



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:10 AM UTC

PDB ID : 2PGZ / pdb\_00002pgz  
Title : Crystal structure of Cocaine bound to an ACh-Binding Protein  
Authors : Hansen, S.B.; Taylor, P.  
Deposited on : 2007-04-10  
Resolution : 1.76 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

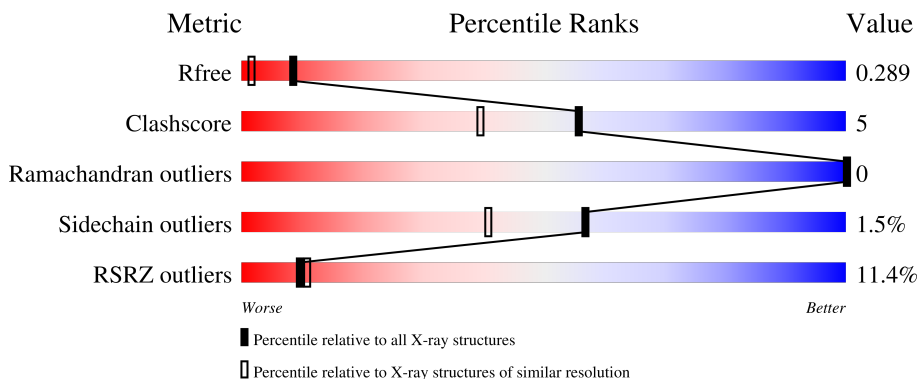
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.76 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.



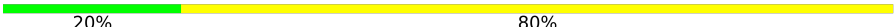
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	
1	B	230	
1	C	230	
1	D	230	
1	E	230	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	F	5	 20% 80%

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
5	PG4	B	403	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9900 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
1	A	211	Total	C	N	O	S	0	6	0
			1721	1085	285	343	8			
1	B	211	Total	C	N	O	S	0	2	0
			1695	1072	276	339	8			
1	C	211	Total	C	N	O	S	0	7	0
			1728	1091	286	341	10			
1	D	214	Total	C	N	O	S	0	5	0
			1742	1100	285	348	9			
1	E	209	Total	C	N	O	S	0	9	0
			1718	1086	282	341	9			

There are 55 discrepancies between the modelled and reference sequences:

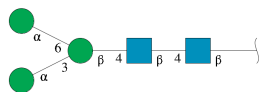
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ASP	-	cloning artifact	UNP Q8WSF8
A	-7	TYR	-	cloning artifact	UNP Q8WSF8
A	-6	LYS	-	cloning artifact	UNP Q8WSF8
A	-5	ASP	-	cloning artifact	UNP Q8WSF8
A	-4	ASP	-	cloning artifact	UNP Q8WSF8
A	-3	ASP	-	cloning artifact	UNP Q8WSF8
A	-2	ASP	-	cloning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

*Continued on next page...*

*Continued from previous page...*

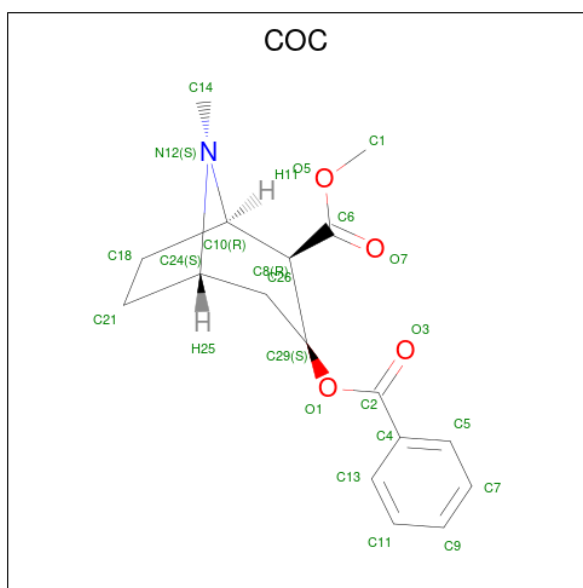
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	LEU	-	cloning artifact	UNP Q8WSF8
B	220	SER	-	cloning artifact	UNP Q8WSF8
B	221	ARG	-	cloning artifact	UNP Q8WSF8
C	-8	ASP	-	cloning artifact	UNP Q8WSF8
C	-7	TYR	-	cloning artifact	UNP Q8WSF8
C	-6	LYS	-	cloning artifact	UNP Q8WSF8
C	-5	ASP	-	cloning artifact	UNP Q8WSF8
C	-4	ASP	-	cloning artifact	UNP Q8WSF8
C	-3	ASP	-	cloning artifact	UNP Q8WSF8
C	-2	ASP	-	cloning artifact	UNP Q8WSF8
C	-1	LYS	-	cloning artifact	UNP Q8WSF8
C	0	LEU	-	cloning artifact	UNP Q8WSF8
C	220	SER	-	cloning artifact	UNP Q8WSF8
C	221	ARG	-	cloning artifact	UNP Q8WSF8
D	-8	ASP	-	cloning artifact	UNP Q8WSF8
D	-7	TYR	-	cloning artifact	UNP Q8WSF8
D	-6	LYS	-	cloning artifact	UNP Q8WSF8
D	-5	ASP	-	cloning artifact	UNP Q8WSF8
D	-4	ASP	-	cloning artifact	UNP Q8WSF8
D	-3	ASP	-	cloning artifact	UNP Q8WSF8
D	-2	ASP	-	cloning artifact	UNP Q8WSF8
D	-1	LYS	-	cloning artifact	UNP Q8WSF8
D	0	LEU	-	cloning artifact	UNP Q8WSF8
D	220	SER	-	cloning artifact	UNP Q8WSF8
D	221	ARG	-	cloning artifact	UNP Q8WSF8
E	-8	ASP	-	cloning artifact	UNP Q8WSF8
E	-7	TYR	-	cloning artifact	UNP Q8WSF8
E	-6	LYS	-	cloning artifact	UNP Q8WSF8
E	-5	ASP	-	cloning artifact	UNP Q8WSF8
E	-4	ASP	-	cloning artifact	UNP Q8WSF8
E	-3	ASP	-	cloning artifact	UNP Q8WSF8
E	-2	ASP	-	cloning artifact	UNP Q8WSF8
E	-1	LYS	-	cloning artifact	UNP Q8WSF8
E	0	LEU	-	cloning artifact	UNP Q8WSF8
E	220	SER	-	cloning artifact	UNP Q8WSF8
E	221	ARG	-	cloning artifact	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 COCAINE (CCD ID: COC) (formula:  $C_{17}H_{21}NO_4$ ).



