



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 4, 2024 – 03:47 am GMT

PDB ID : 9FZ0
Title : Crystal structure of SusG from Bacteroides thetaiotaomicron covalently bound to alpha-1,6 branched pseudo-trisaccharide activity-based probe
Authors : Pickles, I.B.; Moroz, O.; Davies, G.
Deposited on : 2024-07-04
Resolution : 2.65 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

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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

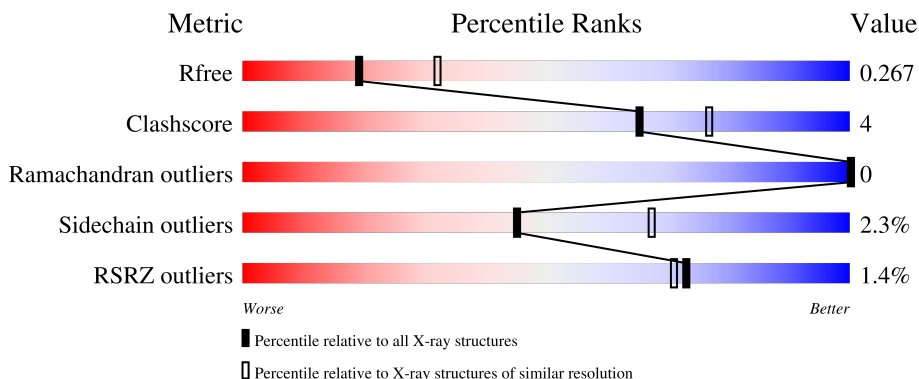
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	164625	1003 (2.66-2.66)
Clashscore	180529	1063 (2.66-2.66)
Ramachandran outliers	177936	1052 (2.66-2.66)
Sidechain outliers	177891	1052 (2.66-2.66)
RSRZ outliers	164620	1003 (2.66-2.66)

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 ≥ 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	690	
1	B	690	
2	C	2	
2	D	2	
2	E	2	

2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 10392 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 Alpha-amylase SusG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	650	5110	3249	825	1020	16	0	0	0
1	B	650	4957	3155	799	987	16	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	MET	-	initiating methionine	UNP Q8A1G3
A	4	GLY	-	expression tag	UNP Q8A1G3
A	5	SER	-	expression tag	UNP Q8A1G3
A	6	SER	-	expression tag	UNP Q8A1G3
A	7	HIS	-	expression tag	UNP Q8A1G3
A	8	HIS	-	expression tag	UNP Q8A1G3
A	9	HIS	-	expression tag	UNP Q8A1G3
A	10	HIS	-	expression tag	UNP Q8A1G3
A	11	HIS	-	expression tag	UNP Q8A1G3
A	12	HIS	-	expression tag	UNP Q8A1G3
A	13	SER	-	expression tag	UNP Q8A1G3
A	14	SER	-	expression tag	UNP Q8A1G3
A	15	GLU	-	expression tag	UNP Q8A1G3
A	16	ASN	-	expression tag	UNP Q8A1G3
A	17	LEU	-	expression tag	UNP Q8A1G3
A	18	TYR	-	expression tag	UNP Q8A1G3
A	19	PHE	-	expression tag	UNP Q8A1G3
A	20	GLN	-	expression tag	UNP Q8A1G3
A	21	GLY	-	expression tag	UNP Q8A1G3
A	22	HIS	-	expression tag	UNP Q8A1G3
A	23	MET	-	expression tag	UNP Q8A1G3
B	3	MET	-	initiating methionine	UNP Q8A1G3
B	4	GLY	-	expression tag	UNP Q8A1G3
B	5	SER	-	expression tag	UNP Q8A1G3
B	6	SER	-	expression tag	UNP Q8A1G3

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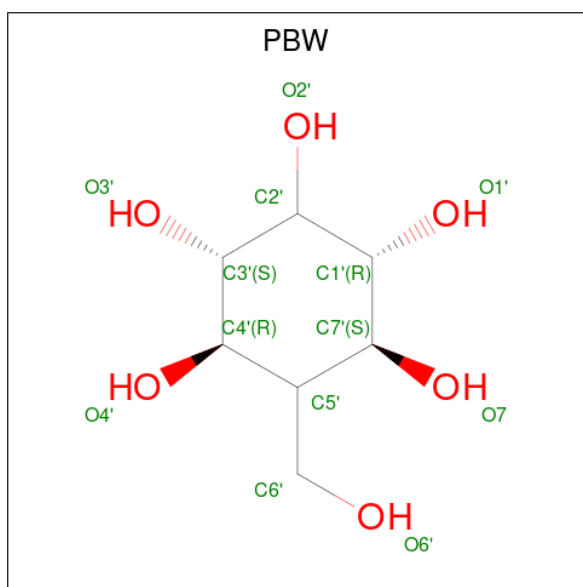
Chain	Residue	Modelled	Actual	Comment	Reference
B	7	HIS	-	expression tag	UNP Q8A1G3
B	8	HIS	-	expression tag	UNP Q8A1G3
B	9	HIS	-	expression tag	UNP Q8A1G3
B	10	HIS	-	expression tag	UNP Q8A1G3
B	11	HIS	-	expression tag	UNP Q8A1G3
B	12	HIS	-	expression tag	UNP Q8A1G3
B	13	SER	-	expression tag	UNP Q8A1G3
B	14	SER	-	expression tag	UNP Q8A1G3
B	15	GLU	-	expression tag	UNP Q8A1G3
B	16	ASN	-	expression tag	UNP Q8A1G3
B	17	LEU	-	expression tag	UNP Q8A1G3
B	18	TYR	-	expression tag	UNP Q8A1G3
B	19	PHE	-	expression tag	UNP Q8A1G3
B	20	GLN	-	expression tag	UNP Q8A1G3
B	21	GLY	-	expression tag	UNP Q8A1G3
B	22	HIS	-	expression tag	UNP Q8A1G3
B	23	MET	-	expression tag	UNP Q8A1G3

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose.



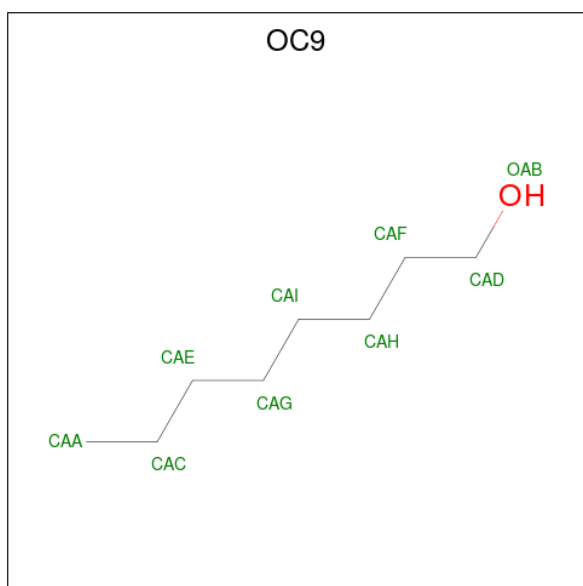
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			22	12	10			
2	D	2	Total	C	O	0	0	0
			22	12	10			
2	E	2	Total	C	O	0	0	0
			22	12	10			

- Molecule 3 is (1 {S},4 {S},5 {R})-6-(hydroxymethyl)cyclohexane-1,2,3,4,5-pentol (three-letter code: PBW) (formula: C₇H₁₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 7 5	0	0
3	B	1	Total C O 12 7 5	0	0

- Molecule 4 is OCTAN-1-OL (three-letter code: OC9) (formula: $C_8H_{18}O$) (labeled as "Ligand of Interest" by depositor).



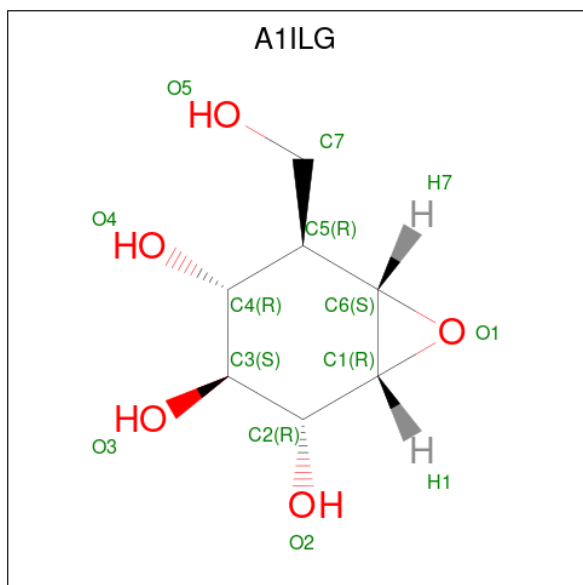
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C 2 2	0	0

- Molecule 5 is (1 {R},2 {R},3 {S},4 {R},5 {R},6 {S})-5-(hydroxymethyl)-7-oxabicyclo[4.1.0]heptane-2,3,4-triol (three-letter code: A1ILG) (formula: C₇H₁₂O₅) (labeled as "Ligand of Interest" by depositor).

