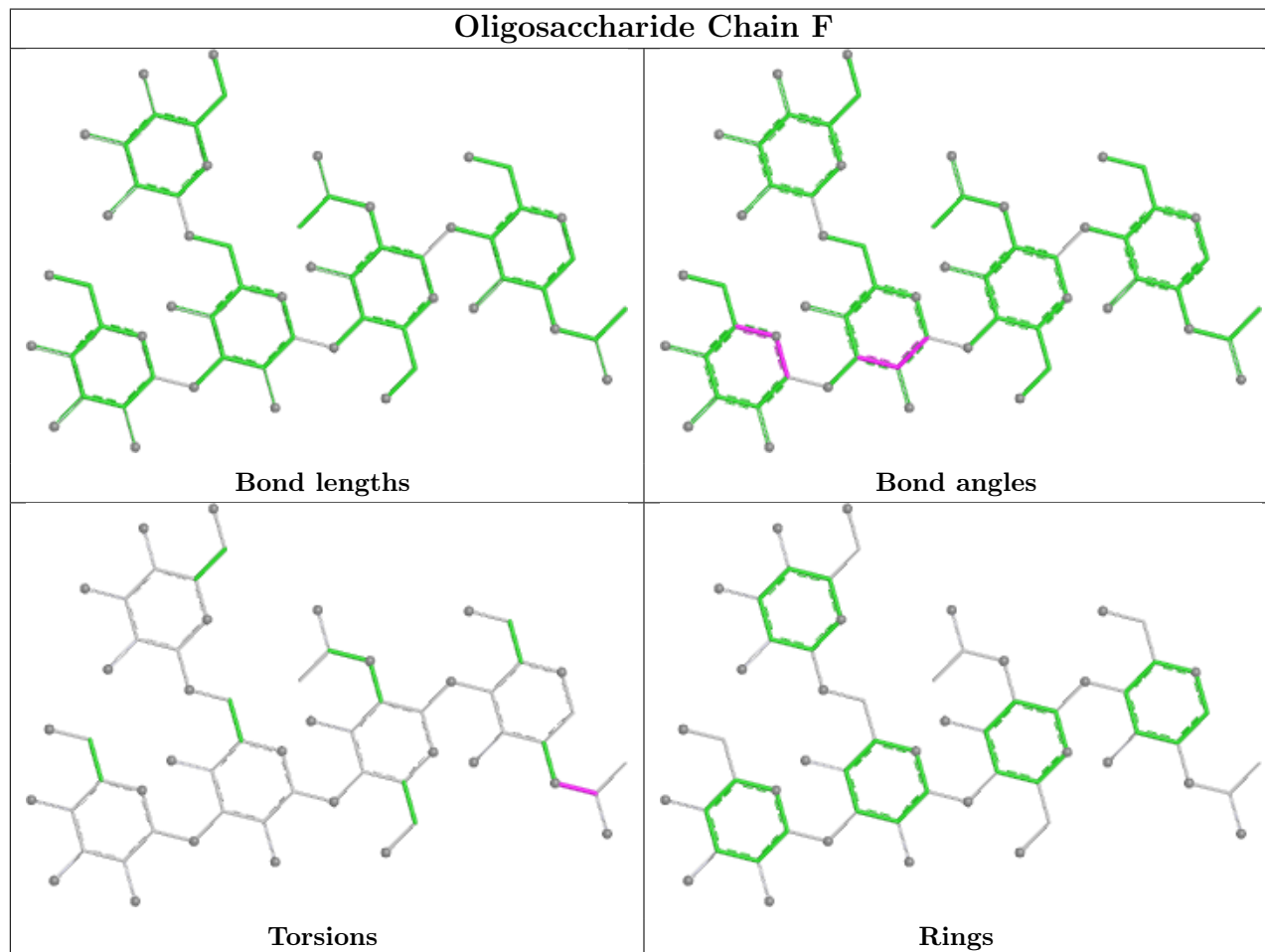
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2

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 [i](#)

6 ligands 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
4	OJ0	B	300	-	32,33,33	5.48	26 (81%)	40,50,50	3.96	20 (50%)
4	OJ0	A	302	-	32,33,33	5.59	27 (84%)	40,50,50	4.22	19 (47%)
3	NAG	A	301	1	14,14,15	0.56	0	17,19,21	0.61	0
4	OJ0	C	300	-	32,33,33	5.35	24 (75%)	40,50,50	4.06	19 (47%)
4	OJ0	D	300	-	32,33,33	5.38	25 (78%)	40,50,50	4.02	18 (45%)
4	OJ0	E	306	-	32,33,33	5.28	24 (75%)	40,50,50	4.23	17 (42%)

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
4	OJ0	B	300	-	-	4/9/34/34	0/6/5/5
4	OJ0	A	302	-	-	3/9/34/34	0/6/5/5
3	NAG	A	301	1	-	3/6/23/26	0/1/1/1
4	OJ0	C	300	-	-	2/9/34/34	0/6/5/5
4	OJ0	D	300	-	-	3/9/34/34	0/6/5/5
4	OJ0	E	306	-	-	4/9/34/34	0/6/5/5