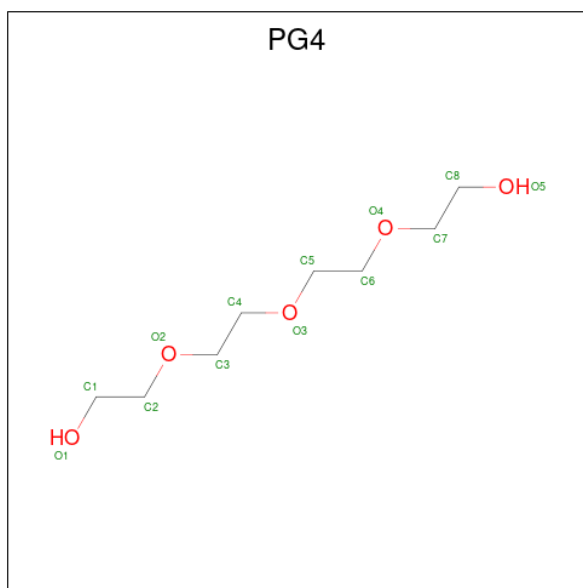
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	22	17	1	4	0	0
3	D	1	22	17	1	4	0	0

- Molecule 4 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
4	B	1	14	8	1	5	0	0

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	B	1	13	8	5	0	0
5	C	1	10	6	4	0	0
5	E	1	13	8	5	0	0

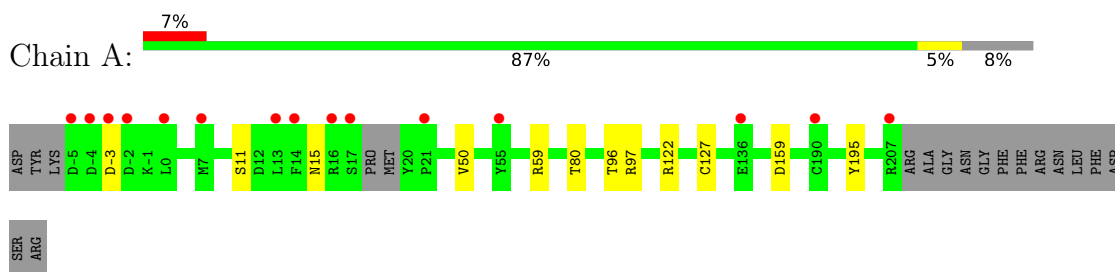
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	251	Total 251	O 251	0	6
6	B	229	Total 229	O 229	0	2
6	C	230	Total 230	O 230	0	8
6	D	223	Total 223	O 223	0	2
6	E	208	Total 208	O 208	0	6

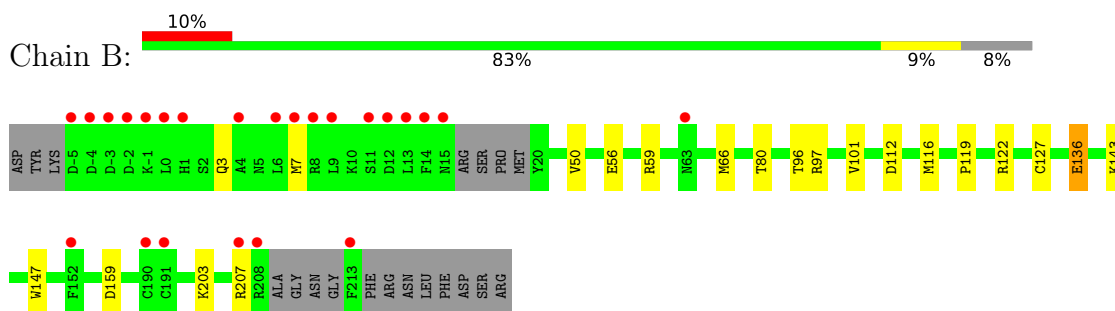
### 3 Residue-property plots [i](#)

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.

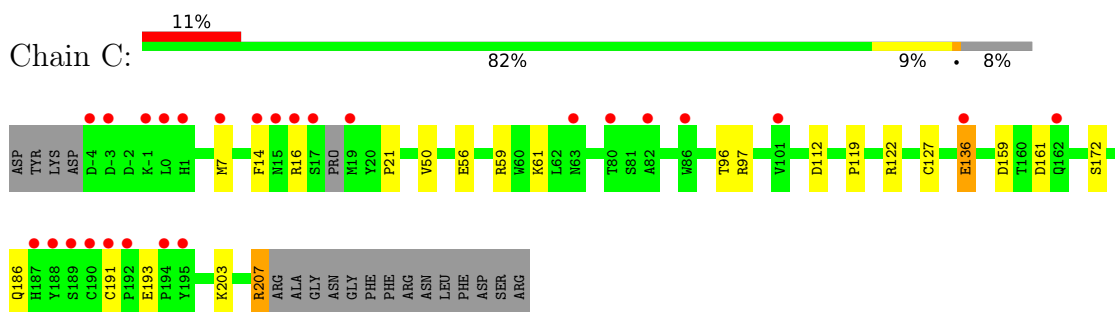
- Molecule 1: Soluble acetylcholine receptor



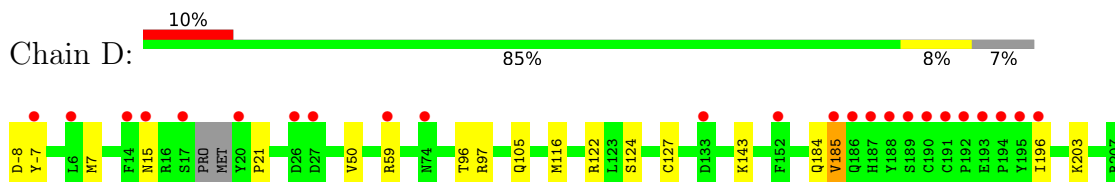
- Molecule 1: Soluble acetylcholine receptor



- Molecule 1: Soluble acetylcholine receptor



- Molecule 1: Soluble acetylcholine receptor



ARG  
ALA  
GLY  
ASN  
GLY  
PHE  
PHE  
ASN  
LEU  
PHE  
ASP  
SER  
SER  
ARG

- Molecule 1: Soluble acetylcholine receptor

Chain E: 13% 80% 10% 9%

ASP TYR LYS D-5 D-4 D-3 D-2 K-1 L0 H1 S2 Q3 A4 N5 L6 M7 R8 L9 K10 S11 D12 L13 F14 N15 ARG SER PRO MET Y20 K25 L29 T30 V31 V50 E56 N63 M67 N74 I75 T80 T86 R97 P119 R122 C127 E136

K143 F152 I154 S172 K173 Q184 V185 Q186 H187 Y188 S189 C190 C191 E193 F194 Y195 R207 ARG ALA GLY ASN GLY PHE PHE ARG ASN LEU PHE ASP SER ARG

- 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

Chain F: 20% 80%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.82Å 115.59Å 130.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.76 50.00 – 1.76	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-1.76) 99.5 (50.00-1.76)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 1.76Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.180 , 0.210 (Not available) , 0.289	Depositor DCC
$R_{free}$ test set	1314 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.8	Xtrriage
Anisotropy	0.057	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 35.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9900	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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, PG4, MAN, COC

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	0.59	0/1777	0.71	0/2418
1	B	0.61	0/1740	0.75	0/2369
1	C	0.57	0/1787	0.72	0/2428
1	D	0.67	1/1796 (0.1%)	0.76	0/2443
1	E	0.72	3/1787 (0.2%)	0.79	2/2430 (0.1%)
All	All	0.63	4/8887 (0.0%)	0.75	2/12088 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	8	ARG	NE-CZ	14.07	1.48	1.33
1	E	8	ARG	CG-CD	6.78	1.72	1.52
1	D	-8	ASP	N-CA	6.77	1.59	1.46
1	E	8	ARG	CZ-NH2	5.12	1.40	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	8	ARG	NE-CZ-NH1	-9.57	111.93	121.50
1	E	8	ARG	NE-CZ-NH2	6.86	125.37	119.20