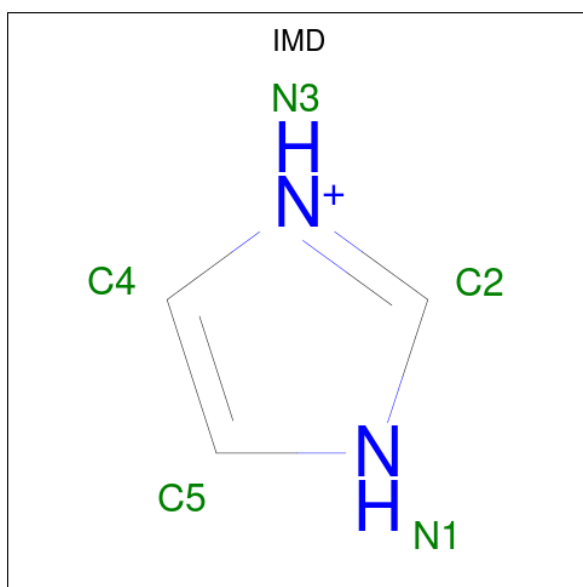


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 12 7 5	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

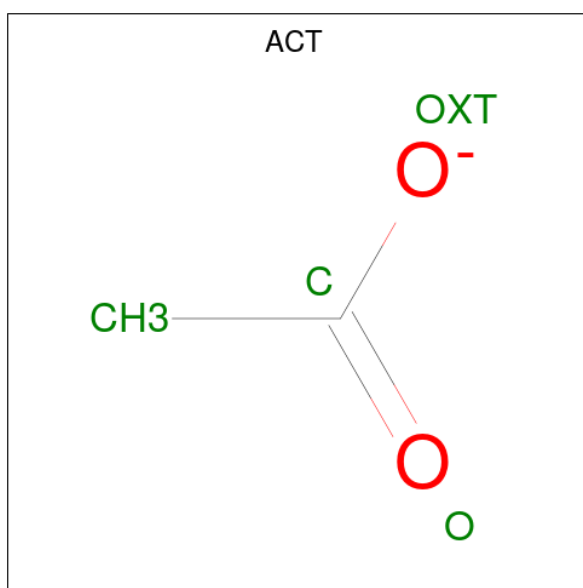
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Ca 2 2	0	0
6	B	2	Total Ca 2 2	0	0

- Molecule 7 is IMIDAZOLE (three-letter code: IMD) (formula: C₃H₅N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	N	0	0
			5	3	2		
7	A	1	Total	C	N	0	0
			5	3	2		

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0


- Molecule 9 is water.

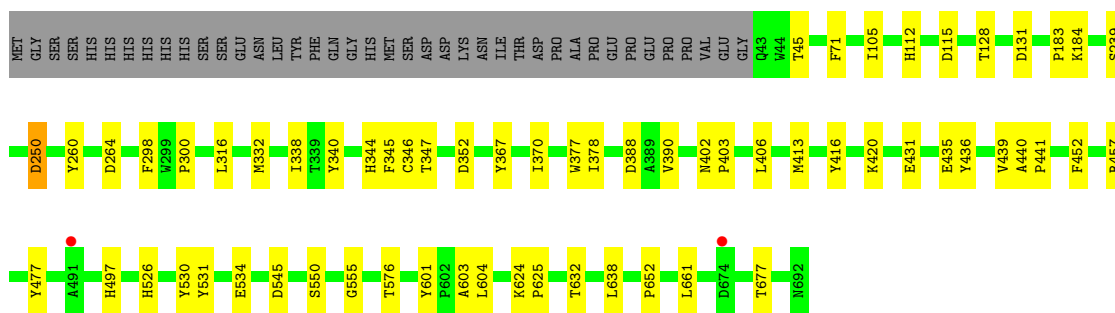
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	120	Total O 120 120	0	0
9	B	65	Total O 65 65	0	0

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.

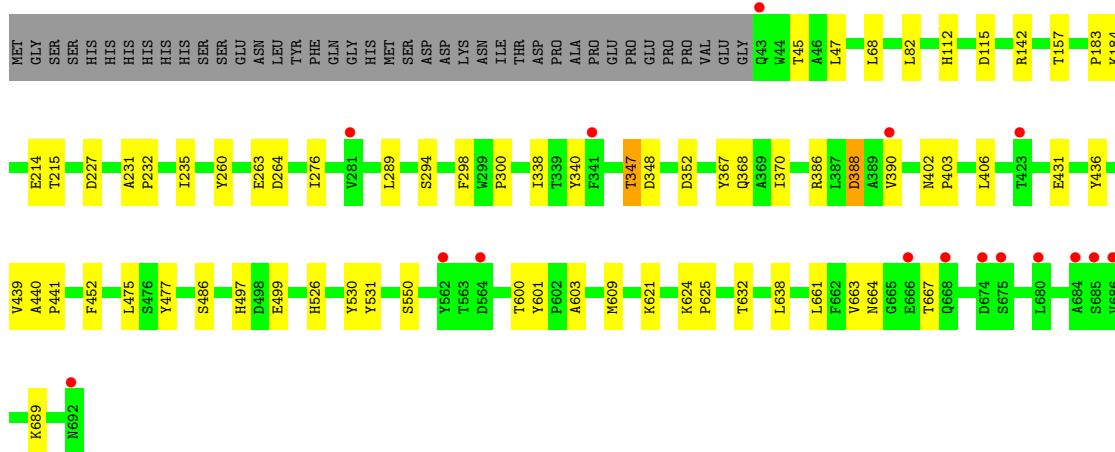
- Molecule 1: Alpha-amylase SusG

Chain A: 



- Molecule 1: Alpha-amylase SusG

Chain B: 



- Molecule 2: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose

Chain C: 



- Molecule 2: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose

Chain D:  100%

GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose

Chain E:  100%

GLC1
GLC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	127.29Å 127.29Å 129.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.65 – 2.65 63.65 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (63.65-2.65) 99.9 (63.65-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.206 , 0.269 0.210 , 0.267	Depositor DCC
R_{free} test set	3010 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	65.1	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k 0.000 for -h,l,k 0.000 for l,-k,h 0.000 for -l,-k,-h 0.020 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10392	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ACT, A1ILG, OC9, GLC, PBW, CA, IMD

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	0.40	0/5249	0.84	5/7151 (0.1%)
1	B	0.38	0/5096	0.81	4/6973 (0.1%)
All	All	0.39	0/10345	0.82	9/14124 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	388	ASP	CB-CG-OD2	-12.80	106.78	118.30
1	A	388	ASP	CB-CG-OD1	10.08	127.38	118.30
1	A	534	GLU	CB-CA-C	-6.70	96.99	110.40
1	A	332	MET	CG-SD-CE	6.15	110.04	100.20
1	B	499	GLU	CG-CD-OE2	-5.80	106.69	118.30
1	B	368	GLN	CB-CA-C	5.57	121.54	110.40
1	B	499	GLU	CG-CD-OE1	5.53	129.35	118.30
1	A	534	GLU	N-CA-CB	5.07	119.73	110.60
1	B	263	GLU	CB-CA-C	5.06	120.52	110.40

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	5110	0	4727	35	0
1	B	4957	0	4423	35	0
2	C	22	0	18	3	0
2	D	22	0	19	0	0
2	E	22	0	18	2	0
3	A	12	0	0	0	0
3	B	12	0	0	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	12	0	0	1	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	A	10	0	10	0	0
8	A	16	0	12	0	0
8	B	4	0	3	0	0
9	A	120	0	0	3	0
9	B	65	0	0	0	0
All	All	10392	0	9230	71	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 4.