All (126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	302	OJ0	C17-N22	-13.05	1.40	1.53
4	A	302	OJ0	C20-N22	-12.77	1.40	1.53
4	B	300	OJ0	C20-N22	-12.70	1.40	1.53
4	C	300	OJ0	C17-N22	-12.56	1.40	1.53
4	D	300	OJ0	C17-N22	-12.30	1.40	1.53
4	E	306	OJ0	C17-N22	-12.12	1.41	1.53
4	D	300	OJ0	C20-N22	-11.95	1.41	1.53
4	B	300	OJ0	C17-N22	-11.67	1.41	1.53
4	C	300	OJ0	C20-N22	-11.58	1.41	1.53
4	E	306	OJ0	C20-N22	-11.15	1.42	1.53
4	D	300	OJ0	C13-C12	9.07	1.51	1.36
4	B	300	OJ0	C13-C12	8.84	1.50	1.36
4	C	300	OJ0	C13-C12	8.81	1.50	1.36
4	B	300	OJ0	C05-C04	8.71	1.53	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	302	OJ0	C13-C12	8.66	1.50	1.36
4	E	306	OJ0	C13-C12	8.60	1.50	1.36
4	A	302	OJ0	C05-C04	8.55	1.53	1.38
4	B	300	OJ0	C07-C08	8.43	1.52	1.39
4	D	300	OJ0	C05-C04	8.30	1.53	1.38
4	C	300	OJ0	C05-C04	8.14	1.52	1.38
4	E	306	OJ0	C07-C08	8.13	1.52	1.39
4	A	302	OJ0	C07-C08	8.11	1.52	1.39
4	E	306	OJ0	C05-C04	8.05	1.52	1.38
4	D	300	OJ0	C07-C08	7.98	1.52	1.39
4	C	300	OJ0	C07-C08	7.88	1.51	1.39
4	A	302	OJ0	C13-N14	7.36	1.47	1.34
4	C	300	OJ0	C13-N14	7.27	1.46	1.34
4	B	300	OJ0	C13-N14	7.22	1.46	1.34
4	D	300	OJ0	C13-N14	7.18	1.46	1.34
4	E	306	OJ0	C13-N14	7.05	1.46	1.34
4	A	302	OJ0	C06-C07	6.65	1.50	1.38
4	B	300	OJ0	C06-C07	6.63	1.50	1.38
4	B	300	OJ0	C08-C03	6.58	1.50	1.41
4	A	302	OJ0	C08-C03	6.55	1.50	1.41
4	C	300	OJ0	C08-C03	6.53	1.50	1.41
4	E	306	OJ0	C06-C07	6.51	1.50	1.38
4	D	300	OJ0	C06-C07	6.42	1.49	1.38
4	E	306	OJ0	C08-C03	6.37	1.50	1.41
4	D	300	OJ0	C08-C03	6.18	1.50	1.41
4	C	300	OJ0	C06-C07	6.17	1.49	1.38
4	B	300	OJ0	C04-C03	6.13	1.49	1.39
4	A	302	OJ0	C04-C03	6.12	1.49	1.39
4	D	300	OJ0	C04-C03	5.96	1.48	1.39
4	E	306	OJ0	C04-C03	5.82	1.48	1.39
4	C	300	OJ0	C04-C03	5.64	1.48	1.39
4	A	302	OJ0	C18-C19	-5.54	1.38	1.54
4	A	302	OJ0	C19-C20	-5.51	1.42	1.53
4	D	300	OJ0	C18-C19	-5.48	1.39	1.54
4	E	306	OJ0	C18-C19	-5.45	1.39	1.54
4	C	300	OJ0	C18-C19	-5.42	1.39	1.54
4	B	300	OJ0	C05-C06	5.40	1.50	1.38
4	E	306	OJ0	C19-C20	-5.28	1.43	1.53
4	B	300	OJ0	C19-C20	-5.20	1.43	1.53
4	C	300	OJ0	C19-C20	-5.19	1.43	1.53
4	A	302	OJ0	C16-C17	-5.19	1.46	1.53
4	A	302	OJ0	C05-C06	5.18	1.49	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	300	OJ0	C19-C20	-5.15	1.43	1.53
4	B	300	OJ0	C18-C19	-5.12	1.40	1.54
4	C	300	OJ0	C05-C06	5.07	1.49	1.38
4	D	300	OJ0	C05-C06	5.05	1.49	1.38
4	E	306	OJ0	C05-C06	5.02	1.49	1.38
4	E	306	OJ0	C16-C17	-4.86	1.47	1.53
4	B	300	OJ0	N26-N25	4.64	1.39	1.32
4	A	302	OJ0	N26-N25	4.59	1.39	1.32
4	A	302	OJ0	C18-C17	-4.54	1.44	1.53
4	B	300	OJ0	C18-C17	-4.51	1.44	1.53
4	C	300	OJ0	N26-N25	4.49	1.39	1.32
4	D	300	OJ0	C16-C17	-4.49	1.47	1.53
4	D	300	OJ0	C18-C17	-4.45	1.44	1.53
4	B	300	OJ0	C12-N26	4.41	1.43	1.36
4	D	300	OJ0	C21-C20	-4.41	1.47	1.53
4	C	300	OJ0	C18-C17	-4.40	1.44	1.53
4	E	306	OJ0	N26-N25	4.40	1.39	1.32
4	E	306	OJ0	C18-C17	-4.37	1.44	1.53
4	D	300	OJ0	N26-N25	4.37	1.39	1.32
4	B	300	OJ0	C16-C17	-4.27	1.48	1.53
4	A	302	OJ0	C12-N26	4.18	1.43	1.36
4	C	300	OJ0	C16-C17	-4.10	1.48	1.53
4	C	300	OJ0	C21-C20	-4.09	1.48	1.53
4	C	300	OJ0	C12-N26	4.07	1.43	1.36
4	B	300	OJ0	C27-C28	4.00	1.53	1.43
4	E	306	OJ0	C12-N26	3.92	1.42	1.36
4	C	300	OJ0	C27-C28	3.89	1.52	1.43
4	B	300	OJ0	C21-C20	-3.84	1.48	1.53
4	C	300	OJ0	C27-C09	3.83	1.47	1.37
4	D	300	OJ0	C12-N26	3.77	1.42	1.36
4	A	302	OJ0	C27-C28	3.71	1.52	1.43
4	A	302	OJ0	C21-C20	-3.70	1.48	1.53
4	E	306	OJ0	C27-C09	3.70	1.47	1.37
4	B	300	OJ0	C27-C09	3.65	1.47	1.37
4	E	306	OJ0	C27-C28	3.63	1.52	1.43
4	A	302	OJ0	C27-C09	3.61	1.46	1.37
4	D	300	OJ0	C27-C09	3.55	1.46	1.37
4	D	300	OJ0	C27-C28	3.50	1.51	1.43
4	E	306	OJ0	C21-C20	-3.43	1.49	1.53
4	C	300	OJ0	C03-N02	3.28	1.47	1.40
4	E	306	OJ0	C03-N02	3.21	1.47	1.40
4	D	300	OJ0	C03-N02	3.13	1.47	1.40

