Full wwPDB X-ray Structure Validation Report (i)

Oct 8, 2023 – 10:09 AM EDT

PDB ID	:	6EA4
Title	:	ERAP2 bound to Aryl Sulfonamide Uncompetitive Inhibitor
Authors	:	Maben, Z.; Stern, L.J.
Deposited on	:	2018-08-02
Resolution	:	2.45 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 (i) 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 (i)) were used in the production of this report:

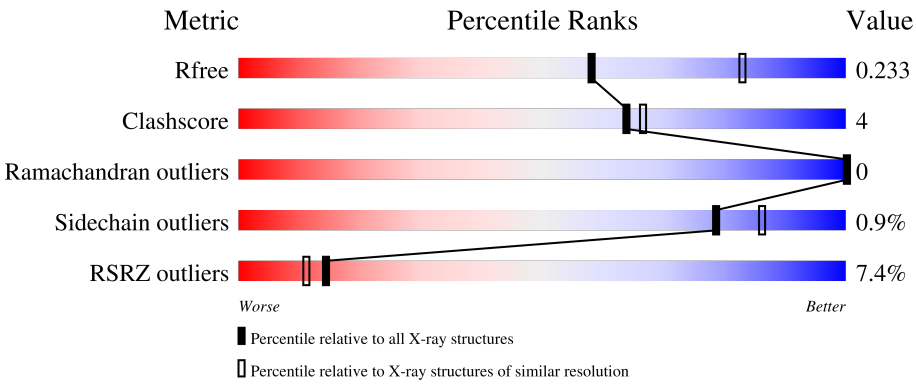
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 <=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	911	2%, 87%, 9%, •
1	B	911	12%, 83%, 12%, 5%
2	C	5	60%, 40%
2	D	5	60%, 40%
2	G	5	60%, 40%

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Mol	Chain	Length	Quality of chain
3	E	2	100%
3	F	2	100%
3	I	2	100%
4	H	3	67% 33%

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
10	IMD	B	1008	-	-	-	X
2	BMA	D	3	-	-	-	X
2	MAN	D	4	-	-	-	X
2	MAN	G	4	-	-	-	X
3	NAG	F	2	-	-	-	X
3	NAG	I	2	-	-	-	X
4	BMA	H	3	-	-	-	X
7	J2G	A	1003[A]	-	-	-	X
7	J2G	A	1003[B]	-	-	-	X
7	J2G	B	1003[A]	-	-	-	X
7	J2G	B	1003[B]	-	-	-	X
8	LYS	B	1010	-	-	-	X

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 15097 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.

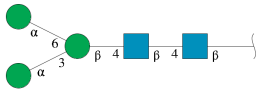
- Molecule 1 is a protein called Endoplasmic reticulum aminopeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	883	7212	4653	1201	1328	30	0	7	0
1	B	869	7054	4550	1169	1306	29	0	2	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	392	ASN	LYS	variant	UNP Q6P179
A	961	ARG	-	expression tag	UNP Q6P179
A	962	HIS	-	expression tag	UNP Q6P179
A	963	HIS	-	expression tag	UNP Q6P179
B	392	ASN	LYS	variant	UNP Q6P179
B	961	ARG	-	expression tag	UNP Q6P179
B	962	HIS	-	expression tag	UNP Q6P179
B	963	HIS	-	expression tag	UNP Q6P179

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

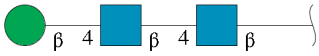


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	5	61	34	2	25	0	0	0
2	D	5	61	34	2	25	0	0	0
2	G	5	61	34	2	25	0	0	0

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

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

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

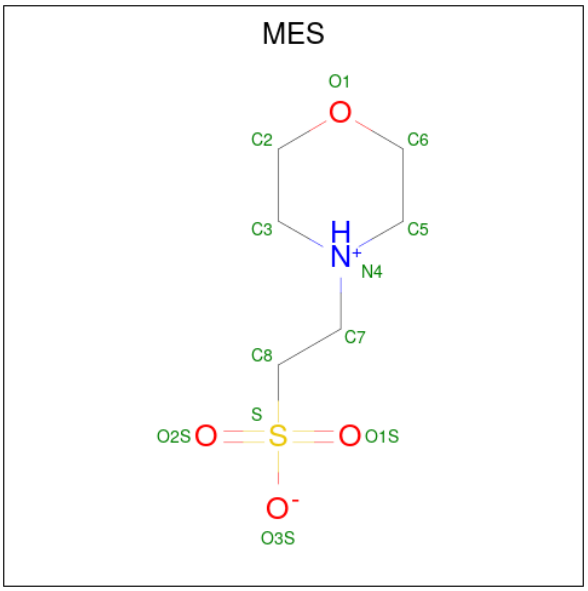


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	H	3	39	22	2	15	0	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

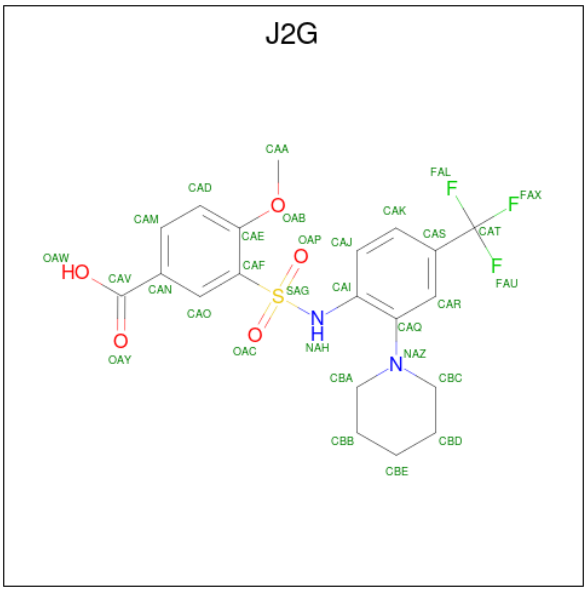
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
5	A	1	1	1	0	0
5	B	1	1	1	0	0

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
6	A	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
6	B	1	12	6	1	4	1	0	0

- Molecule 7 is 4-methoxy-3-{[2-(piperidin-1-yl)-4-(trifluoromethyl)phenyl]sulfamoyl}benzoic acid (three-letter code: J2G) (formula: $C_{20}H_{21}F_3N_2O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	S		
7	A	1	62	40	6	4	10	2	0	1

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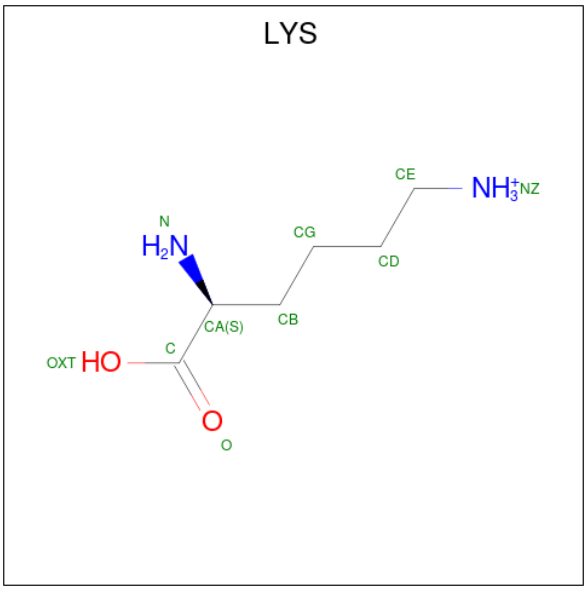
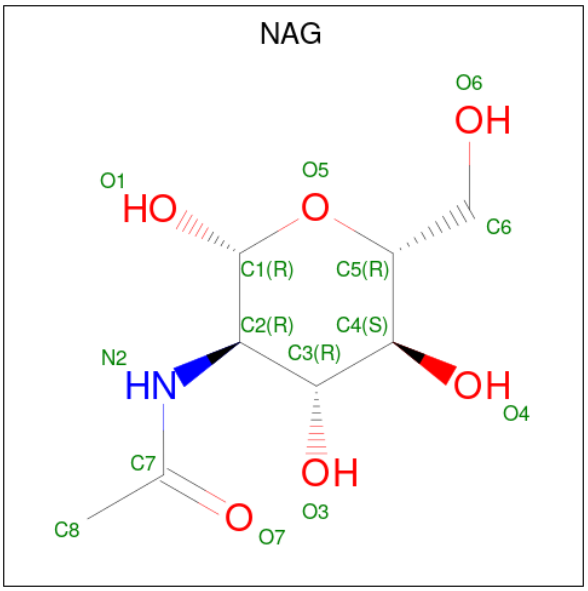
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	S		
7	B	1	62	40	6	4	10	2	0	1