All (71) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ALA:N	1:B:232:PRO:HD2	2.13	0.63
1:B:298:PHE:O	1:B:300:PRO:HD3	1.99	0.63
1:A:298:PHE:O	1:A:300:PRO:HD3	2.02	0.60
1:A:390:VAL:HB	1:A:406:LEU:HD11	1.85	0.58
1:B:603:ALA:HB3	1:B:638:LEU:HD22	1.86	0.58
1:B:112:HIS:CD2	2:E:1:GLC:H2	2.40	0.57
1:A:260:TYR:OH	1:A:264:ASP:OD1	2.18	0.56
1:A:603:ALA:HB3	1:A:638:LEU:HD22	1.87	0.56
1:B:663:VAL:HG13	1:B:667:THR:HG21	1.87	0.55
1:A:435:GLU:O	1:A:439:VAL:HG23	2.07	0.54
1:B:475:LEU:CD2	1:B:609:MET:HE2	2.38	0.54
1:B:347:THR:OG1	2:E:2:GLC:H62	2.10	0.51
1:A:112:HIS:CD2	2:C:1:GLC:H2	2.45	0.50
1:A:71:PHE:HB3	9:A:909:HOH:O	2.11	0.50
1:B:390:VAL:HB	1:B:406:LEU:HD11	1.93	0.49
1:A:545:ASP:OD2	2:C:1:GLC:O3	2.16	0.49
1:A:431:GLU:HG3	1:A:452:PHE:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:GLU:HG3	1:A:452:PHE:HZ	1.79	0.47
1:B:68:LEU:HD22	1:B:82:LEU:HD23	1.95	0.47
1:B:367:TYR:HA	1:B:370:ILE:HG22	1.97	0.47
1:B:214:GLU:HG2	1:B:215:THR:N	2.30	0.47
1:A:652:PRO:HA	1:A:677:THR:HG22	1.97	0.47
1:B:227:ASP:OD1	1:B:276:ILE:HD11	2.16	0.46
1:B:436:TYR:CD1	1:B:477:TYR:CE1	3.04	0.46
1:B:601:TYR:OH	1:B:661:LEU:HD22	2.15	0.46
1:B:436:TYR:CG	1:B:477:TYR:CD1	3.04	0.46
1:A:402:ASN:HB2	1:A:403:PRO:HD3	1.98	0.46
1:B:386:ARG:NH1	1:B:388:ASP:HB2	2.30	0.46
1:A:530:TYR:O	1:A:531:TYR:C	2.55	0.46
1:A:239:SER:HA	1:A:316:LEU:HD23	1.98	0.45
1:A:378:ILE:HD12	1:A:413:MET:HE3	1.99	0.45
1:B:600:THR:HG22	1:B:601:TYR:CD1	2.52	0.45
1:A:416:TYR:CZ	1:A:420:LYS:HE3	2.52	0.45
1:B:47:LEU:HD12	1:B:47:LEU:N	2.32	0.45
1:A:345:PHE:O	1:A:346:CYS:HB2	2.16	0.45
1:A:105:ILE:CD1	1:A:377:TRP:CH2	3.00	0.44
1:A:601:TYR:OH	1:A:661:LEU:HD22	2.17	0.44
1:B:402:ASN:HB2	1:B:403:PRO:HD3	2.00	0.44
1:A:457:ARG:HD3	5:A:803:A1ILG:O3	2.17	0.44
1:A:555:GLY:N	1:A:576:THR:OG1	2.50	0.44
1:A:624:LYS:N	1:A:625:PRO:CD	2.81	0.44
1:B:183:PRO:O	1:B:184:LYS:C	2.56	0.44
1:B:436:TYR:HA	1:B:439:VAL:HG12	1.98	0.44
1:B:663:VAL:HG12	1:B:664:ASN:N	2.32	0.44
1:B:530:TYR:O	1:B:531:TYR:C	2.56	0.44
1:B:436:TYR:HA	1:B:439:VAL:CG1	2.48	0.43
1:B:440:ALA:HB3	1:B:441:PRO:HD3	2.00	0.43
1:A:440:ALA:HB3	1:A:441:PRO:HD3	2.00	0.43
1:A:604:LEU:HD13	1:A:638:LEU:HD23	2.00	0.43
1:A:344:HIS:HD2	9:A:921:HOH:O	2.02	0.42
1:B:475:LEU:HD21	1:B:609:MET:HE2	2.01	0.42
1:A:128:THR:HA	9:A:907:HOH:O	2.19	0.42
1:B:260:TYR:OH	1:B:264:ASP:OD1	2.17	0.42
2:C:1:GLC:H61	2:C:2:GLC:H5	2.02	0.42
1:A:531:TYR:O	1:A:531:TYR:CG	2.73	0.42
1:B:338:ILE:HG22	1:B:340:TYR:CE1	2.54	0.42
1:B:388:ASP:OD1	3:B:801:PBW:O7	2.37	0.42
1:B:624:LYS:N	1:B:625:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ASP:OD1	1:A:250:ASP:C	2.59	0.41
1:A:367:TYR:HA	1:A:370:ILE:HG22	2.01	0.41
1:A:338:ILE:HG22	1:A:340:TYR:CE1	2.55	0.41
1:A:105:ILE:HD11	1:A:377:TRP:CH2	2.55	0.41
1:A:183:PRO:O	1:A:184:LYS:C	2.58	0.41
1:A:128:THR:HG23	1:A:131:ASP:H	1.86	0.41
1:B:388:ASP:OD1	3:B:801:PBW:C7'	2.68	0.41
1:B:142:ARG:HH11	1:B:142:ARG:HG3	1.85	0.41
1:B:157:THR:HG21	1:B:348:ASP:O	2.21	0.41
1:B:289:LEU:HD12	1:B:289:LEU:C	2.41	0.41
1:A:436:TYR:CD1	1:A:477:TYR:CE1	3.09	0.41
1:B:431:GLU:HG3	1:B:452:PHE:CZ	2.56	0.40
1:A:436:TYR:CG	1:A:477:TYR:CD1	3.09	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	648/690 (94%)	617 (95%)	31 (5%)	0	100	100
1	B	648/690 (94%)	615 (95%)	33 (5%)	0	100	100
All	All	1296/1380 (94%)	1232 (95%)	64 (5%)	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	532/587 (91%)	523 (98%)	9 (2%)	56	75
1	B	490/587 (84%)	476 (97%)	14 (3%)	37	58
All	All	1022/1174 (87%)	999 (98%)	23 (2%)	45	67

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	THR
1	A	115	ASP
1	A	250	ASP
1	A	347	THR
1	A	352	ASP
1	A	497	HIS
1	A	526	HIS
1	A	550	SER
1	A	632	THR
1	B	45	THR
1	B	115	ASP
1	B	235	ILE
1	B	294	SER
1	B	347	THR
1	B	352	ASP
1	B	388	ASP
1	B	486	SER
1	B	497	HIS
1	B	526	HIS
1	B	550	SER
1	B	621	LYS
1	B	632	THR
1	B	689	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	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](#)

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

5.5 Carbohydrates [i](#)

6 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	GLC	C	1	3,2,4	11,11,12	1.11	1 (9%)	15,15,17	1.41	2 (13%)
2	GLC	C	2	2	11,11,12	0.42	0	15,15,17	0.82	1 (6%)
2	GLC	D	1	2,5	11,11,12	0.58	0	15,15,17	1.20	2 (13%)
2	GLC	D	2	2	11,11,12	0.45	0	15,15,17	1.14	2 (13%)
2	GLC	E	1	3,2,4	11,11,12	0.70	0	15,15,17	1.07	2 (13%)
2	GLC	E	2	2	11,11,12	0.91	1 (9%)	15,15,17	1.36	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	GLC	C	1	3,2,4	-	0/2/19/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	D	1	2,5	-	0/2/19/22	0/1/1/1
2	GLC	D	2	2	-	2/2/19/22	0/1/1/1
2	GLC	E	1	3,2,4	-	0/2/19/22	0/1/1/1
2	GLC	E	2	2	-	1/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	GLC	C2-C3	-2.77	1.48	1.52
2	C	1	GLC	O5-C5	2.18	1.47	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	GLC	C1-C2-C3	-3.05	105.91	109.67
2	C	1	GLC	O5-C1-C2	-3.05	106.06	110.77
2	E	2	GLC	C3-C4-C5	2.81	115.26	110.24
2	C	2	GLC	C1-C2-C3	2.79	113.09	109.67
2	D	1	GLC	C1-O5-C5	2.58	115.68	112.19
2	E	1	GLC	O5-C1-C2	-2.50	106.92	110.77
2	D	2	GLC	C1-O5-C5	2.43	115.48	112.19
2	D	1	GLC	O2-C2-C3	2.28	114.70	110.14
2	D	2	GLC	C1-C2-C3	2.25	112.43	109.67
2	E	1	GLC	O2-C2-C1	2.14	113.53	109.15
2	E	2	GLC	C1-O5-C5	2.03	114.94	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