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	306	OJ0	C08-C09	3.11	1.50	1.45
4	A	302	OJ0	C03-N02	3.09	1.47	1.40
4	B	300	OJ0	C03-N02	2.99	1.46	1.40
4	A	302	OJ0	C08-C09	2.87	1.50	1.45
4	C	300	OJ0	C16-C15	2.83	1.58	1.53
4	A	302	OJ0	C16-C15	2.82	1.58	1.53
4	C	300	OJ0	C08-C09	2.81	1.50	1.45
4	D	300	OJ0	C08-C09	2.76	1.50	1.45
4	D	300	OJ0	C16-C15	2.73	1.58	1.53
4	B	300	OJ0	C08-C09	2.72	1.50	1.45
4	B	300	OJ0	C16-C15	2.71	1.58	1.53
4	E	306	OJ0	C16-C15	2.62	1.58	1.53
4	A	302	OJ0	C01-N02	-2.52	1.42	1.46
4	B	300	OJ0	C11-C12	2.51	1.53	1.49
4	A	302	OJ0	C23-N22	-2.47	1.46	1.51
4	B	300	OJ0	C24-N22	-2.47	1.46	1.51
4	B	300	OJ0	C23-N22	-2.38	1.46	1.51
4	D	300	OJ0	C01-N02	-2.37	1.42	1.46
4	D	300	OJ0	C23-N22	-2.33	1.46	1.51
4	A	302	OJ0	C24-N22	-2.31	1.46	1.51
4	A	302	OJ0	C11-C12	2.23	1.53	1.49
4	B	300	OJ0	C01-N02	-2.22	1.43	1.46
4	E	306	OJ0	C01-N02	-2.20	1.43	1.46
4	C	300	OJ0	C01-N02	-2.20	1.43	1.46
4	A	302	OJ0	N14-N25	-2.18	1.32	1.35
4	D	300	OJ0	C24-N22	-2.10	1.47	1.51
4	C	300	OJ0	C24-N22	-2.07	1.47	1.51
4	E	306	OJ0	C23-N22	-2.03	1.47	1.51

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	306	OJ0	O10-C09-C08	12.79	125.67	113.56
4	A	302	OJ0	O10-C09-C08	12.25	125.15	113.56
4	D	300	OJ0	O10-C09-C08	11.99	124.91	113.56
4	C	300	OJ0	O10-C09-C08	11.43	124.38	113.56
4	C	300	OJ0	C18-C17-N22	-10.88	94.36	102.31
4	A	302	OJ0	C19-C20-N22	-10.42	94.70	102.31
4	B	300	OJ0	C18-C17-N22	-10.40	94.72	102.31
4	B	300	OJ0	C19-C20-N22	-9.87	95.10	102.31
4	D	300	OJ0	C18-C17-N22	-9.80	95.15	102.31
4	A	302	OJ0	C18-C17-N22	-9.49	95.38	102.31

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	306	OJ0	C19-C20-N22	-9.12	95.65	102.31
4	E	306	OJ0	C18-C17-N22	-8.84	95.85	102.31
4	E	306	OJ0	O10-C09-C27	-8.65	115.53	125.47
4	C	300	OJ0	C19-C20-N22	-8.57	96.05	102.31
4	D	300	OJ0	O10-C09-C27	-8.30	115.93	125.47
4	D	300	OJ0	C19-C20-N22	-8.13	96.37	102.31
4	A	302	OJ0	O10-C09-C27	-7.94	116.34	125.47
4	B	300	OJ0	O10-C09-C08	7.67	120.82	113.56
4	E	306	OJ0	N14-N25-N26	7.59	113.50	107.09
4	C	300	OJ0	O10-C09-C27	-7.36	117.01	125.47
4	C	300	OJ0	N14-N25-N26	7.35	113.30	107.09
4	B	300	OJ0	N14-N25-N26	7.22	113.19	107.09
4	D	300	OJ0	N14-N25-N26	7.19	113.16	107.09
4	E	306	OJ0	C15-N14-N25	7.01	130.45	120.94
4	B	300	OJ0	C15-N14-N25	6.98	130.41	120.94
4	A	302	OJ0	C15-N14-N25	6.76	130.11	120.94
4	B	300	OJ0	C16-C17-C18	-6.73	106.97	113.14
4	A	302	OJ0	N14-N25-N26	6.62	112.69	107.09
4	E	306	OJ0	C16-C17-C18	-6.47	107.21	113.14
4	C	300	OJ0	C15-N14-N25	6.46	129.71	120.94
4	B	300	OJ0	C20-N22-C17	5.96	111.28	100.87
4	A	302	OJ0	C20-N22-C17	5.95	111.27	100.87
4	D	300	OJ0	C15-N14-N25	5.73	128.72	120.94
4	A	302	OJ0	C16-C17-C18	-5.53	108.07	113.14
4	D	300	OJ0	C16-C17-C18	-5.52	108.08	113.14
4	D	300	OJ0	C20-N22-C17	5.35	110.22	100.87
4	B	300	OJ0	C27-C28-N02	5.35	120.66	115.44
4	C	300	OJ0	C20-N22-C17	4.95	109.51	100.87
4	E	306	OJ0	C20-N22-C17	4.92	109.47	100.87
4	A	302	OJ0	C15-N14-C13	-4.63	121.10	128.77
4	A	302	OJ0	C27-C28-N02	4.52	119.86	115.44
4	D	300	OJ0	C27-C28-N02	4.45	119.79	115.44
4	B	300	OJ0	C15-N14-C13	-4.29	121.67	128.77
4	C	300	OJ0	C21-C20-C19	-4.29	109.21	113.14
4	E	306	OJ0	C15-N14-C13	-4.28	121.67	128.77
4	B	300	OJ0	O10-C09-C27	-4.28	120.55	125.47
4	E	306	OJ0	C27-C28-N02	4.24	119.58	115.44
4	C	300	OJ0	C16-C17-C18	-4.21	109.28	113.14
4	C	300	OJ0	C27-C28-N02	4.19	119.54	115.44
4	B	300	OJ0	C18-C19-C20	4.01	109.25	104.58
4	C	300	OJ0	C15-N14-C13	-3.98	122.17	128.77
4	E	306	OJ0	C19-C18-C17	3.97	109.20	104.58