- Molecule 8 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



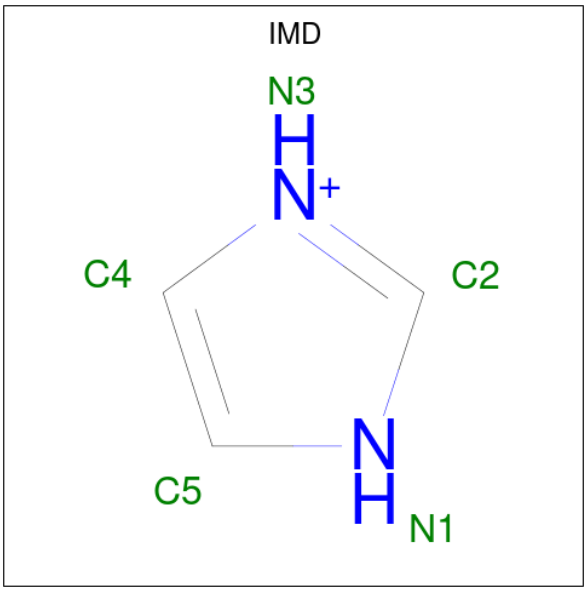
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	A	1	10	6	2	2	0	0
			Total	C	N	O		
8	A	1	10	6	2	2	0	0
			Total	C	N	O		
8	B	1	10	6	2	2	0	0
			Total	C	N	O		
8	B	1	10	6	2	2	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



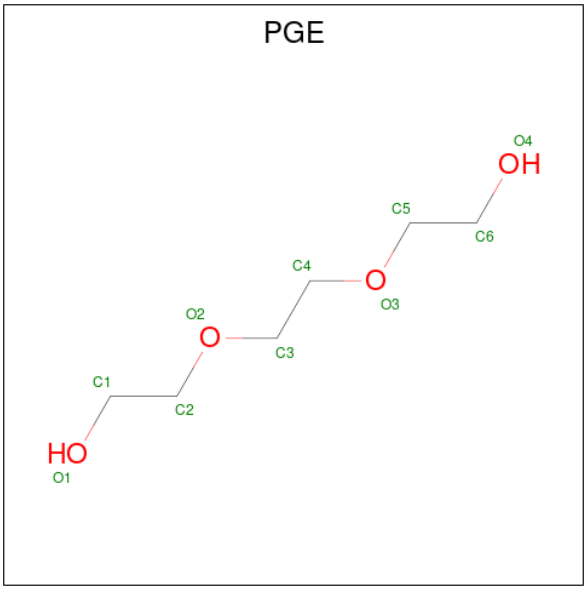
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
9	A	1	14	8	1	5	0	0
			Total	C	N	O		
9	A	1	14	8	1	5	0	0
			Total	C	N	O		
9	A	1	14	8	1	5	0	0
			Total	C	N	O		
9	A	1	14	8	1	5	0	0
			Total	C	N	O		
9	B	1	14	8	1	5	0	0
			Total	C	N	O		
9	B	1	14	8	1	5	0	0
			Total	C	N	O		
9	B	1	14	8	1	5	0	0

- Molecule 10 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



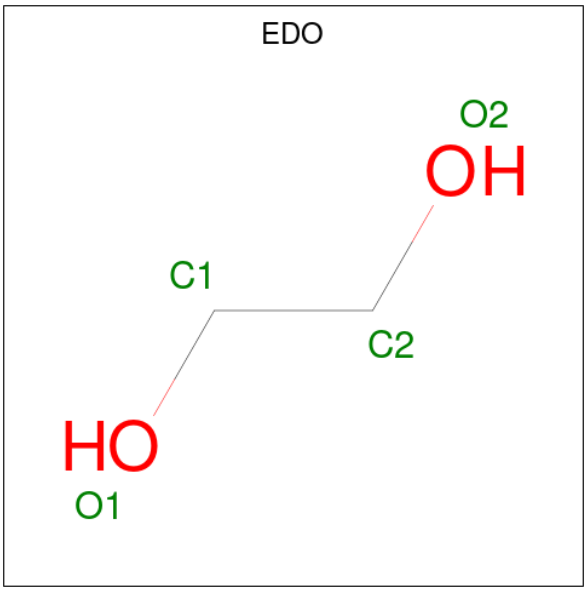
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
10	A	1	5	3	2	0	0
			Total	C	N		
10	B	1	5	3	2	0	0

- Molecule 11 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
11	A	1	10	6	4	0	0

- Molecule 12 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 13 is water.

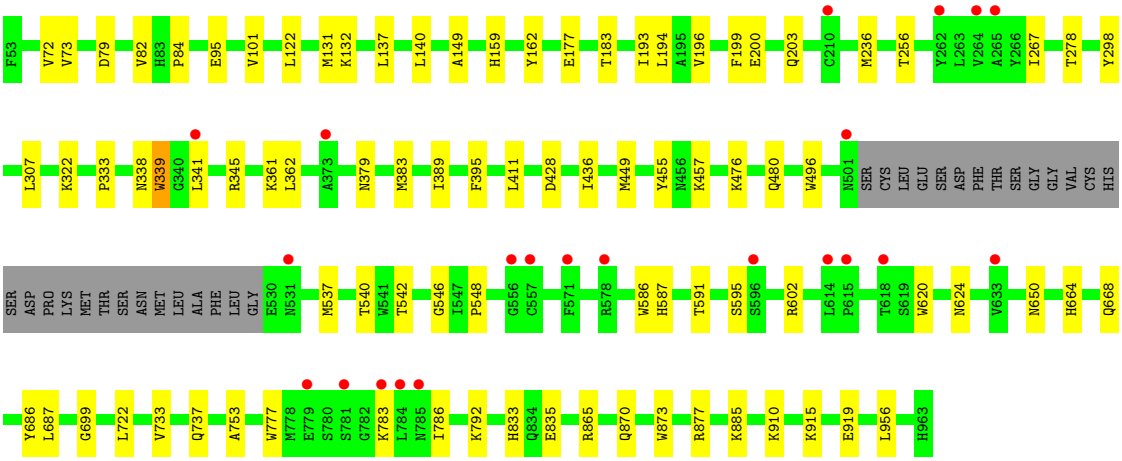
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
13	A	175	175	175	0	0
			Total	O		
13	B	34	34	34	0	0

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.

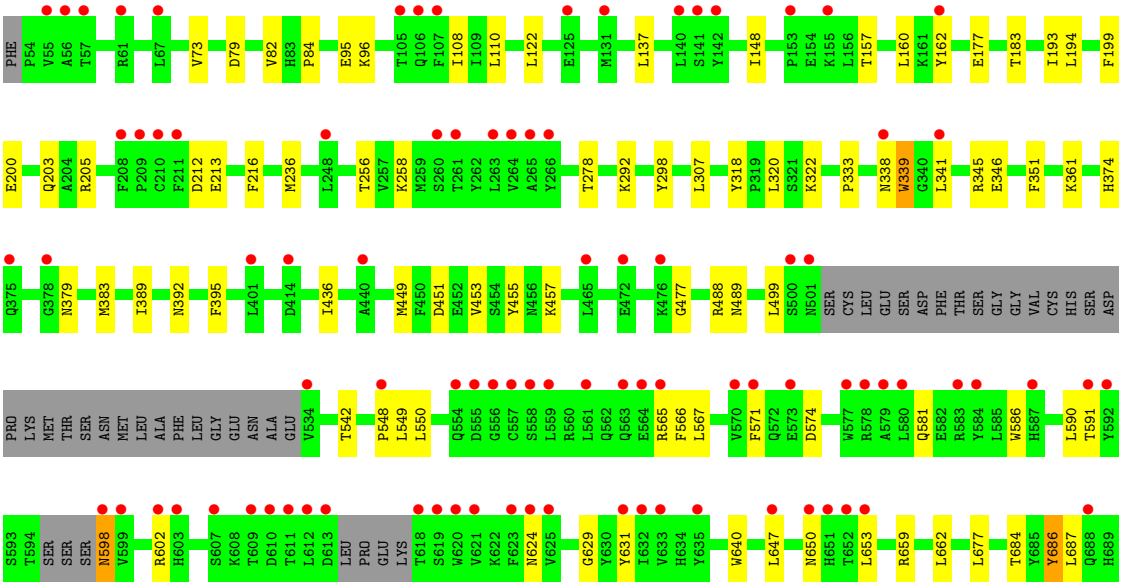
• Molecule 1: Endoplasmic reticulum aminopeptidase 2