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	1721	0	1659	9	0
1	B	1695	0	1615	19	0
1	C	1728	0	1675	22	0
1	D	1742	0	1675	17	1
1	E	1718	0	1661	17	1
2	F	61	0	52	0	0
3	A	22	0	21	1	0
3	D	22	0	21	0	0
4	B	14	0	13	0	0
5	B	13	0	18	3	0
5	C	10	0	13	0	0
5	E	13	0	18	2	0
6	A	251	0	0	3	0
6	B	229	0	0	8	0
6	C	230	0	0	7	0
6	D	223	0	0	2	0
6	E	208	0	0	4	0
All	All	9900	0	8441	80	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (80) 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:C:97[B]:ARG:HG3	6:C:633[B]:HOH:O	1.45	1.12
1:A:97[B]:ARG:NE	6:A:650[B]:HOH:O	1.65	1.00
1:B:59:ARG:HD3	1:B:116:MET:HE2	1.47	0.97
1:D:7:MET:HE2	1:D:7:MET:HA	1.53	0.88
5:B:403:PG4:H62	6:B:611:HOH:O	1.78	0.83
1:C:21:PRO:HB3	1:D:7:MET:HE3	1.60	0.83
1:A:97[B]:ARG:CZ	6:A:650[B]:HOH:O	2.16	0.79
1:C:207[A]:ARG:HD3	6:C:635[A]:HOH:O	1.82	0.78
1:C:207[A]:ARG:CG	1:C:207[A]:ARG:HH11	1.97	0.78
1:C:207[A]:ARG:HH11	1:C:207[A]:ARG:HG2	1.49	0.78
1:A:97[B]:ARG:NH2	6:A:650[B]:HOH:O	2.17	0.75
1:C:59[B]:ARG:NH1	1:C:159:ASP:OD2	2.17	0.75
1:D:105:GLN:OE1	6:D:580:HOH:O	2.04	0.74
1:B:101:VAL:HG13	6:B:632:HOH:O	1.87	0.73
1:B:59:ARG:NH1	1:B:159:ASP:OD2	2.21	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:PRO:HD3	1:E:7:MET:HE3	1.71	0.72
1:A:59[A]:ARG:NH1	1:A:159:ASP:OD2	2.23	0.71
1:C:191:CYS:HB3	1:C:193:GLU:OE2	1.93	0.68
1:D:105:GLN:OE1	6:D:594:HOH:O	2.12	0.67
5:E:403:PG4:H32	6:E:587:HOH:O	1.95	0.67
1:B:147:TRP:O	5:B:403:PG4:H82	1.95	0.66
1:D:185:VAL:HG13	1:D:196:ILE:CD1	2.27	0.65
1:A:11:SER:HA	1:A:15:ASN:HD22	1.62	0.63
1:E:29:LEU:HD21	1:E:31:VAL:HG23	1.80	0.63
1:D:97[A]:ARG:HH21	1:D:124:SER:CB	2.13	0.62
1:C:203[B]:LYS:HG3	6:C:565:HOH:O	1.99	0.61
1:D:143:LYS:HZ2	1:D:184:GLN:HE22	1.50	0.60
5:E:403:PG4:H21	6:E:587:HOH:O	2.01	0.59
1:D:143:LYS:NZ	1:D:184:GLN:HE22	2.00	0.59
1:B:136:GLU:H	1:B:136:GLU:CD	2.12	0.58
1:E:29:LEU:HD21	1:E:31:VAL:CG2	2.34	0.57
1:B:203[B]:LYS:HG3	6:B:623:HOH:O	2.05	0.57
1:C:21:PRO:HB3	1:D:7:MET:CE	2.31	0.57
1:C:97[B]:ARG:CG	6:C:633[B]:HOH:O	2.24	0.56
1:E:143[A]:LYS:HE2	1:E:184:GLN:HE22	1.70	0.56
1:C:161[A]:ASP:HB3	6:C:624:HOH:O	2.05	0.56
1:B:59:ARG:HG2	1:B:116:MET:HG3	1.88	0.56
1:B:96:THR:O	1:C:122:ARG:HD2	2.06	0.56
1:C:7:MET:HG2	6:C:505:HOH:O	2.06	0.55
1:C:207[A]:ARG:CG	1:C:207[A]:ARG:NH1	2.66	0.55
1:C:97[A]:ARG:NH1	6:C:442:HOH:O	2.39	0.54
1:B:59:ARG:CG	1:B:116:MET:HG3	2.40	0.52
1:C:96:THR:O	1:D:122:ARG:HD2	2.10	0.52
1:E:29:LEU:CD2	1:E:31:VAL:HG23	2.39	0.52
1:D:50:VAL:HG21	1:D:127:CYS:SG	2.50	0.51
1:A:96:THR:O	1:B:122:ARG:HD2	2.11	0.51
1:A:122:ARG:HD2	1:E:96:THR:O	2.12	0.50
1:B:3:GLN:O	1:B:7:MET:HG3	2.11	0.50
1:B:3:GLN:HB3	1:B:7:MET:HE3	1.94	0.49
1:C:50:VAL:HG21	1:C:127:CYS:SG	2.52	0.49
1:D:96:THR:O	1:E:122:ARG:HD2	2.13	0.49
1:B:97[B]:ARG:HD3	6:B:476:HOH:O	2.13	0.48
1:B:143:LYS:NZ	6:B:532:HOH:O	2.45	0.48
1:E:25:LYS:HE2	1:E:152:PHE:CD2	2.48	0.48
1:B:50:VAL:HG21	1:B:127:CYS:SG	2.54	0.47
1:A:195:TYR:CG	3:A:401:COC:H15	2.50	0.47

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:ARG:HD3	1:D:116[A]:MET:HE1	1.96	0.47
1:C:14:PHE:C	1:C:16:ARG:H	2.23	0.46
1:E:25:LYS:HG3	1:E:152:PHE:HB3	1.96	0.46
1:C:61:LYS:HE3	1:C:112:ASP:O	2.15	0.46
1:E:50:VAL:HG21	1:E:127:CYS:SG	2.56	0.46
1:E:29:LEU:HD22	1:E:154:ILE:HG12	1.97	0.45
1:D:7:MET:HA	1:D:7:MET:CE	2.34	0.45
1:E:97[A]:ARG:HD2	6:E:609[A]:HOH:O	2.17	0.45
1:B:56:GLU:O	1:B:119:PRO:HD2	2.16	0.44
5:B:403:PG4:H12	6:B:611:HOH:O	2.18	0.44
1:E:97[A]:ARG:HD3	6:E:476:HOH:O	2.17	0.44
1:E:172:SER:O	1:E:207[A]:ARG:NH2	2.50	0.44
1:C:136:GLU:CD	1:C:136:GLU:H	2.26	0.43
1:A:50:VAL:HG21	1:A:127:CYS:SG	2.59	0.43
1:D:185:VAL:HG13	1:D:196:ILE:HD13	2.01	0.42
1:B:7:MET:HG2	6:B:597:HOH:O	2.19	0.41
1:B:66:MET:HG2	1:B:112:ASP:C	2.45	0.41
1:E:193:GLU:HG2	1:E:195:TYR:CE2	2.55	0.41
1:E:56:GLU:O	1:E:119:PRO:HD2	2.21	0.41
1:B:207:ARG:HD3	6:B:523:HOH:O	2.20	0.40
1:C:172:SER:N	1:C:207[B]:ARG:HH11	2.18	0.40
1:C:56:GLU:O	1:C:119:PRO:HD2	2.22	0.40
1:E:136:GLU:H	1:E:136:GLU:CD	2.29	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:-7:TYR:OH	1:E:173:LYS:O[2_554]	2.12	0.08