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	300	OJ0	C21-C20-C19	-3.88	109.58	113.14
4	B	300	OJ0	C11-C12-N26	3.79	127.76	121.49
4	D	300	OJ0	C18-C19-C20	3.76	108.96	104.58
4	B	300	OJ0	C03-N02-C28	-3.74	119.38	122.93
4	E	306	OJ0	C21-C20-C19	-3.67	109.78	113.14
4	C	300	OJ0	C18-C19-C20	3.65	108.83	104.58
4	D	300	OJ0	C15-N14-C13	-3.63	122.76	128.77
4	A	302	OJ0	C19-C18-C17	3.61	108.78	104.58
4	A	302	OJ0	C18-C19-C20	3.54	108.70	104.58
4	C	300	OJ0	C03-N02-C28	-3.43	119.68	122.93
4	D	300	OJ0	C19-C18-C17	3.27	108.39	104.58
4	B	300	OJ0	C19-C18-C17	3.27	108.39	104.58
4	A	302	OJ0	C03-N02-C28	-3.25	119.85	122.93
4	E	306	OJ0	C11-C12-N26	3.20	126.78	121.49
4	A	302	OJ0	C11-C12-N26	3.12	126.66	121.49
4	D	300	OJ0	C03-N02-C28	-3.08	120.01	122.93
4	A	302	OJ0	C16-C15-C21	3.07	114.01	110.27
4	E	306	OJ0	C03-N02-C28	-3.05	120.04	122.93
4	B	300	OJ0	C16-C15-C21	3.02	113.96	110.27
4	C	300	OJ0	C11-C12-N26	3.02	126.50	121.49
4	B	300	OJ0	C24-N22-C20	-2.99	107.48	112.88
4	E	306	OJ0	C13-N14-N25	-2.93	107.87	110.63
4	E	306	OJ0	C18-C19-C20	2.88	107.94	104.58
4	C	300	OJ0	C19-C18-C17	2.88	107.93	104.58
4	B	300	OJ0	C13-N14-N25	-2.87	107.93	110.63
4	C	300	OJ0	C16-C15-N14	2.67	114.42	111.06
4	C	300	OJ0	C13-N14-N25	-2.67	108.12	110.63
4	E	306	OJ0	O29-C28-C27	-2.51	119.41	125.61
4	D	300	OJ0	C16-C15-N14	2.50	114.20	111.06
4	B	300	OJ0	O29-C28-C27	-2.47	119.52	125.61
4	D	300	OJ0	C11-C12-N26	2.44	125.53	121.49
4	D	300	OJ0	O29-C28-C27	-2.36	119.78	125.61
4	C	300	OJ0	O29-C28-C27	-2.33	119.86	125.61
4	A	302	OJ0	C21-C20-C19	-2.27	111.06	113.14
4	D	300	OJ0	C13-N14-N25	-2.23	108.53	110.63
4	A	302	OJ0	C13-C12-N26	-2.23	105.41	108.12
4	C	300	OJ0	C24-N22-C20	-2.21	108.88	112.88
4	B	300	OJ0	C13-C12-N26	-2.16	105.49	108.12
4	A	302	OJ0	O29-C28-C27	-2.05	120.55	125.61
4	A	302	OJ0	C08-C09-C27	-2.02	118.50	121.45
4	B	300	OJ0	C11-C12-C13	-2.01	126.75	130.22

There are no chirality outliers.

All (19) torsion outliers are listed below:

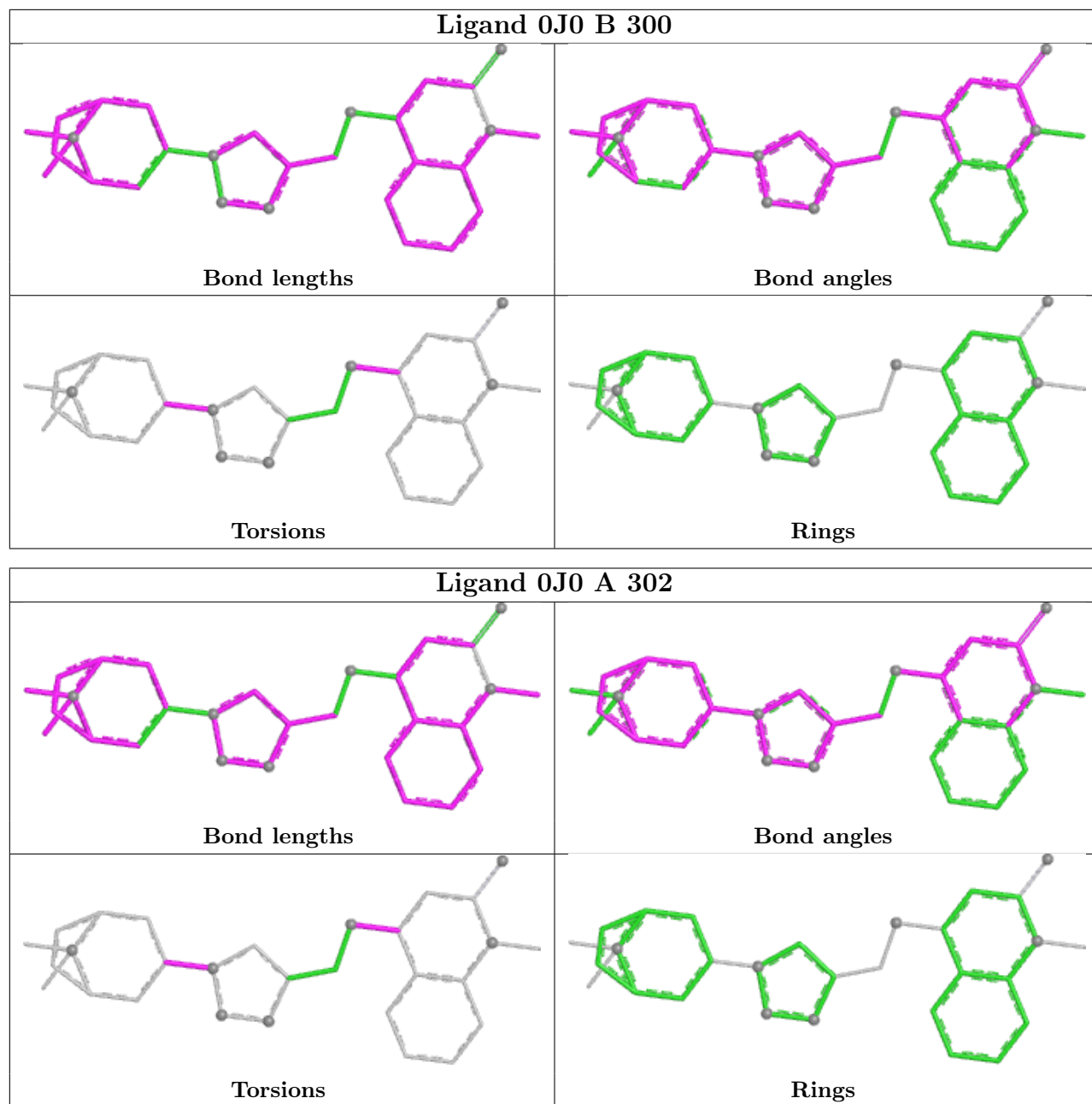
Mol	Chain	Res	Type	Atoms
3	A	301	NAG	C3-C2-N2-C7
4	A	302	OJ0	C27-C09-O10-C11
4	A	302	OJ0	C08-C09-O10-C11
4	B	300	OJ0	C08-C09-O10-C11
4	C	300	OJ0	C27-C09-O10-C11
4	C	300	OJ0	C08-C09-O10-C11
4	D	300	OJ0	C27-C09-O10-C11
4	D	300	OJ0	C08-C09-O10-C11
4	E	306	OJ0	C27-C09-O10-C11
4	E	306	OJ0	C08-C09-O10-C11
3	A	301	NAG	C4-C5-C6-O6
3	A	301	NAG	O5-C5-C6-O6
4	B	300	OJ0	C16-C15-N14-N25
4	B	300	OJ0	C27-C09-O10-C11
4	B	300	OJ0	C16-C15-N14-C13
4	E	306	OJ0	C21-C15-N14-C13
4	A	302	OJ0	C21-C15-N14-N25
4	D	300	OJ0	C16-C15-N14-C13
4	E	306	OJ0	C21-C15-N14-N25