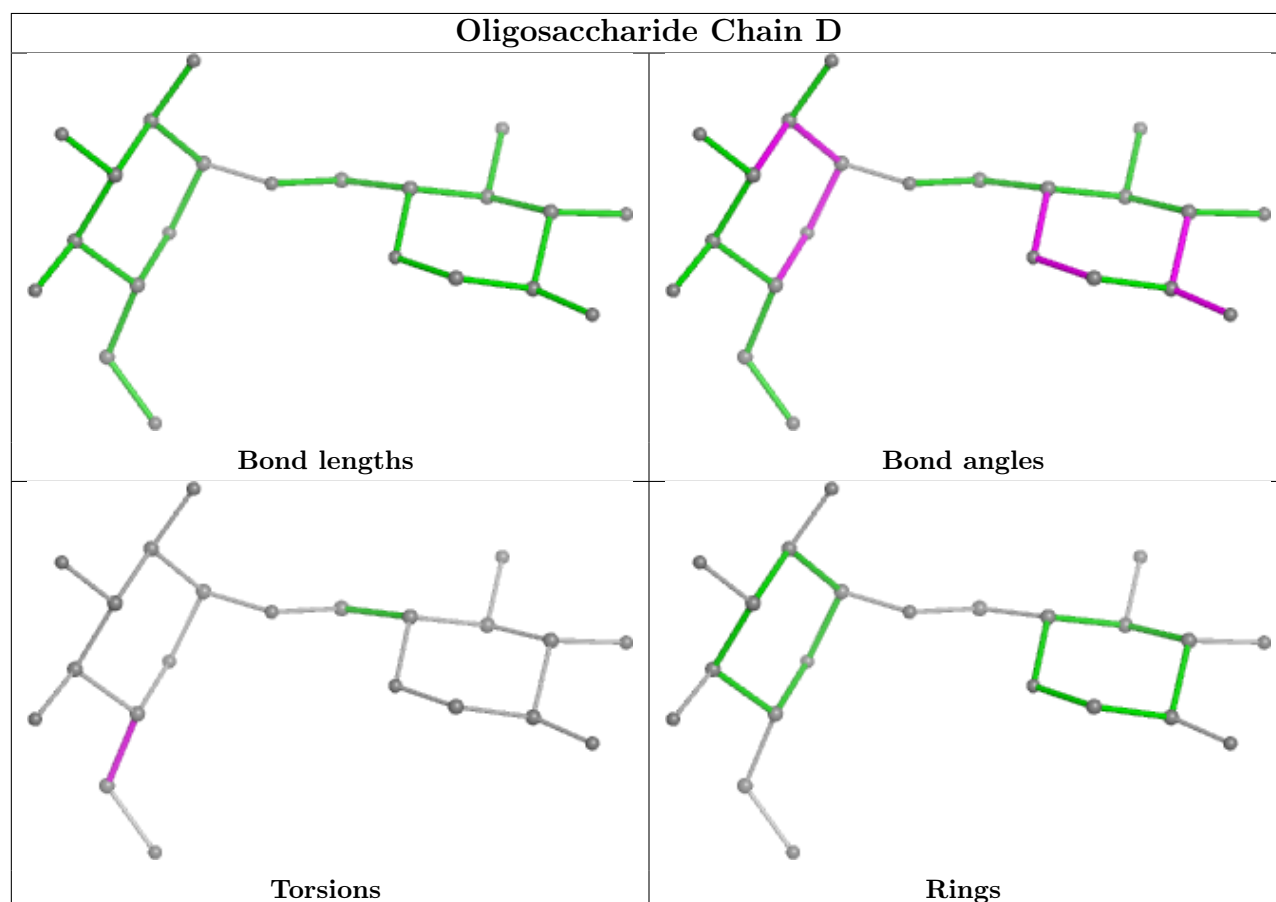
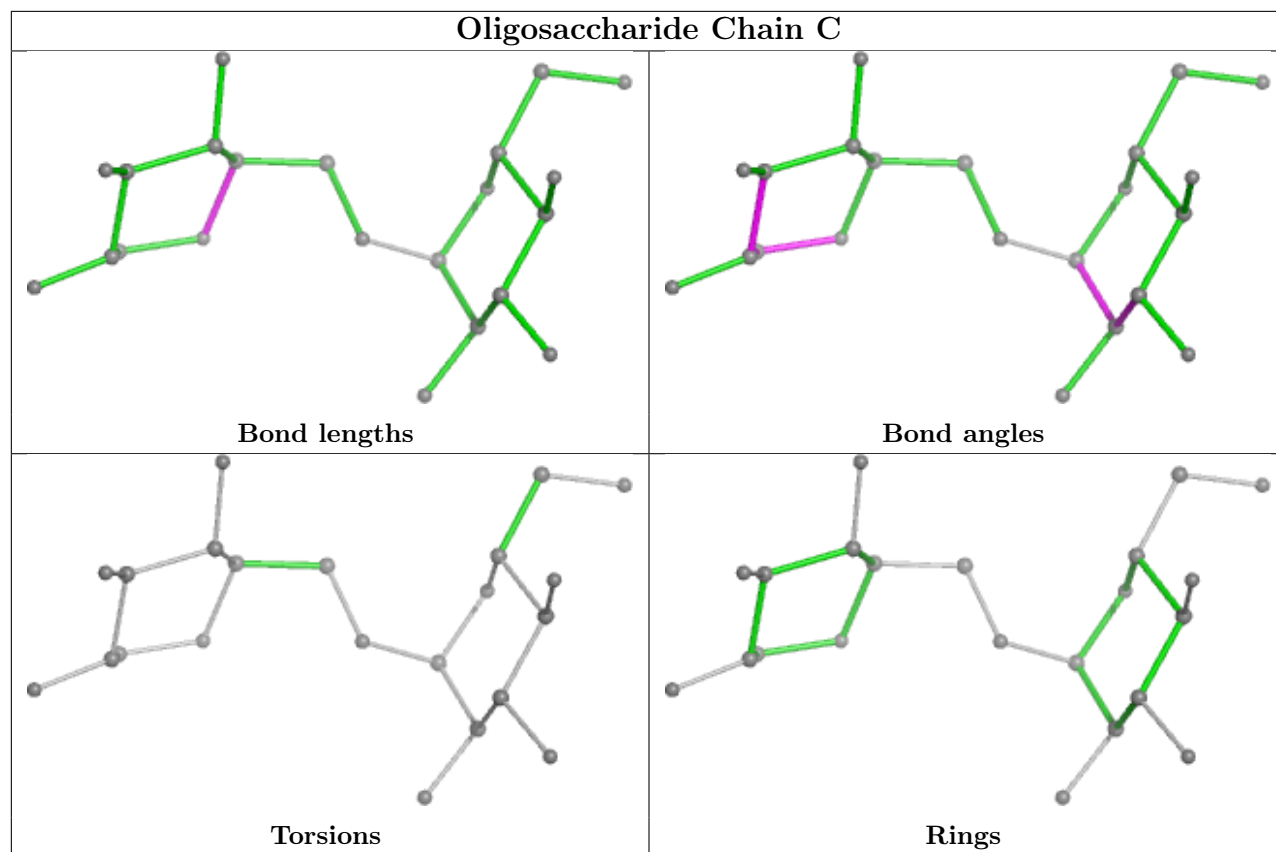
Mol	Chain	Res	Type	Atoms
2	D	2	GLC	C4-C5-C6-O6
2	D	2	GLC	O5-C5-C6-O6
2	E	2	GLC	O5-C5-C6-O6

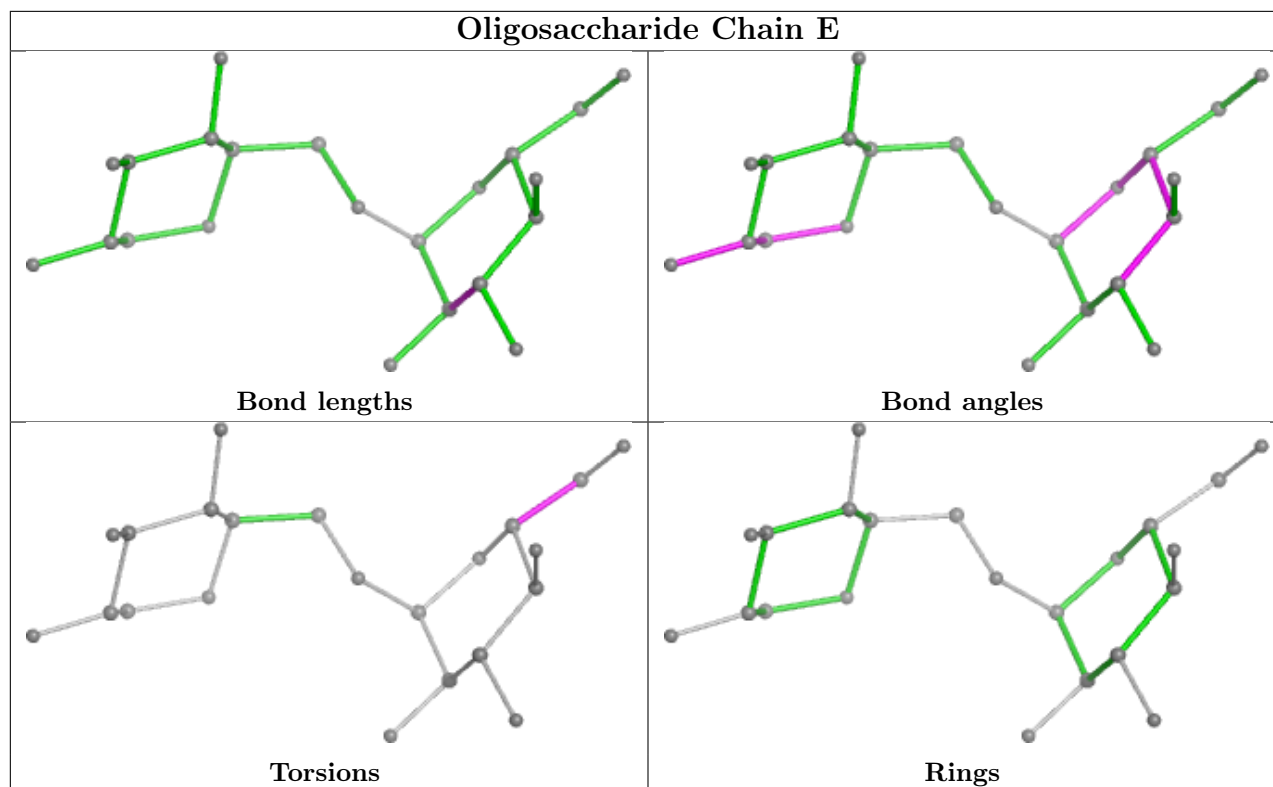
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	GLC	3	0
2	E	1	GLC	1	0
2	C	2	GLC	1	0
2	E	2	GLC	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 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	ACT	B	805	-	3,3,3	1.23	0	3,3,3	0.72	0
7	IMD	A	807	-	3,5,5	0.20	0	4,5,5	0.62	0
3	PBW	B	801	1,2	12,12,13	0.41	0	14,17,19	1.01	1 (7%)
8	ACT	A	811	-	3,3,3	1.49	1 (33%)	3,3,3	0.63	0
8	ACT	A	809	-	3,3,3	1.32	0	3,3,3	0.42	0
7	IMD	A	806	-	3,5,5	0.25	0	4,5,5	0.70	0
4	OC9	A	802	2	1,1,8	1.13	0	-		
8	ACT	A	810	-	3,3,3	1.30	0	3,3,3	0.60	0
3	PBW	A	801	1,2	12,12,13	0.58	0	14,17,19	0.62	0
5	A1ILG	A	803	2	13,13,13	0.35	0	16,20,20	1.09	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	ACT	A	808	-	3,3,3	1.17	0	3,3,3	0.88	0
4	OC9	B	802	2	1,1,8	1.08	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
7	IMD	A	807	-	-	-	0/1/1/1
3	PBW	B	801	1,2	-	0/2/22/26	0/1/1/1
7	IMD	A	806	-	-	-	0/1/1/1
3	PBW	A	801	1,2	-	0/2/22/26	0/1/1/1
5	A1ILG	A	803	2	-	0/2/27/27	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	811	ACT	CH3-C	2.17	1.58	1.49