## 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	46/230 (20%)	45 (98%)	1 (2%)	0	100	100
1	E	149/230 (65%)	148 (99%)	1 (1%)	0	100	100
All	All	195/460 (42%)	193 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	198/208 (95%)	196 (99%)	2 (1%)	68	56
1	B	193/208 (93%)	191 (99%)	2 (1%)	68	56
1	C	199/208 (96%)	195 (98%)	4 (2%)	48	29
1	D	200/208 (96%)	198 (99%)	2 (1%)	68	56
1	E	199/208 (96%)	194 (98%)	5 (2%)	42	22
All	All	989/1040 (95%)	974 (98%)	15 (2%)	57	41

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	ASP
1	A	80	THR
1	B	80	THR
1	B	136	GLU
1	C	136	GLU
1	C	186	GLN
1	C	207[A]	ARG
1	C	207[B]	ARG
1	D	15	ASN
1	D	185	VAL
1	E	0	LEU
1	E	29	LEU
1	E	80	THR
1	E	136	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	186	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	63	ASN
1	A	162	GLN
1	B	3	GLN
1	B	58	GLN
1	B	184	GLN
1	C	184	GLN
1	C	186	GLN
1	D	3	GLN
1	D	15	ASN
1	D	58	GLN
1	D	74	ASN
1	D	184	GLN
1	E	3	GLN
1	E	15	ASN
1	E	58	GLN
1	E	184	GLN
1	E	186	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	0.46	0	17,19,21	1.29	1 (5%)
2	NAG	F	2	2	14,14,15	0.33	0	17,19,21	1.04	1 (5%)
2	BMA	F	3	2	11,11,12	0.40	0	15,15,17	0.63	0
2	MAN	F	4	2	11,11,12	0.47	0	15,15,17	1.17	1 (6%)
2	MAN	F	5	2	11,11,12	0.52	0	15,15,17	0.90	2 (13%)

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	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C2-N2-C7	4.24	128.58	122.90
2	F	4	MAN	C1-O5-C5	4.04	117.60	112.19
2	F	2	NAG	C1-C2-N2	-3.43	105.02	110.43
2	F	5	MAN	C1-O5-C5	2.45	115.46	112.19
2	F	5	MAN	C1-C2-C3	2.02	112.59	109.64

There are no chirality outliers.

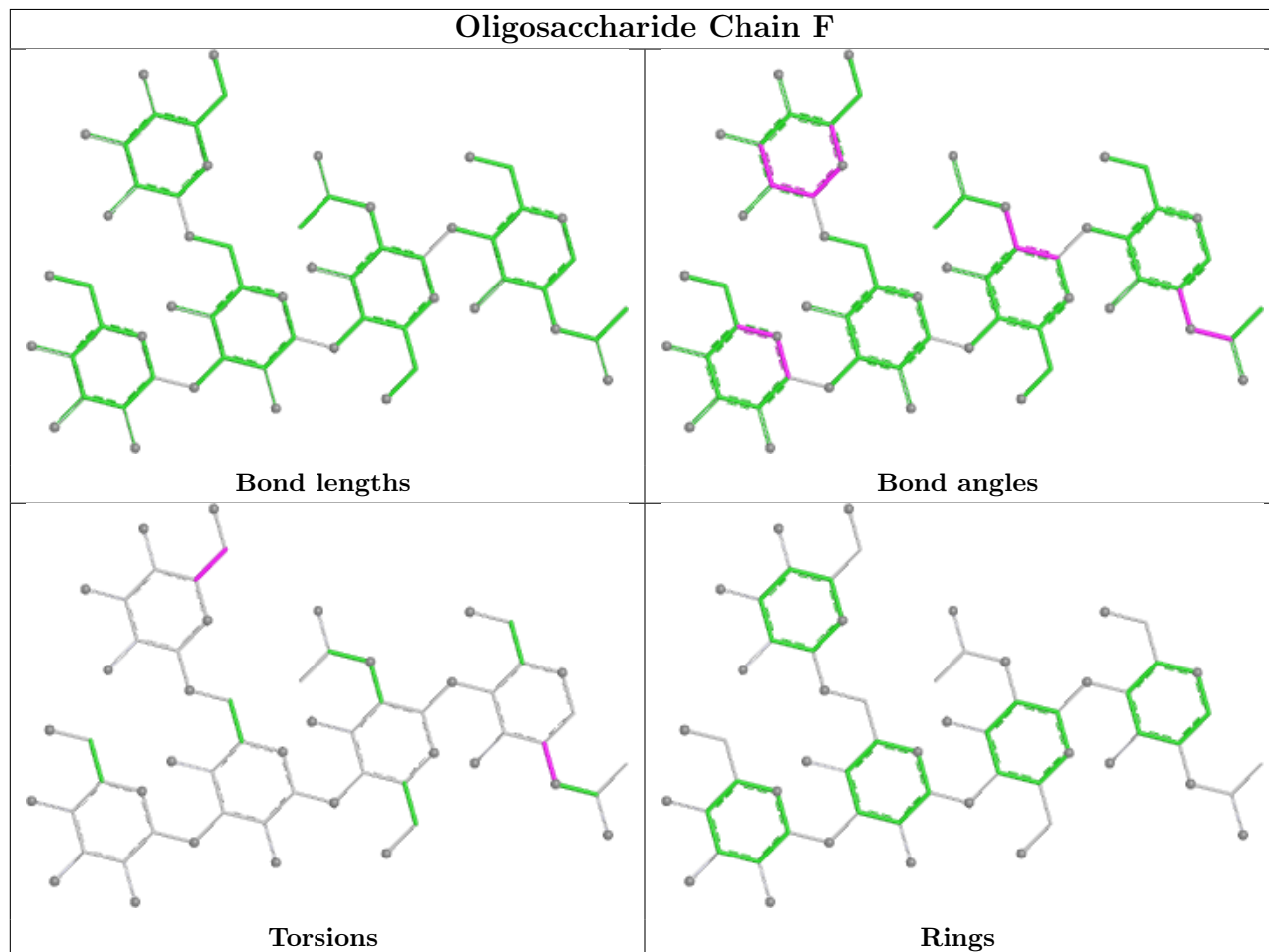
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1	NAG	C1-C2-N2-C7
2	F	5	MAN	C4-C5-C6-O6
2	F	1	NAG	C3-C2-N2-C7

