



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:30 AM UTC

PDB ID : 8BXL / pdb_00008bxl
Title : Patulin Synthase from *Penicillium expansum*
Authors : Tjallinks, G.; Boverio, A.; Rozeboom, H.J.; Fraaije, M.W.
Deposited on : 2022-12-09
Resolution : 2.40 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (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

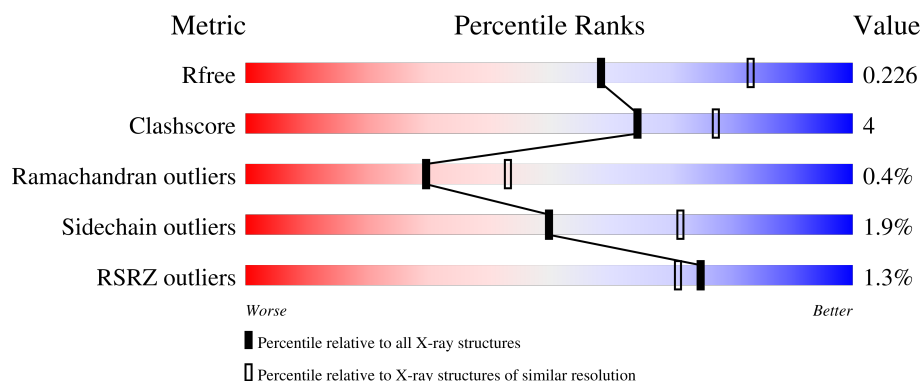
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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.



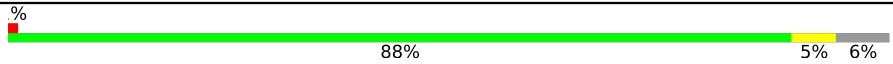
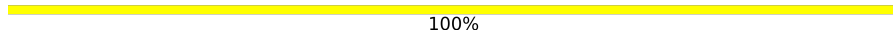
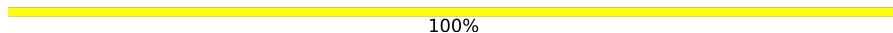
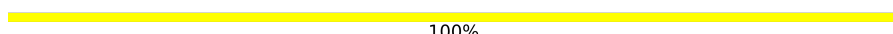
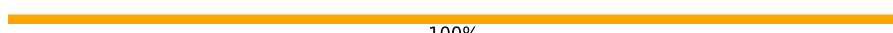
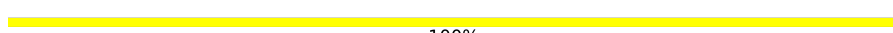
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	628	
1	B	628	
1	C	628	
1	D	628	
1	E	628	

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Mol	Chain	Length	Quality of chain
1	F	628	 88% 5% 6%
2	G	3	 100%
2	H	3	 100%
2	I	3	 100%
2	J	3	 100%
2	K	3	 100%
3	L	2	 100%

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
6	PEG	F	610	-	-	X	-
7	GOL	E	607	-	-	X	-

2 Entry composition [i](#)

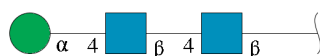
There are 8 unique types of molecules in this entry. The entry contains 29074 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Patulin synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	590	Total	C	N	O	S	0	0	0
			4526	2865	785	862	14			
1	C	590	Total	C	N	O	S	0	0	0
			4490	2846	778	852	14			
1	D	590	Total	C	N	O	S	0	0	0
			4446	2822	764	846	14			
1	A	590	Total	C	N	O	S	0	0	0
			4530	2867	785	864	14			
1	F	590	Total	C	N	O	S	0	0	0
			4506	2852	781	859	14			
1	E	590	Total	C	N	O	S	0	0	0
			4530	2867	785	864	14			

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



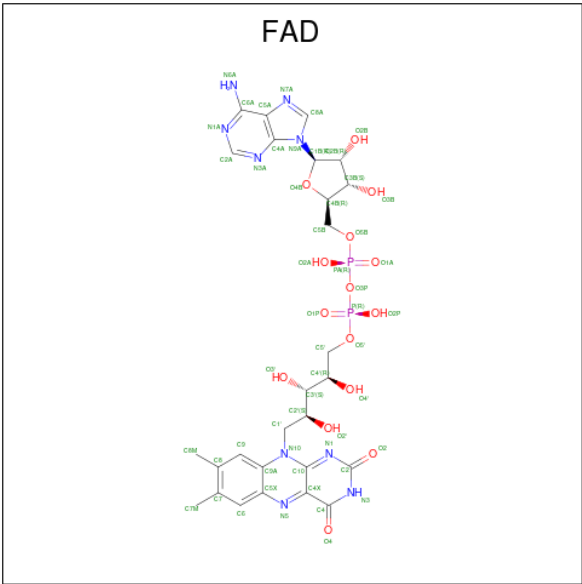
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	K	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



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

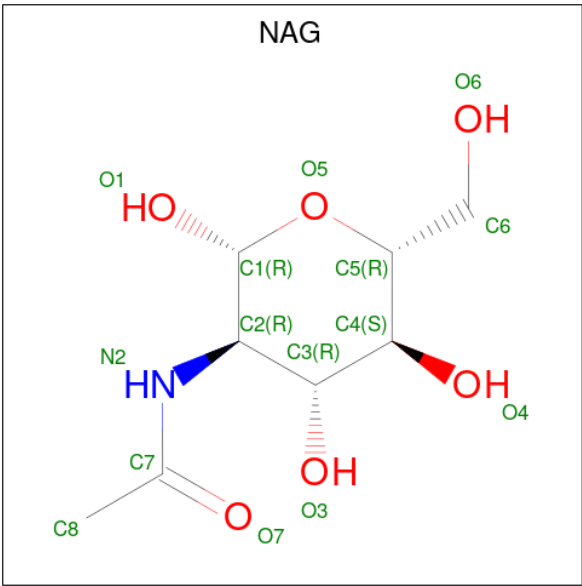
- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

C₈H₁₅NO₆).



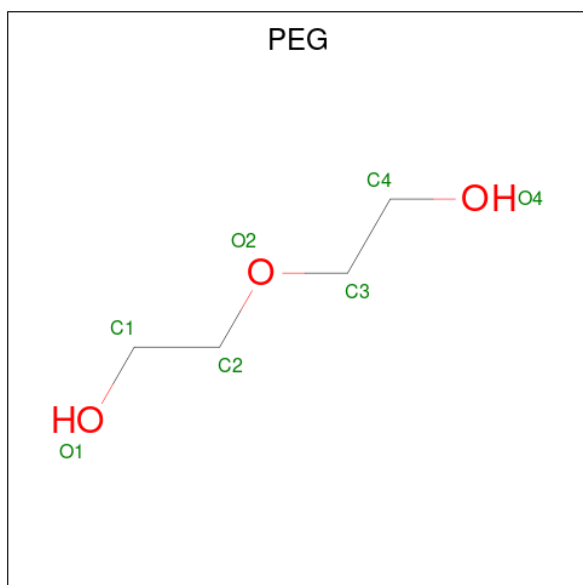
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1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

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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	C	1	Total C O 7 4 3	0	0
6	C	1	Total C O 7 4 3	0	0
6	D	1	Total C O 7 4 3	0	0
6	D	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	F	1	Total C O 7 4 3	0	0
6	F	1	Total C O 7 4 3	0	0
6	F	1	Total C O 7 4 3	0	0
6	F	1	Total C O 7 4 3	0	0
6	F	1	Total C O 7 4 3	0	0
6	F	1	Total C O 7 4 3	0	0
6	E	1	Total C O 7 4 3	0	0
6	E	1	Total C O 7 4 3	0	0
6	E	1	Total C O 7 4 3	0	0
6	E	1	Total C O 7 4 3	0	0

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	F	1	Total	C	O	0	0
			6	3	3		
7	F	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	199	Total	O	0	1
			200	200		
8	C	170	Total	O	0	0
			170	170		
8	D	63	Total	O	0	0
			63	63		
8	A	154	Total	O	0	4
			158	158		
8	F	187	Total	O	0	0
			187	187		

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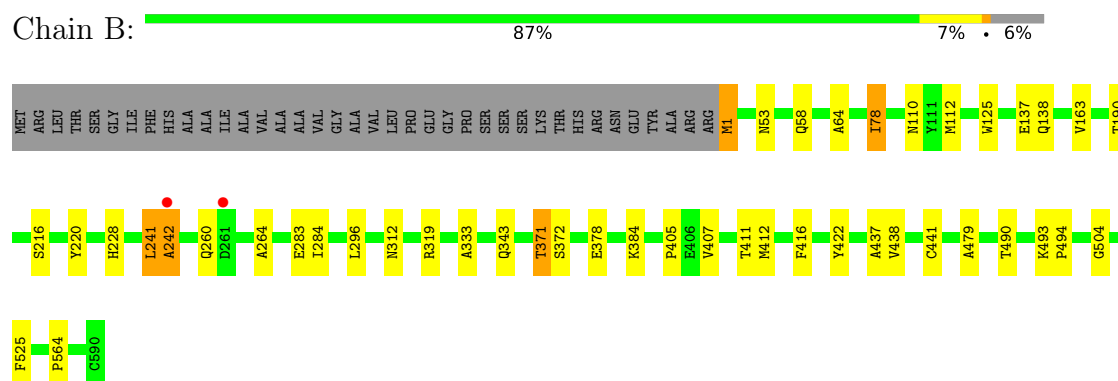
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	206	Total 209	O 209	0	3

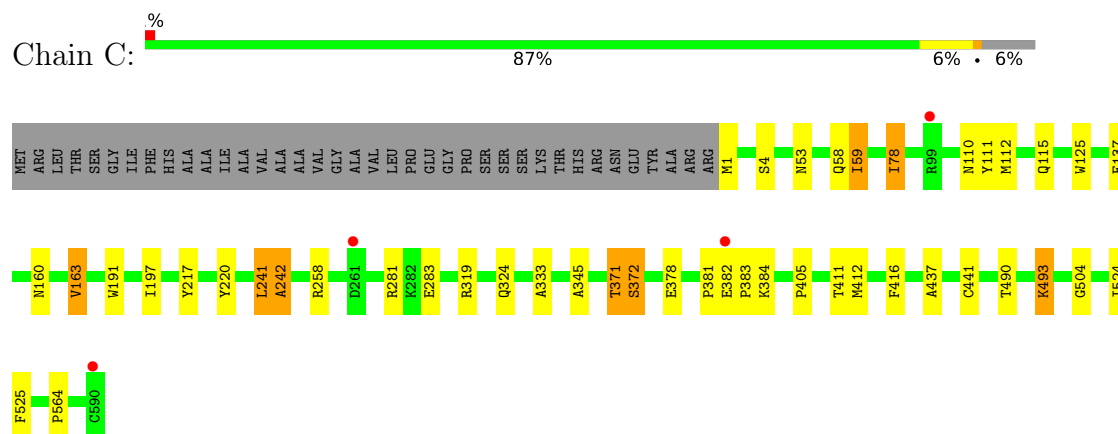
3 Residue-property plots [i](#)

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.

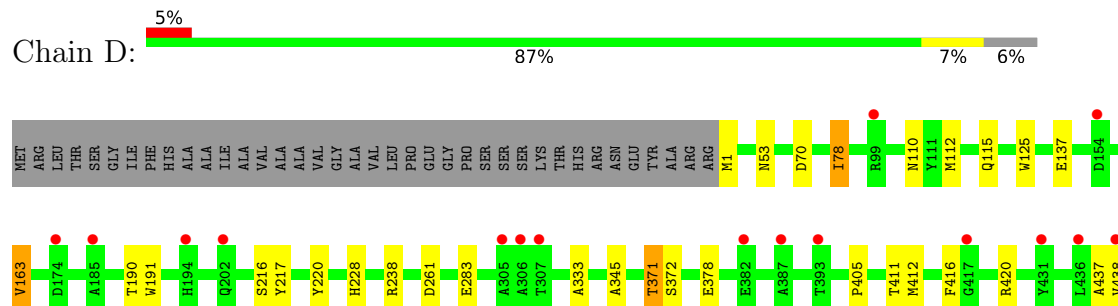
- Molecule 1: Patulin synthase

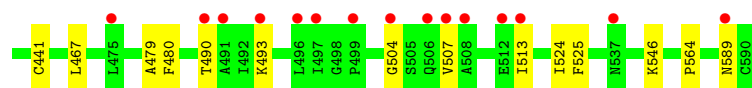


- Molecule 1: Patulin synthase



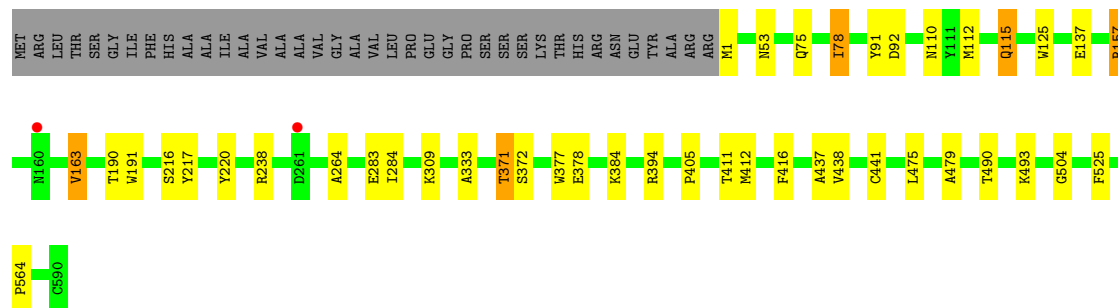
- Molecule 1: Patulin synthase





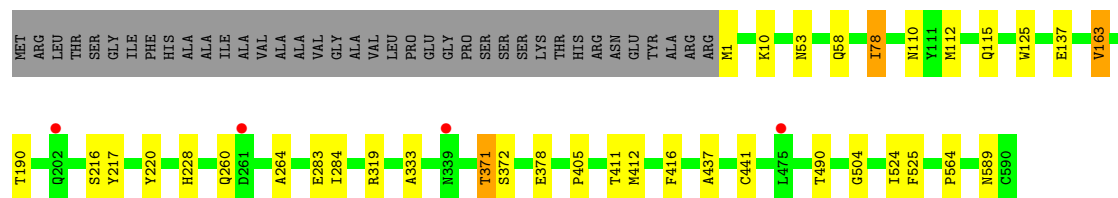
• Molecule 1: Patulin synthase

Chain A: 87% 6% • 6%



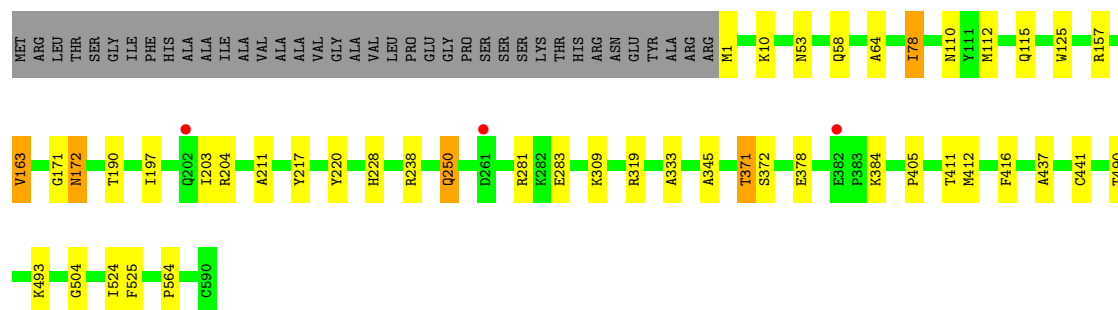
• Molecule 1: Patulin synthase

Chain F: 88% 5% 6%



• Molecule 1: Patulin synthase

Chain E: 87% 7% • 6%



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

Chain G: 100%



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

Chain H:  100%

MAG1
MAG2
MAN3

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

Chain I:  100%

MAG1
MAG2
MAN3

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

Chain J:  100%

MAG1
MAG2
MAN3

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

Chain K:  100%

MAG1
MAG2
MAN3

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

Chain L:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	104.84Å 144.16Å 155.24Å 90.00° 91.53° 90.00°	Depositor
Resolution (Å)	48.74 – 2.40 48.74 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.74-2.40) 100.0 (48.74-2.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.39Å)	Xtriage
Refinement program	REFMAC v7.1.018	Depositor
R, R_{free}	0.182 , 0.222 0.188 , 0.226	Depositor DCC
R_{free} test set	9411 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	29074	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.4539e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MAN, PEG, GOL, FAD

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	0.99	0/4646	1.29	3/6332 (0.0%)
1	B	1.00	0/4642	1.30	3/6327 (0.0%)
1	C	1.00	1/4606 (0.0%)	1.30	6/6284 (0.1%)
1	D	1.00	0/4562	1.29	3/6233 (0.0%)
1	E	1.00	0/4646	1.30	7/6332 (0.1%)
1	F	0.99	0/4622	1.28	3/6305 (0.0%)
All	All	1.00	1/27724 (0.0%)	1.29	25/37813 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	2
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	59	ILE	N-CA	5.07	1.50	1.46

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	241	LEU	N-CA-C	-9.53	96.17	110.28
1	C	241	LEU	N-CA-C	-8.96	97.01	110.28
1	E	172	ASN	N-CA-C	-8.72	96.19	109.79
1	F	504	GLY	CA-C-O	-7.28	117.48	122.22
1	C	160	ASN	CB-CA-C	-7.13	96.22	110.42
1	A	504	GLY	CA-C-O	-6.70	117.87	122.22
1	C	160	ASN	OD1-CG-ND2	6.64	129.24	122.60
1	D	504	GLY	CA-C-O	-6.53	117.97	122.22
1	C	504	GLY	CA-C-O	-6.16	118.22	122.22
1	E	157	ARG	NE-CZ-NH2	6.08	124.67	119.20
1	B	504	GLY	CA-C-O	-6.05	118.29	122.22
1	A	157	ARG	NE-CZ-NH2	5.91	124.52	119.20
1	E	504	GLY	CA-C-O	-5.88	118.39	122.22
1	E	319	ARG	CB-CG-CD	5.59	124.17	111.30
1	D	137	GLU	CB-CG-CD	5.42	121.81	112.60
1	E	172	ASN	CB-CA-C	5.36	125.45	113.33
1	F	137	GLU	CB-CG-CD	5.27	121.56	112.60
1	E	524	ILE	N-CA-C	-5.25	107.18	112.17
1	B	137	GLU	CB-CG-CD	5.14	121.34	112.60
1	C	524	ILE	N-CA-C	-5.13	107.30	112.17
1	F	524	ILE	N-CA-C	-5.10	107.32	112.17
1	C	137	GLU	CB-CG-CD	5.09	121.25	112.60
1	A	137	GLU	CB-CG-CD	5.08	121.23	112.60
1	E	250	GLN	CB-CA-C	5.05	118.14	109.80
1	D	524	ILE	N-CA-C	-5.04	107.38	112.17