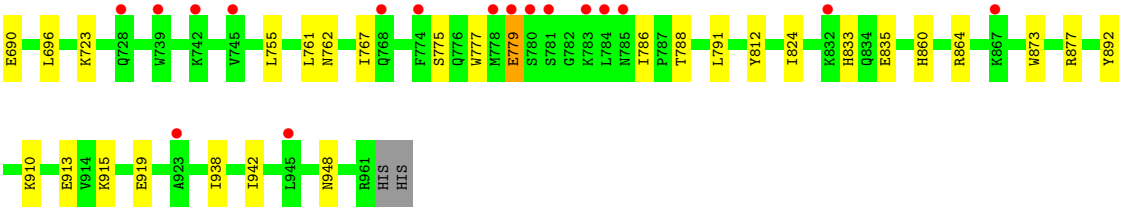
Chain A:



• Molecule 1: Endoplasmic reticulum aminopeptidase 2

Chain B:





• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 60% 40%

• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 60% 40%

• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 60% 40%

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

Chain E: 100%

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

Chain F: 100%

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

Chain I:

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

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.23Å 135.45Å 127.28Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	29.29 – 2.45 29.89 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.1 (29.29-2.45) 87.2 (29.89-2.45)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.17 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.208 , 0.236 0.208 , 0.233	Depositor DCC
R_{free} test set	2027 reflections (2.23%)	wwPDB-VP
Wilson B-factor (Å^2)	48.0	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 43.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15097	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: MAN, BMA, EDO, IMD, J2G, ZN, PGE, NAG, MES

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	0.24	0/7408	0.44	0/10041
1	B	0.23	0/7233	0.45	0/9808
All	All	0.23	0/14641	0.45	0/19849

There are no bond length outliers.

There are no bond angle outliers.

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	7212	0	7151	51	0
1	B	7054	0	6957	68	0
2	C	61	0	52	0	0
2	D	61	0	52	0	0
2	G	61	0	52	0	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
3	I	28	0	25	0	0
4	H	39	0	34	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	12	0	12	3	0
6	B	12	0	12	2	0
7	A	62	0	0	1	0
7	B	62	0	0	0	0
8	A	20	0	24	2	0
8	B	20	0	24	2	0
9	A	56	0	52	0	0
9	B	42	0	39	0	0
10	A	5	0	5	0	0
10	B	5	0	5	2	0
11	A	10	0	14	2	0
12	A	4	0	6	0	0
12	B	4	0	6	0	0
13	A	175	0	0	3	0
13	B	34	0	0	0	0
All	All	15097	0	14572	123	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 (123) 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:777:TRP:HE1	1:A:783:LYS:HD2	1.42	0.83
1:A:383:MET:HE2	1:A:389:ILE:HA	1.66	0.77
1:A:177[B]:GLU:HB3	1:A:203:GLN:HG2	1.67	0.76
1:B:177[B]:GLU:HB3	1:B:203:GLN:HG2	1.72	0.72
1:B:200:GLU:OE1	8:B:1004:LYS:N	2.23	0.71
1:A:177[A]:GLU:HB2	1:A:203:GLN:HG2	1.71	0.71
1:B:565:ARG:H	1:B:581:GLN:HE22	1.37	0.69
1:B:910:LYS:HD3	1:B:913:GLU:OE2	1.95	0.67
1:A:753:ALA:HB2	11:A:1011:PGE:H62	1.76	0.66
1:B:383:MET:HE2	1:B:389:ILE:HA	1.79	0.64
1:A:131:MET:HG2	1:A:132:LYS:H	1.65	0.62
1:A:278:THR:HG21	1:A:307:LEU:HD23	1.82	0.61
1:A:183:THR:HG22	1:A:193:ILE:HD13	1.82	0.61
1:B:650:ASN:HB3	1:B:653:LEU:HD13	1.84	0.60
1:A:915:LYS:HE3	1:A:919:GLU:OE2	2.02	0.59
1:B:177[A]:GLU:HB2	1:B:203:GLN:HG2	1.83	0.59
1:B:374:HIS:HE1	1:B:392:ASN:HB3	1.69	0.58
1:B:183:THR:HG22	1:B:193:ILE:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:LEU:HG	1:A:956:LEU:HD11	1.87	0.55
1:B:339:TRP:CD2	1:B:379:ASN:HB3	2.42	0.55
1:A:298:TYR:CZ	1:A:361:LYS:HD2	2.42	0.55
1:A:540:THR:HG21	1:A:587:HIS:H	1.70	0.55
1:A:199:PHE:HA	1:A:203:GLN:HB2	1.89	0.54
1:B:565:ARG:H	1:B:581:GLN:NE2	2.05	0.54
1:A:777:TRP:HB2	1:A:786:ILE:HD11	1.89	0.54
1:A:537:MET:O	1:A:540:THR:HG22	2.09	0.53
8:A:1009:LYS:OXT	13:A:1101:HOH:O	2.18	0.53
1:A:362:LEU:HD13	1:A:411:LEU:HB3	1.89	0.53
1:B:915:LYS:HE3	1:B:919:GLU:OE2	2.09	0.53
1:A:72:VAL:HG23	1:A:73:VAL:HG23	1.90	0.52
1:B:549:LEU:HB2	1:B:566:PHE:HB2	1.91	0.52
1:B:777:TRP:HB2	1:B:786:ILE:HD11	1.91	0.52
1:B:892:TYR:CD2	10:B:1008:IMD:H5	2.45	0.52
1:A:476:LYS:O	1:A:480[A]:GLN:HG2	2.10	0.51
1:B:677:LEU:HD22	1:B:948:ASN:HB3	1.92	0.51
1:A:200:GLU:OE1	8:A:1004:LYS:N	2.43	0.51
1:A:436:ILE:HG22	1:A:542:THR:HA	1.91	0.51
1:B:82:VAL:HG12	1:B:84:PRO:HD3	1.93	0.50
1:B:298:TYR:CZ	1:B:361:LYS:HD2	2.45	0.50
1:B:451:ASP:HA	6:B:1002:MES:H62	1.93	0.50
1:A:82:VAL:HG12	1:A:84:PRO:HD3	1.93	0.50
1:A:122:LEU:HB2	1:A:137:LEU:HD11	1.94	0.49
1:B:684:THR:HA	1:B:687:LEU:HD23	1.93	0.49
1:B:598:ASN:HD22	1:B:598:ASN:N	2.11	0.49
1:A:389:ILE:HG21	1:A:449:MET:HB3	1.93	0.49
1:A:792:LYS:HE3	11:A:1011:PGE:H1	1.95	0.48
1:B:199:PHE:HA	1:B:203:GLN:HB2	1.95	0.47
1:B:477:GLY:HA3	1:B:499:LEU:HD23	1.97	0.47
1:B:122:LEU:HB2	1:B:137:LEU:HD11	1.94	0.47
1:B:236:MET:HG2	1:B:256:THR:HG22	1.96	0.47
1:A:591:THR:O	1:A:624:ASN:N	2.47	0.47
1:A:338:ASN:HB2	1:A:341:LEU:O	2.15	0.46
1:B:122:LEU:HD11	1:B:162:TYR:HB3	1.97	0.46
1:B:205:ARG:HH21	1:B:212:ASP:HB3	1.81	0.46
1:B:550:LEU:HD22	1:B:590:LEU:HD11	1.98	0.46
1:A:122:LEU:HD11	1:A:162:TYR:HB3	1.96	0.46
1:B:892:TYR:HD2	10:B:1008:IMD:H5	1.81	0.46
1:B:333:PRO:O	1:B:345:ARG:HG3	2.16	0.46
1:A:236:MET:HG2	1:A:256:THR:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:PHE:CZ	1:B:361:LYS:HE3	2.51	0.46
1:A:865:ARG:NE	13:A:1119:HOH:O	2.48	0.46
1:B:723:LYS:HG3	1:B:761:LEU:HB3	1.98	0.46
6:A:1002:MES:H51	6:A:1002:MES:H81	1.71	0.45
1:A:885:LYS:HA	1:A:885:LYS:HE2	1.98	0.45
1:B:455:TYR:OH	8:B:1004:LYS:OXT	2.25	0.45
1:B:73:VAL:HG11	1:B:108:ILE:HG23	1.98	0.45
1:B:591:THR:HG22	1:B:602:ARG:HG2	1.99	0.45
1:B:788:THR:HA	1:B:791:LEU:HB2	1.99	0.45
1:B:833:HIS:HB3	1:B:835:GLU:OE2	2.16	0.45
1:A:339:TRP:CD2	1:A:379:ASN:HB3	2.52	0.45
1:A:591:THR:HG22	1:A:602:ARG:HG2	1.99	0.45
1:B:591:THR:O	1:B:624:ASN:N	2.49	0.45
1:B:640:TRP:HZ3	1:B:662:LEU:HD22	1.82	0.45
1:A:496:TRP:HZ2	1:A:542:THR:HG21	1.82	0.45
1:A:687:LEU:HD11	1:A:699:GLY:HA3	1.99	0.44
1:B:436:ILE:HG22	1:B:542:THR:HA	1.98	0.44
1:B:860:HIS:NE2	1:B:864:ARG:HD2	2.32	0.44
1:A:457:LYS:NZ	13:A:1110:HOH:O	2.34	0.44
1:B:762:ASN:HA	1:B:767:ILE:HD11	2.00	0.44
1:A:540:THR:HG21	1:A:586:TRP:HA	2.00	0.44
1:B:775:SER:O	1:B:779:GLU:HB3	2.16	0.44
1:A:595:SER:HB3	1:A:620:TRP:CE2	2.53	0.44
1:A:664:HIS:O	1:A:668:GLN:HG2	2.18	0.44
1:A:833:HIS:HB3	1:A:835:GLU:OE2	2.17	0.44
1:B:374:HIS:CE1	1:B:392:ASN:HB3	2.50	0.43
6:B:1002:MES:H51	6:B:1002:MES:H81	1.73	0.43
1:B:110:LEU:HD11	1:B:148:ILE:HD11	2.01	0.43
1:A:548:PRO:HB3	1:A:586:TRP:CE3	2.54	0.43
1:B:389:ILE:HG21	1:B:449:MET:HB3	2.01	0.43
1:A:870:GLN:OE1	1:A:910:LYS:NZ	2.50	0.42
1:A:333:PRO:O	1:A:345:ARG:HG3	2.19	0.42
1:B:213:GLU:HB2	1:B:216:PHE:CD1	2.54	0.42
1:B:278:THR:HG21	1:B:307:LEU:HD23	2.01	0.42
1:B:157:THR:HB	1:B:160:LEU:HD12	2.01	0.42
1:B:213:GLU:HB2	1:B:216:PHE:HD1	1.84	0.42
1:A:101:VAL:O	1:A:159:HIS:N	2.47	0.42
1:B:338:ASN:HB2	1:B:341:LEU:O	2.19	0.42
6:A:1002:MES:H72	7:A:1003[B]:J2G:OAP	2.19	0.42
1:B:567:LEU:HD13	1:B:567:LEU:HA	1.93	0.42
1:B:629:GLY:HA3	1:B:631:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:733:VAL:O	1:A:737:GLN:HG2	2.19	0.42
1:A:873:TRP:CZ2	1:A:877:ARG:HD3	2.54	0.41
1:B:647:LEU:HB3	1:B:686:TYR:CG	2.55	0.41
1:B:659:ARG:NE	1:B:690:GLU:OE1	2.53	0.41
1:A:777:TRP:NE1	1:A:783:LYS:HD2	2.22	0.41
1:B:488:ARG:HG2	1:B:489:ASN:H	1.86	0.41
1:B:938:ILE:O	1:B:942:ILE:HG12	2.21	0.41
1:A:79:ASP:O	1:A:95:GLU:HA	2.21	0.41
1:A:196:VAL:HG23	1:A:267:ILE:HG12	2.03	0.41
1:A:428:ASP:O	1:A:546:GLY:HA2	2.21	0.41
1:A:455:TYR:CD2	6:A:1002:MES:H31	2.56	0.41
1:B:318:TYR:CE2	1:B:320:LEU:HB2	2.55	0.41
1:B:571:PHE:N	1:B:574:ASP:OD2	2.39	0.41
1:B:812:TYR:HB2	1:B:824:ILE:HG21	2.03	0.41
1:B:548:PRO:HB3	1:B:586:TRP:CE3	2.56	0.41
1:B:687:LEU:HD12	1:B:696:LEU:HA	2.02	0.41
1:B:873:TRP:CZ2	1:B:877:ARG:HD3	2.56	0.41
1:A:140:LEU:HB2	1:A:149:ALA:HB3	2.03	0.40
1:B:79:ASP:O	1:B:95:GLU:HA	2.21	0.40
1:B:79:ASP:HB2	1:B:96:LYS:HB3	2.04	0.40
1:B:292:LYS:NZ	1:B:346:GLU:OE1	2.53	0.40
1:B:258:LYS:H	4:H:1:NAG:H62	1.85	0.40
1:B:453:VAL:O	1:B:457:LYS:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	886/911 (97%)	859 (97%)	27 (3%)	0	100	100
1	B	863/911 (95%)	835 (97%)	28 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1749/1822 (96%)	1694 (97%)	55 (3%)	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	792/819 (97%)	786 (99%)	6 (1%)	81	88
1	B	772/819 (94%)	764 (99%)	8 (1%)	76	84
All	All	1564/1638 (96%)	1550 (99%)	14 (1%)	78	86