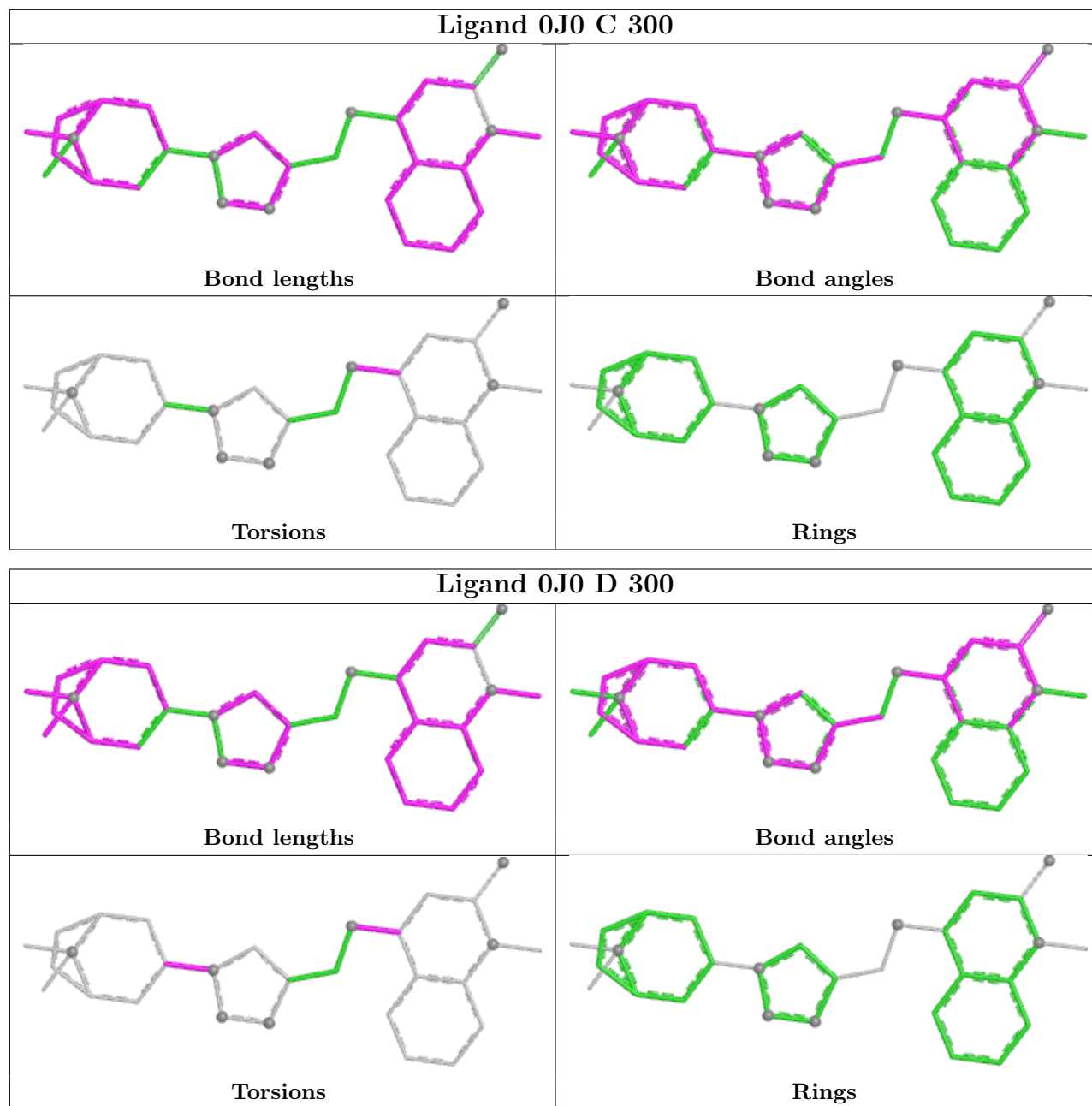
There are no ring outliers.