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	378	GLU	Peptide
1	B	378	GLU	Peptide
1	C	378	GLU	Peptide
1	C	381	PRO	Peptide
1	D	378	GLU	Peptide
1	E	378	GLU	Peptide
1	F	378	GLU	Peptide

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	4530	0	4370	35	0
1	B	4526	0	4366	36	0
1	C	4490	0	4310	42	0
1	D	4446	0	4227	41	0
1	E	4530	0	4370	40	0
1	F	4506	0	4324	38	0
2	G	39	0	34	0	0
2	H	39	0	34	0	0
2	I	39	0	34	2	0
2	J	39	0	34	0	0
2	K	39	0	34	2	0
3	L	28	0	25	0	0
4	A	53	0	31	5	0
4	B	53	0	31	5	0
4	C	53	0	31	6	0
4	D	53	0	31	6	0
4	E	53	0	31	5	0
4	F	53	0	31	5	0
5	A	56	0	52	3	0
5	B	56	0	52	1	0
5	C	56	0	52	5	0
5	D	56	0	52	2	0
5	E	56	0	52	3	0
5	F	56	0	52	1	0
6	A	21	0	30	2	0
6	B	28	0	40	1	0
6	C	14	0	20	2	0
6	D	14	0	20	2	0
6	E	28	0	40	3	0
6	F	35	0	50	12	0
7	A	6	0	8	2	0
7	B	6	0	8	3	0
7	C	6	0	8	3	0
7	D	6	0	8	1	0
7	E	6	0	8	4	0
7	F	12	0	16	4	0
8	A	158	0	0	4	0
8	B	200	0	0	5	0
8	C	170	0	0	3	0
8	D	63	0	0	3	0
8	E	209	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	187	0	0	1	0
All	All	29074	0	26916	214	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 (214) 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:438:VAL:HG21	1:A:479:ALA:HB1	1.47	0.96
1:D:438:VAL:HG21	1:D:479:ALA:HB1	1.48	0.94
1:B:438:VAL:HG21	1:B:479:ALA:HB1	1.48	0.93
1:A:157:ARG:NH1	8:A:744[B]:HOH:O	1.91	0.91
1:A:371:THR:HG21	7:A:606:GOL:H2	1.52	0.91
1:E:1:MET:N	6:E:605:PEG:O4	2.07	0.88
1:D:507:VAL:HG12	1:D:513:ILE:HD13	1.58	0.86
1:F:589:ASN:ND2	6:F:610:PEG:C3	2.39	0.85
1:B:1:MET:N	6:B:603:PEG:O4	2.11	0.84
1:A:1:MET:N	6:A:603:PEG:O4	2.12	0.83
6:A:605:PEG:H21	8:A:835:HOH:O	1.79	0.83
1:D:261:ASP:CB	8:D:759:HOH:O	2.27	0.81
1:F:589:ASN:HD21	6:F:610:PEG:H22	1.43	0.81
1:D:110:ASN:HA	4:D:601:FAD:C6	2.11	0.80
1:C:58:GLN:HB2	1:D:1:MET:HE2	1.64	0.79
1:D:70:ASP:OD1	1:D:420:ARG:HG2	1.82	0.79
1:C:110:ASN:HA	4:C:601:FAD:C6	2.13	0.78
1:E:371:THR:HG21	7:E:607:GOL:H2	1.66	0.78
1:F:110:ASN:HA	4:F:601:FAD:C6	2.12	0.78
1:F:589:ASN:ND2	6:F:610:PEG:H31	2.01	0.76
1:F:228:HIS:CD2	1:E:1:MET:HE3	2.21	0.76
1:C:412:MET:CE	7:C:606:GOL:H2	2.18	0.74
1:D:480:PHE:CD2	1:D:513:ILE:HD12	2.23	0.74
1:E:110:ASN:HA	4:E:603:FAD:C6	2.16	0.74
7:F:609:GOL:H31	6:F:610:PEG:O2	1.86	0.73
1:C:319:ARG:HD2	8:C:705:HOH:O	1.87	0.73
1:C:1:MET:HE3	1:D:228:HIS:NE2	2.04	0.72
1:A:110:ASN:HA	4:A:601:FAD:C6	2.19	0.72
1:B:58:GLN:CB	1:A:1:MET:HE2	2.20	0.72
1:B:319:ARG:HD2	8:B:741:HOH:O	1.90	0.72
1:B:110:ASN:HA	4:B:601:FAD:C6	2.20	0.71
1:C:110:ASN:HB2	4:C:601:FAD:C4X	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:GLN:NE2	1:A:377:TRP:CH2	2.58	0.71
1:F:1:MET:HE3	1:E:228:HIS:CD2	2.26	0.71
1:F:589:ASN:HD21	6:F:610:PEG:C2	2.03	0.70
1:C:59:ILE:HG13	1:D:1:MET:HE1	1.73	0.70
1:B:241:LEU:O	1:B:242:ALA:HB3	1.92	0.69
1:C:1:MET:HE3	1:D:228:HIS:CD2	2.27	0.69
1:E:281:ARG:HD3	8:E:785:HOH:O	1.92	0.69
1:F:589:ASN:ND2	6:F:610:PEG:H32	2.06	0.69
1:C:241:LEU:O	1:C:242:ALA:HB3	1.93	0.69
1:A:115:GLN:NE2	1:A:377:TRP:CZ2	2.60	0.69
1:C:191:TRP:CE2	5:C:604:NAG:H61	2.28	0.68
1:D:110:ASN:HB2	4:D:601:FAD:C4X	2.23	0.68
1:A:110:ASN:HB2	4:A:601:FAD:C4X	2.24	0.68
1:D:1:MET:N	6:D:603:PEG:O4	2.27	0.68
1:E:190:THR:HG22	5:E:609:NAG:H82	1.76	0.68
1:B:58:GLN:HB2	1:A:1:MET:HE2	1.76	0.67
1:B:110:ASN:HB2	4:B:601:FAD:C4X	2.26	0.66
1:F:110:ASN:HB2	4:F:601:FAD:C4X	2.27	0.65
1:E:110:ASN:HB2	4:E:603:FAD:C4X	2.27	0.65
1:F:319:ARG:HD2	8:F:715:HOH:O	1.95	0.65
1:C:191:TRP:CZ2	5:C:604:NAG:H61	2.31	0.64
1:F:589:ASN:HD22	6:F:610:PEG:H31	1.63	0.63
1:C:241:LEU:O	1:C:242:ALA:CB	2.47	0.63
1:B:241:LEU:O	1:B:242:ALA:CB	2.46	0.63
1:B:407:VAL:HG13	1:B:438:VAL:CG2	2.29	0.62
1:F:371:THR:HG21	7:F:606:GOL:H2	1.81	0.62
1:D:190:THR:HG22	5:D:604:NAG:H82	1.82	0.62
1:F:58:GLN:HB3	1:E:1:MET:HE2	1.80	0.62
1:A:371:THR:HG21	7:A:606:GOL:C2	2.30	0.61
1:A:190:THR:HG22	5:A:604:NAG:H82	1.82	0.61
1:C:281:ARG:NH2	8:C:702:HOH:O	2.33	0.60
1:F:58:GLN:CB	1:E:1:MET:HE2	2.31	0.60
1:B:58:GLN:HB3	1:A:1:MET:HE2	1.84	0.59
1:D:546:LYS:CB	8:D:763:HOH:O	2.51	0.59
1:C:412:MET:HE1	7:C:606:GOL:H2	1.83	0.59
1:D:507:VAL:CG1	1:D:513:ILE:HD13	2.32	0.58
1:F:190:THR:HG22	5:F:604:NAG:H82	1.86	0.58
1:F:228:HIS:NE2	1:E:1:MET:HE3	2.19	0.57
1:D:110:ASN:HB2	4:D:601:FAD:N5	2.20	0.57
1:B:138:GLN:HG3	8:B:826:HOH:O	2.03	0.57
1:B:407:VAL:HG13	1:B:438:VAL:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:ASN:HB2	4:C:601:FAD:N5	2.19	0.56
1:E:64:ALA:HB2	7:E:607:GOL:H12	1.86	0.56
1:B:296:LEU:HG	8:B:850:HOH:O	2.05	0.56
1:F:1:MET:N	6:F:603:PEG:O4	2.37	0.56
1:E:64:ALA:HB2	7:E:607:GOL:C1	2.35	0.56
1:B:228:HIS:CD2	1:A:1:MET:HE3	2.42	0.55
1:F:110:ASN:HB2	4:F:601:FAD:N5	2.22	0.55
1:C:58:GLN:HB2	1:D:1:MET:CE	2.36	0.55
1:F:1:MET:HE2	1:E:58:GLN:CB	2.37	0.54
1:D:110:ASN:HB2	4:D:601:FAD:C5X	2.37	0.54
2:I:2:NAG:H4	2:I:3:MAN:O2	2.06	0.54
1:B:372:SER:HB3	8:B:880:HOH:O	2.08	0.54
1:F:1:MET:HE2	1:E:58:GLN:HB3	1.89	0.54
1:D:480:PHE:CE2	1:D:513:ILE:HD12	2.43	0.53
1:B:110:ASN:HB2	4:B:601:FAD:N5	2.23	0.53
1:D:589:ASN:ND2	8:D:703:HOH:O	2.41	0.53
1:E:345:ALA:HA	6:E:606:PEG:H31	1.90	0.53
1:F:589:ASN:HD21	6:F:610:PEG:C3	2.20	0.52
1:B:319:ARG:CD	8:B:741:HOH:O	2.52	0.52
1:F:110:ASN:HB2	4:F:601:FAD:C5X	2.40	0.52
1:A:110:ASN:HB2	4:A:601:FAD:N5	2.24	0.52
1:C:59:ILE:CG1	1:D:1:MET:HE1	2.40	0.52
1:C:110:ASN:HB2	4:C:601:FAD:C5X	2.40	0.52
1:C:191:TRP:NE1	5:C:604:NAG:H61	2.24	0.51
1:B:64:ALA:CB	7:B:606:GOL:H11	2.40	0.51
1:C:110:ASN:HA	4:C:601:FAD:C5X	2.40	0.51
7:F:609:GOL:H12	6:F:610:PEG:H12	1.92	0.51
1:D:333:ALA:HB2	1:D:437:ALA:HA	1.93	0.51
1:A:333:ALA:HB2	1:A:437:ALA:HA	1.93	0.51
1:A:91:TYR:CD1	1:E:203:ILE:HD12	2.46	0.50
1:C:58:GLN:CB	1:D:1:MET:HE2	2.38	0.50
1:D:371:THR:HG21	7:D:606:GOL:H2	1.93	0.50
1:C:1:MET:N	6:C:603:PEG:O4	2.45	0.49
1:C:345:ALA:HA	6:C:605:PEG:H31	1.93	0.49
1:D:110:ASN:HA	4:D:601:FAD:C5X	2.42	0.49
1:E:110:ASN:HB2	4:E:603:FAD:N5	2.27	0.49
1:B:110:ASN:HB2	4:B:601:FAD:C5X	2.43	0.49
1:B:333:ALA:HB2	1:B:437:ALA:HA	1.94	0.49
1:F:1:MET:HE3	1:E:228:HIS:NE2	2.28	0.48
1:C:333:ALA:HB2	1:C:437:ALA:HA	1.95	0.48
1:D:371:THR:CG2	1:D:412:MET:HE3	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:333:ALA:HB2	1:F:437:ALA:HA	1.95	0.48
1:A:371:THR:CG2	1:A:412:MET:HE3	2.44	0.48
1:A:475:LEU:HD13	8:A:703:HOH:O	2.12	0.48
1:E:110:ASN:HA	4:E:603:FAD:C5X	2.44	0.48
1:E:333:ALA:HB2	1:E:437:ALA:HA	1.95	0.48
1:C:324:GLN:HE22	5:C:608:NAG:H81	1.79	0.47
1:B:190:THR:HG22	5:B:604:NAG:H82	1.95	0.47
1:E:10:LYS:HE2	6:E:602:PEG:H22	1.96	0.47
1:D:507:VAL:HG12	1:D:513:ILE:CD1	2.37	0.47
1:A:92:ASP:HB2	1:E:197:ILE:HD13	1.96	0.47
1:A:110:ASN:HB2	4:A:601:FAD:C5X	2.44	0.47
1:B:371:THR:CG2	1:B:412:MET:HE3	2.45	0.47
1:B:407:VAL:CG1	1:B:438:VAL:HG23	2.45	0.46
1:E:125:TRP:CD1	1:E:564:PRO:HG3	2.50	0.46
1:C:371:THR:CG2	1:C:412:MET:HE3	2.45	0.46
1:E:171:GLY:C	1:E:172:ASN:O	2.58	0.46
1:C:125:TRP:CD1	1:C:564:PRO:HG3	2.51	0.46
1:A:110:ASN:HA	4:A:601:FAD:C5X	2.44	0.46
1:C:111:TYR:CE1	7:C:606:GOL:H12	2.50	0.46
1:F:371:THR:CG2	1:F:412:MET:HE3	2.45	0.46
1:D:125:TRP:CD1	1:D:564:PRO:HG3	2.50	0.46
1:B:343:GLN:HE22	7:B:606:GOL:C1	2.29	0.46
1:E:372:SER:HA	1:E:411:THR:O	2.16	0.46
1:B:53:ASN:CG	1:B:78:ILE:HG12	2.41	0.46
1:A:125:TRP:CD1	1:A:564:PRO:HG3	2.50	0.46
1:E:110:ASN:HB2	4:E:603:FAD:C5X	2.45	0.45
1:B:125:TRP:CD1	1:B:564:PRO:HG3	2.51	0.45
1:C:382:GLU:N	1:C:383:PRO:CD	2.79	0.45
1:A:53:ASN:CG	1:A:78:ILE:HG12	2.41	0.45
1:F:125:TRP:CD1	1:F:564:PRO:HG3	2.52	0.45
1:E:53:ASN:CG	1:E:78:ILE:HG12	2.42	0.45
1:D:345:ALA:HA	6:D:605:PEG:H31	1.99	0.45
1:A:372:SER:HA	1:A:411:THR:O	2.17	0.45
1:E:371:THR:CG2	1:E:412:MET:HE3	2.46	0.45
1:A:163:VAL:HG22	1:A:217:TYR:HB2	1.99	0.44
1:C:372:SER:HA	1:C:411:THR:O	2.17	0.44
1:D:53:ASN:CG	1:D:78:ILE:HG12	2.41	0.44
1:C:53:ASN:CG	1:C:78:ILE:HG12	2.42	0.44
1:F:10:LYS:HE2	6:F:608:PEG:H12	1.99	0.44
1:F:112:MET:O	1:F:220:TYR:HA	2.18	0.44
1:F:110:ASN:HA	4:F:601:FAD:C5X	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:493:LYS:HE2	8:C:731:HOH:O	2.18	0.44
1:F:372:SER:HA	1:F:411:THR:O	2.18	0.44
1:E:112:MET:O	1:E:220:TYR:HA	2.17	0.44
1:E:371:THR:HG21	7:E:607:GOL:C2	2.42	0.44
1:B:112:MET:O	1:B:220:TYR:HA	2.18	0.43
1:C:110:ASN:CB	4:C:601:FAD:C5X	2.96	0.43
1:C:112:MET:O	1:C:220:TYR:HA	2.18	0.43
1:D:372:SER:HA	1:D:411:THR:O	2.18	0.43
1:A:112:MET:O	1:A:220:TYR:HA	2.18	0.43
1:B:405:PRO:O	1:B:441:CYS:HB2	2.19	0.43
1:D:110:ASN:CB	4:D:601:FAD:C5X	2.96	0.43
1:C:258:ARG:NH2	5:C:607:NAG:O6	2.52	0.43
1:F:163:VAL:HG22	1:F:217:TYR:HB2	2.01	0.43
1:F:53:ASN:CG	1:F:78:ILE:HG12	2.42	0.43
1:E:163:VAL:HG22	1:E:217:TYR:HB2	2.00	0.43
1:D:163:VAL:HG22	1:D:217:TYR:HB2	2.00	0.42
1:F:58:GLN:HB2	1:E:1:MET:HE2	1.99	0.42
1:D:112:MET:O	1:D:220:TYR:HA	2.19	0.42
1:D:191:TRP:CE2	5:D:604:NAG:H83	2.55	0.42
7:F:609:GOL:C1	6:F:610:PEG:H12	2.49	0.42
1:B:412:MET:HE2	1:B:416:PHE:CE1	2.55	0.42
1:E:405:PRO:O	1:E:441:CYS:HB2	2.20	0.42
1:B:372:SER:HA	1:B:411:THR:O	2.18	0.42
1:B:412:MET:HE2	1:B:416:PHE:CZ	2.55	0.42
1:A:412:MET:HE2	1:A:416:PHE:CE1	2.55	0.42
2:K:1:NAG:H62	2:K:2:NAG:C1	2.50	0.42
1:E:412:MET:HE2	1:E:416:PHE:CE1	2.54	0.42
1:F:405:PRO:O	1:F:441:CYS:HB2	2.20	0.42
1:D:405:PRO:O	1:D:441:CYS:HB2	2.20	0.41
1:D:467:LEU:HD23	1:D:467:LEU:HA	1.89	0.41
1:B:264:ALA:HB1	1:B:284:ILE:HD12	2.02	0.41
1:C:405:PRO:O	1:C:441:CYS:HB2	2.20	0.41
1:A:191:TRP:CE2	5:A:604:NAG:H83	2.55	0.41
1:F:412:MET:HE2	1:F:416:PHE:CE1	2.56	0.41
1:B:110:ASN:HA	4:B:601:FAD:C5X	2.50	0.41
1:B:422:TYR:CD2	7:B:606:GOL:H31	2.55	0.41
1:C:58:GLN:CB	1:D:1:MET:CE	2.99	0.41
1:E:190:THR:HG22	5:E:609:NAG:C8	2.48	0.41
1:D:412:MET:HE2	1:D:416:PHE:CE1	2.55	0.41
1:D:412:MET:HE2	1:D:416:PHE:CZ	2.56	0.41
1:E:190:THR:HG21	5:E:609:NAG:N2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:LYS:N	1:B:494:PRO:CD	2.84	0.41
1:A:190:THR:HG21	5:A:604:NAG:N2	2.36	0.41
1:A:264:ALA:HB1	1:A:284:ILE:HD12	2.02	0.41
1:A:405:PRO:O	1:A:441:CYS:HB2	2.20	0.41
1:F:1:MET:HE2	1:E:58:GLN:HB2	2.03	0.41
1:E:204:ARG:NH2	1:E:211:ALA:HB3	2.36	0.41
1:C:1:MET:CE	1:D:228:HIS:CD2	3.00	0.41
1:C:412:MET:HE2	1:C:416:PHE:CE1	2.55	0.41
1:A:394:ARG:HD2	8:A:841:HOH:O	2.20	0.41
1:A:412:MET:HE2	1:A:416:PHE:CZ	2.56	0.41
1:E:412:MET:HE2	1:E:416:PHE:CZ	2.56	0.41
1:F:412:MET:HE2	1:F:416:PHE:CZ	2.56	0.40
1:C:4:SER:O	2:I:1:NAG:H61	2.21	0.40
1:A:75:GLN:HG3	1:A:78:ILE:HD11	2.03	0.40
1:F:264:ALA:HB1	1:F:284:ILE:HD12	2.04	0.40
1:C:163:VAL:HG22	1:C:217:TYR:HB2	2.02	0.40
2:K:2:NAG:H4	2:K:3:MAN:O2	2.21	0.40
1:C:382:GLU:N	1:C:383:PRO:HD2	2.36	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	588/628 (94%)	570 (97%)	16 (3%)	2 (0%)	36	50
1	B	588/628 (94%)	569 (97%)	16 (3%)	3 (0%)	24	37
1	C	588/628 (94%)	568 (97%)	17 (3%)	3 (0%)	24	37
1	D	588/628 (94%)	570 (97%)	16 (3%)	2 (0%)	36	50
1	E	588/628 (94%)	570 (97%)	16 (3%)	2 (0%)	36	50
1	F	588/628 (94%)	569 (97%)	17 (3%)	2 (0%)	36	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3528/3768 (94%)	3416 (97%)	98 (3%)	14 (0%)	30	43