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	194	LEU
1	A	322	LYS
1	A	339	TRP
1	A	395	PHE
1	A	650	ASN
1	A	686	TYR
1	B	194	LEU
1	B	322	LYS
1	B	339	TRP
1	B	395	PHE
1	B	598	ASN
1	B	686	TYR
1	B	755	LEU
1	B	779	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	869	GLN

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Mol	Chain	Res	Type
1	B	581	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

24 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	C	1	2,1	14,14,15	0.28	0	17,19,21	0.37	0
2	NAG	C	2	2	14,14,15	0.26	0	17,19,21	0.44	0
2	BMA	C	3	2	11,11,12	0.54	0	15,15,17	0.83	0
2	MAN	C	4	2	11,11,12	0.76	1 (9%)	15,15,17	1.61	3 (20%)
2	MAN	C	5	2	11,11,12	0.57	0	15,15,17	1.03	2 (13%)
2	NAG	D	1	2,1	14,14,15	0.27	0	17,19,21	0.38	0
2	NAG	D	2	2	14,14,15	0.21	0	17,19,21	0.48	0
2	BMA	D	3	2	11,11,12	0.69	0	15,15,17	0.78	0
2	MAN	D	4	2	11,11,12	0.88	1 (9%)	15,15,17	1.63	3 (20%)
2	MAN	D	5	2	11,11,12	0.66	0	15,15,17	1.03	2 (13%)
3	NAG	E	1	1,3	14,14,15	0.23	0	17,19,21	0.41	0
3	NAG	E	2	3	14,14,15	0.23	0	17,19,21	0.40	0
3	NAG	F	1	1,3	14,14,15	0.20	0	17,19,21	0.38	0
3	NAG	F	2	3	14,14,15	0.23	0	17,19,21	0.41	0
2	NAG	G	1	2,1	14,14,15	0.27	0	17,19,21	0.37	0
2	NAG	G	2	2	14,14,15	0.31	0	17,19,21	0.44	0
2	BMA	G	3	2	11,11,12	0.60	0	15,15,17	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MAN	G	4	2	11,11,12	0.92	1 (9%)	15,15,17	1.64	3 (20%)
2	MAN	G	5	2	11,11,12	0.67	0	15,15,17	1.04	2 (13%)
4	NAG	H	1	1,4	14,14,15	0.17	0	17,19,21	0.40	0
4	NAG	H	2	4	14,14,15	0.24	0	17,19,21	0.44	0
4	BMA	H	3	4	11,11,12	0.63	0	15,15,17	0.70	0
3	NAG	I	1	1,3	14,14,15	0.25	0	17,19,21	0.44	0
3	NAG	I	2	3	14,14,15	0.24	0	17,19,21	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	MAN	D	4	2	-	0/2/19/22	0/1/1/1
2	MAN	D	5	2	-	1/2/19/22	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	BMA	G	3	2	-	0/2/19/22	0/1/1/1
2	MAN	G	4	2	-	2/2/19/22	0/1/1/1
2	MAN	G	5	2	-	2/2/19/22	0/1/1/1
4	NAG	H	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	BMA	H	3	4	-	0/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	MAN	C1-C2	2.43	1.57	1.52
2	G	4	MAN	C1-C2	2.43	1.57	1.52
2	C	4	MAN	C1-C2	2.09	1.57	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	4	MAN	C1-O5-C5	5.08	119.07	112.19
2	D	4	MAN	C1-O5-C5	4.93	118.88	112.19
2	C	4	MAN	C1-O5-C5	4.79	118.68	112.19
2	G	5	MAN	C1-O5-C5	2.77	115.95	112.19
2	D	5	MAN	C1-O5-C5	2.68	115.82	112.19
2	C	5	MAN	C1-O5-C5	2.66	115.79	112.19
2	C	4	MAN	O5-C1-C2	2.42	114.50	110.77
2	D	5	MAN	O2-C2-C3	-2.25	105.64	110.14
2	C	5	MAN	O2-C2-C3	-2.22	105.69	110.14
2	G	5	MAN	O2-C2-C3	-2.21	105.72	110.14
2	C	4	MAN	O2-C2-C3	-2.19	105.75	110.14
2	D	4	MAN	O2-C2-C3	-2.19	105.75	110.14
2	G	4	MAN	O2-C2-C3	-2.16	105.81	110.14
2	D	4	MAN	O5-C1-C2	2.14	114.07	110.77
2	G	4	MAN	O5-C1-C2	2.03	113.91	110.77