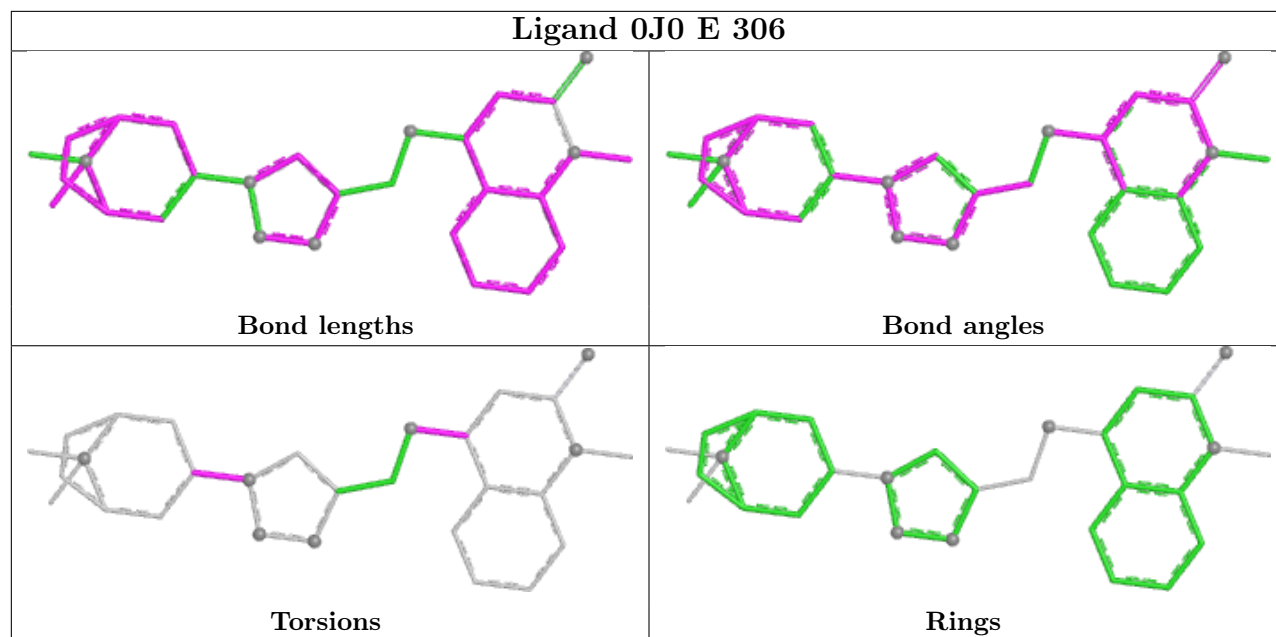
5 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	300	OJ0	1	0
3	A	301	NAG	1	0
4	C	300	OJ0	8	0
4	D	300	OJ0	12	0
4	E	306	OJ0	7	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	211/230 (91%)	-0.04	6 (2%) 55 57	14, 36, 64, 93	1 (0%)
1	B	209/230 (90%)	-0.05	3 (1%) 73 75	17, 38, 61, 105	1 (0%)
1	C	206/230 (89%)	0.06	11 (5%) 32 34	14, 36, 73, 91	2 (0%)
1	D	213/230 (92%)	0.08	7 (3%) 49 51	15, 37, 64, 76	2 (0%)
1	E	209/230 (90%)	-0.09	7 (3%) 49 51	17, 37, 59, 80	1 (0%)
All	All	1048/1150 (91%)	-0.01	34 (3%) 50 52	14, 37, 66, 105	7 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	18	PRO	5.3
1	A	16	ARG	5.1
1	A	17	SER	4.9
1	E	17	SER	4.3
1	D	191	CYS	4.1
1	C	0	LEU	3.8
1	E	19	MET	3.7
1	C	29	LEU	3.4
1	A	18	PRO	3.4
1	E	0	LEU	3.3
1	C	15	ASN	3.1
1	E	55	TYR	3.0
1	C	55	TYR	3.0
1	B	19	MET	2.9
1	E	1	HIS	2.9
1	B	16	ARG	2.9
1	C	72	TYR	2.8
1	D	15	ASN	2.8
1	E	16	ARG	2.8
1	D	190	CYS	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	-2	ASP	2.6
1	C	71	GLU	2.5
1	D	26	ASP	2.5
1	D	186	GLN	2.5
1	D	19	MET	2.4
1	C	2	SER	2.4
1	A	19	MET	2.4
1	A	190	CYS	2.3
1	C	1	HIS	2.3
1	D	72	TYR	2.3
1	C	14	PHE	2.2
1	A	116	MET	2.2
1	C	59	ARG	2.2
1	C	-1	LYS	2.1

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

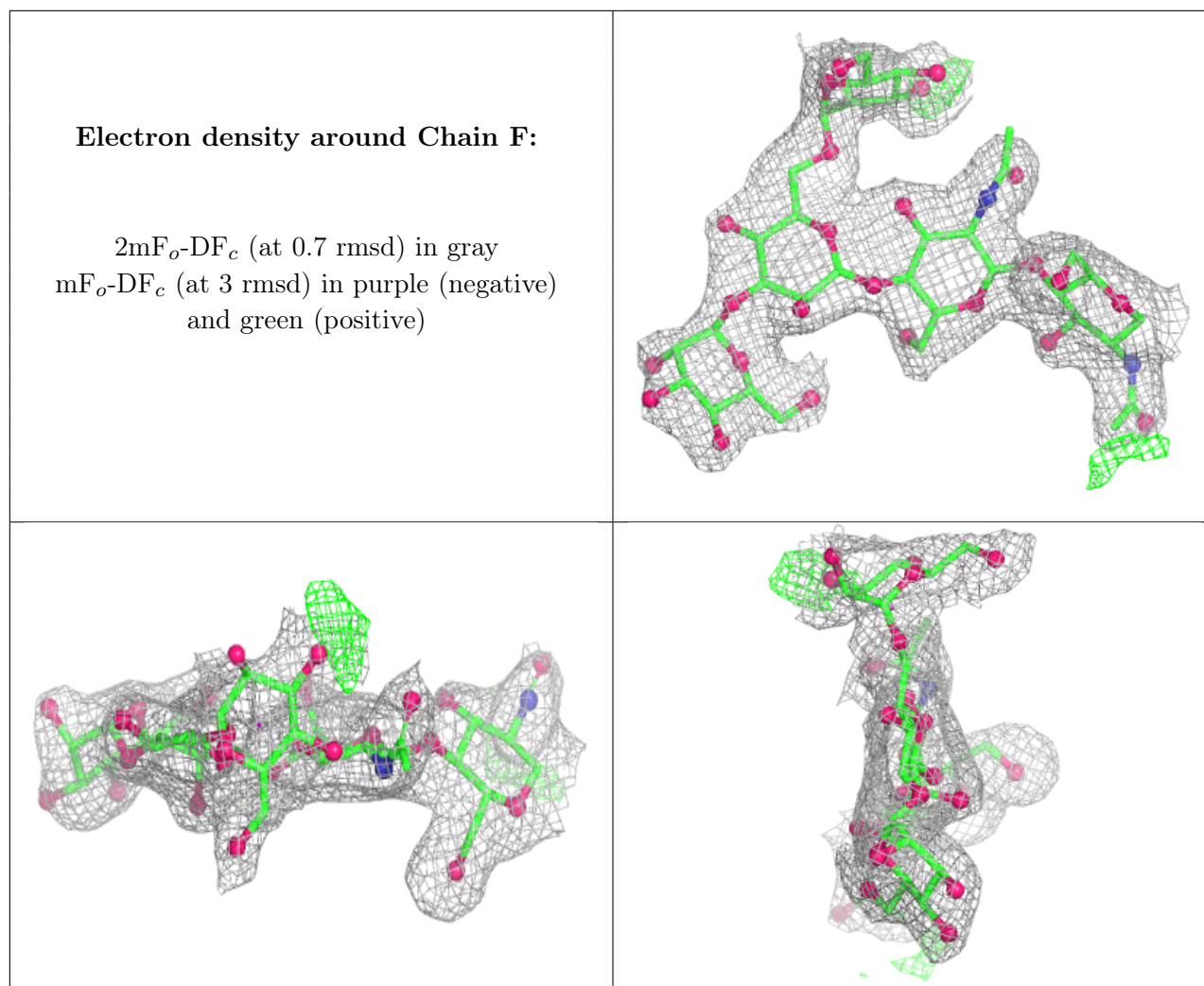
There are no non-standard protein/DNA/RNA residues in this entry.