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	371	THR
1	C	371	THR
1	D	371	THR
1	A	371	THR
1	F	371	THR
1	E	371	THR
1	B	242	ALA
1	E	525	PHE
1	B	525	PHE
1	C	242	ALA
1	C	525	PHE
1	D	525	PHE
1	A	525	PHE
1	F	525	PHE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	472/500 (94%)	462 (98%)	10 (2%)	47	69
1	B	471/500 (94%)	462 (98%)	9 (2%)	50	71
1	C	462/500 (92%)	453 (98%)	9 (2%)	50	71
1	D	452/500 (90%)	444 (98%)	8 (2%)	51	73
1	E	472/500 (94%)	462 (98%)	10 (2%)	47	69
1	F	466/500 (93%)	459 (98%)	7 (2%)	57	77
All	All	2795/3000 (93%)	2742 (98%)	53 (2%)	50	71

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1	MET
1	B	78	ILE
1	B	163	VAL
1	B	216	SER
1	B	260	GLN
1	B	283	GLU
1	B	312	ASN
1	B	384	LYS
1	B	490	THR
1	C	78	ILE
1	C	115	GLN
1	C	163	VAL
1	C	197	ILE
1	C	283	GLU
1	C	372	SER
1	C	384	LYS
1	C	490	THR
1	C	493	LYS
1	D	78	ILE
1	D	115	GLN
1	D	163	VAL
1	D	216	SER
1	D	238	ARG
1	D	283	GLU
1	D	490	THR
1	D	493	LYS
1	A	78	ILE
1	A	115	GLN
1	A	163	VAL
1	A	216	SER
1	A	238	ARG
1	A	283	GLU
1	A	309	LYS
1	A	384	LYS
1	A	490	THR
1	A	493	LYS
1	F	78	ILE
1	F	115	GLN
1	F	163	VAL
1	F	216	SER
1	F	260	GLN
1	F	283	GLU
1	F	490	THR

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Mol	Chain	Res	Type
1	E	78	ILE
1	E	115	GLN
1	E	163	VAL
1	E	238	ARG
1	E	250	GLN
1	E	283	GLU
1	E	309	LYS
1	E	384	LYS
1	E	490	THR
1	E	493	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	343	GLN
1	B	589	ASN
1	C	324	GLN
1	C	343	GLN
1	D	343	GLN
1	D	516	HIS
1	A	115	GLN
1	A	343	GLN
1	A	516	HIS
1	F	83	HIS
1	F	343	GLN
1	F	516	HIS
1	F	589	ASN
1	E	250	GLN
1	E	260	GLN
1	E	343	GLN
1	E	516	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

17 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	G	1	1,2	14,14,15	0.73	0	17,19,21	1.99	3 (17%)
2	NAG	G	2	2	14,14,15	0.78	0	17,19,21	1.81	3 (17%)
2	MAN	G	3	2	11,11,12	0.80	0	15,15,17	2.00	4 (26%)
2	NAG	H	1	1,2	14,14,15	0.46	0	17,19,21	2.97	4 (23%)
2	NAG	H	2	2	14,14,15	0.61	0	17,19,21	1.72	3 (17%)
2	MAN	H	3	2	11,11,12	0.86	0	15,15,17	1.51	3 (20%)
2	NAG	I	1	1,2	14,14,15	0.55	0	17,19,21	2.27	4 (23%)
2	NAG	I	2	2	14,14,15	0.51	0	17,19,21	1.80	3 (17%)
2	MAN	I	3	2	11,11,12	0.67	0	15,15,17	1.64	2 (13%)
2	NAG	J	1	1,2	14,14,15	0.79	1 (7%)	17,19,21	2.02	4 (23%)
2	NAG	J	2	2	14,14,15	0.61	0	17,19,21	1.15	1 (5%)
2	MAN	J	3	2	11,11,12	0.69	0	15,15,17	1.43	2 (13%)
2	NAG	K	1	1,2	14,14,15	0.76	0	17,19,21	2.66	4 (23%)
2	NAG	K	2	2	14,14,15	0.74	0	17,19,21	1.98	7 (41%)
2	MAN	K	3	2	11,11,12	0.84	0	15,15,17	1.66	3 (20%)
3	NAG	L	1	1,3	14,14,15	0.57	0	17,19,21	2.21	4 (23%)
3	NAG	L	2	3	14,14,15	0.98	1 (7%)	17,19,21	2.02	7 (41%)

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	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	MAN	G	3	2	-	2/2/19/22	1/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	MAN	H	3	2	-	2/2/19/22	1/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	MAN	I	3	2	-	1/2/19/22	1/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	4/6/23/26	0/1/1/1
2	MAN	J	3	2	-	2/2/19/22	0/1/1/1
2	NAG	K	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	1/6/23/26	0/1/1/1
2	MAN	K	3	2	-	1/2/19/22	1/1/1/1
3	NAG	L	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	2	NAG	C4-C5	2.32	1.58	1.53
2	J	1	NAG	O7-C7	-2.18	1.18	1.23

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	NAG	C1-O5-C5	10.22	125.89	112.19
2	K	1	NAG	C1-O5-C5	9.23	124.56	112.19
3	L	1	NAG	C1-O5-C5	7.49	122.22	112.19
2	I	1	NAG	C1-O5-C5	7.30	121.96	112.19
2	G	3	MAN	C1-O5-C5	5.98	120.19	112.19
2	J	1	NAG	C1-O5-C5	5.48	119.53	112.19
2	G	1	NAG	C1-O5-C5	5.03	118.93	112.19
2	I	2	NAG	O5-C1-C2	-5.00	103.56	111.29
2	I	3	MAN	C1-O5-C5	4.69	118.47	112.19
2	G	1	NAG	C6-C5-C4	-4.13	102.89	113.02
2	K	3	MAN	C1-O5-C5	4.06	117.63	112.19
2	H	3	MAN	C1-O5-C5	4.03	117.58	112.19
2	G	2	NAG	C2-N2-C7	-3.93	117.64	122.90
2	G	2	NAG	O3-C3-C2	-3.80	101.51	109.40
2	H	2	NAG	C4-C3-C2	3.75	116.52	111.02
2	J	3	MAN	C1-O5-C5	3.75	117.21	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	2	NAG	C1-O5-C5	3.73	117.18	112.19
2	I	1	NAG	C6-C5-C4	-3.72	103.89	113.02
2	K	2	NAG	O5-C5-C6	-3.69	100.48	107.66
2	H	1	NAG	C6-C5-C4	-3.62	104.13	113.02
2	H	2	NAG	O4-C4-C3	-3.58	101.95	110.38
2	G	1	NAG	O5-C5-C6	3.56	114.60	107.66
2	K	1	NAG	O3-C3-C4	-3.52	102.09	110.38
2	I	2	NAG	C4-C3-C2	3.42	116.03	111.02
3	L	2	NAG	C1-O5-C5	3.42	116.76	112.19
3	L	2	NAG	C4-C3-C2	-3.24	106.28	111.02
2	H	2	NAG	O4-C4-C5	3.19	117.18	109.32
2	H	1	NAG	O5-C5-C4	3.19	118.58	110.83
3	L	2	NAG	O5-C5-C6	-3.02	101.78	107.66
2	K	3	MAN	O5-C5-C6	2.97	113.44	107.66
2	I	3	MAN	C1-C2-C3	2.92	113.90	109.64
2	J	1	NAG	C6-C5-C4	-2.92	105.85	113.02
2	J	1	NAG	O3-C3-C2	-2.91	103.36	109.40
2	K	1	NAG	C6-C5-C4	-2.79	106.16	113.02
2	G	3	MAN	C1-C2-C3	2.76	113.67	109.64
2	J	3	MAN	O5-C5-C6	2.72	112.95	107.66
2	G	3	MAN	O5-C5-C6	2.71	112.93	107.66
3	L	2	NAG	O5-C5-C4	2.70	117.39	110.83
2	I	1	NAG	O5-C5-C4	2.66	117.29	110.83
2	H	3	MAN	O4-C4-C3	2.60	116.50	110.38
2	I	2	NAG	O6-C6-C5	-2.52	102.75	111.33
2	K	2	NAG	C4-C3-C2	2.49	114.67	111.02
3	L	2	NAG	O3-C3-C4	2.48	116.22	110.38
2	K	2	NAG	O4-C4-C3	-2.48	104.53	110.38
3	L	2	NAG	C2-N2-C7	2.46	126.19	122.90
2	G	2	NAG	C4-C3-C2	2.44	114.59	111.02
2	I	1	NAG	O3-C3-C4	-2.32	104.90	110.38
2	K	2	NAG	O4-C4-C5	2.24	114.85	109.32
2	K	2	NAG	O6-C6-C5	-2.23	103.73	111.33
3	L	1	NAG	C4-C3-C2	-2.21	107.78	111.02
2	J	1	NAG	O6-C6-C5	-2.18	103.92	111.33
3	L	1	NAG	C3-C4-C5	2.17	114.17	110.23
2	K	3	MAN	O4-C4-C3	2.15	115.44	110.38
3	L	1	NAG	O3-C3-C4	-2.13	105.35	110.38
2	H	3	MAN	O5-C5-C6	2.13	111.81	107.66
2	G	3	MAN	O2-C2-C3	-2.11	105.79	110.15
2	K	1	NAG	O6-C6-C5	-2.10	104.17	111.33
2	K	2	NAG	O5-C5-C4	2.10	115.93	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	NAG	C2-N2-C7	-2.08	120.11	122.90
2	J	2	NAG	C4-C3-C2	2.08	114.07	111.02
3	L	2	NAG	O3-C3-C2	-2.05	105.14	109.40

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	3	MAN	O5-C5-C6-O6
2	G	3	MAN	C4-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	J	3	MAN	C4-C5-C6-O6
2	J	3	MAN	O5-C5-C6-O6
2	H	3	MAN	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	H	3	MAN	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	K	3	MAN	O5-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
2	I	3	MAN	O5-C5-C6-O6
2	J	2	NAG	C8-C7-N2-C2
2	H	2	NAG	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O7-C7-N2-C2
2	J	2	NAG	C4-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	L	2	NAG	C3-C2-N2-C7
2	J	2	NAG	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6

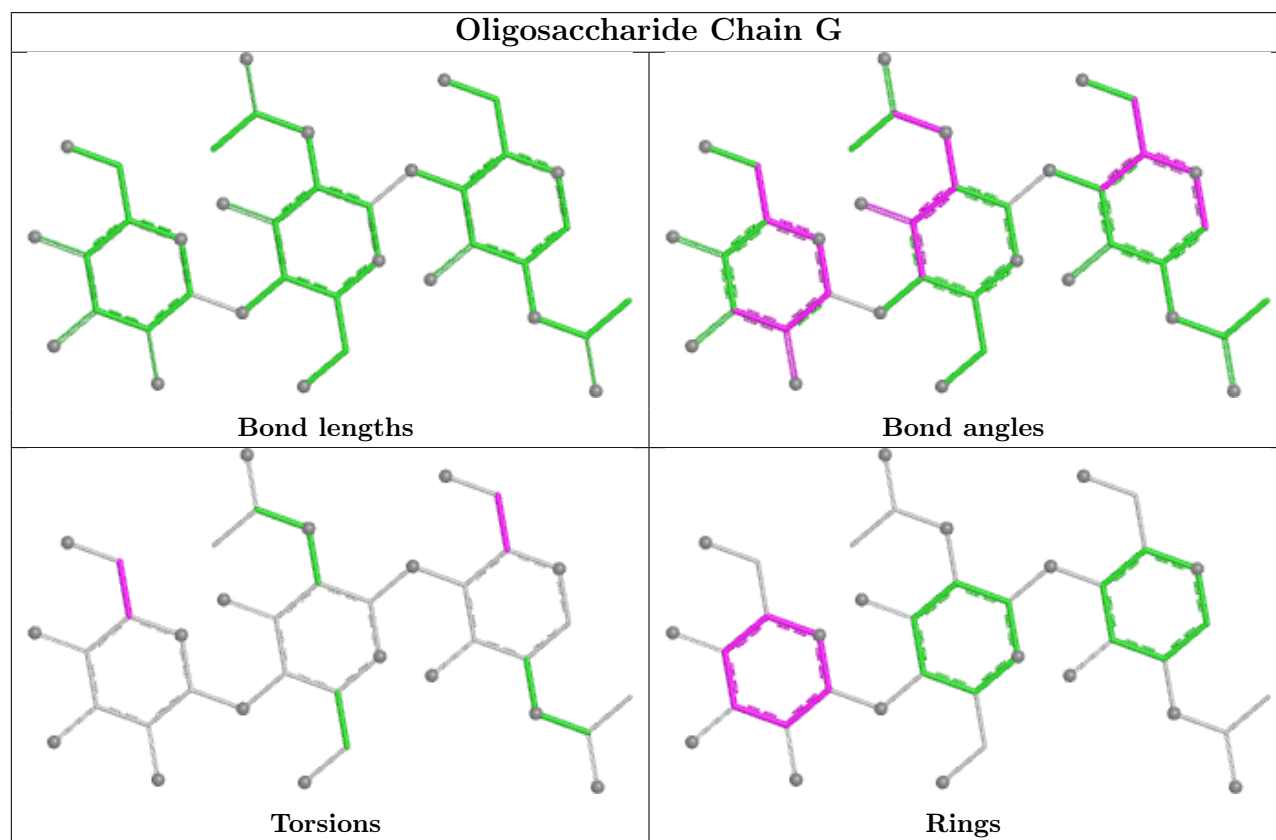
All (4) ring outliers are listed below:

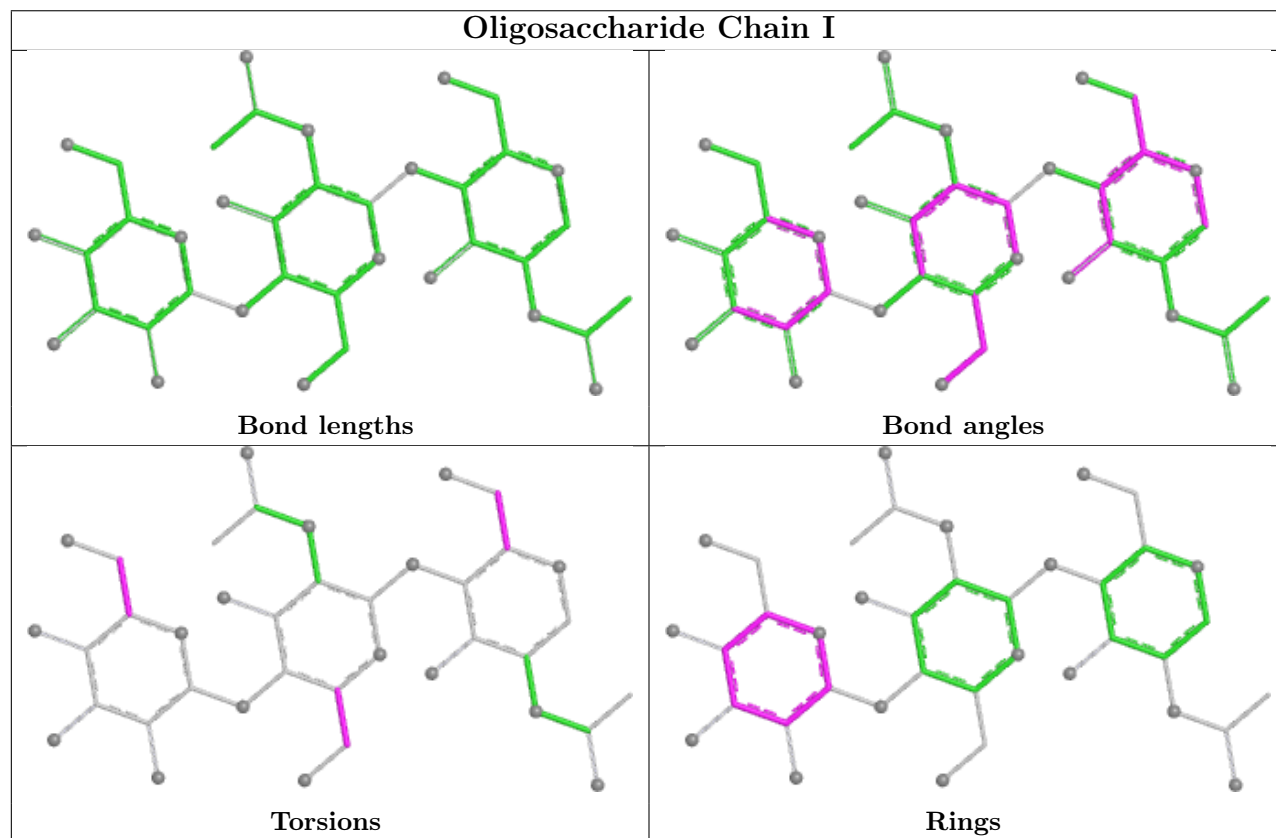
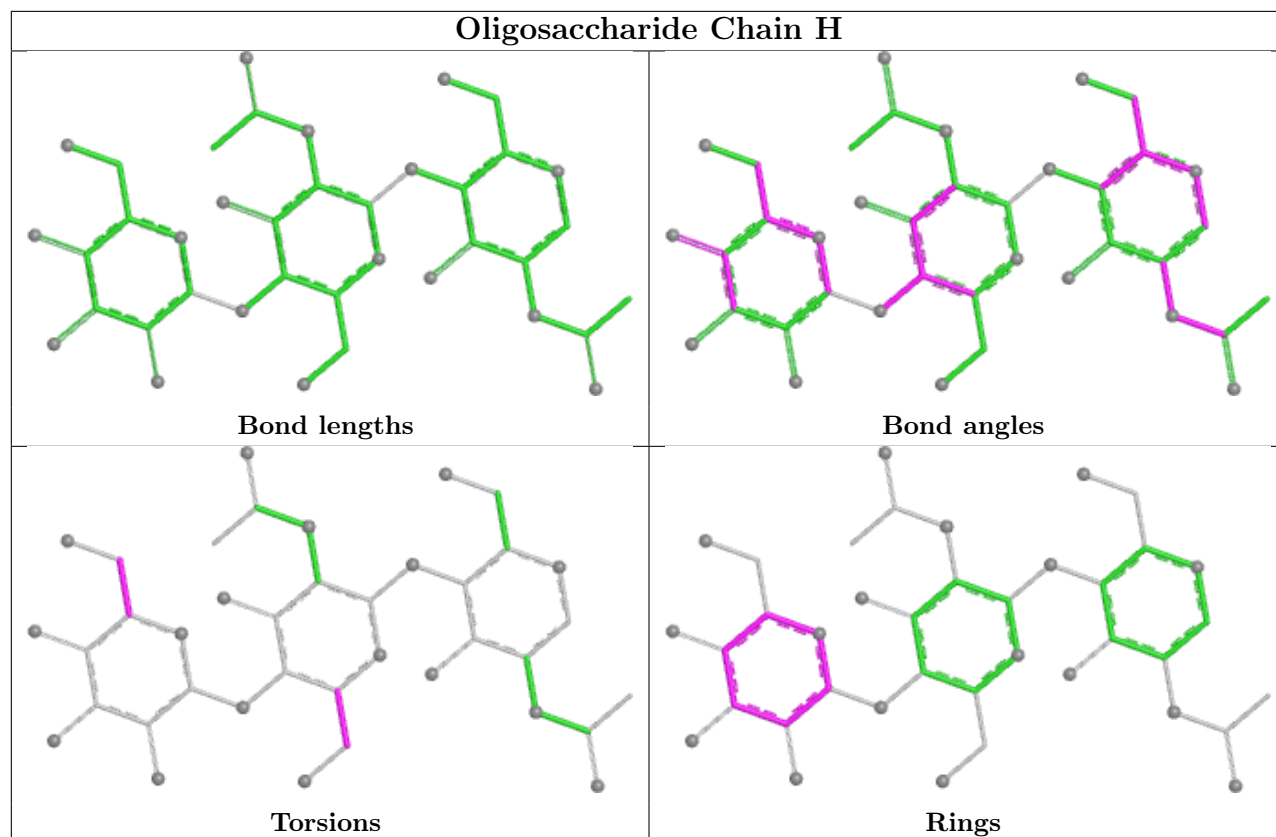
Mol	Chain	Res	Type	Atoms
2	G	3	MAN	C1-C2-C3-C4-C5-O5
2	I	3	MAN	C1-C2-C3-C4-C5-O5
2	H	3	MAN	C1-C2-C3-C4-C5-O5
2	K	3	MAN	C1-C2-C3-C4-C5-O5