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	4	MAN	C4-C5-C6-O6
2	G	4	MAN	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
2	G	5	MAN	C4-C5-C6-O6
2	C	4	MAN	O5-C5-C6-O6
2	D	5	MAN	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
2	G	5	MAN	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6

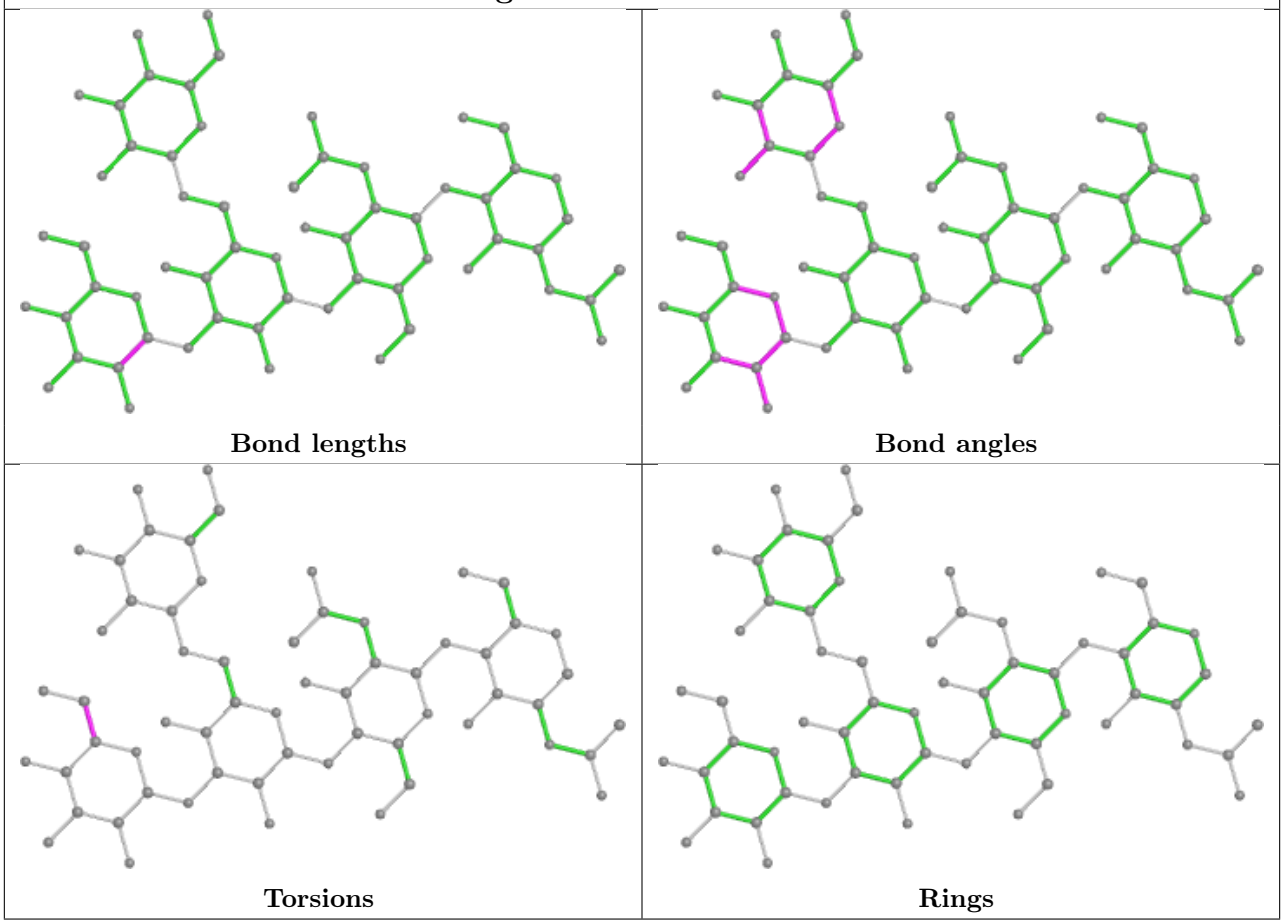
There are no ring outliers.

1 monomer is involved in 1 short contact:

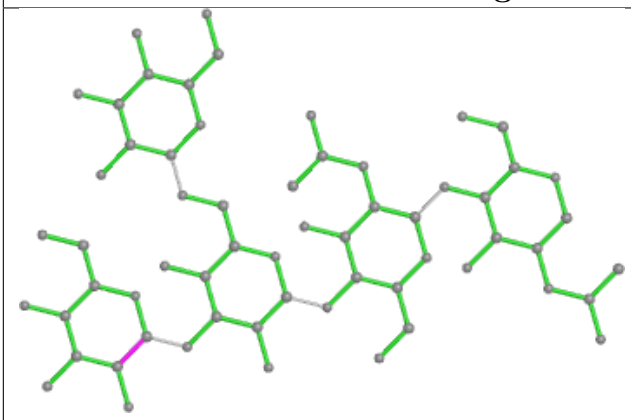
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	NAG	1	0