## 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
2	MAN	F	5	11/12	0.55	0.17	74,92,98,98	0
2	NAG	F	1	14/15	0.74	0.13	60,73,79,81	0
2	BMA	F	3	11/12	0.87	0.08	62,69,76,87	0
2	MAN	F	4	11/12	0.87	0.11	54,63,69,69	0
2	NAG	F	2	14/15	0.87	0.10	70,76,79,80	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.



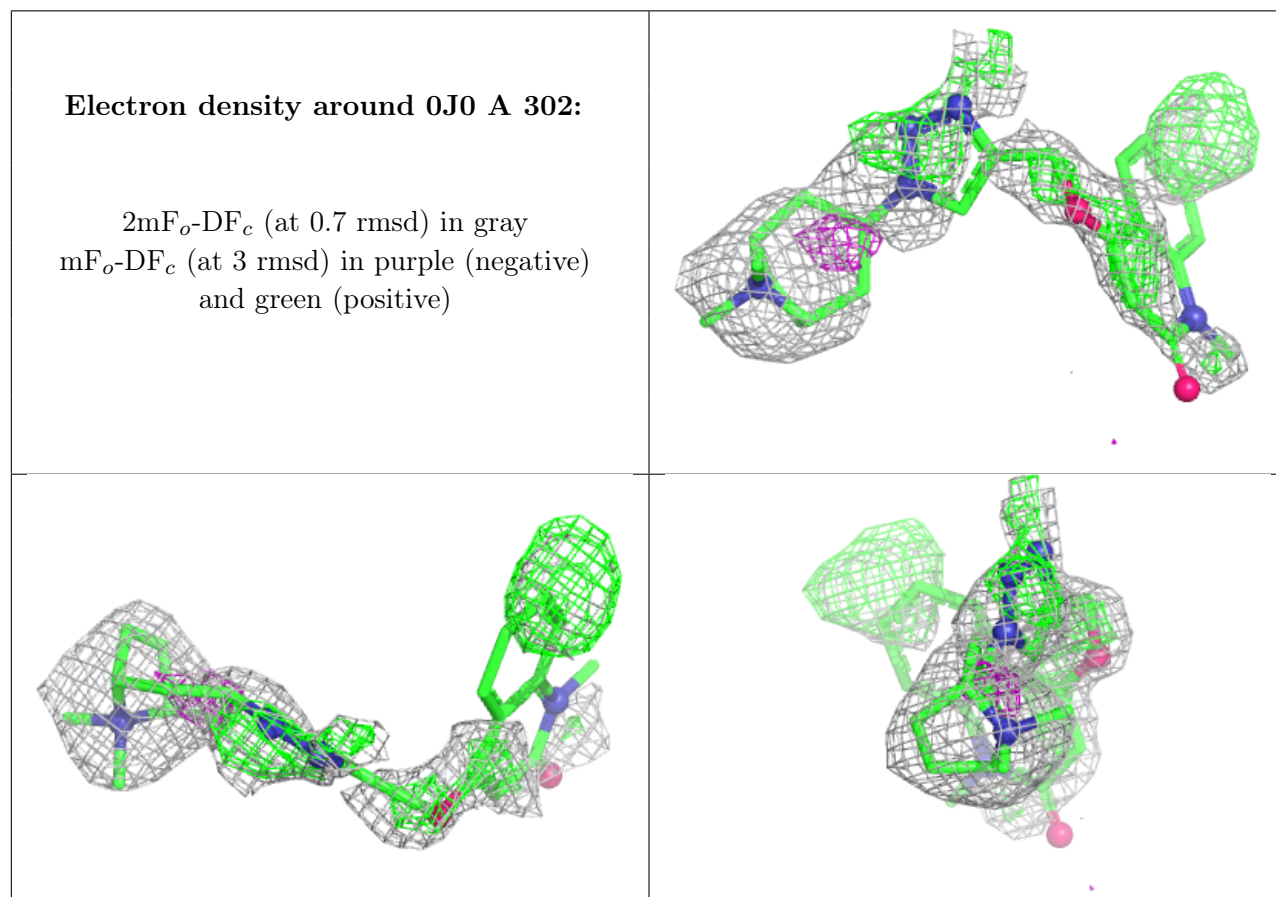
## 6.4 Ligands [i](#)

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
3	NAG	A	301	14/15	0.61	0.17	77,81,88,94	0
4	OJ0	A	302	29/29	0.79	0.15	44,50,56,59	18
4	OJ0	E	306	29/29	0.79	0.17	42,55,72,76	0
4	OJ0	B	300	29/29	0.83	0.16	39,58,91,99	19
4	OJ0	D	300	29/29	0.88	0.11	36,50,67,73	0
4	OJ0	C	300	29/29	0.88	0.12	39,48,65,67	0

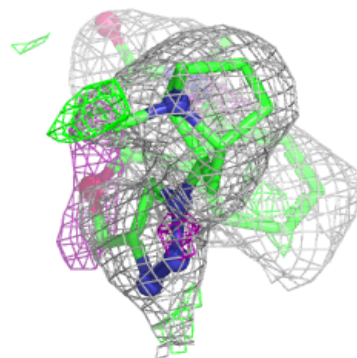
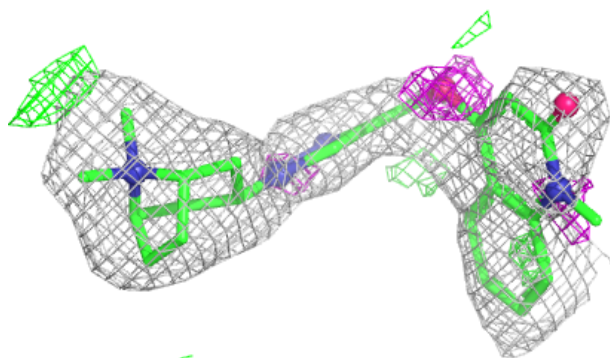
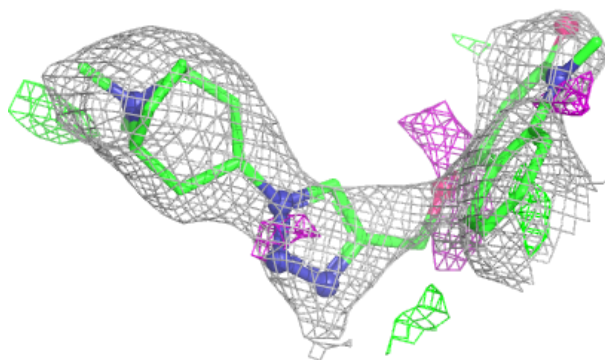
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