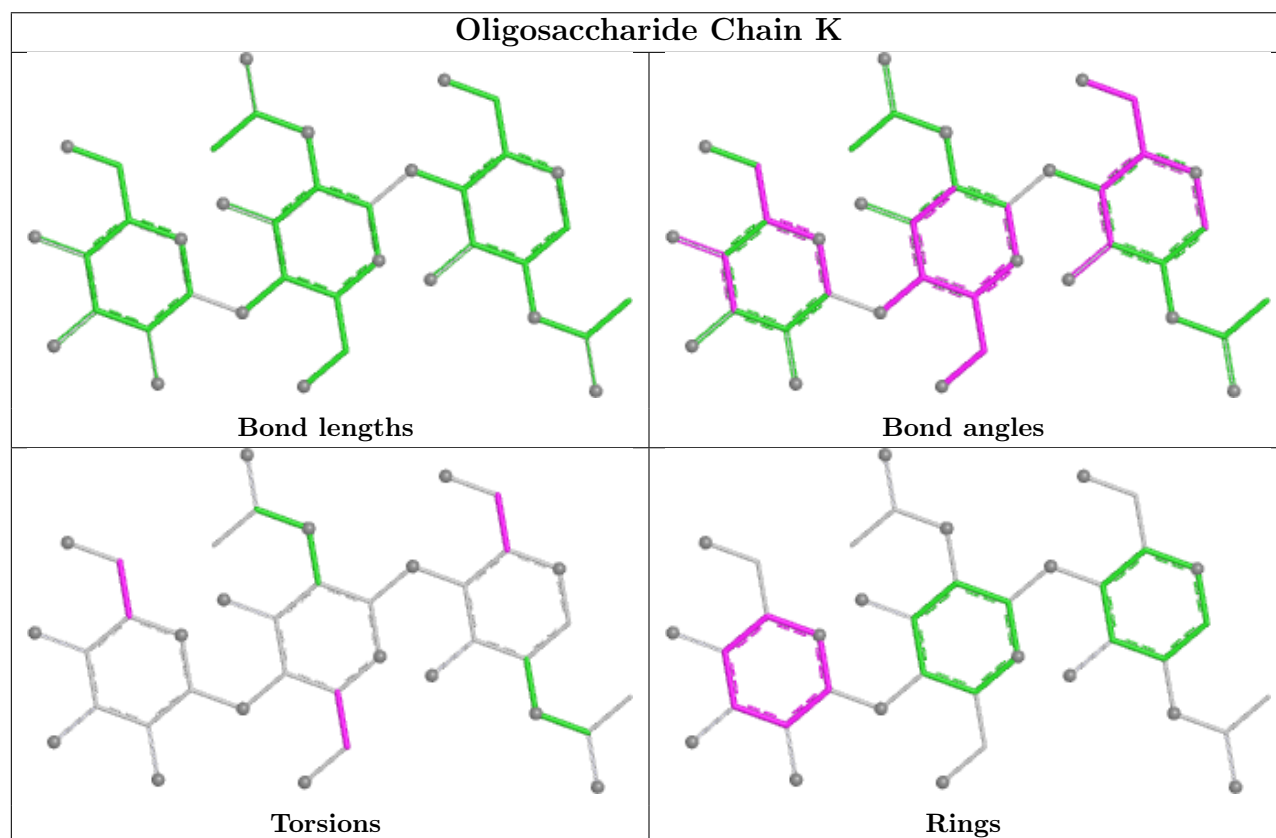
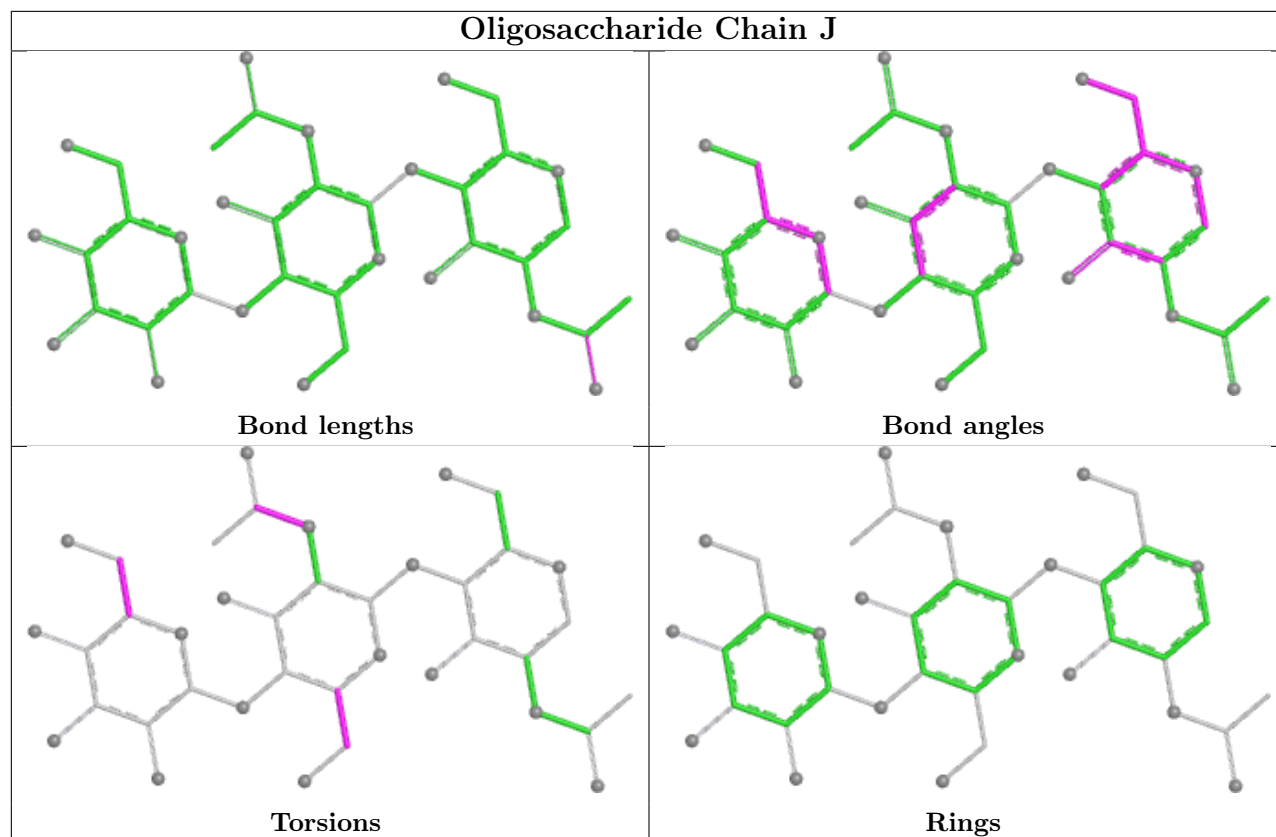
6 monomers are involved in 4 short contacts:

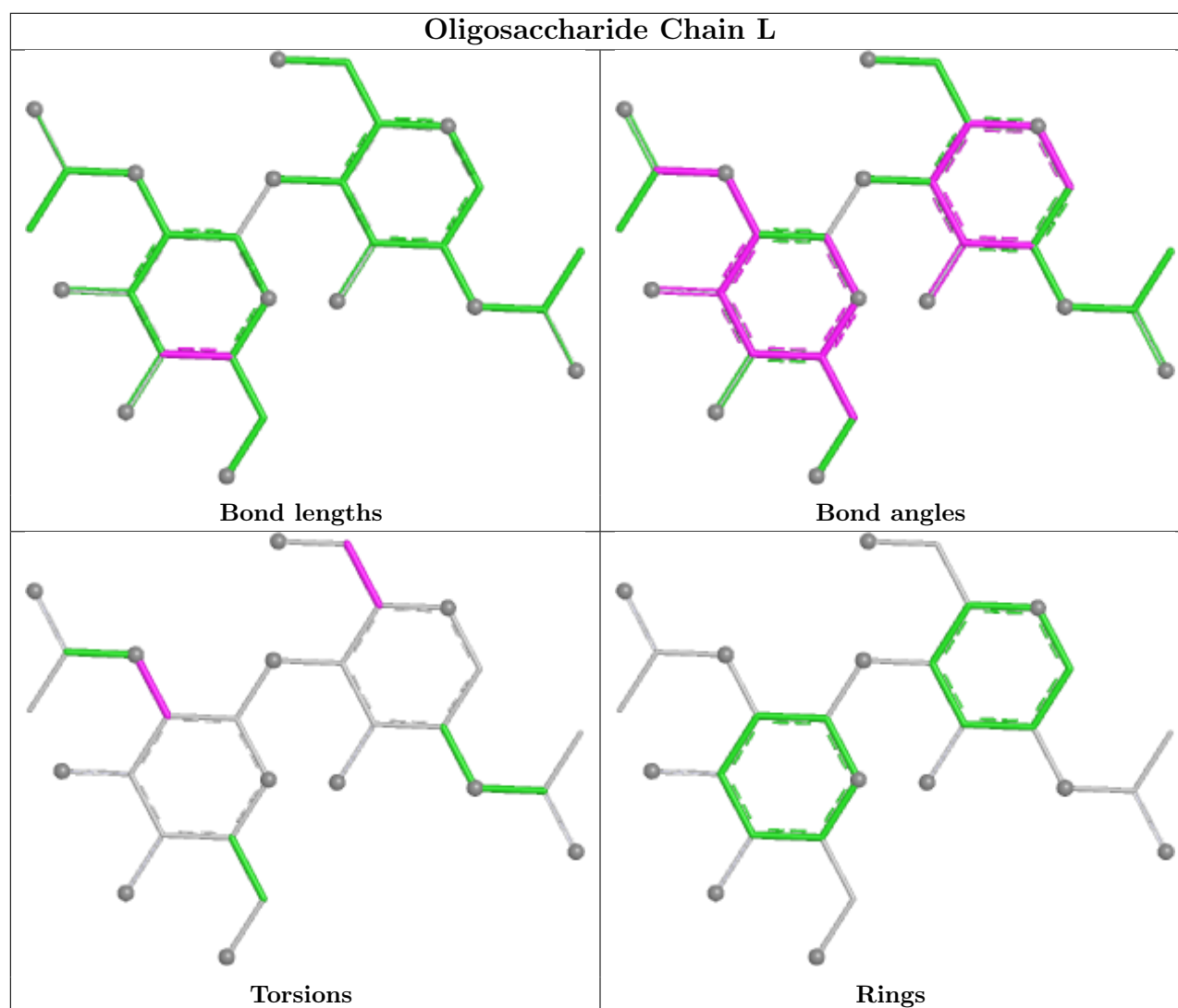
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	2	NAG	2	0
2	I	2	NAG	1	0
2	I	3	MAN	1	0
2	K	1	NAG	1	0
2	I	1	NAG	1	0
2	K	3	MAN	1	0

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](#)

57 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	$\# Z > 2$
6	PEG	B	605	-	6,6,6	0.52	0	5,5,5	0.37	0
5	NAG	C	607	1	14,14,15	0.29	0	17,19,21	1.31	2 (11%)
5	NAG	E	604	1	14,14,15	0.75	0	17,19,21	2.74	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	D	607	1	14,14,15	0.24	0	17,19,21	1.37	2 (11%)
5	NAG	F	607	1	14,14,15	0.47	0	17,19,21	2.25	5 (29%)
6	PEG	B	610	-	6,6,6	0.39	0	5,5,5	0.29	0
6	PEG	C	605	-	6,6,6	0.22	0	5,5,5	0.25	0
6	PEG	D	605	-	6,6,6	0.18	0	5,5,5	0.17	0
4	FAD	A	601	-	58,58,58	0.67	0	85,89,89	0.78	1 (1%)
5	NAG	D	602	1	14,14,15	0.78	0	17,19,21	1.63	5 (29%)
5	NAG	D	604	1	14,14,15	0.59	0	17,19,21	2.43	3 (17%)
5	NAG	E	609	1	14,14,15	0.53	0	17,19,21	1.59	4 (23%)
5	NAG	A	607	1	14,14,15	0.60	0	17,19,21	2.05	7 (41%)
5	NAG	D	608	1	14,14,15	0.62	0	17,19,21	1.52	3 (17%)
6	PEG	A	608	-	6,6,6	0.33	0	5,5,5	0.35	0
7	GOL	F	609	-	5,5,5	0.21	0	5,5,5	0.61	0
5	NAG	A	604	1	14,14,15	0.83	1 (7%)	17,19,21	1.58	3 (17%)
7	GOL	C	606	-	5,5,5	0.16	0	5,5,5	0.41	0
6	PEG	F	608	-	6,6,6	0.33	0	5,5,5	0.34	0
6	PEG	F	605	-	6,6,6	0.41	0	5,5,5	0.32	0
6	PEG	E	601	-	6,6,6	0.18	0	5,5,5	0.13	0
6	PEG	C	603	-	6,6,6	0.29	0	5,5,5	0.32	0
7	GOL	F	606	-	5,5,5	0.26	0	5,5,5	0.52	0
6	PEG	F	603	-	6,6,6	0.30	0	5,5,5	0.21	0
6	PEG	B	603	-	6,6,6	0.32	0	5,5,5	0.25	0
5	NAG	A	609	1	14,14,15	0.44	0	17,19,21	1.18	1 (5%)
7	GOL	A	606	-	5,5,5	0.40	0	5,5,5	0.57	0
7	GOL	E	607	-	5,5,5	0.33	0	5,5,5	0.55	0
4	FAD	D	601	-	58,58,58	0.65	1 (1%)	85,89,89	0.74	2 (2%)
5	NAG	C	602	1	14,14,15	0.91	0	17,19,21	2.04	6 (35%)
6	PEG	E	605	-	6,6,6	0.28	0	5,5,5	0.13	0
4	FAD	B	601	-	58,58,58	0.83	1 (1%)	85,89,89	0.82	1 (1%)
6	PEG	B	608	-	6,6,6	0.38	0	5,5,5	0.22	0
4	FAD	F	601	-	58,58,58	0.69	1 (1%)	85,89,89	0.79	1 (1%)
5	NAG	F	602	1	14,14,15	0.74	0	17,19,21	2.06	6 (35%)
6	PEG	F	610	-	6,6,6	0.32	0	5,5,5	0.50	0
5	NAG	A	602	1	14,14,15	0.84	0	17,19,21	1.60	5 (29%)
6	PEG	E	606	-	6,6,6	0.38	0	5,5,5	0.33	0
5	NAG	B	602	1	14,14,15	0.66	0	17,19,21	1.72	4 (23%)
5	NAG	E	610	1	14,14,15	0.48	0	17,19,21	1.79	5 (29%)
7	GOL	B	606	-	5,5,5	0.18	0	5,5,5	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	609	1	14,14,15	0.61	0	17,19,21	1.81	4 (23%)
7	GOL	D	606	-	5,5,5	0.13	0	5,5,5	0.34	0
5	NAG	C	608	1	14,14,15	0.50	0	17,19,21	0.84	1 (5%)
6	PEG	E	602	-	6,6,6	0.45	0	5,5,5	0.31	0
4	FAD	C	601	-	58,58,58	0.64	1 (1%)	85,89,89	0.76	2 (2%)
5	NAG	E	608	1	14,14,15	0.29	0	17,19,21	1.32	3 (17%)
6	PEG	A	605	-	6,6,6	0.32	0	5,5,5	0.30	0
5	NAG	B	607	1	14,14,15	0.47	0	17,19,21	1.46	3 (17%)
4	FAD	E	603	-	58,58,58	0.64	0	85,89,89	0.85	3 (3%)
6	PEG	A	603	-	6,6,6	0.22	0	5,5,5	0.14	0
5	NAG	B	604	1	14,14,15	0.94	1 (7%)	17,19,21	1.76	3 (17%)
5	NAG	C	604	1	14,14,15	0.42	0	17,19,21	1.36	2 (11%)
5	NAG	F	604	1	14,14,15	0.45	0	17,19,21	1.85	1 (5%)
6	PEG	F	611	-	6,6,6	0.20	0	5,5,5	0.12	0
6	PEG	D	603	-	6,6,6	0.37	0	5,5,5	0.24	0
5	NAG	F	612	1	14,14,15	0.67	0	17,19,21	1.52	3 (17%)