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

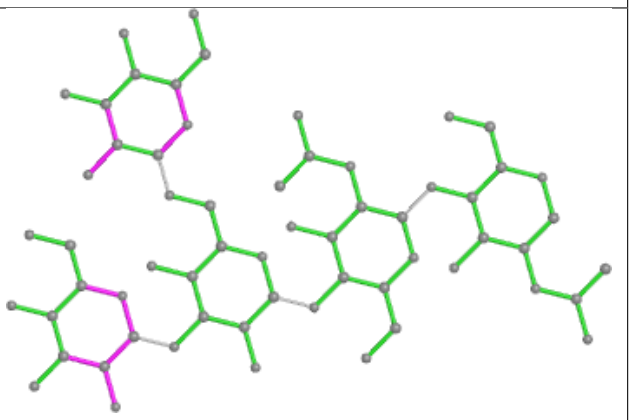
Oligosaccharide Chain C



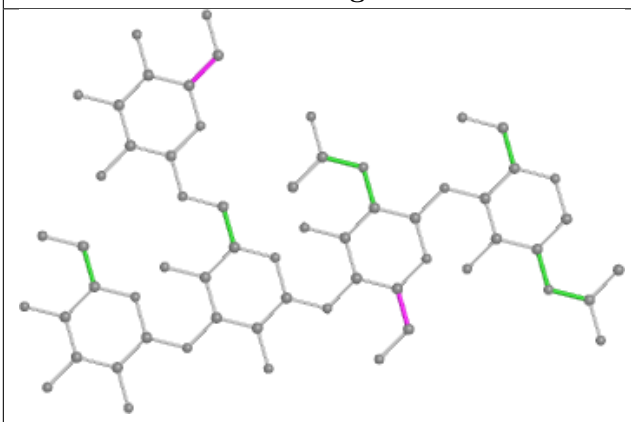
Oligosaccharide Chain D



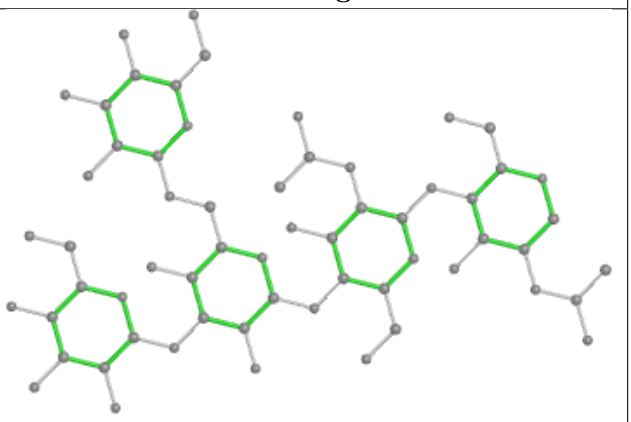
Bond lengths



Bond angles

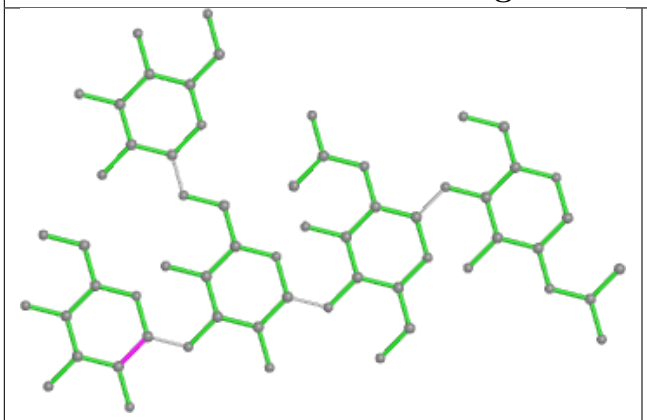


Torsions

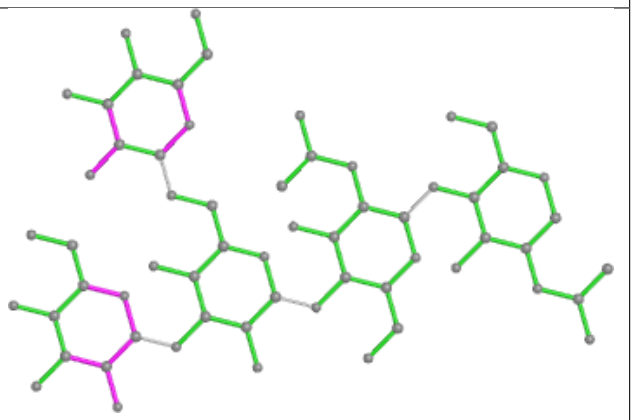


Rings

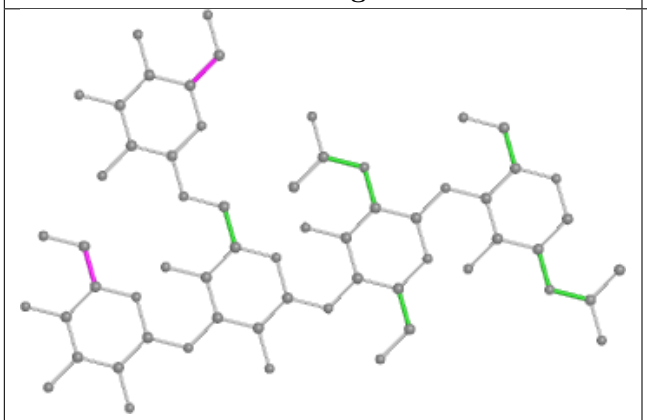
Oligosaccharide Chain G



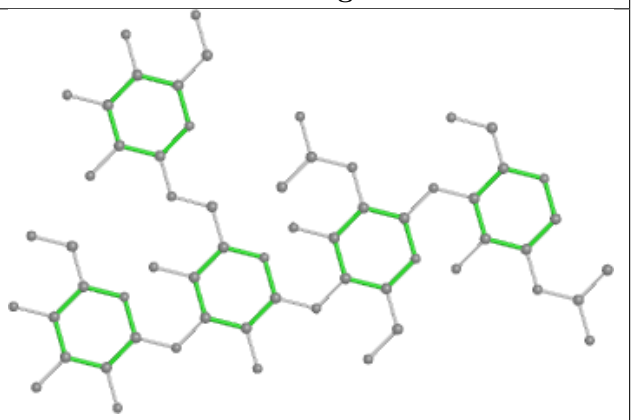
Bond lengths



Bond angles

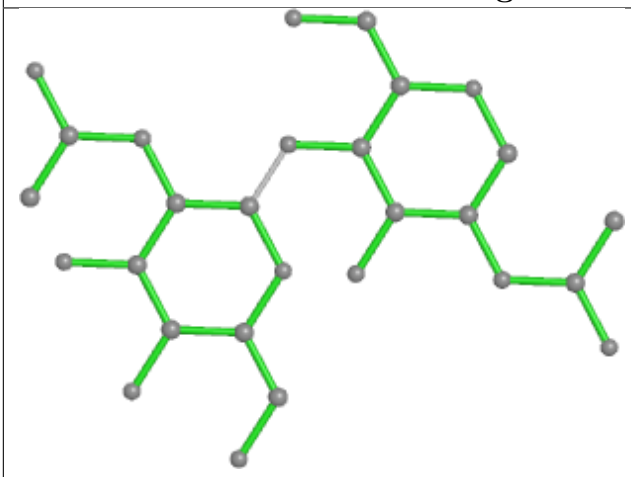


Torsions

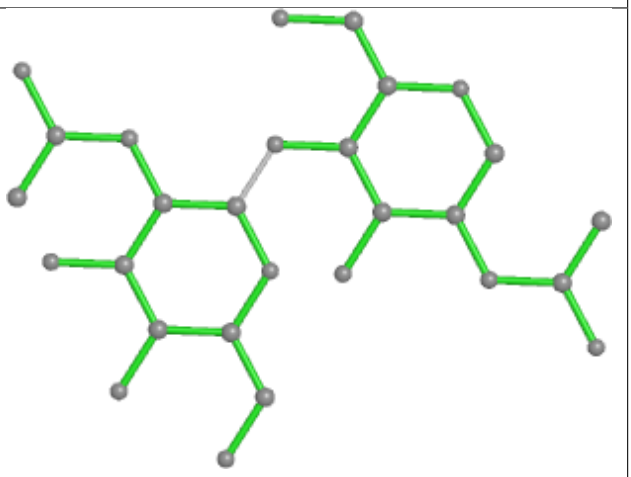


Rings

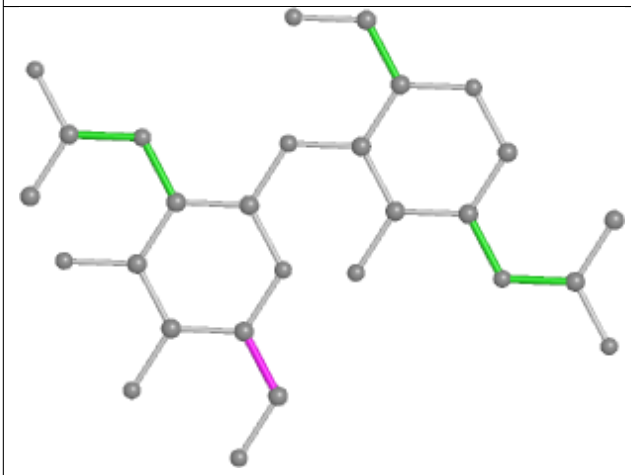
Oligosaccharide Chain E



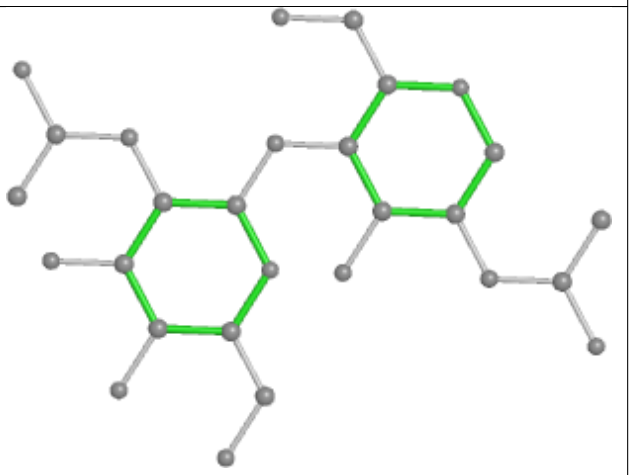
Bond lengths



Bond angles

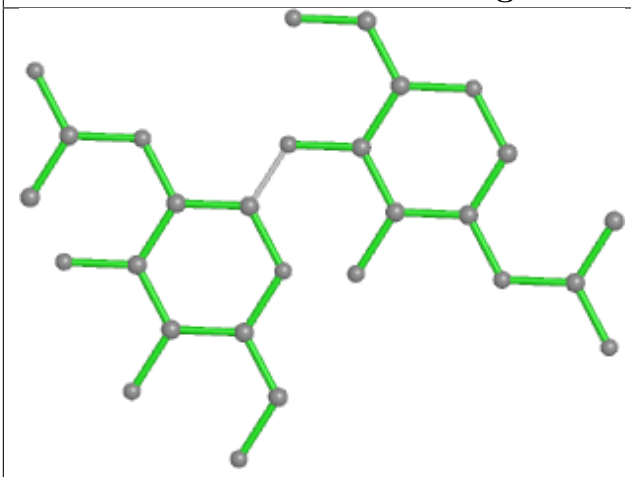


Torsions

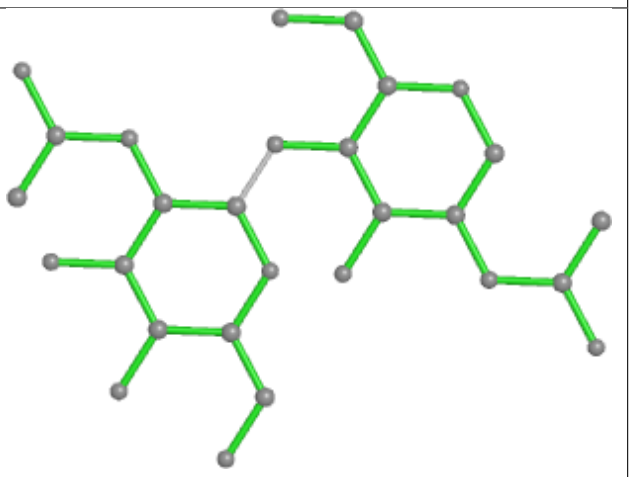


Rings

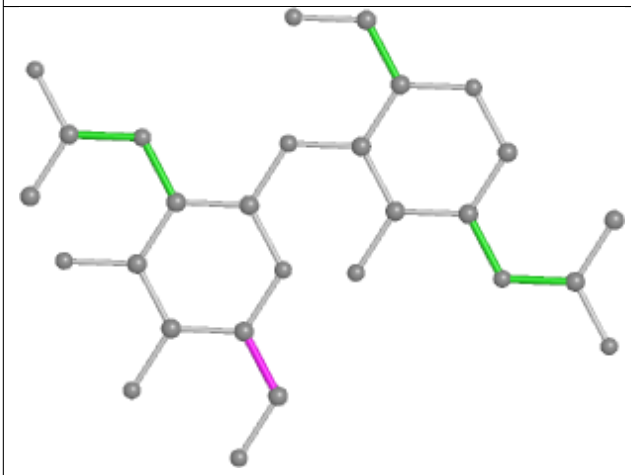
Oligosaccharide Chain F



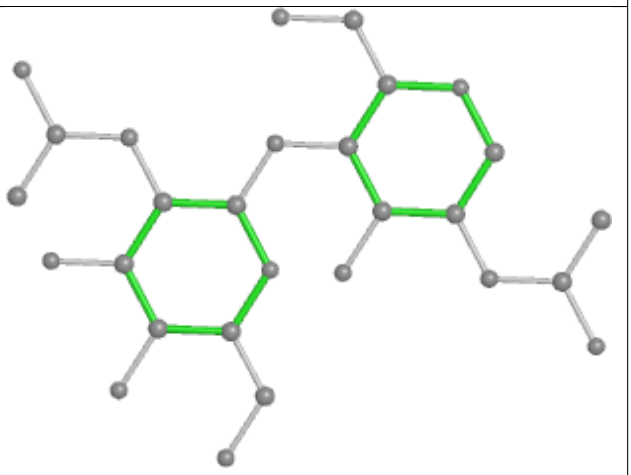
Bond lengths



Bond angles

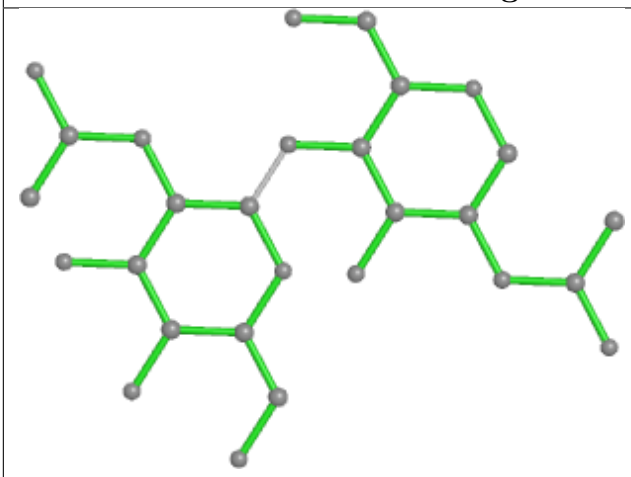


Torsions

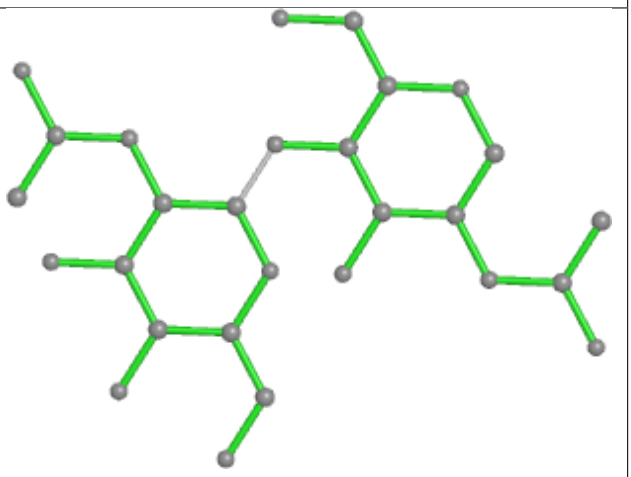


Rings

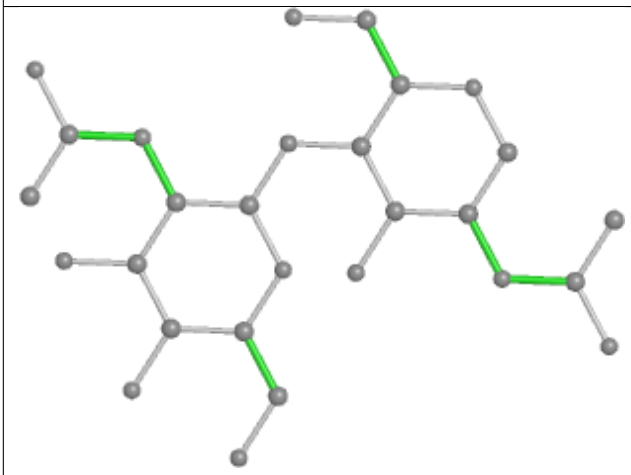
Oligosaccharide Chain I



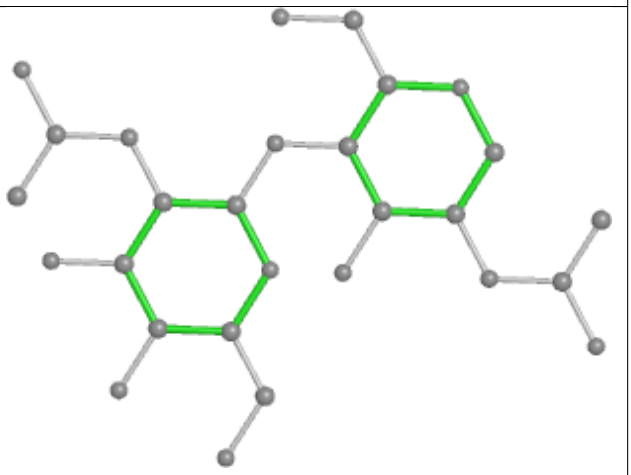
Bond lengths



Bond angles

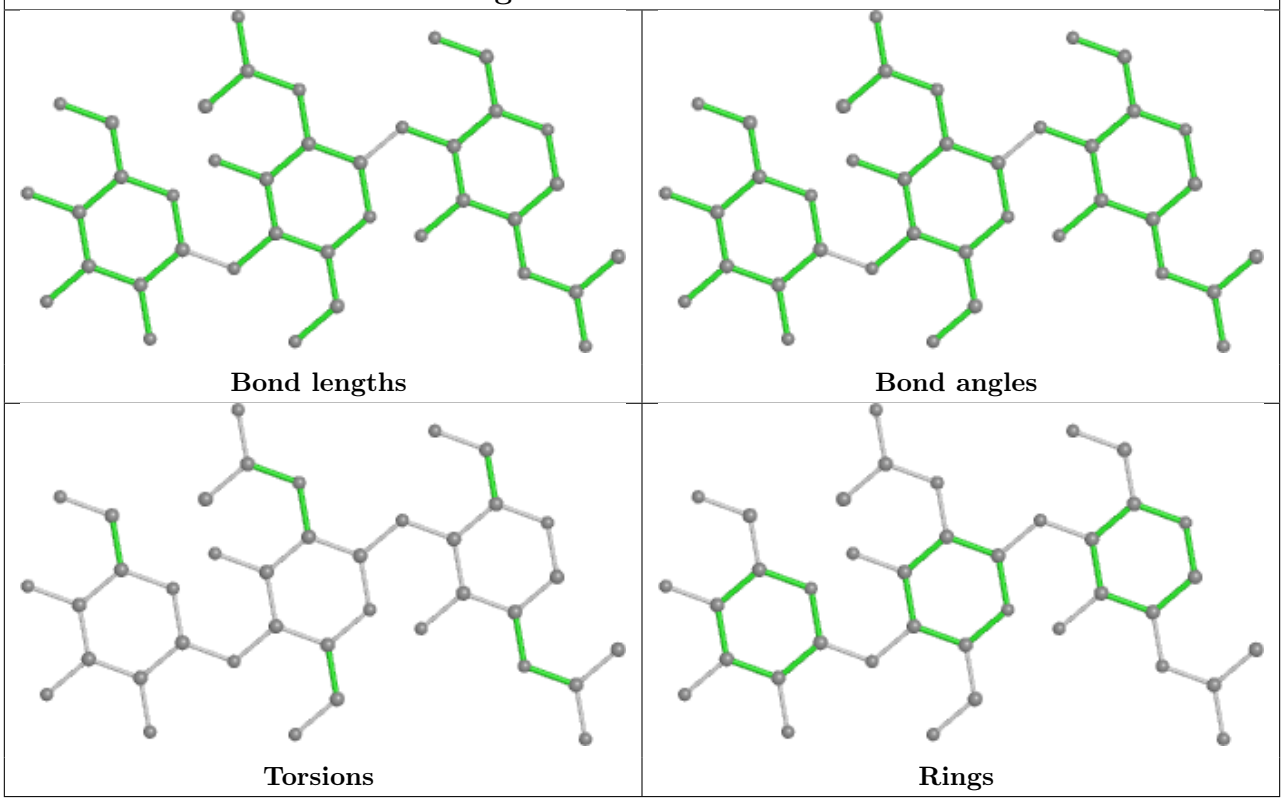


Torsions



Rings

Oligosaccharide Chain H



5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 2 are monoatomic - leaving 22 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	LYS	B	1004	5	8,9,9	0.82	1 (12%)	9,10,10	1.23	2 (22%)
7	J2G	A	1003[B]	-	33,33,33	0.93	1 (3%)	48,49,49	1.26	3 (6%)
6	MES	A	1002	-	12,12,12	2.32	1 (8%)	14,16,16	1.83	5 (35%)
7	J2G	A	1003[A]	-	33,33,33	0.93	2 (6%)	48,49,49	1.26	6 (12%)
11	PGE	A	1011	-	9,9,9	0.30	0	8,8,8	0.29	0
9	NAG	B	1007	1	14,14,15	0.24	0	17,19,21	0.46	0
7	J2G	B	1003[B]	-	33,33,33	0.92	1 (3%)	48,49,49	1.26	4 (8%)