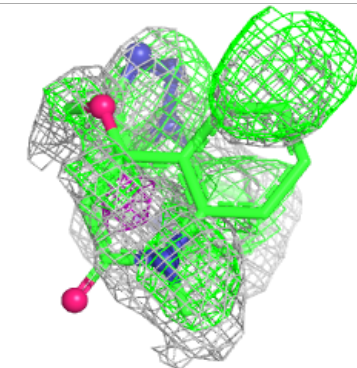
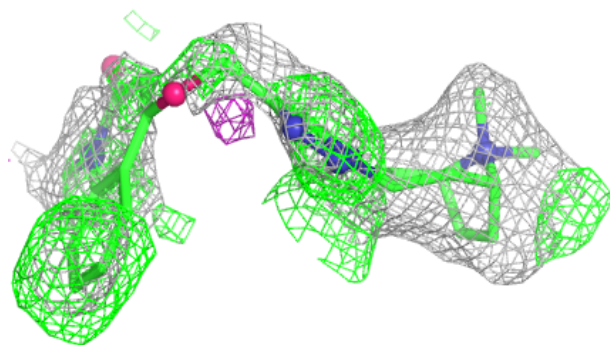
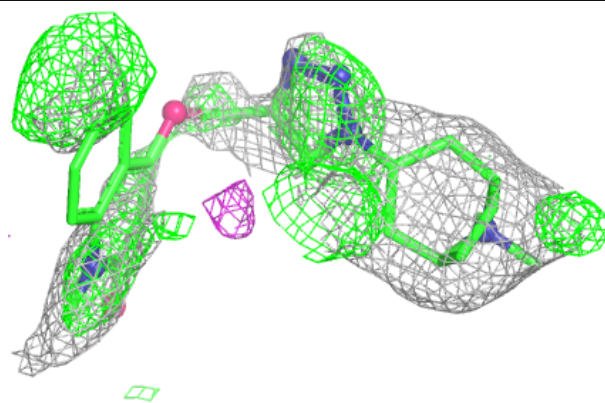


**Electron density around 0J0 E 306:**

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

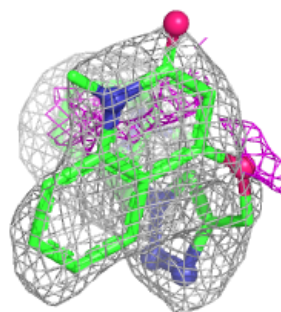
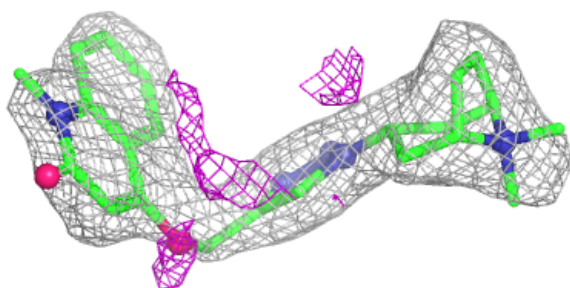
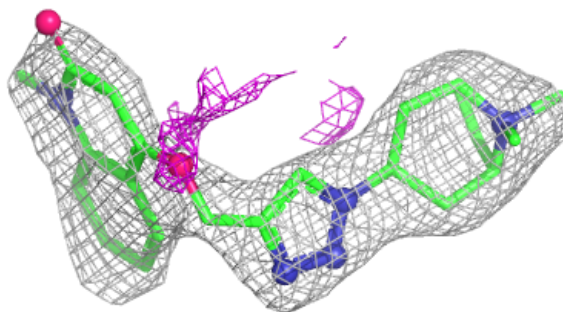
**Electron density around 0J0 B 300:**

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

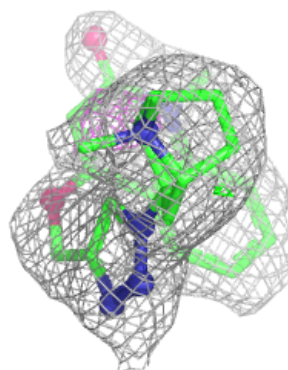
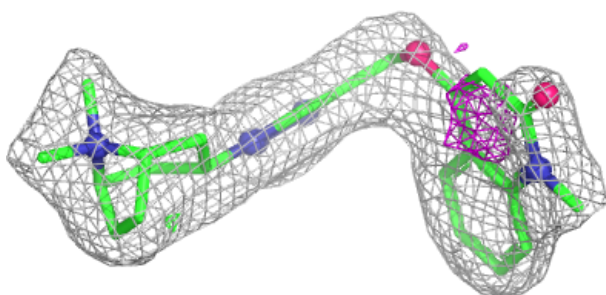
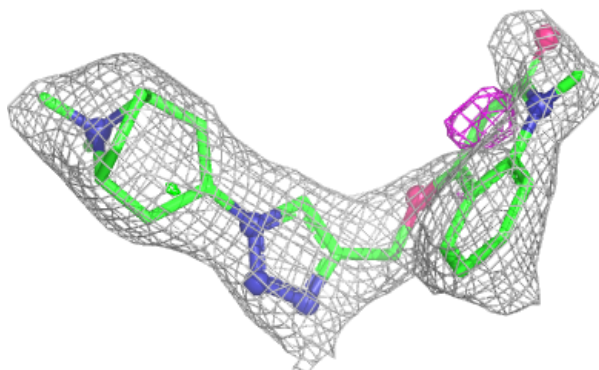


**Electron density around 0J0 D 300:**

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

**Electron density around 0J0 C 300:**

$2mF_o-DF_c$  (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.