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	$\# Z  > 2$
5	PG4	E	403	-	12,12,12	0.52	0	11,11,11	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PG4	C	407	-	9,9,12	1.18	1 (11%)	8,8,11	0.81	0
3	COC	D	401	-	24,24,24	1.76	3 (12%)	32,34,34	3.64	13 (40%)
5	PG4	B	403	-	12,12,12	1.54	3 (25%)	11,11,11	0.63	0
3	COC	A	401	-	24,24,24	1.62	3 (12%)	32,34,34	3.99	9 (28%)
4	NAG	B	402	1	14,14,15	3.52	4 (28%)	17,19,21	3.19	5 (29%)

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	PG4	E	403	-	-	8/10/10/10	-
5	PG4	C	407	-	-	3/7/7/10	-
3	COC	D	401	-	-	1/14/39/39	0/4/3/3
5	PG4	B	403	-	-	7/10/10/10	-
3	COC	A	401	-	-	0/14/39/39	0/4/3/3
4	NAG	B	402	1	-	2/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	402	NAG	C7-N2	9.53	1.65	1.34
4	B	402	NAG	O7-C7	7.13	1.39	1.23
3	D	401	COC	O5-C6	5.34	1.46	1.33
3	D	401	COC	O1-C2	5.27	1.45	1.34
3	A	401	COC	O1-C2	4.57	1.44	1.34
4	B	402	NAG	O6-C6	4.33	1.60	1.42
3	A	401	COC	O5-C6	4.33	1.43	1.33
5	B	403	PG4	O3-C5	3.31	1.56	1.42
3	A	401	COC	O1-C29	-3.05	1.40	1.46
3	D	401	COC	O1-C29	-2.28	1.42	1.46
5	C	407	PG4	O3-C4	2.23	1.51	1.42
4	B	402	NAG	C8-C7	2.18	1.55	1.50
5	B	403	PG4	C4-C3	2.16	1.59	1.49
5	B	403	PG4	O2-C3	2.06	1.51	1.42

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	COC	C24-N12-C10	15.11	114.71	101.14
3	D	401	COC	C24-N12-C10	14.63	114.28	101.14
3	A	401	COC	C18-C10-N12	-12.54	92.26	105.18
4	B	402	NAG	C2-N2-C7	-10.02	109.47	122.90
3	D	401	COC	C18-C10-N12	-8.16	96.77	105.18
4	B	402	NAG	C8-C7-N2	-6.57	105.23	116.12
3	D	401	COC	O5-C6-C8	5.86	119.38	111.03
3	A	401	COC	C21-C24-N12	-5.54	93.77	104.49
3	A	401	COC	O5-C6-C8	4.86	117.95	111.03
3	D	401	COC	C14-N12-C24	4.19	123.06	113.21
3	D	401	COC	C14-N12-C10	3.84	122.60	113.61
4	B	402	NAG	C1-C2-N2	-3.81	104.43	110.43
3	D	401	COC	O1-C2-C4	3.62	117.72	111.90
3	A	401	COC	C14-N12-C10	3.57	121.97	113.61
3	D	401	COC	C21-C24-N12	-3.52	97.67	104.49
3	A	401	COC	C14-N12-C24	3.45	121.33	113.21
3	D	401	COC	C1-O5-C6	2.97	122.66	115.92
3	A	401	COC	O5-C6-O7	-2.95	118.11	123.85
3	A	401	COC	O1-C2-C4	2.55	116.00	111.90
3	D	401	COC	O5-C6-O7	-2.54	118.91	123.85
3	D	401	COC	C21-C18-C10	2.35	107.83	104.08
3	D	401	COC	C26-C29-C8	2.31	116.17	111.88
4	B	402	NAG	O6-C6-C5	-2.29	103.53	111.33
3	D	401	COC	O1-C2-O3	-2.25	119.89	123.55
3	A	401	COC	C21-C18-C10	2.20	107.59	104.08
4	B	402	NAG	C1-O5-C5	2.10	115.00	112.19
3	D	401	COC	C26-C24-N12	-2.09	104.69	107.54

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	402	NAG	O7-C7-N2-C2
5	E	403	PG4	O2-C3-C4-O3
5	C	407	PG4	O2-C3-C4-O3
5	C	407	PG4	O4-C7-C8-O5
4	B	402	NAG	O5-C5-C6-O6
5	B	403	PG4	O4-C7-C8-O5
5	E	403	PG4	O1-C1-C2-O2
5	E	403	PG4	O3-C5-C6-O4
5	B	403	PG4	O1-C1-C2-O2
5	E	403	PG4	O4-C7-C8-O5
5	B	403	PG4	O2-C3-C4-O3