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	803	A1ILG	C3-C2-C1	2.32	114.98	109.68
3	B	801	PBW	O7-C7'-C5'	-2.07	103.83	110.14
5	A	803	A1ILG	O4-C4-C5	-2.03	105.84	110.05
5	A	803	A1ILG	O3-C3-C2	-2.02	105.67	110.35

There are no chirality outliers.

There are no torsion outliers.

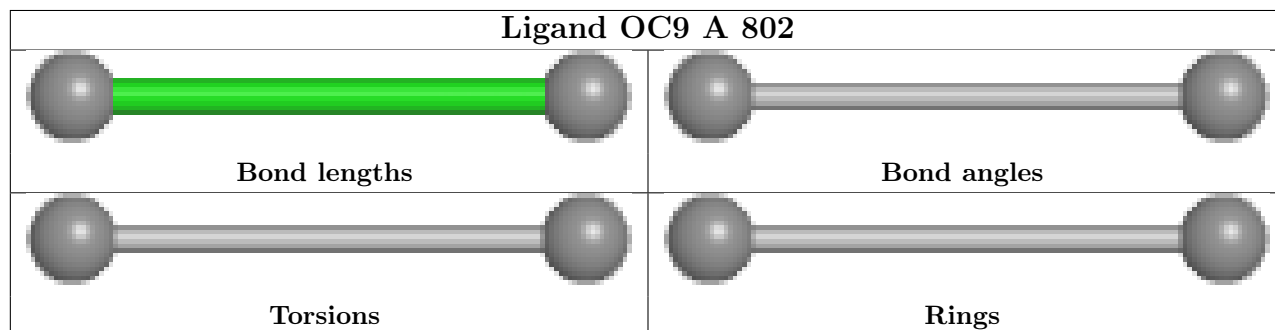
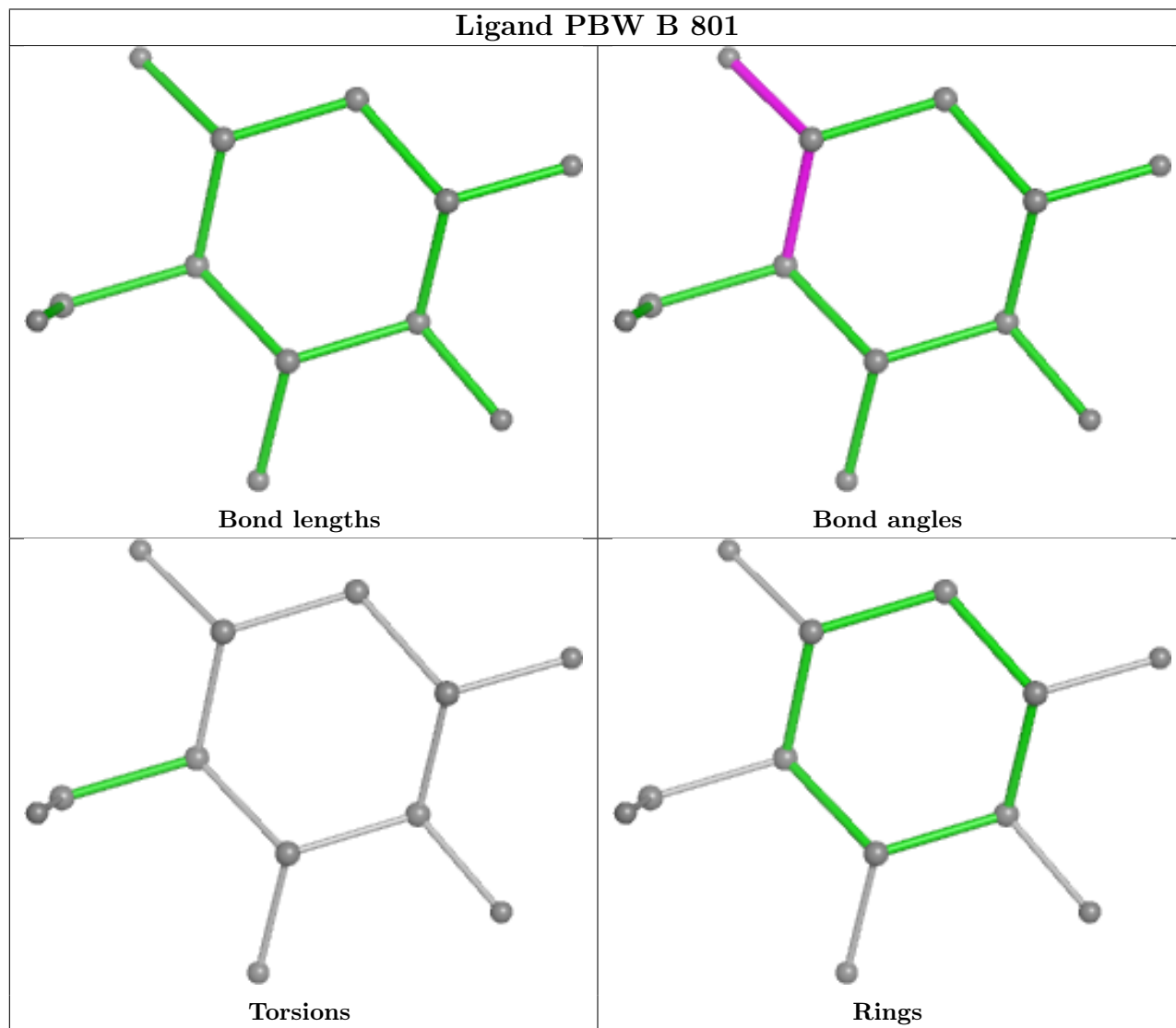
There are no ring outliers.

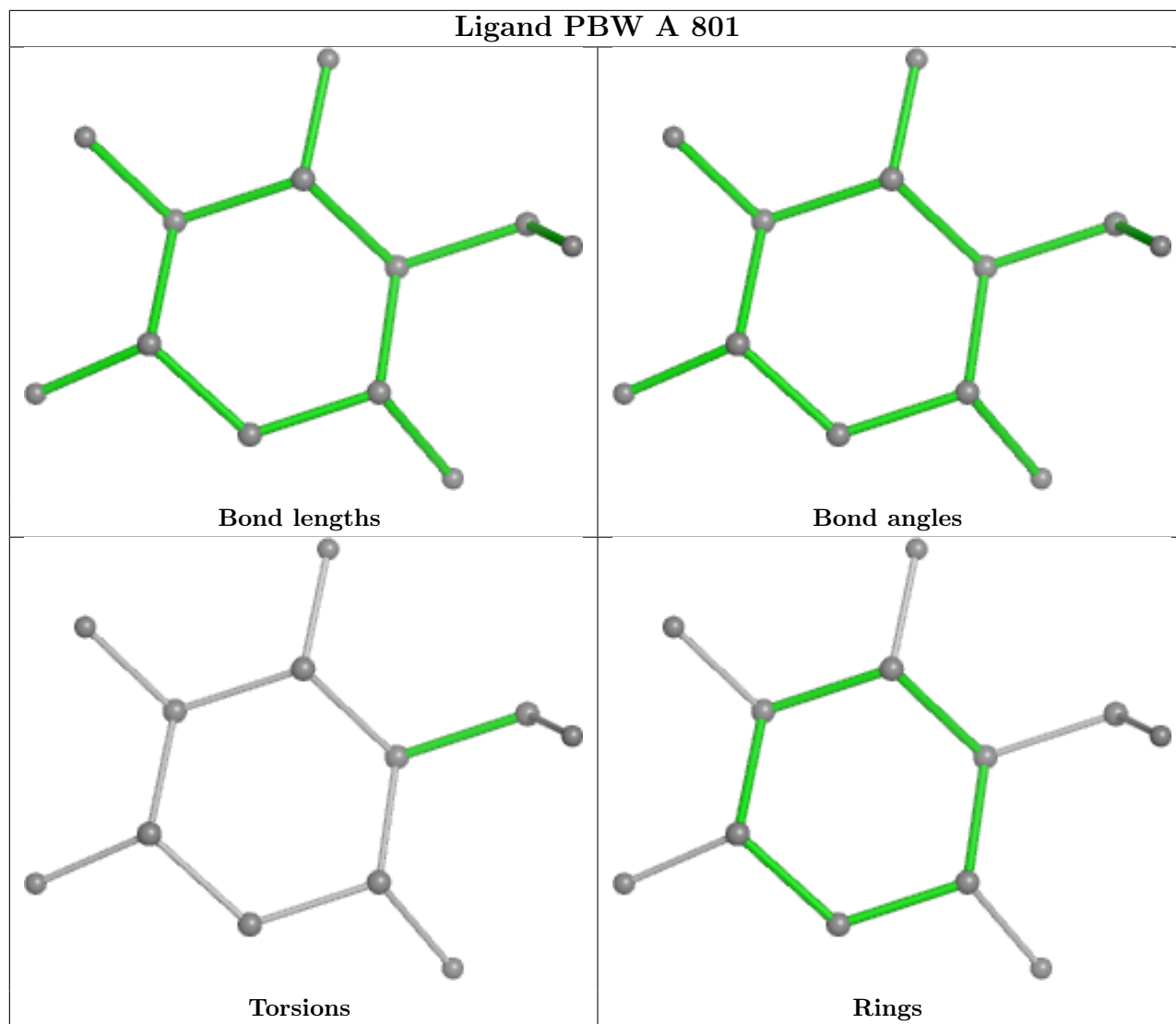
2 monomers are involved in 3 short contacts:

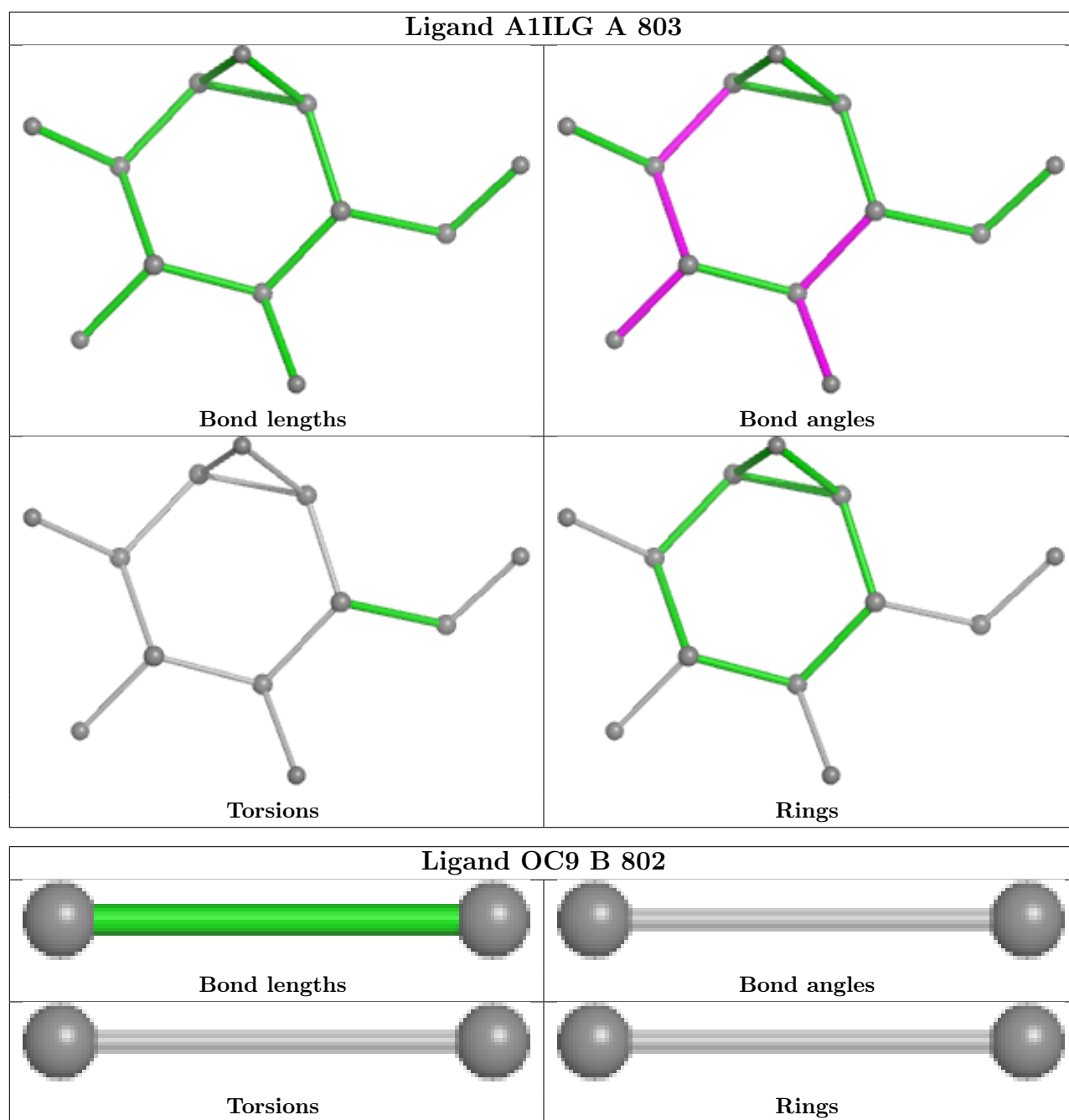
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	801	PBW	2	0
5	A	803	A1ILG	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	650/690 (94%)	-0.35	2 (0%) 90 90	40, 64, 90, 140	0
1	B	650/690 (94%)	0.22	16 (2%) 58 56	47, 84, 122, 143	0
All	All	1300/1380 (94%)	-0.06	18 (1%) 73 71	40, 73, 117, 143	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	692	ASN	3.5
1	B	680	LEU	3.4
1	B	674	ASP	3.1
1	B	43	GLN	2.9
1	A	491	ALA	2.9
1	A	674	ASP	2.6
1	B	685	SER	2.6
1	B	668	GLN	2.5
1	B	562	TYR	2.5
1	B	341	PHE	2.4
1	B	684	ALA	2.4
1	B	564	ASP	2.3
1	B	390	VAL	2.3
1	B	423	THR	2.2
1	B	281	VAL	2.1
1	B	686	VAL	2.1
1	B	666	GLU	2.0
1	B	675	SER	2.0

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

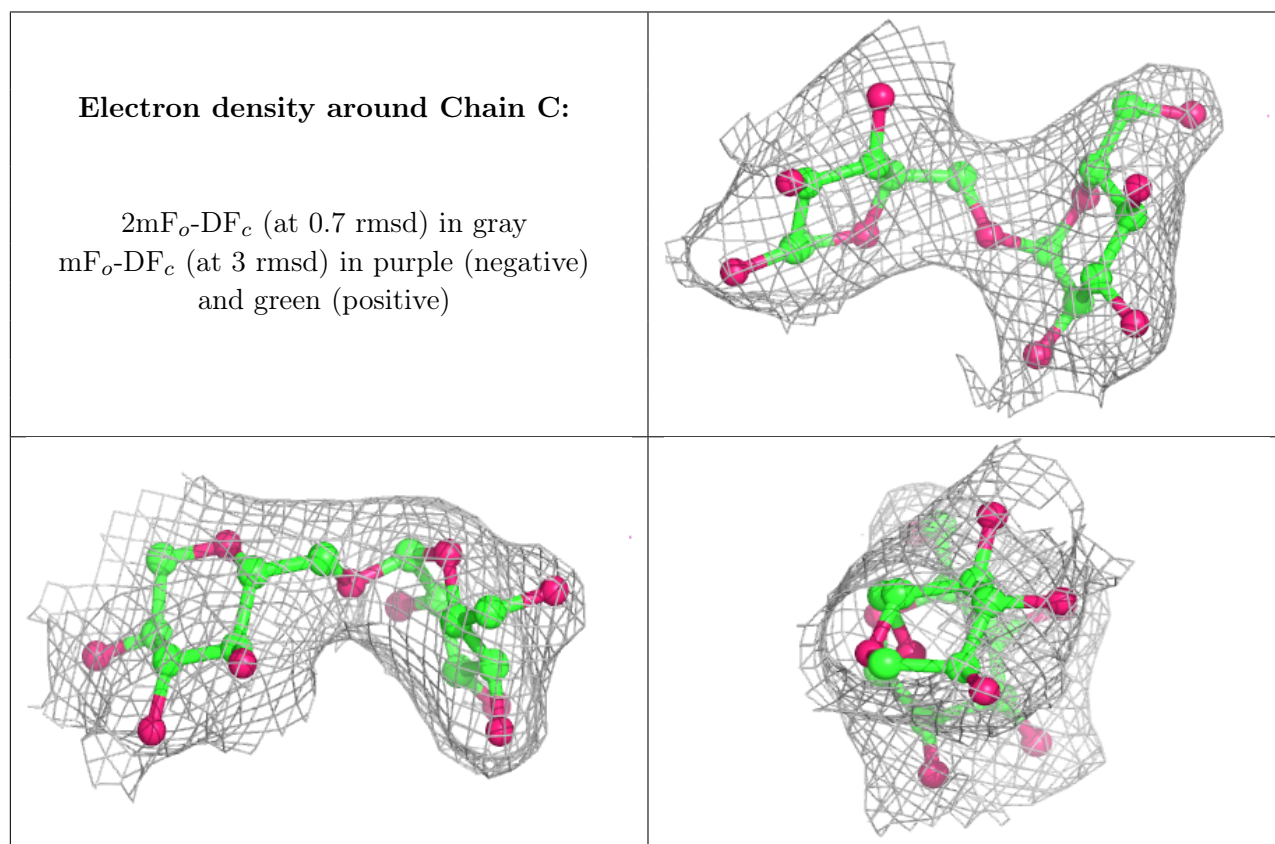
There are no non-standard protein/DNA/RNA residues in this entry.