7	J2G	B	1003[A]	-	33,33,33	0.93	2 (6%)	48,49,49	1.25	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	NAG	A	1008	1	14,14,15	0.31	0	17,19,21	0.45	0
10	IMD	A	1010	-	3,5,5	0.41	0	4,5,5	0.58	0
8	LYS	B	1010	-	8,9,9	0.82	1 (12%)	9,10,10	1.13	2 (22%)
9	NAG	A	1005	1	14,14,15	0.23	0	17,19,21	0.42	0
9	NAG	B	1006	1	14,14,15	0.23	0	17,19,21	0.42	0
6	MES	B	1002	-	12,12,12	2.26	1 (8%)	14,16,16	1.98	5 (35%)
12	EDO	B	1009	-	3,3,3	0.46	0	2,2,2	0.32	0
9	NAG	B	1005	1	14,14,15	0.21	0	17,19,21	0.40	0
10	IMD	B	1008	-	3,5,5	0.42	0	4,5,5	0.58	0
8	LYS	A	1009	-	8,9,9	0.84	1 (12%)	9,10,10	1.08	2 (22%)
9	NAG	A	1006	1	14,14,15	0.23	0	17,19,21	0.44	0
8	LYS	A	1004	5	8,9,9	0.83	1 (12%)	9,10,10	1.22	2 (22%)
12	EDO	A	1012	-	3,3,3	0.46	0	2,2,2	0.34	0
9	NAG	A	1007	1	14,14,15	0.30	0	17,19,21	0.45	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
8	LYS	B	1004	5	-	4/9/9/9	-
7	J2G	A	1003[B]	-	-	13/27/35/35	0/3/3/3
6	MES	A	1002	-	-	3/6/14/14	0/1/1/1
7	J2G	A	1003[A]	-	-	18/27/35/35	0/3/3/3
11	PGE	A	1011	-	-	3/7/7/7	-
9	NAG	B	1007	1	-	4/6/23/26	0/1/1/1
7	J2G	B	1003[B]	-	-	13/27/35/35	0/3/3/3
7	J2G	B	1003[A]	-	-	18/27/35/35	0/3/3/3
9	NAG	A	1008	1	-	0/6/23/26	0/1/1/1
10	IMD	A	1010	-	-	-	0/1/1/1
8	LYS	B	1010	-	-	2/9/9/9	-
9	NAG	A	1005	1	-	2/6/23/26	0/1/1/1
9	NAG	B	1006	1	-	1/6/23/26	0/1/1/1
6	MES	B	1002	-	-	0/6/14/14	0/1/1/1
12	EDO	B	1009	-	-	0/1/1/1	-
9	NAG	B	1005	1	-	2/6/23/26	0/1/1/1
10	IMD	B	1008	-	-	-	0/1/1/1
8	LYS	A	1009	-	-	2/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	A	1006	1	-	2/6/23/26	0/1/1/1
8	LYS	A	1004	5	-	4/9/9/9	-
12	EDO	A	1012	-	-	0/1/1/1	-
9	NAG	A	1007	1	-	1/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1002	MES	C8-S	-7.75	1.66	1.77
6	B	1002	MES	C8-S	-7.55	1.66	1.77
7	A	1003[A]	J2G	SAG-NAH	2.47	1.67	1.63
7	B	1003[A]	J2G	SAG-NAH	2.41	1.67	1.63