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
6	PEG	B	605	-	-	1/4/4/4	-
5	NAG	C	607	1	-	2/6/23/26	0/1/1/1
5	NAG	E	604	1	-	2/6/23/26	0/1/1/1
5	NAG	D	607	1	-	2/6/23/26	0/1/1/1
5	NAG	F	607	1	-	0/6/23/26	0/1/1/1
6	PEG	B	610	-	-	4/4/4/4	-
6	PEG	C	605	-	-	3/4/4/4	-
6	PEG	D	605	-	-	2/4/4/4	-
4	FAD	A	601	-	-	4/34/50/50	0/6/6/6
5	NAG	D	602	1	-	1/6/23/26	0/1/1/1
5	NAG	D	604	1	-	2/6/23/26	0/1/1/1
5	NAG	E	609	1	-	2/6/23/26	0/1/1/1
5	NAG	A	607	1	-	2/6/23/26	0/1/1/1
5	NAG	D	608	1	-	2/6/23/26	0/1/1/1
6	PEG	A	608	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	F	609	-	-	2/4/4/4	-
5	NAG	A	604	1	-	2/6/23/26	0/1/1/1
7	GOL	C	606	-	-	0/4/4/4	-
6	PEG	F	608	-	-	2/4/4/4	-
6	PEG	F	605	-	-	3/4/4/4	-
6	PEG	E	601	-	-	4/4/4/4	-
6	PEG	C	603	-	-	1/4/4/4	-
7	GOL	F	606	-	-	0/4/4/4	-
6	PEG	F	603	-	-	3/4/4/4	-
6	PEG	B	603	-	-	2/4/4/4	-
5	NAG	A	609	1	-	1/6/23/26	0/1/1/1
7	GOL	A	606	-	-	3/4/4/4	-
7	GOL	E	607	-	-	4/4/4/4	-
4	FAD	D	601	-	-	2/34/50/50	0/6/6/6
5	NAG	C	602	1	-	2/6/23/26	0/1/1/1
6	PEG	E	605	-	-	2/4/4/4	-
4	FAD	B	601	-	-	2/34/50/50	0/6/6/6
6	PEG	B	608	-	-	2/4/4/4	-
4	FAD	F	601	-	-	4/34/50/50	0/6/6/6
5	NAG	F	602	1	-	2/6/23/26	0/1/1/1
6	PEG	F	610	-	-	2/4/4/4	-
5	NAG	A	602	1	-	2/6/23/26	0/1/1/1
6	PEG	E	606	-	-	3/4/4/4	-
5	NAG	B	602	1	-	0/6/23/26	0/1/1/1
5	NAG	E	610	1	-	2/6/23/26	0/1/1/1
7	GOL	B	606	-	-	0/4/4/4	-
5	NAG	B	609	1	-	0/6/23/26	0/1/1/1
7	GOL	D	606	-	-	2/4/4/4	-
5	NAG	C	608	1	-	4/6/23/26	0/1/1/1
6	PEG	E	602	-	-	4/4/4/4	-
4	FAD	C	601	-	-	2/34/50/50	0/6/6/6
5	NAG	E	608	1	-	2/6/23/26	0/1/1/1
6	PEG	A	605	-	-	3/4/4/4	-
5	NAG	B	607	1	-	2/6/23/26	0/1/1/1
4	FAD	E	603	-	-	3/34/50/50	0/6/6/6
6	PEG	A	603	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	604	1	-	2/6/23/26	0/1/1/1
5	NAG	C	604	1	-	5/6/23/26	0/1/1/1
5	NAG	F	604	1	-	2/6/23/26	0/1/1/1
6	PEG	F	611	-	-	1/4/4/4	-
6	PEG	D	603	-	-	2/4/4/4	-
5	NAG	F	612	1	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	FAD	C1'-C2'	-3.45	1.47	1.52
5	B	604	NAG	C1-C2	2.98	1.56	1.52
4	C	601	FAD	C1'-C2'	-2.28	1.49	1.52
5	A	604	NAG	C1-C2	2.27	1.55	1.52
4	D	601	FAD	P-O3P	2.00	1.61	1.59
4	F	601	FAD	C8A-N9A	2.00	1.40	1.37

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	604	NAG	C1-O5-C5	8.33	123.35	112.19
5	F	607	NAG	C1-O5-C5	7.28	121.94	112.19
5	F	604	NAG	C1-O5-C5	6.05	120.30	112.19
5	E	604	NAG	C2-N2-C7	5.81	130.68	122.90
5	B	604	NAG	C2-N2-C7	5.24	129.92	122.90
5	B	609	NAG	C3-C4-C5	-4.83	101.47	110.23
5	E	604	NAG	O5-C1-C2	-4.63	104.13	111.29
5	E	610	NAG	C1-O5-C5	4.46	118.16	112.19
5	E	604	NAG	C8-C7-N2	-4.45	108.73	116.12
5	A	609	NAG	C1-O5-C5	4.20	117.82	112.19
5	D	608	NAG	C1-O5-C5	4.18	117.79	112.19
5	E	609	NAG	O5-C1-C2	-4.02	105.07	111.29
5	E	604	NAG	O7-C7-N2	3.95	128.97	121.98
5	C	602	NAG	O5-C1-C2	-3.89	105.27	111.29
5	F	602	NAG	O5-C1-C2	-3.86	105.31	111.29
5	F	602	NAG	O7-C7-N2	3.84	128.76	121.98
5	E	604	NAG	C3-C4-C5	-3.73	103.47	110.23
5	B	602	NAG	O5-C1-C2	-3.66	105.62	111.29
5	C	602	NAG	O7-C7-N2	3.63	128.40	121.98
5	A	604	NAG	C1-O5-C5	3.58	116.99	112.19
5	C	604	NAG	C1-O5-C5	3.47	116.84	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	602	NAG	C1-C2-N2	3.38	115.76	110.43
4	E	603	FAD	O2P-P-O1P	3.37	128.12	112.44
5	F	612	NAG	C1-O5-C5	3.36	116.69	112.19
5	C	607	NAG	C1-O5-C5	3.29	116.59	112.19
5	B	607	NAG	C1-O5-C5	3.27	116.56	112.19
5	A	604	NAG	O5-C1-C2	-3.22	106.31	111.29
5	D	602	NAG	O5-C1-C2	-3.22	106.31	111.29
5	D	607	NAG	O5-C1-C2	-3.16	106.41	111.29
5	A	607	NAG	C4-C3-C2	3.15	115.63	111.02
5	B	602	NAG	C4-C3-C2	3.11	115.57	111.02
5	D	604	NAG	C3-C4-C5	3.10	115.85	110.23
5	D	607	NAG	C1-C2-N2	3.08	115.29	110.43
5	E	604	NAG	C4-C3-C2	3.07	115.52	111.02
5	A	607	NAG	C1-O5-C5	3.05	116.27	112.19
5	A	607	NAG	O5-C5-C6	-3.00	101.81	107.66
5	A	607	NAG	C1-C2-N2	-2.97	105.75	110.43
5	F	607	NAG	C6-C5-C4	-2.96	105.75	113.02
5	D	604	NAG	O5-C5-C4	2.85	117.77	110.83
5	C	604	NAG	C4-C3-C2	-2.84	106.86	111.02
5	B	604	NAG	C1-O5-C5	2.82	115.97	112.19
5	F	602	NAG	C4-C3-C2	2.82	115.15	111.02
5	A	607	NAG	C3-C4-C5	2.79	115.30	110.23
4	A	601	FAD	O2P-P-O1P	2.77	125.34	112.44
5	A	602	NAG	O4-C4-C5	2.77	116.14	109.32
5	A	602	NAG	O5-C1-C2	-2.77	107.01	111.29
5	C	602	NAG	C3-C4-C5	-2.70	105.34	110.23
5	F	602	NAG	C2-N2-C7	2.69	126.51	122.90
5	B	609	NAG	O4-C4-C5	2.68	115.93	109.32
5	C	607	NAG	C3-C4-C5	2.65	115.03	110.23
5	E	608	NAG	C4-C3-C2	-2.62	107.18	111.02
5	B	602	NAG	C8-C7-N2	-2.60	111.81	116.12
5	D	602	NAG	C1-C2-N2	2.56	114.47	110.43
5	E	610	NAG	C4-C3-C2	-2.52	107.32	111.02
5	A	607	NAG	O4-C4-C3	-2.52	104.44	110.38
5	D	602	NAG	C4-C3-C2	2.52	114.71	111.02
5	C	602	NAG	C8-C7-N2	-2.51	111.95	116.12
5	F	602	NAG	C8-C7-N2	-2.46	112.04	116.12
5	E	609	NAG	O4-C4-C5	2.45	115.35	109.32
5	E	609	NAG	C3-C4-C5	-2.42	105.84	110.23
5	D	602	NAG	O4-C4-C5	2.42	115.27	109.32
4	D	601	FAD	O2P-P-O1P	2.41	123.66	112.44
4	F	601	FAD	O2P-P-O1P	2.40	123.60	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	602	NAG	O7-C7-N2	2.39	126.20	121.98
5	A	607	NAG	C2-N2-C7	-2.38	119.70	122.90
5	F	612	NAG	O4-C4-C5	2.35	115.11	109.32
5	B	604	NAG	O5-C1-C2	-2.34	107.67	111.29
5	D	608	NAG	O5-C1-C2	2.32	114.88	111.29
5	D	602	NAG	C8-C7-N2	-2.32	112.27	116.12
5	F	607	NAG	C1-C2-N2	2.29	114.04	110.43
5	B	609	NAG	O5-C1-C2	-2.27	107.78	111.29
5	E	608	NAG	C3-C4-C5	-2.26	106.13	110.23
5	C	602	NAG	O4-C4-C5	2.22	114.79	109.32
5	D	608	NAG	C3-C4-C5	2.20	114.22	110.23
5	B	609	NAG	C4-C3-C2	-2.20	107.80	111.02
5	E	610	NAG	C3-C4-C5	-2.19	106.26	110.23
5	E	610	NAG	O4-C4-C5	2.17	114.67	109.32
5	B	607	NAG	O5-C1-C2	-2.16	107.95	111.29
4	C	601	FAD	O2P-P-O1P	2.16	122.49	112.44
5	B	607	NAG	C2-N2-C7	-2.16	120.01	122.90
5	E	610	NAG	O5-C5-C6	2.15	111.85	107.66
4	B	601	FAD	C4-N3-C2	-2.15	121.83	125.64
5	A	602	NAG	C8-C7-N2	-2.12	112.60	116.12
5	E	609	NAG	C4-C3-C2	-2.11	107.92	111.02
4	E	603	FAD	O5'-P-O1P	-2.10	100.61	108.94
4	E	603	FAD	C4-N3-C2	-2.10	121.92	125.64
5	A	602	NAG	C3-C4-C5	-2.09	106.44	110.23
5	F	612	NAG	O6-C6-C5	-2.07	104.27	111.33
5	F	602	NAG	C3-C4-C5	-2.07	106.47	110.23
5	A	604	NAG	C1-C2-N2	2.07	113.69	110.43
5	E	608	NAG	C1-C2-N2	2.06	113.69	110.43
5	A	602	NAG	O7-C7-N2	2.04	125.59	121.98
5	F	607	NAG	C3-C4-C5	2.03	113.92	110.23
4	D	601	FAD	C4-N3-C2	-2.02	122.06	125.64
5	C	608	NAG	C2-N2-C7	-2.01	120.20	122.90
4	C	601	FAD	C4-N3-C2	-2.00	122.08	125.64
5	F	607	NAG	O5-C5-C4	2.00	115.70	110.83

There are no chirality outliers.

All (118) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	601	FAD	PA-O3P-P-O5'
4	D	601	FAD	PA-O3P-P-O5'
4	E	603	FAD	PA-O3P-P-O5'

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Mol	Chain	Res	Type	Atoms
5	C	604	NAG	C3-C2-N2-C7
5	C	604	NAG	C8-C7-N2-C2
5	C	604	NAG	O7-C7-N2-C2
5	C	608	NAG	C8-C7-N2-C2
5	C	608	NAG	O7-C7-N2-C2
7	D	606	GOL	O1-C1-C2-C3
7	E	607	GOL	O1-C1-C2-C3
7	E	607	GOL	C1-C2-C3-O3
5	E	610	NAG	O5-C5-C6-O6
5	A	607	NAG	C4-C5-C6-O6
5	D	607	NAG	O5-C5-C6-O6
5	E	609	NAG	O5-C5-C6-O6
5	D	608	NAG	O5-C5-C6-O6
5	E	610	NAG	C4-C5-C6-O6
5	A	607	NAG	O5-C5-C6-O6
6	F	605	PEG	C4-C3-O2-C2
5	A	604	NAG	C4-C5-C6-O6
6	B	605	PEG	C4-C3-O2-C2
5	B	607	NAG	O5-C5-C6-O6
5	F	604	NAG	O5-C5-C6-O6
5	C	607	NAG	C4-C5-C6-O6
5	B	607	NAG	C4-C5-C6-O6
5	D	608	NAG	C4-C5-C6-O6
5	C	604	NAG	O5-C5-C6-O6
5	E	609	NAG	C4-C5-C6-O6
5	A	604	NAG	O5-C5-C6-O6
5	D	607	NAG	C4-C5-C6-O6
5	F	604	NAG	C4-C5-C6-O6
7	E	607	GOL	O1-C1-C2-O2
6	B	608	PEG	O2-C3-C4-O4
6	C	605	PEG	O1-C1-C2-O2
6	F	603	PEG	O1-C1-C2-O2
6	E	605	PEG	O2-C3-C4-O4
5	C	604	NAG	C4-C5-C6-O6
5	D	604	NAG	C4-C5-C6-O6
5	E	604	NAG	C4-C5-C6-O6
5	C	607	NAG	O5-C5-C6-O6
6	F	610	PEG	O2-C3-C4-O4
6	E	606	PEG	O1-C1-C2-O2
5	B	604	NAG	C4-C5-C6-O6
7	A	606	GOL	O1-C1-C2-C3
5	E	604	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	B	603	PEG	O1-C1-C2-O2
6	F	611	PEG	O2-C3-C4-O4
6	E	602	PEG	O1-C1-C2-O2
7	D	606	GOL	O1-C1-C2-O2
7	A	606	GOL	O1-C1-C2-O2
5	C	602	NAG	O5-C5-C6-O6
5	C	602	NAG	C4-C5-C6-O6
5	B	604	NAG	O5-C5-C6-O6
6	B	608	PEG	O1-C1-C2-O2
6	A	605	PEG	O2-C3-C4-O4
6	A	608	PEG	O2-C3-C4-O4
6	B	603	PEG	O2-C3-C4-O4
6	B	610	PEG	O1-C1-C2-O2
6	B	610	PEG	O2-C3-C4-O4
6	C	603	PEG	O2-C3-C4-O4
6	C	605	PEG	O2-C3-C4-O4
6	D	605	PEG	O2-C3-C4-O4
6	A	605	PEG	O1-C1-C2-O2
6	F	608	PEG	O1-C1-C2-O2
6	F	608	PEG	O2-C3-C4-O4
7	E	607	GOL	O2-C2-C3-O3
5	E	608	NAG	O5-C5-C6-O6
6	E	601	PEG	O1-C1-C2-O2
6	E	601	PEG	O2-C3-C4-O4
5	A	602	NAG	C4-C5-C6-O6
7	A	606	GOL	O2-C2-C3-O3
5	E	608	NAG	C4-C5-C6-O6
6	E	602	PEG	O2-C3-C4-O4
4	B	601	FAD	PA-O3P-P-O5'
4	A	601	FAD	PA-O3P-P-O5'
4	F	601	FAD	PA-O3P-P-O5'
6	E	602	PEG	C4-C3-O2-C2
6	F	605	PEG	O2-C3-C4-O4
6	F	603	PEG	C1-C2-O2-C3
6	D	603	PEG	C4-C3-O2-C2
6	A	603	PEG	C4-C3-O2-C2
6	C	605	PEG	C4-C3-O2-C2
6	E	601	PEG	C4-C3-O2-C2
5	F	602	NAG	C4-C5-C6-O6
4	F	601	FAD	N10-C1'-C2'-O2'
6	D	605	PEG	O1-C1-C2-O2
6	E	606	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
5	A	602	NAG	O5-C5-C6-O6
6	B	610	PEG	C4-C3-O2-C2
5	C	608	NAG	O5-C5-C6-O6
4	A	601	FAD	O4B-C4B-C5B-O5B
6	A	608	PEG	C1-C2-O2-C3
6	F	605	PEG	O1-C1-C2-O2
6	F	610	PEG	C1-C2-O2-C3
6	E	605	PEG	C1-C2-O2-C3
5	F	602	NAG	O5-C5-C6-O6
4	B	601	FAD	O4B-C4B-C5B-O5B
5	C	608	NAG	C4-C5-C6-O6
5	D	604	NAG	O5-C5-C6-O6
7	F	609	GOL	O1-C1-C2-C3
6	F	603	PEG	C4-C3-O2-C2
6	E	606	PEG	C4-C3-O2-C2
6	E	602	PEG	C1-C2-O2-C3
6	A	605	PEG	C4-C3-O2-C2
7	F	609	GOL	O1-C1-C2-O2
6	B	610	PEG	C1-C2-O2-C3
6	D	603	PEG	O1-C1-C2-O2
5	A	609	NAG	C4-C5-C6-O6
4	D	601	FAD	O4B-C4B-C5B-O5B
4	F	601	FAD	P-O3P-PA-O1A
4	F	601	FAD	P-O3P-PA-O2A
6	E	601	PEG	C1-C2-O2-C3
4	A	601	FAD	C3B-C4B-C5B-O5B
5	D	602	NAG	C4-C5-C6-O6
4	C	601	FAD	P-O3P-PA-O2A
4	A	601	FAD	P-O3P-PA-O2A
4	E	603	FAD	P-O3P-PA-O1A
4	E	603	FAD	P-O3P-PA-O2A

There are no ring outliers.