*Continued on next page...*

*Continued from previous page...*

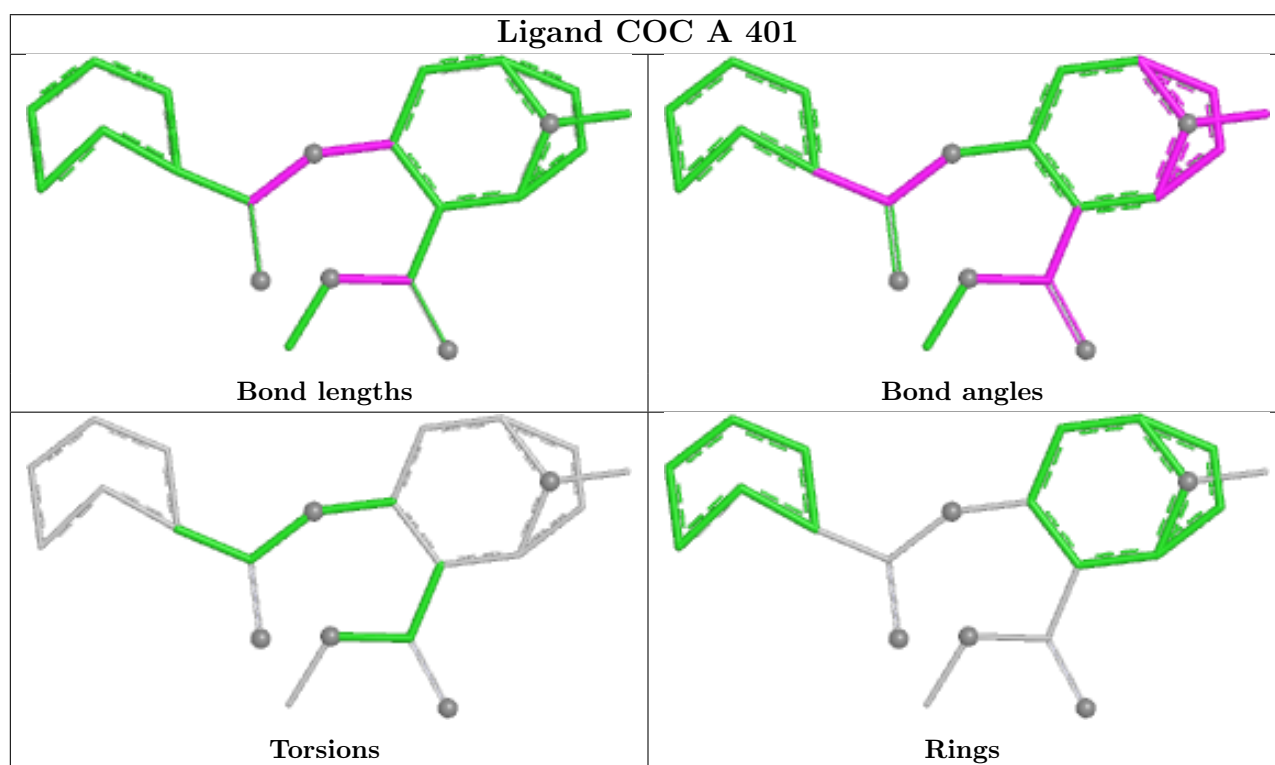
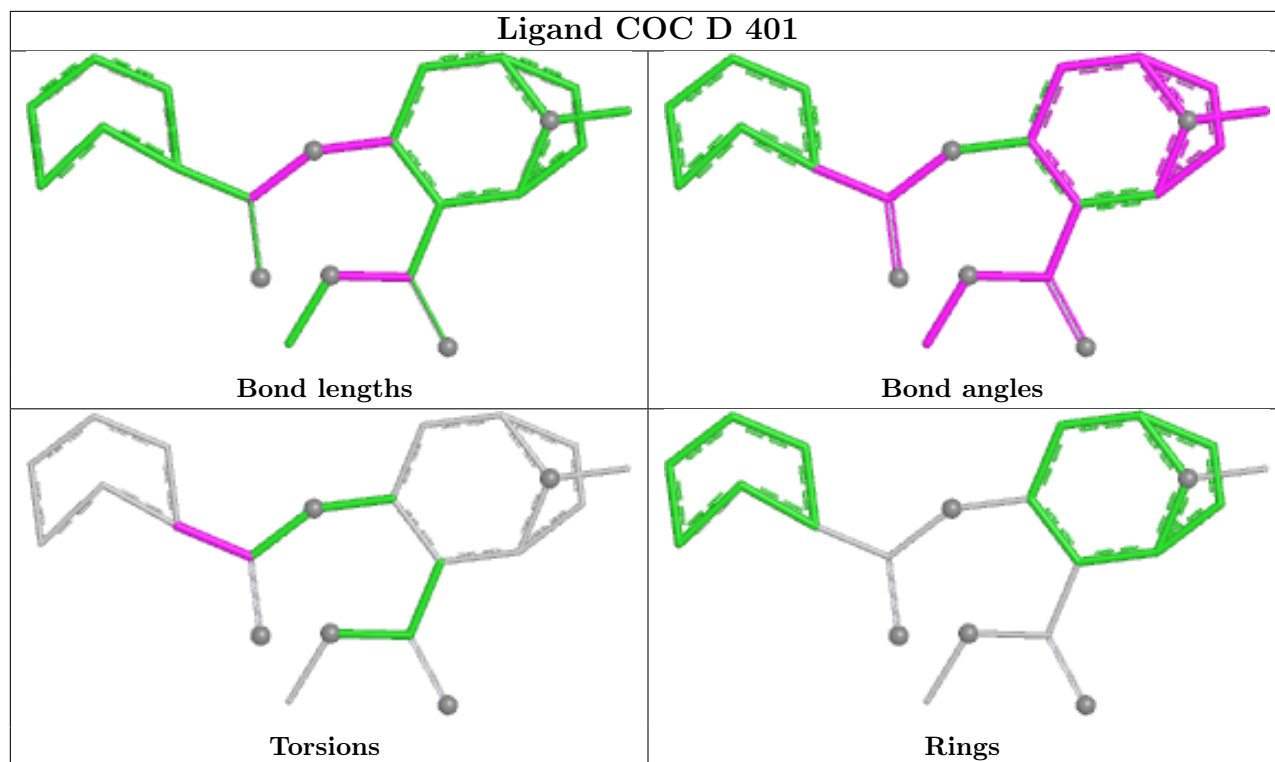
Mol	Chain	Res	Type	Atoms
5	B	403	PG4	C1-C2-O2-C3
5	B	403	PG4	C3-C4-O3-C5
5	E	403	PG4	C1-C2-O2-C3
5	B	403	PG4	C6-C5-O3-C4
5	C	407	PG4	O3-C5-C6-O4
5	B	403	PG4	C8-C7-O4-C6
5	E	403	PG4	C8-C7-O4-C6
5	E	403	PG4	C6-C5-O3-C4
5	E	403	PG4	C3-C4-O3-C5
3	D	401	COC	O1-C2-C4-C5

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	403	PG4	2	0
5	B	403	PG4	3	0
3	A	401	COC	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

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%)	0.74	15 (7%) 22 25	15, 26, 34, 46	6 (2%)
1	B	211/230 (91%)	0.87	24 (11%) 10 11	15, 27, 43, 51	2 (0%)
1	C	211/230 (91%)	1.06	26 (12%) 8 9	15, 28, 47, 57	7 (3%)
1	D	214/230 (93%)	0.88	24 (11%) 10 11	15, 27, 43, 57	5 (2%)
1	E	209/230 (90%)	1.00	31 (14%) 5 6	13, 26, 54, 60	9 (4%)
All	All	1056/1150 (91%)	0.91	120 (11%) 10 11	13, 27, 46, 60	29 (2%)

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	13	LEU	6.1
1	E	15	ASN	6.0
1	E	13	LEU	5.9
1	E	14	PHE	5.5
1	C	190	CYS	5.4
1	D	187	HIS	5.4
1	E	9	LEU	5.3
1	D	192	PRO	5.2
1	E	190	CYS	5.1
1	B	14	PHE	5.0
1	D	189	SER	4.9
1	E	6	LEU	4.9
1	D	188	TYR	4.8
1	E	10	LYS	4.7
1	B	-3	ASP	4.7
1	A	17	SER	4.6
1	D	152	PHE	4.4
1	E	191	CYS	4.2
1	B	7	MET	4.1
1	C	187	HIS	4.1