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, 95th 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.

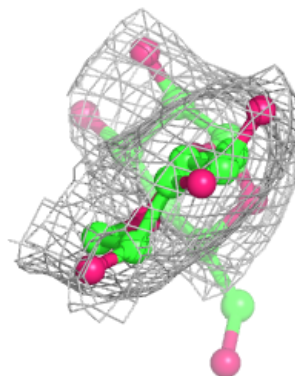
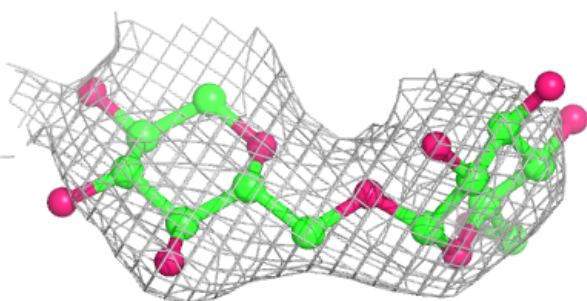
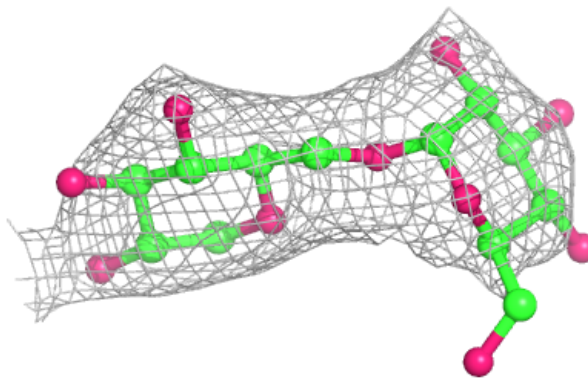
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	D	2	11/12	0.86	0.10	122,136,145,145	0
2	GLC	D	1	11/12	0.93	0.09	88,105,115,120	0
2	GLC	E	1	11/12	0.93	0.08	57,62,71,75	0
2	GLC	E	2	11/12	0.93	0.07	55,67,80,83	0
2	GLC	C	1	11/12	0.96	0.06	49,55,65,66	0
2	GLC	C	2	11/12	0.96	0.07	53,59,63,72	0

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

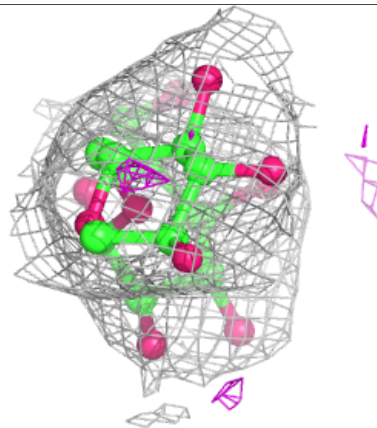
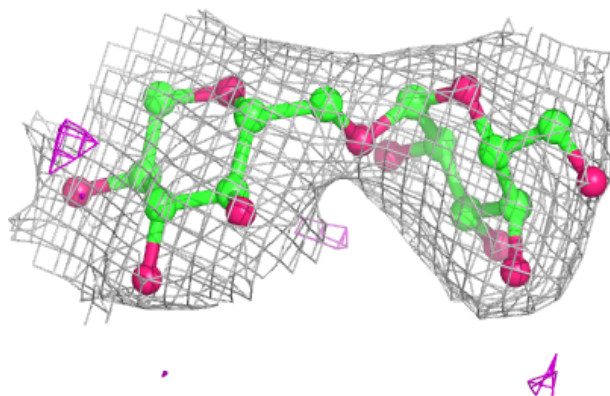
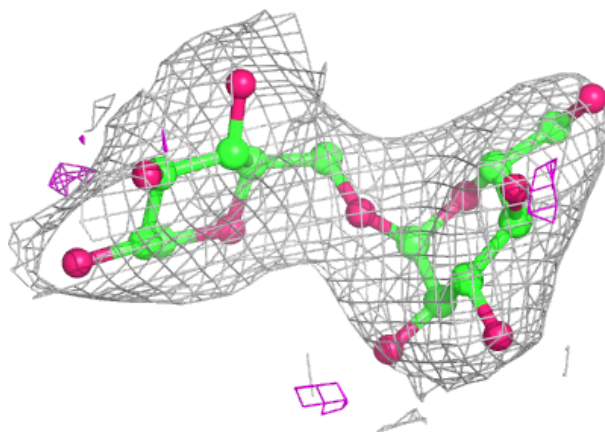


Electron density around Chain D:

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

**Electron density around Chain 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](#)

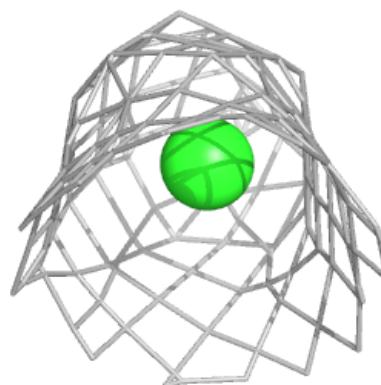
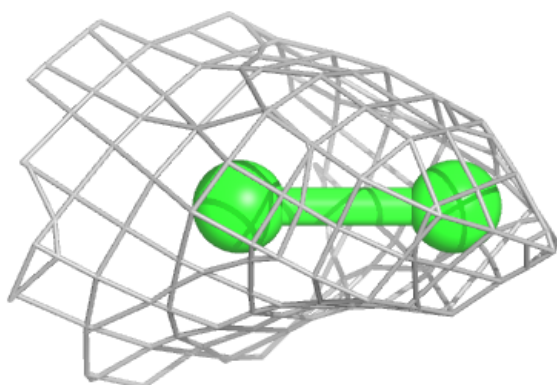
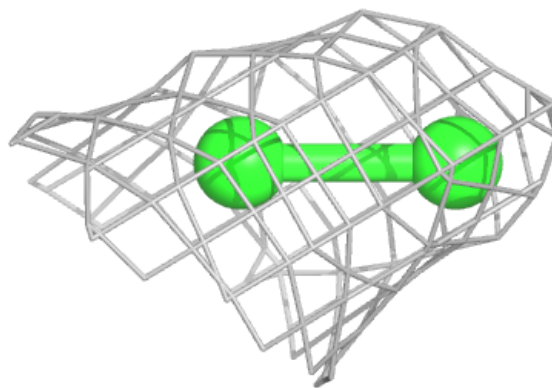
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	ACT	B	805	4/4	0.67	0.17	84,86,87,99	0
8	ACT	A	811	4/4	0.70	0.23	73,75,75,92	0
8	ACT	A	809	4/4	0.75	0.18	79,86,97,101	0
8	ACT	A	808	4/4	0.84	0.15	80,85,91,102	0
4	OC9	B	802	2/9	0.86	0.21	59,59,59,73	0
4	OC9	A	802	2/9	0.89	0.17	53,53,53,57	0
7	IMD	A	806	5/5	0.89	0.16	94,99,102,111	0
5	A1ILG	A	803	12/12	0.90	0.08	77,95,103,104	0
8	ACT	A	810	4/4	0.90	0.17	63,68,79,85	0
7	IMD	A	807	5/5	0.91	0.14	107,108,114,115	0
6	CA	B	804	1/1	0.95	0.05	124,124,124,124	0
3	PBW	B	801	12/13	0.95	0.07	57,66,73,78	0
3	PBW	A	801	12/13	0.97	0.05	49,56,61,63	0
6	CA	B	803	1/1	0.98	0.04	79,79,79,79	0
6	CA	A	805	1/1	0.99	0.03	69,69,69,69	0
6	CA	A	804	1/1	1.00	0.02	49,49,49,49	0