34 monomers are involved in 83 short contacts:

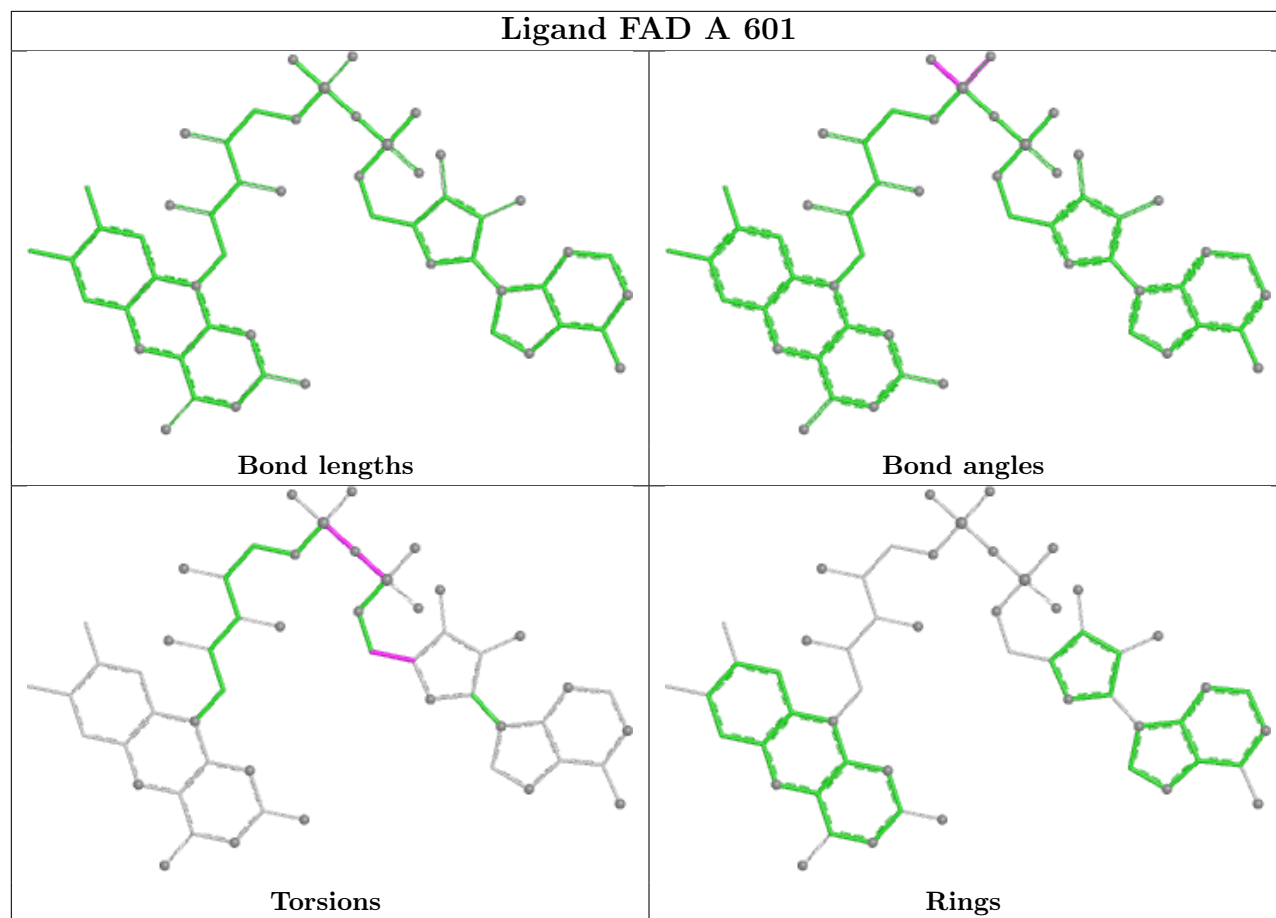
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	607	NAG	1	0
6	C	605	PEG	1	0
6	D	605	PEG	1	0
4	A	601	FAD	5	0
5	D	604	NAG	2	0
5	E	609	NAG	3	0

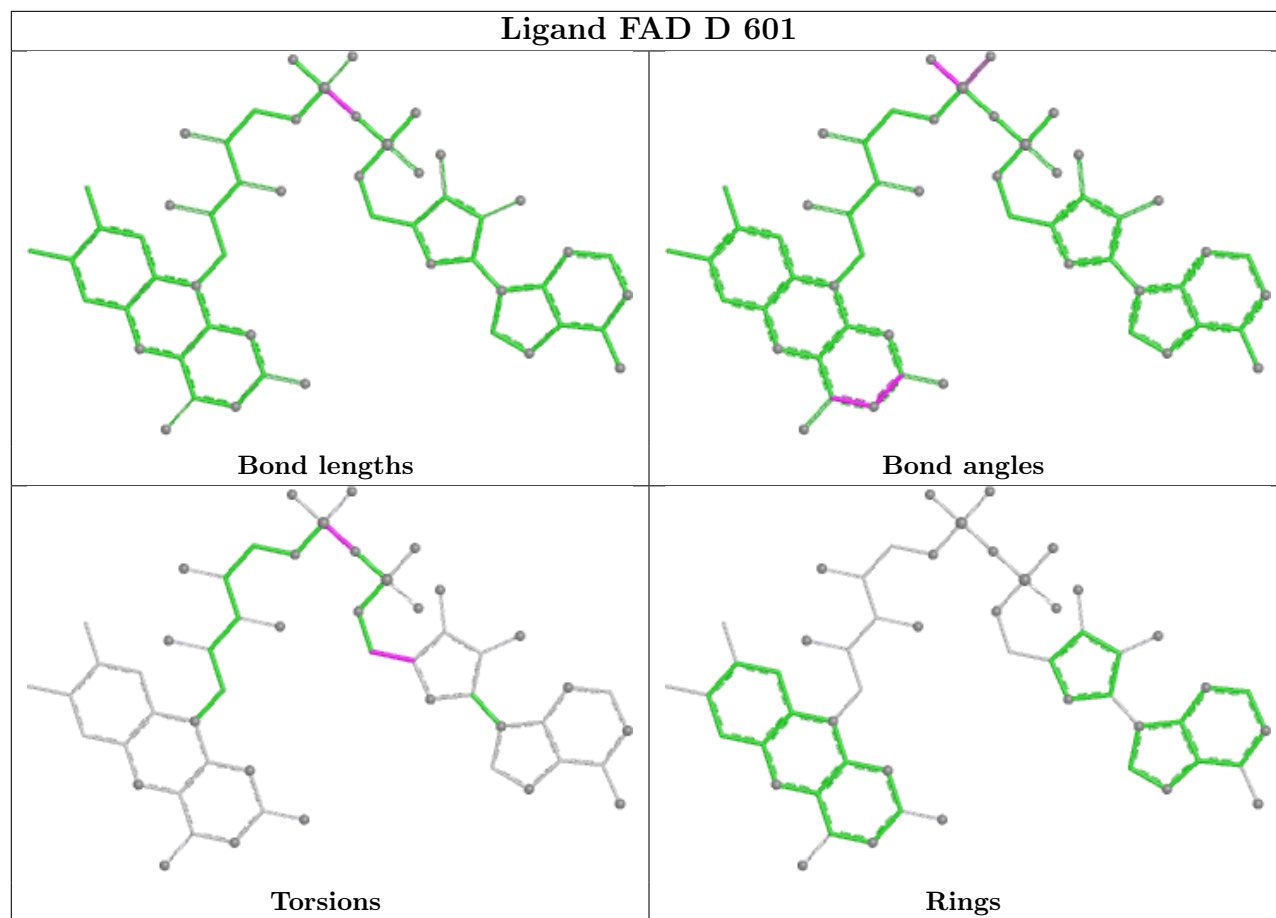
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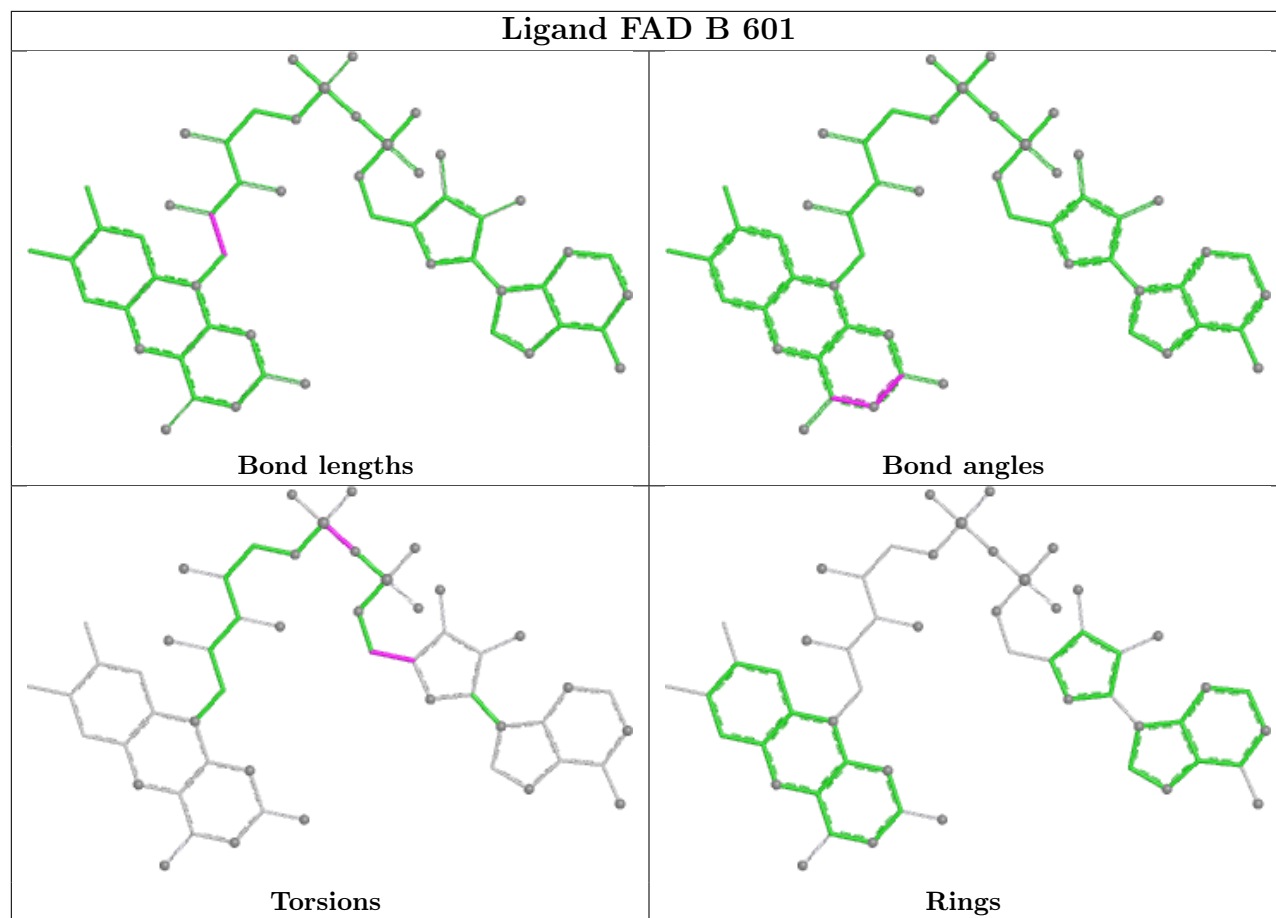
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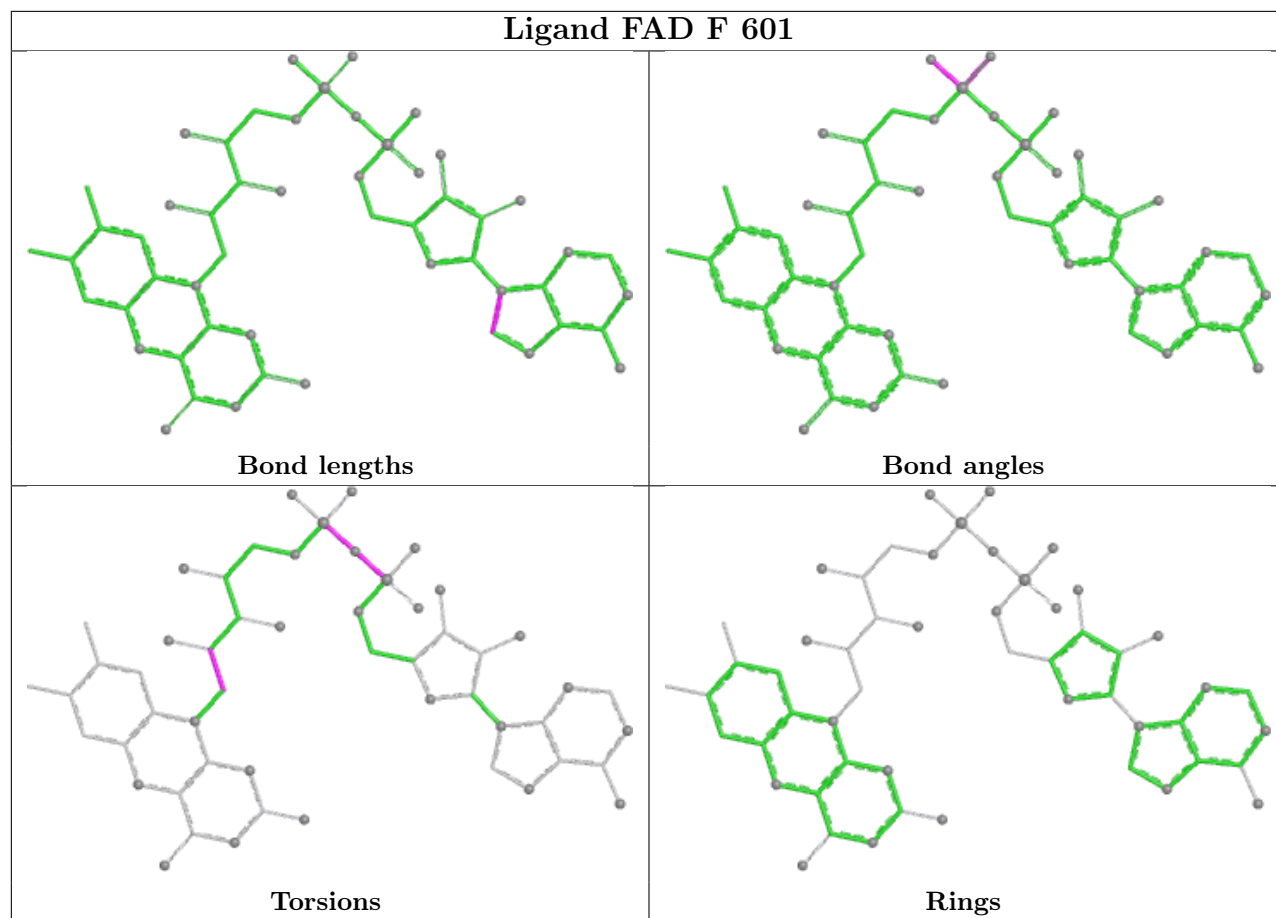
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	609	GOL	3	0
5	A	604	NAG	3	0
7	C	606	GOL	3	0
6	F	608	PEG	1	0
6	C	603	PEG	1	0
7	F	606	GOL	1	0
6	F	603	PEG	1	0
6	B	603	PEG	1	0
7	A	606	GOL	2	0
7	E	607	GOL	4	0
4	D	601	FAD	6	0
6	E	605	PEG	1	0
4	B	601	FAD	5	0
4	F	601	FAD	5	0
6	F	610	PEG	10	0
6	E	606	PEG	1	0
7	B	606	GOL	3	0
7	D	606	GOL	1	0
5	C	608	NAG	1	0
6	E	602	PEG	1	0
4	C	601	FAD	6	0
6	A	605	PEG	1	0
4	E	603	FAD	5	0
6	A	603	PEG	1	0
5	B	604	NAG	1	0
5	C	604	NAG	3	0
5	F	604	NAG	1	0
6	D	603	PEG	1	0

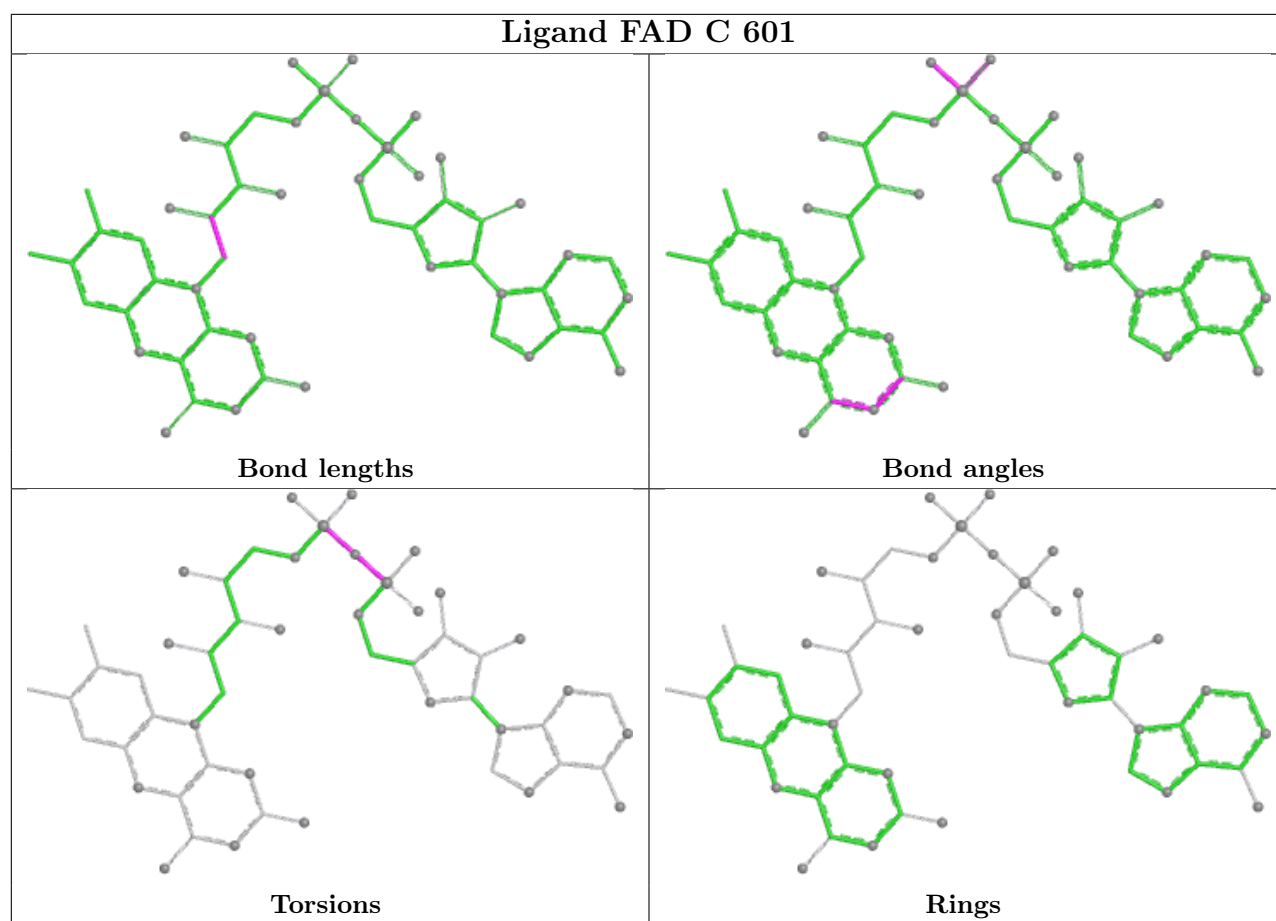
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