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	8	ARG	4.0
1	B	15	ASN	4.0
1	B	213	PHE	4.0
1	E	1	HIS	4.0
1	B	-5	ASP	4.0
1	E	-5	ASP	3.9
1	D	191	CYS	3.9
1	B	9	LEU	3.9
1	D	195	TYR	3.9
1	E	-4	ASP	3.8
1	E	7	MET	3.8
1	C	188	TYR	3.7
1	C	189	SER	3.5
1	D	186	GLN	3.5
1	D	17	SER	3.4
1	D	26	ASP	3.4
1	E	-2	ASP	3.4
1	E	189	SER	3.4
1	C	15	ASN	3.4
1	B	207	ARG	3.4
1	A	-5	ASP	3.3
1	D	190	CYS	3.3
1	D	20	TYR	3.2
1	E	11	SER	3.2
1	B	6	LEU	3.2
1	C	0	LEU	3.2
1	C	19	MET	3.2
1	C	17	SER	3.2
1	E	75	ILE	3.2
1	D	194	PRO	3.1
1	D	-7	TYR	3.1
1	B	-4	ASP	3.1
1	A	13	LEU	3.1
1	A	-4	ASP	3.0
1	D	185	VAL	3.0
1	E	4	ALA	3.0
1	E	-3	ASP	2.9
1	E	0	LEU	2.9
1	C	191	CYS	2.9
1	C	-3	ASP	2.9
1	C	192	PRO	2.9
1	D	14	PHE	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	136	GLU	2.8
1	E	5	ASN	2.8
1	A	190	CYS	2.8
1	B	0	LEU	2.8
1	B	1	HIS	2.8
1	A	0	LEU	2.7
1	E	187	HIS	2.7
1	C	136	GLU	2.7
1	E	207[A]	ARG	2.7
1	C	-1	LYS	2.7
1	C	16	ARG	2.7
1	A	7	MET	2.7
1	E	67	TRP	2.6
1	E	12	ASP	2.6
1	B	190	CYS	2.6
1	A	207[A]	ARG	2.6
1	C	194	PRO	2.5
1	B	8	ARG	2.5
1	D	74	ASN	2.5
1	E	2	SER	2.4
1	B	208	ARG	2.4
1	C	1	HIS	2.4
1	C	82	ALA	2.4
1	B	12	ASP	2.4
1	C	-4	ASP	2.4
1	D	59	ARG	2.4
1	E	25	LYS	2.3
1	A	21	PRO	2.3
1	E	63	ASN	2.3
1	A	-2	ASP	2.3
1	B	4	ALA	2.3
1	D	193	GLU	2.3
1	B	63	ASN	2.3
1	C	14	PHE	2.3
1	C	195	TYR	2.3
1	C	101	VAL	2.3
1	B	-1	LYS	2.2
1	C	7	MET	2.2
1	D	6	LEU	2.2
1	C	86	TRP	2.2
1	C	162	GLN	2.2
1	A	14	PHE	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	188	TYR	2.2
1	B	-2	ASP	2.1
1	E	74	ASN	2.1
1	B	11	SER	2.1
1	A	-3	ASP	2.1
1	A	55	TYR	2.1
1	D	15	ASN	2.1
1	D	27	ASP	2.1
1	D	196	ILE	2.1
1	D	133	ASP	2.0
1	C	80	THR	2.0
1	C	63	ASN	2.0
1	A	16	ARG	2.0
1	B	152	PHE	2.0
1	E	20	TYR	2.0
1	B	191	CYS	2.0

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

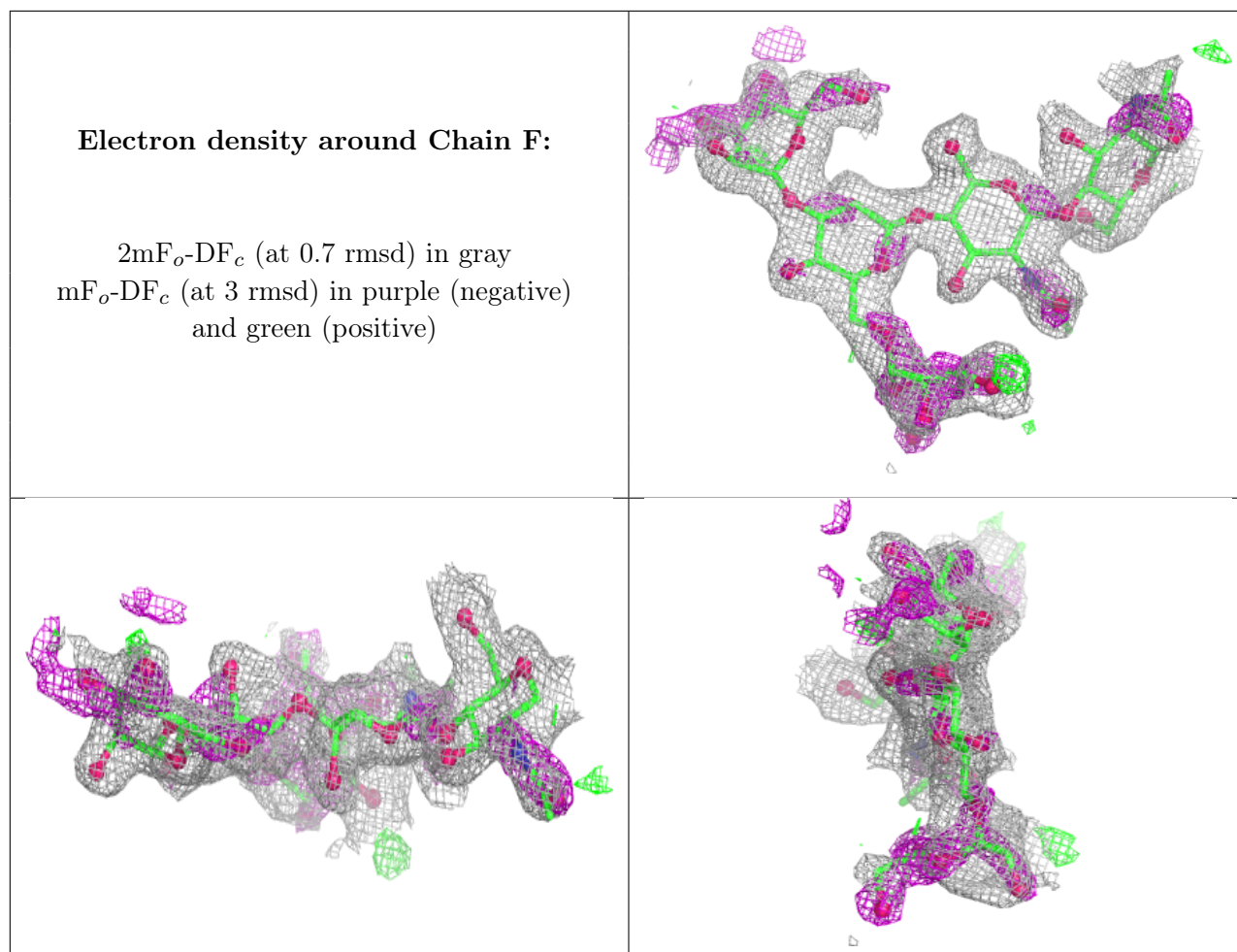
There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MAN	F	5	11/12	0.46	0.20	43,44,44,44	0
2	NAG	F	1	14/15	0.68	0.16	44,47,49,49	0
2	NAG	F	2	14/15	0.73	0.15	44,47,50,50	0
2	MAN	F	4	11/12	0.75	0.15	39,40,42,42	0
2	BMA	F	3	11/12	0.81	0.12	39,40,41,42	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.