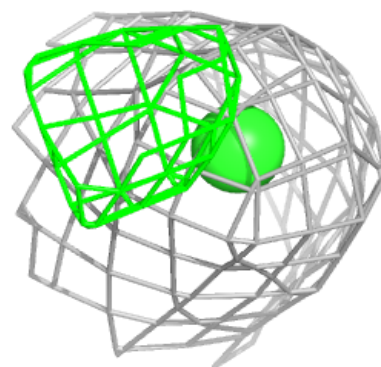
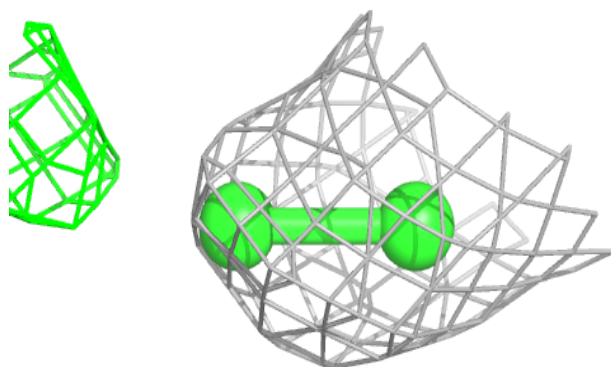
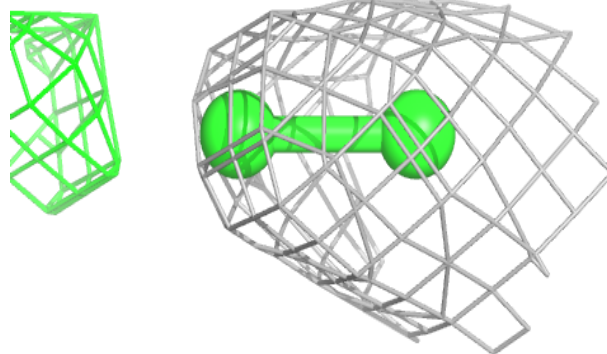
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OC9 B 802:

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

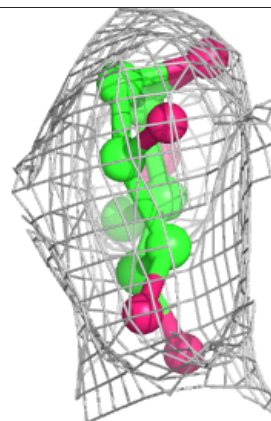
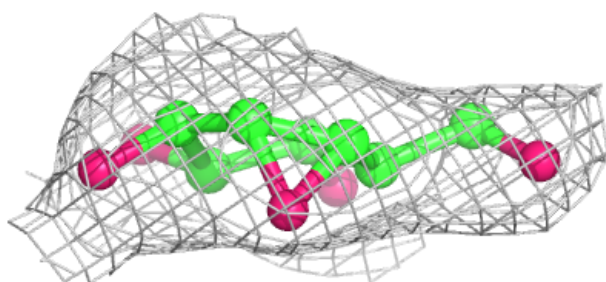
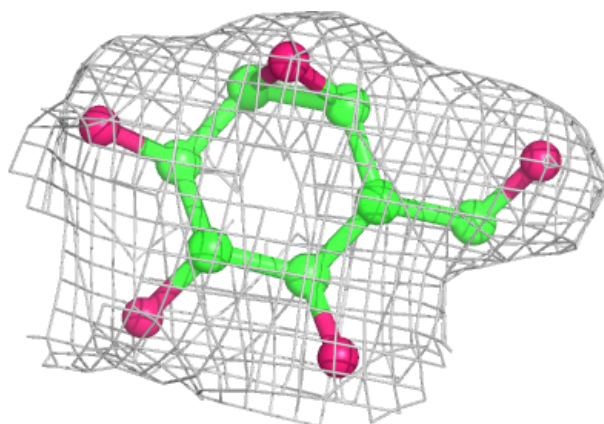
**Electron density around OC9 A 802:**

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



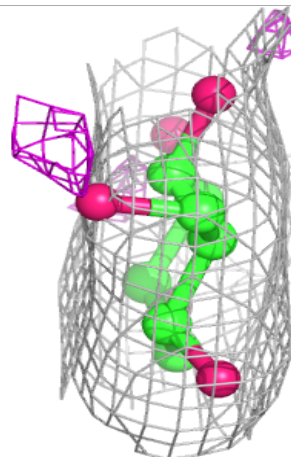
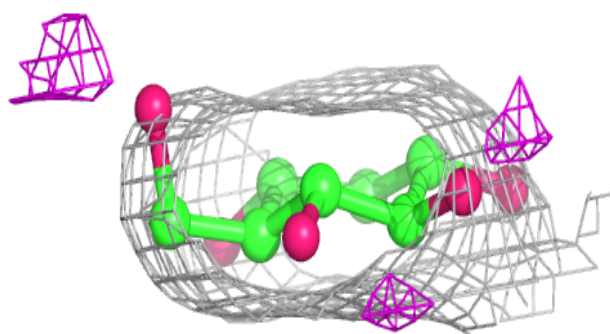
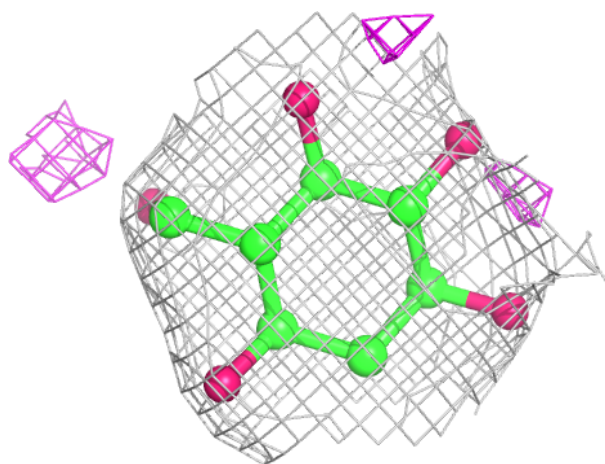
Electron density around A1ILG A 803:

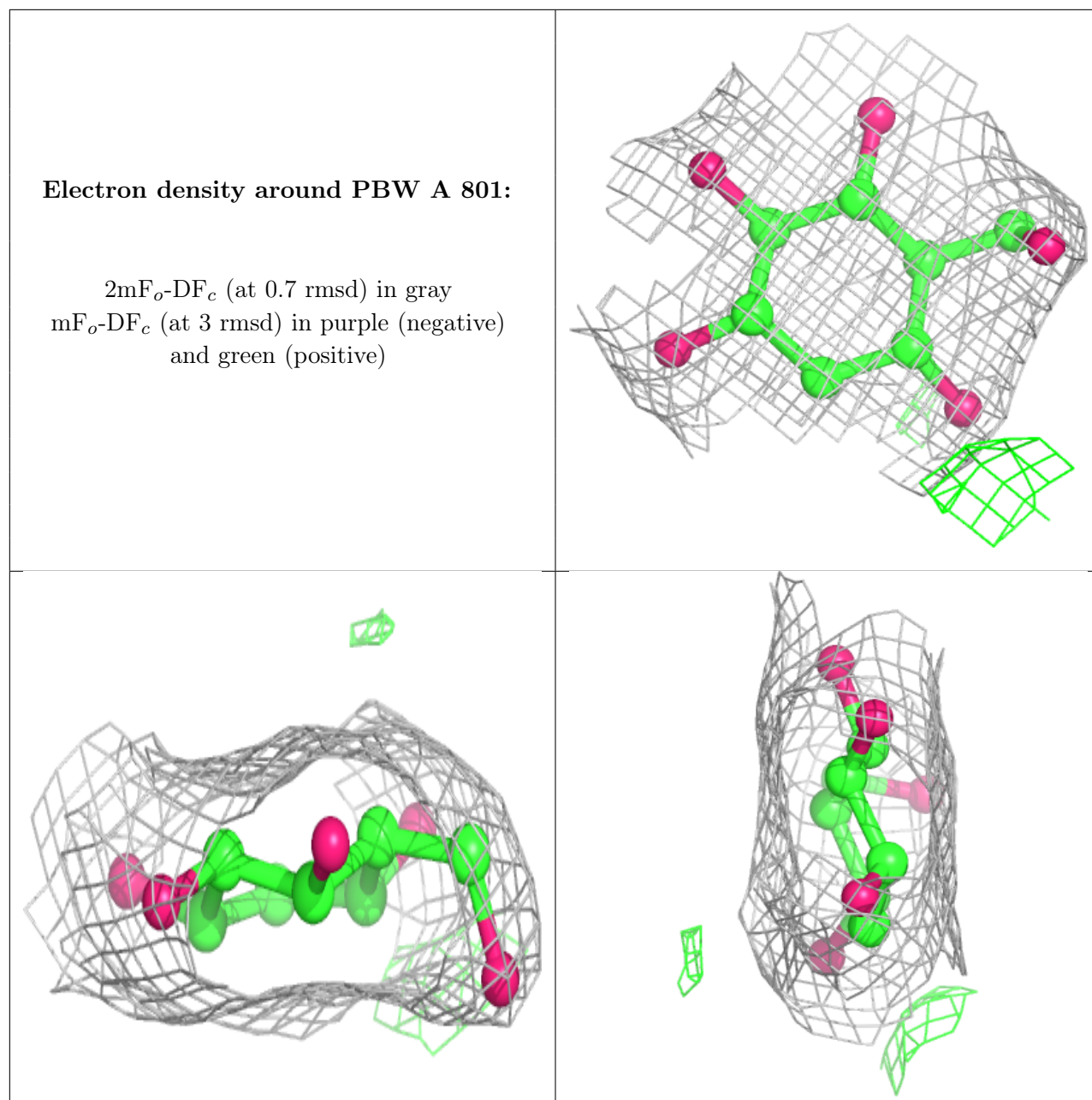
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PBW B 801:

$2mF_o-DF_c$ (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.