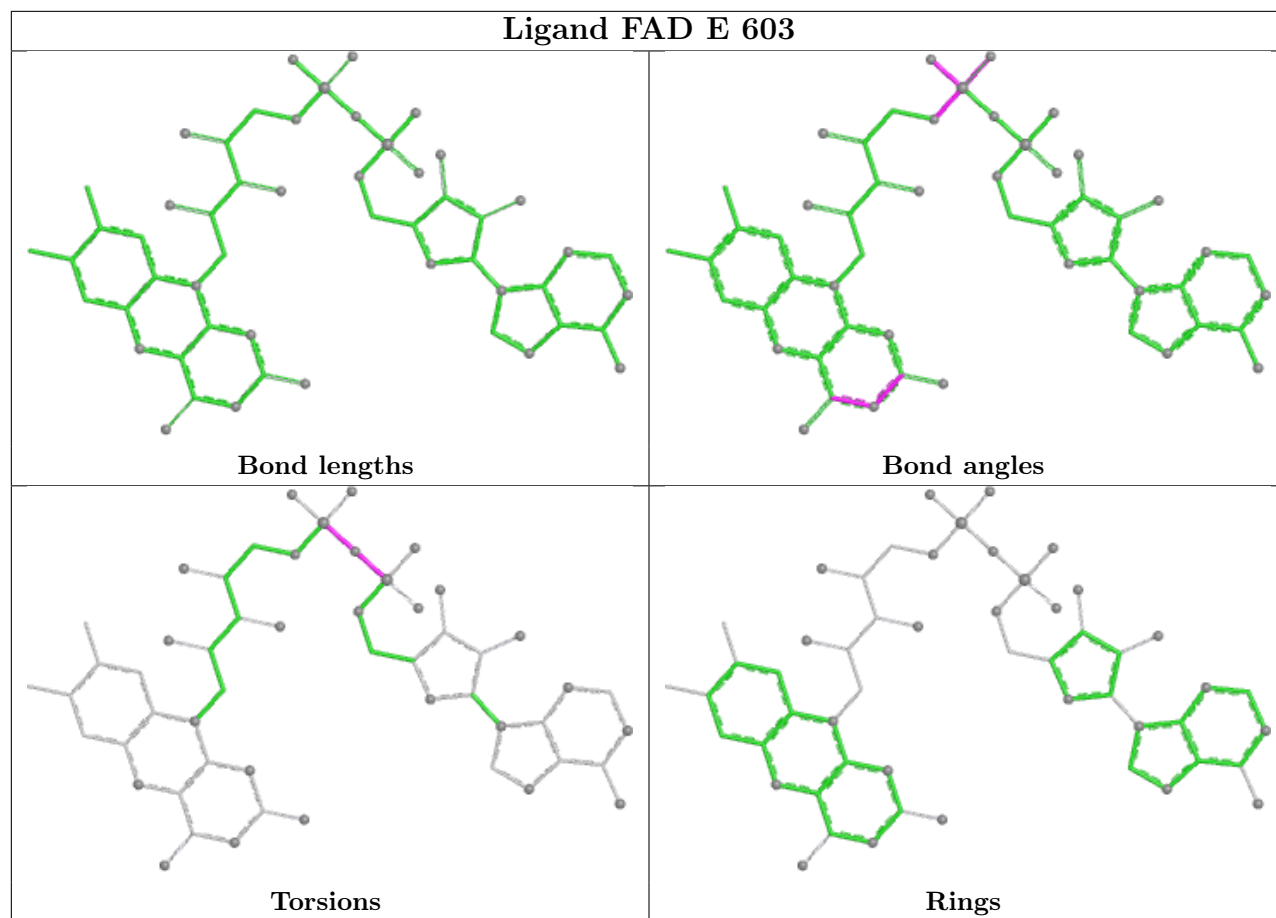












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	590/628 (93%)	-0.21	2 (0%) 90 88	19, 32, 52, 86	0
1	B	590/628 (93%)	-0.32	2 (0%) 90 88	19, 31, 50, 71	0
1	C	590/628 (93%)	-0.09	4 (0%) 84 81	26, 39, 61, 87	0
1	D	590/628 (93%)	0.65	31 (5%) 32 28	28, 53, 80, 104	0
1	E	590/628 (93%)	-0.23	3 (0%) 87 85	20, 32, 54, 80	0
1	F	590/628 (93%)	-0.06	4 (0%) 84 81	23, 38, 58, 87	0
All	All	3540/3768 (93%)	-0.04	46 (1%) 75 71	19, 37, 66, 104	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	261	ASP	3.9
1	A	261	ASP	3.7
1	E	261	ASP	3.6
1	D	475	LEU	3.4
1	D	387	ALA	3.4
1	F	261	ASP	3.3
1	D	154	ASP	3.2
1	F	475	LEU	3.2
1	D	202	GLN	3.0
1	D	493	LYS	2.8
1	D	436	LEU	2.7
1	E	202	GLN	2.7
1	D	508	ALA	2.7
1	D	431	TYR	2.6
1	D	194	HIS	2.6
1	D	537	ASN	2.6
1	D	393	THR	2.6
1	B	242	ALA	2.6
1	D	174	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	382	GLU	2.5
1	D	506	GLN	2.5
1	D	438	VAL	2.5
1	D	491	ALA	2.5
1	D	504	GLY	2.4
1	D	497	ILE	2.4
1	F	339	ASN	2.4
1	D	99	ARG	2.4
1	A	160	ASN	2.4
1	D	185	ALA	2.4
1	D	490	THR	2.3
1	B	261	ASP	2.3
1	C	590	CYS	2.3
1	D	499	PRO	2.3
1	C	99	ARG	2.3
1	D	306	ALA	2.2
1	D	496	LEU	2.2
1	D	513	ILE	2.2
1	D	512	GLU	2.2
1	E	382	GLU	2.2
1	D	305	ALA	2.2
1	D	589	ASN	2.2
1	F	202	GLN	2.1
1	D	507	VAL	2.1
1	D	382	GLU	2.0
1	D	417	GLY	2.0
1	D	307	THR	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.

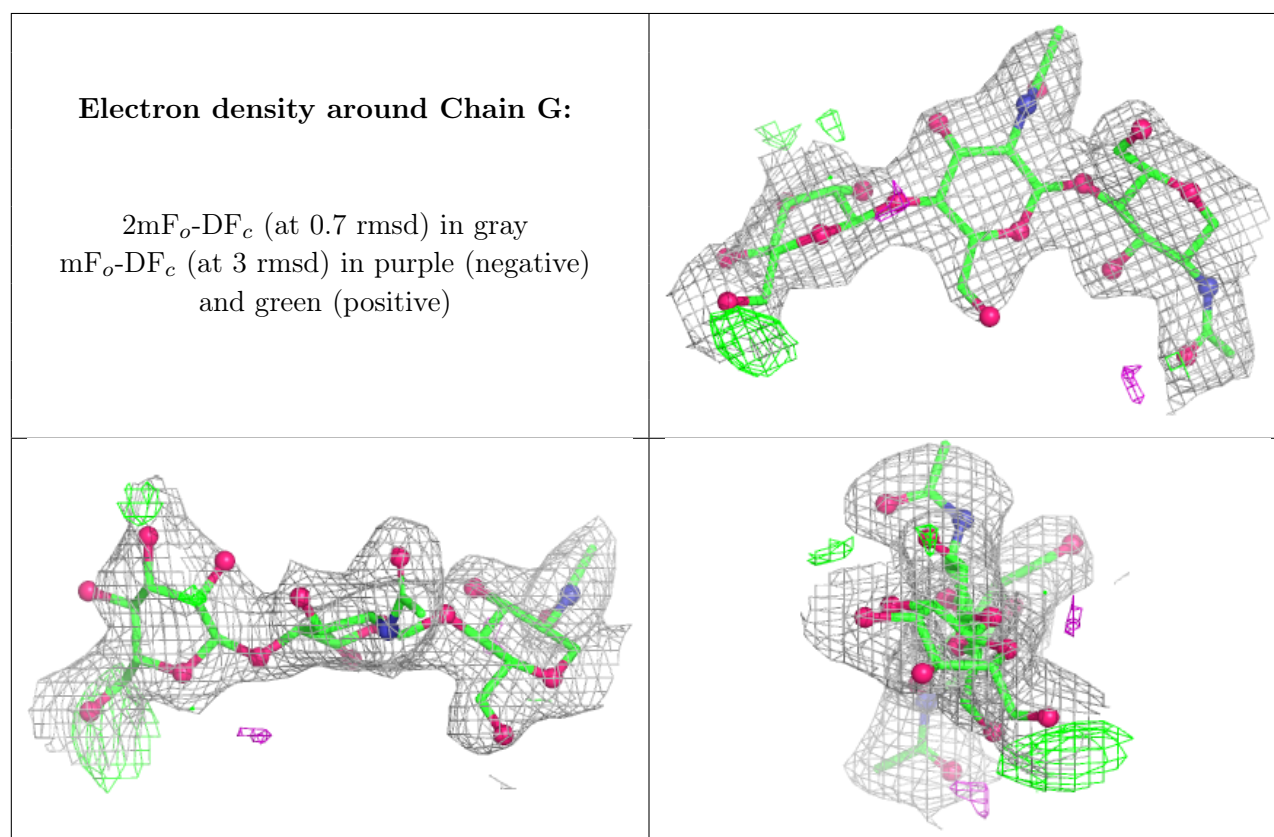
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	I	3	11/12	0.61	0.17	70,89,104,105	0

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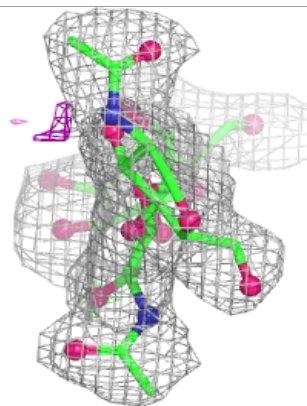
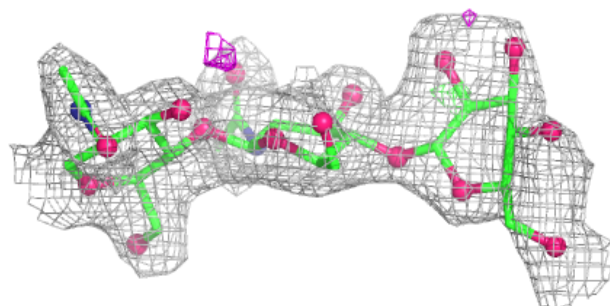
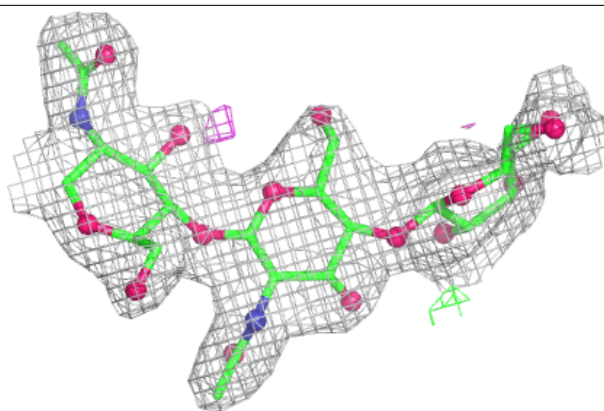
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MAN	G	3	11/12	0.67	0.18	57,84,93,95	0
2	MAN	J	3	11/12	0.71	0.17	55,74,92,95	0
2	MAN	K	3	11/12	0.73	0.16	54,76,91,99	0
2	MAN	H	3	11/12	0.80	0.15	53,76,105,108	0
3	NAG	L	2	14/15	0.84	0.12	41,52,59,61	0
2	NAG	I	2	14/15	0.87	0.13	53,66,82,99	0
2	NAG	J	2	14/15	0.89	0.12	44,54,74,85	0
2	NAG	H	2	14/15	0.89	0.10	50,62,74,74	0
2	NAG	H	1	14/15	0.91	0.10	26,37,45,46	0
2	NAG	G	2	14/15	0.92	0.11	36,49,64,67	0
2	NAG	I	1	14/15	0.93	0.09	37,42,53,55	0
3	NAG	L	1	14/15	0.93	0.08	23,33,42,54	0
2	NAG	K	2	14/15	0.93	0.09	38,45,55,73	0
2	NAG	J	1	14/15	0.94	0.08	24,28,34,52	0
2	NAG	K	1	14/15	0.94	0.08	22,29,34,47	0
2	NAG	G	1	14/15	0.95	0.07	22,28,36,46	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.

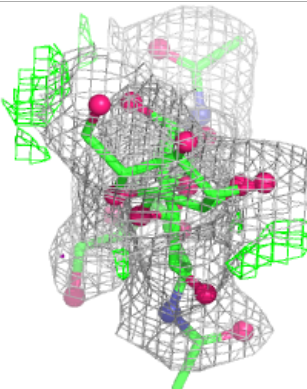
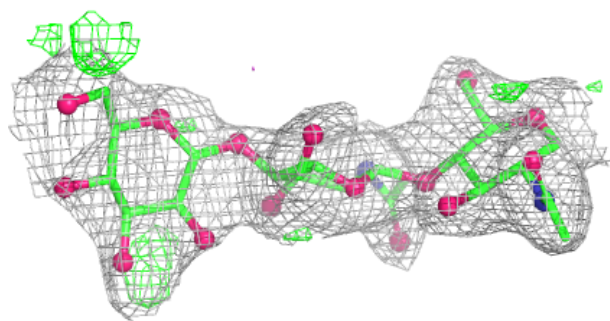
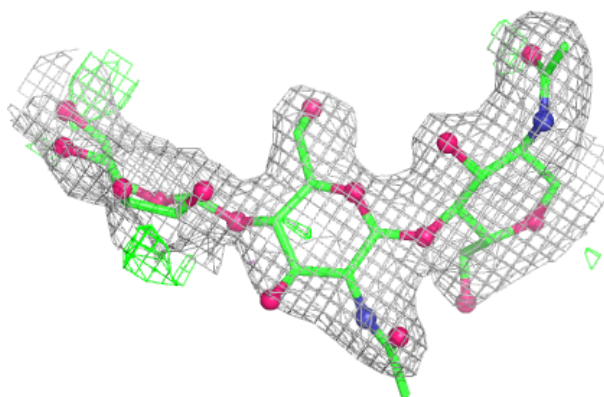


Electron density around Chain H:

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

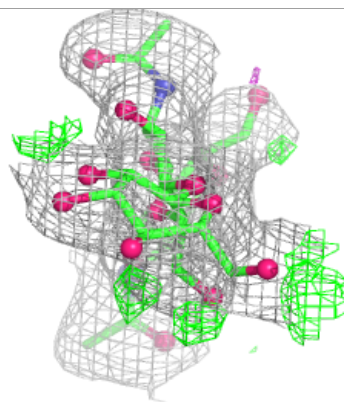
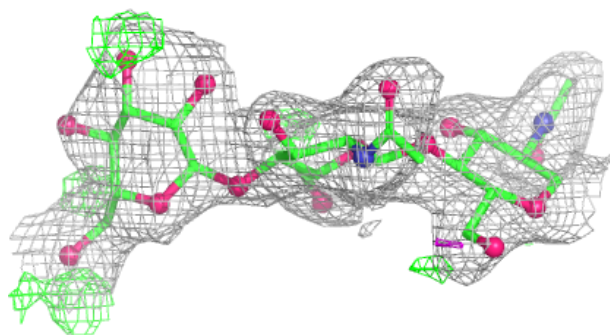
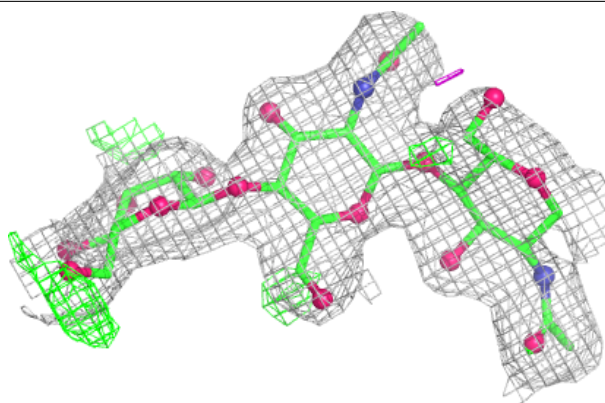
**Electron density around Chain I:**

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

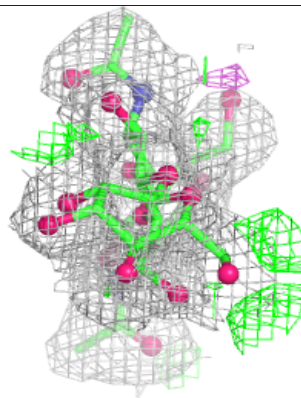
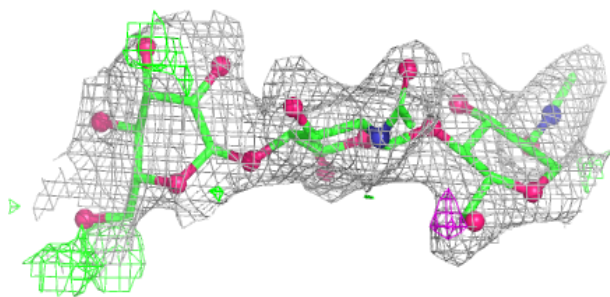
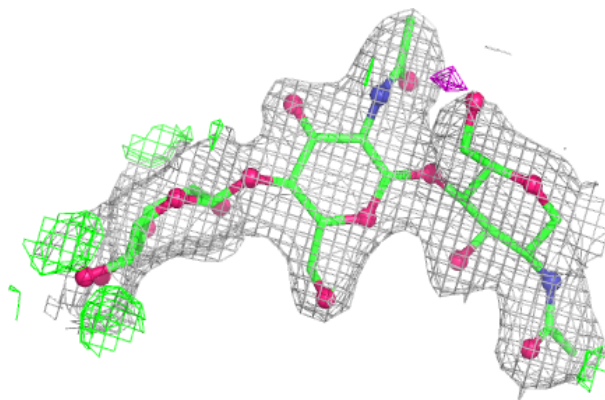