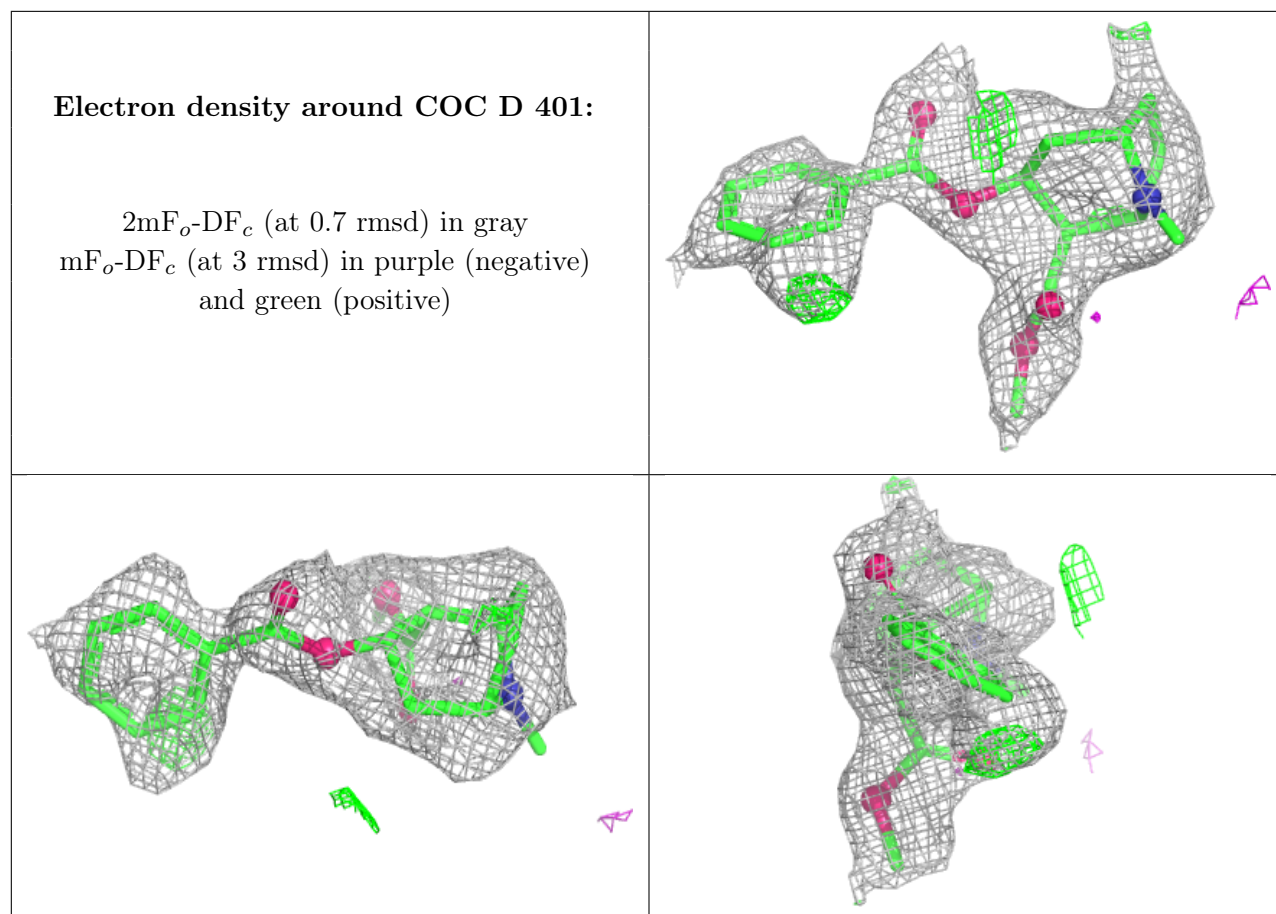


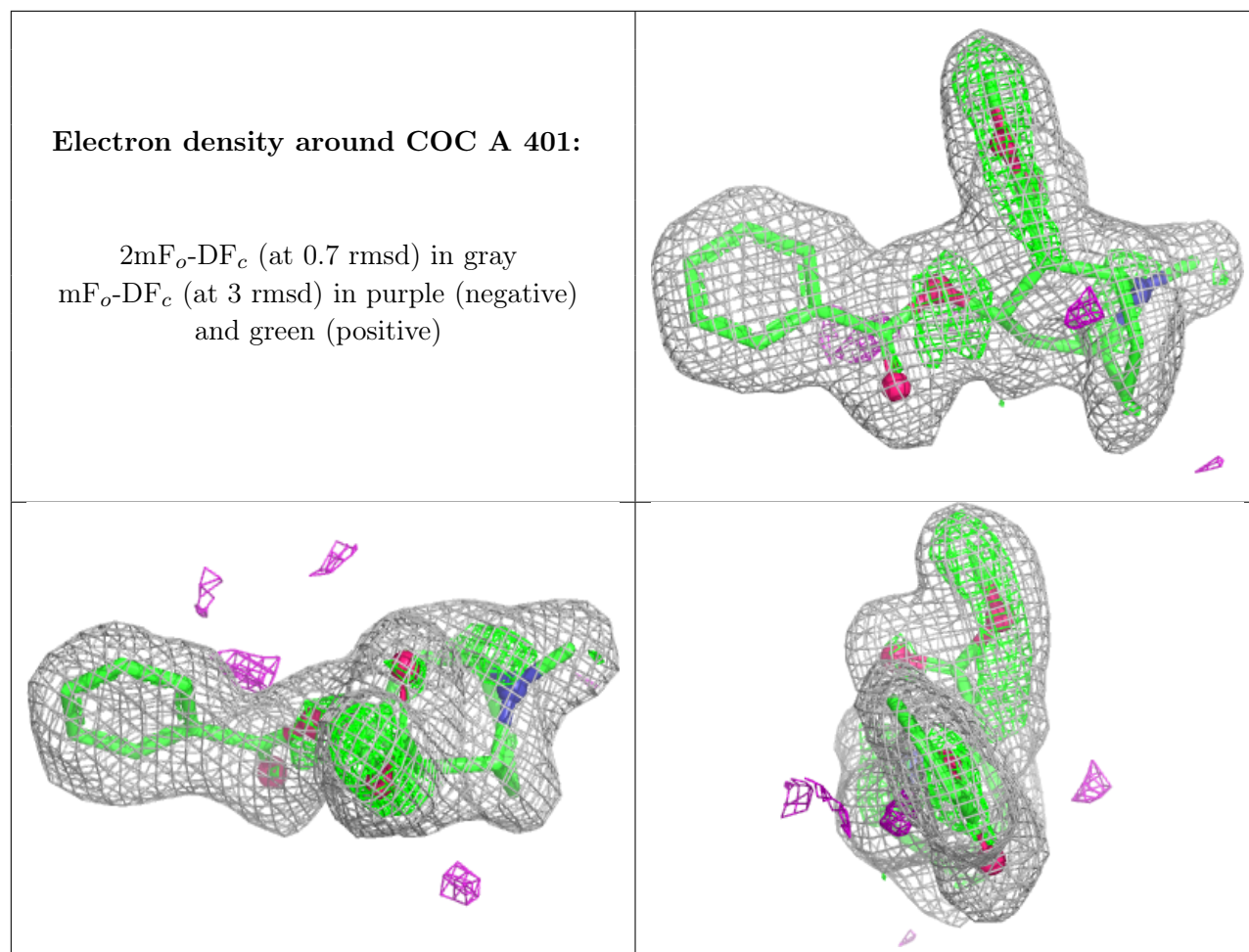
## 6.4 Ligands [i](#)

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
4	NAG	B	402	14/15	0.60	0.17	42,43,44,44	0
3	COC	D	401	22/22	0.76	0.16	32,34,37,38	0
5	PG4	B	403	13/13	0.76	0.54	78,85,88,88	0
5	PG4	E	403	13/13	0.76	0.23	57,58,60,60	0
5	PG4	C	407	10/13	0.79	0.21	44,45,47,47	0
3	COC	A	401	22/22	0.89	0.13	20,22,26,27	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.