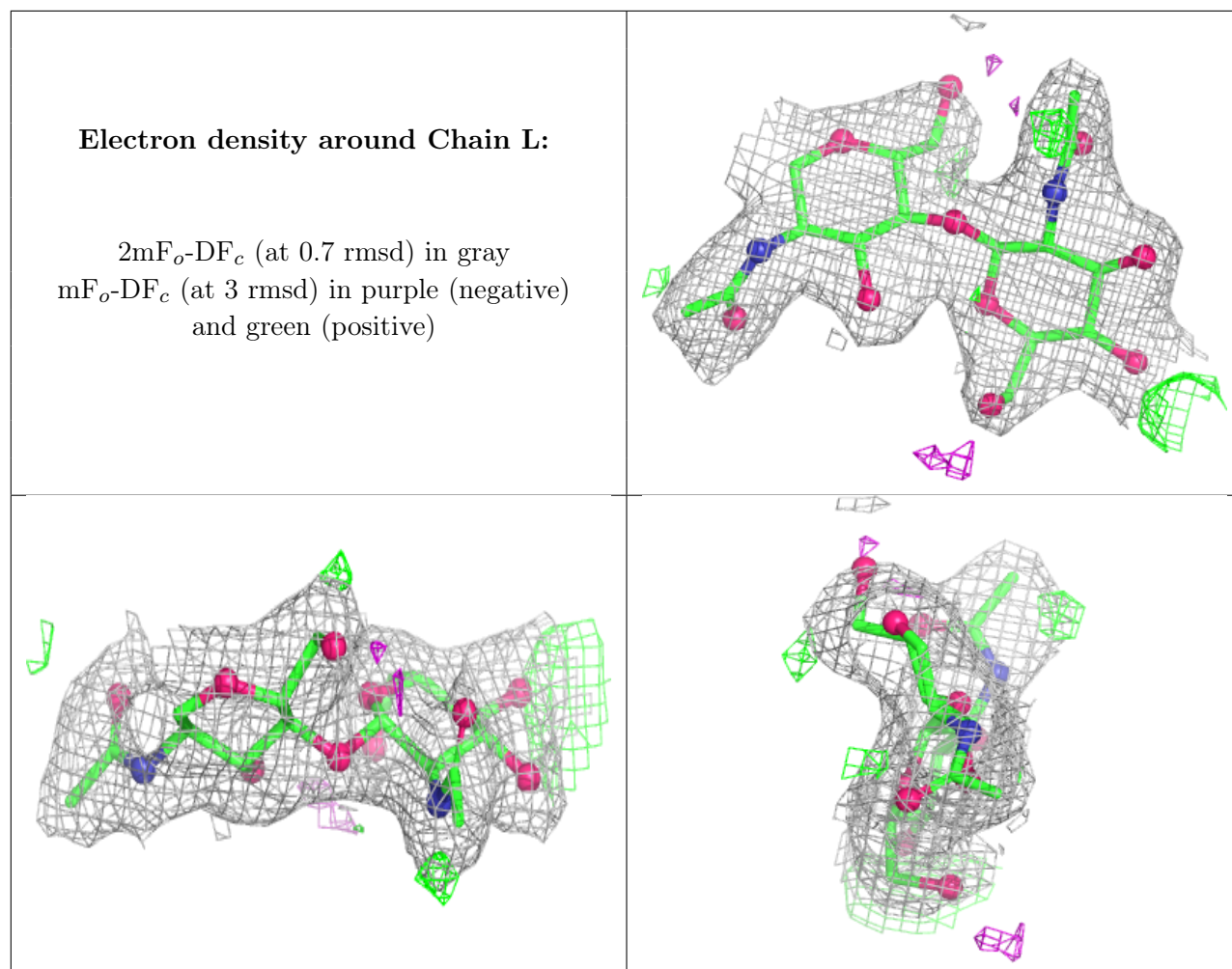
Electron density around Chain J:

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

**Electron density around Chain K:**

$2mF_o-DF_c$ (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
6	PEG	F	611	7/7	0.59	0.23	62,85,98,100	0
6	PEG	F	610	7/7	0.61	0.23	67,86,106,122	0
6	PEG	B	608	7/7	0.72	0.26	56,68,83,100	0
5	NAG	C	604	14/15	0.73	0.23	51,69,112,130	0
5	NAG	C	602	14/15	0.73	0.15	36,56,68,79	0
7	GOL	F	606	6/6	0.78	0.26	56,68,78,80	0
7	GOL	F	609	6/6	0.78	0.17	61,73,86,89	0
5	NAG	D	602	14/15	0.80	0.13	38,53,62,71	0
5	NAG	F	602	14/15	0.81	0.14	37,54,63,75	0
5	NAG	D	604	14/15	0.81	0.13	61,93,104,110	0

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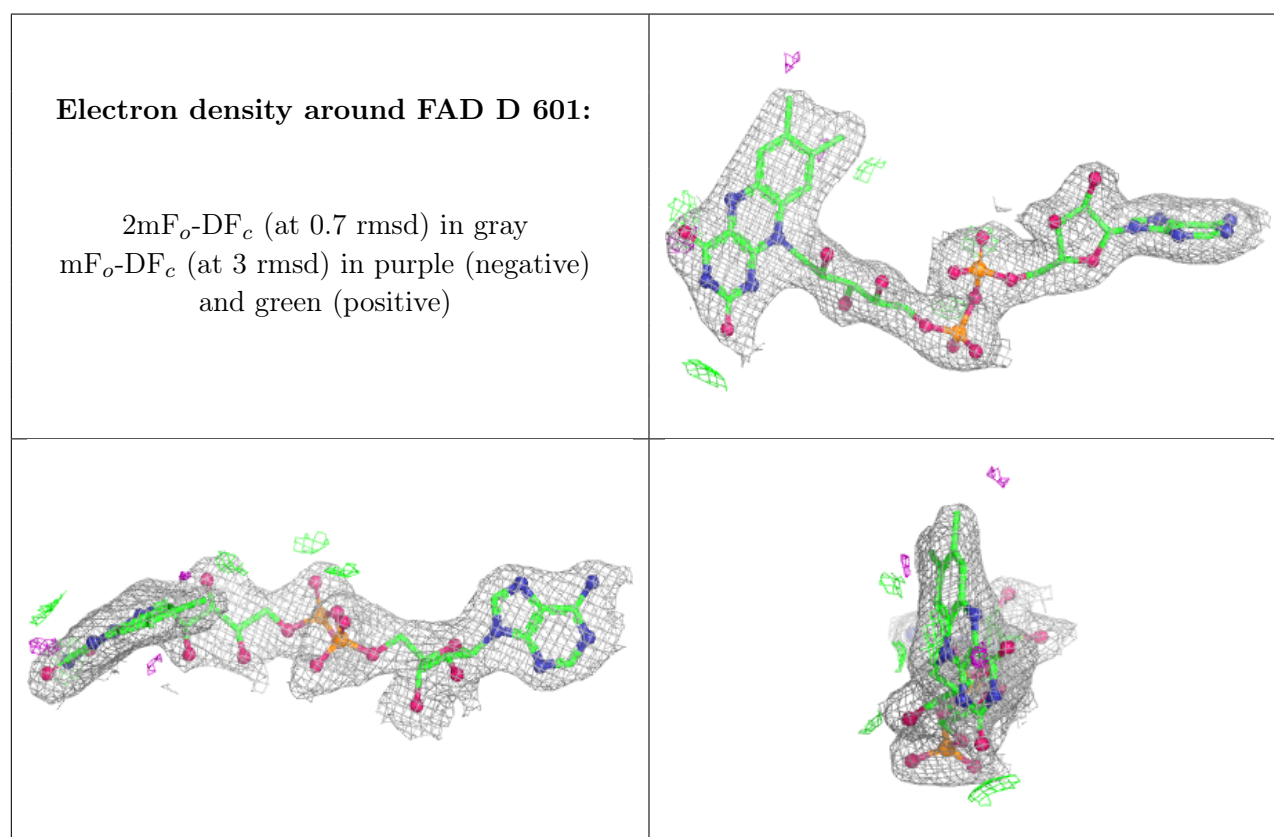
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	D	608	14/15	0.81	0.15	55,73,100,113	0
7	GOL	A	606	6/6	0.82	0.17	43,52,53,56	0
5	NAG	A	607	14/15	0.82	0.16	51,73,106,159	0
6	PEG	A	608	7/7	0.82	0.22	40,50,58,70	0
5	NAG	C	607	14/15	0.83	0.14	59,78,85,86	0
7	GOL	E	607	6/6	0.83	0.25	41,64,88,88	0
6	PEG	E	601	7/7	0.84	0.20	47,53,58,60	0
7	GOL	B	606	6/6	0.84	0.16	40,52,76,79	0
5	NAG	C	608	14/15	0.84	0.15	58,79,89,94	0
5	NAG	A	602	14/15	0.85	0.11	34,41,53,74	0
7	GOL	D	606	6/6	0.86	0.20	78,89,97,98	0
6	PEG	B	610	7/7	0.86	0.16	45,48,54,55	0
6	PEG	F	605	7/7	0.86	0.18	47,49,54,67	0
6	PEG	C	603	7/7	0.86	0.18	42,58,63,76	0
7	GOL	C	606	6/6	0.86	0.19	66,73,84,94	0
5	NAG	B	602	14/15	0.87	0.11	31,43,60,65	0
5	NAG	D	607	14/15	0.87	0.12	62,77,88,94	0
5	NAG	F	604	14/15	0.87	0.13	45,62,73,92	0
6	PEG	B	605	7/7	0.87	0.14	43,43,50,51	0
6	PEG	E	606	7/7	0.87	0.17	46,50,56,66	0
6	PEG	F	603	7/7	0.87	0.16	39,45,62,65	0
5	NAG	E	604	14/15	0.88	0.10	35,42,55,60	0
6	PEG	A	603	7/7	0.89	0.14	37,45,60,61	0
5	NAG	F	612	14/15	0.89	0.11	38,50,64,65	0
5	NAG	B	607	14/15	0.89	0.11	45,57,71,81	0
5	NAG	A	609	14/15	0.90	0.12	44,63,75,84	0
6	PEG	D	603	7/7	0.90	0.15	51,54,70,72	0
5	NAG	B	604	14/15	0.90	0.10	47,58,73,76	0
6	PEG	E	605	7/7	0.90	0.13	35,40,55,56	0
5	NAG	A	604	14/15	0.91	0.09	33,42,53,59	0
5	NAG	F	607	14/15	0.91	0.10	44,55,67,71	0
6	PEG	F	608	7/7	0.91	0.13	38,42,55,59	0
6	PEG	A	605	7/7	0.91	0.15	37,45,51,54	0
6	PEG	C	605	7/7	0.91	0.15	45,51,58,65	0
5	NAG	B	609	14/15	0.92	0.10	33,46,56,58	0
5	NAG	E	608	14/15	0.92	0.10	45,64,74,74	0
5	NAG	E	610	14/15	0.92	0.09	38,51,62,62	0
6	PEG	B	603	7/7	0.93	0.12	26,43,53,53	0
5	NAG	E	609	14/15	0.93	0.07	31,44,58,61	0
6	PEG	E	602	7/7	0.93	0.14	49,52,64,71	0
6	PEG	D	605	7/7	0.94	0.10	55,62,66,68	0
4	FAD	D	601	53/53	0.96	0.07	24,37,46,54	0

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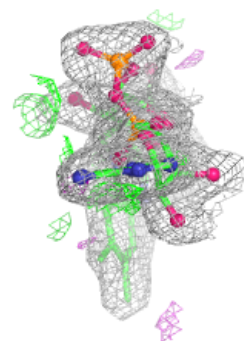
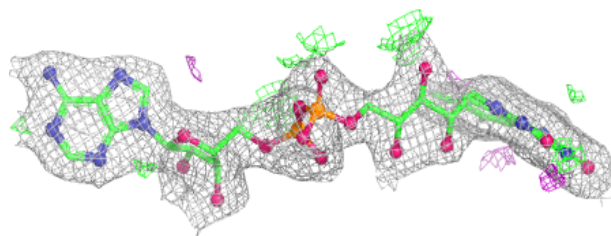
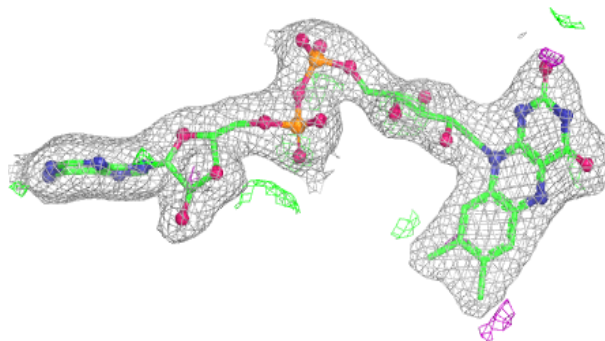
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FAD	F	601	53/53	0.97	0.06	18,27,40,42	0
4	FAD	C	601	53/53	0.97	0.07	25,36,44,49	0
4	FAD	A	601	53/53	0.98	0.06	18,24,32,39	0
4	FAD	B	601	53/53	0.98	0.06	17,25,32,35	0
4	FAD	E	603	53/53	0.98	0.06	18,26,35,39	0

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.

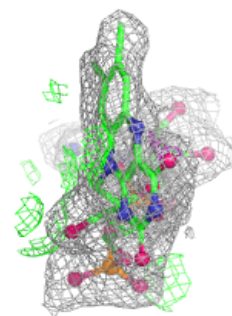
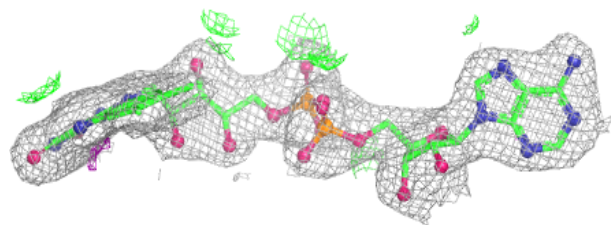
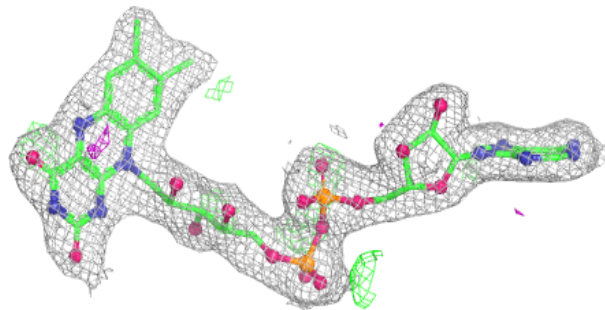


Electron density around FAD F 601:

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

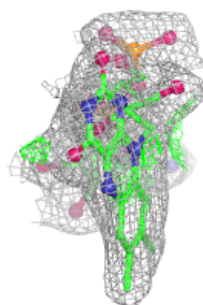
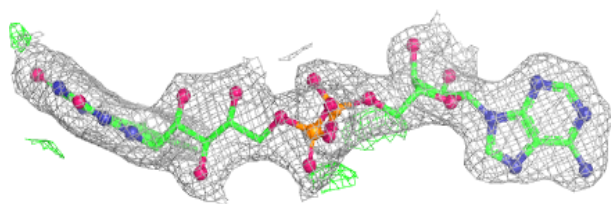
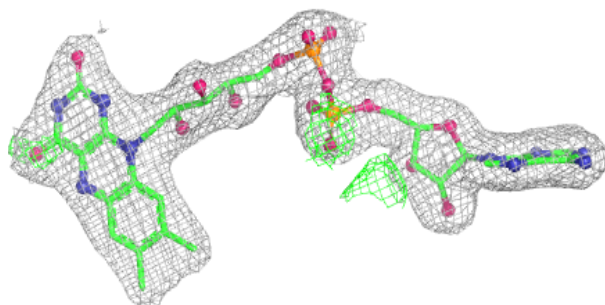
**Electron density around FAD C 601:**

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

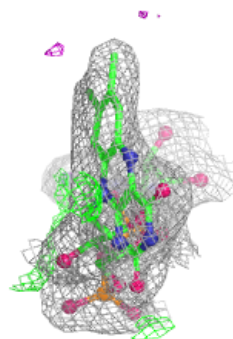
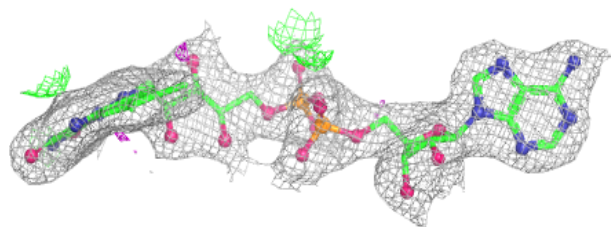
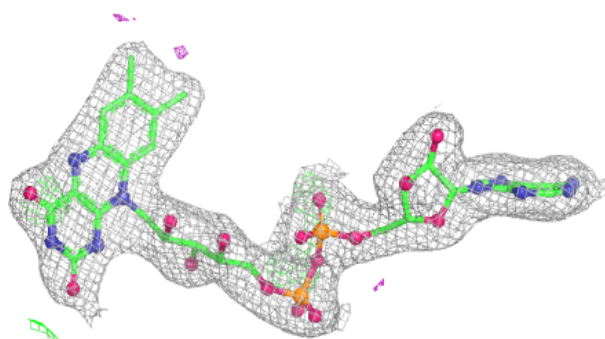


Electron density around FAD A 601:

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

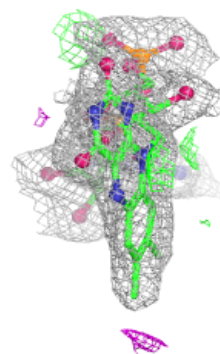
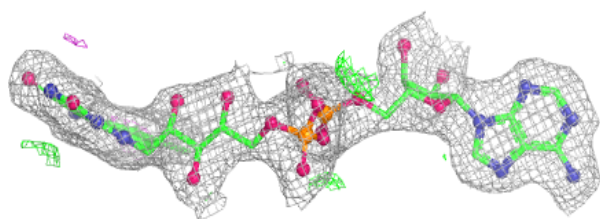
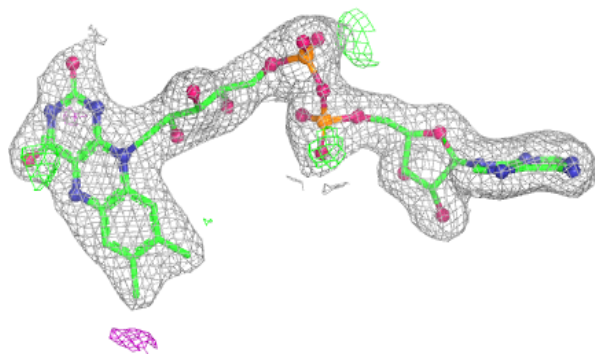
**Electron density around FAD B 601:**

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



Electron density around FAD E 603:

$2mF_o - DF_c$ (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.