7	B	1003[B]	J2G	OAB-CAE	-2.40	1.33	1.37
7	A	1003[B]	J2G	OAB-CAE	-2.30	1.33	1.37
7	B	1003[A]	J2G	OAB-CAE	-2.26	1.33	1.37
8	A	1009	LYS	OXT-C	-2.19	1.23	1.30
8	A	1004	LYS	OXT-C	-2.18	1.23	1.30
7	A	1003[A]	J2G	OAB-CAE	-2.17	1.33	1.37
8	B	1010	LYS	OXT-C	-2.16	1.23	1.30
8	B	1004	LYS	OXT-C	-2.14	1.23	1.30

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1002	MES	C5-N4-C3	3.92	117.66	108.83
7	A	1003[B]	J2G	CAF-SAG-NAH	-3.86	102.76	107.27
7	B	1003[B]	J2G	CBC-NAZ-CBA	3.72	119.73	111.52
7	B	1003[B]	J2G	OAC-SAG-CAF	3.60	113.58	107.66
7	A	1003[B]	J2G	OAC-SAG-CAF	3.49	113.40	107.66
7	B	1003[B]	J2G	CAF-SAG-NAH	-3.45	103.24	107.27
6	A	1002	MES	C5-N4-C3	3.35	116.37	108.83
7	B	1003[A]	J2G	CBC-NAZ-CBA	3.29	118.77	111.52
7	A	1003[A]	J2G	CBC-NAZ-CBA	3.09	118.33	111.52
6	B	1002	MES	C6-C5-N4	-3.08	105.43	110.10
7	B	1003[A]	J2G	OAC-SAG-CAF	3.03	112.65	107.66
7	A	1003[B]	J2G	CBC-NAZ-CBA	2.97	118.07	111.52
7	A	1003[A]	J2G	OAC-SAG-CAF	2.90	112.43	107.66
6	A	1002	MES	C6-C5-N4	-2.81	105.84	110.10
8	A	1004	LYS	OXT-C-O	-2.74	117.87	124.09
8	B	1004	LYS	OXT-C-O	-2.73	117.90	124.09
7	A	1003[A]	J2G	OAB-CAE-CAF	2.68	118.58	116.50
7	A	1003[A]	J2G	CBB-CBA-NAZ	2.66	116.24	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1002	MES	O3S-S-C8	2.66	110.07	105.77
6	A	1002	MES	O1S-S-C8	2.58	110.02	106.92
6	B	1002	MES	O2S-S-C8	2.46	109.87	106.92
6	B	1002	MES	O3S-S-C8	2.44	109.72	105.77
7	B	1003[A]	J2G	OAB-CAE-CAF	2.40	118.36	116.50
8	B	1010	LYS	OXT-C-O	-2.38	118.69	124.09
8	A	1009	LYS	OXT-C-O	-2.33	118.80	124.09
8	B	1004	LYS	OXT-C-CA	2.32	121.28	113.38
8	A	1004	LYS	OXT-C-CA	2.31	121.25	113.38
6	A	1002	MES	C7-N4-C5	2.24	116.95	111.23
7	B	1003[A]	J2G	CBB-CBA-NAZ	2.24	115.41	111.05
8	B	1010	LYS	OXT-C-CA	2.21	120.91	113.38
7	B	1003[B]	J2G	CBD-CBC-NAZ	2.19	115.33	111.05
7	B	1003[A]	J2G	CBD-CBE-CBB	-2.17	104.50	111.18
7	B	1003[A]	J2G	OAP-SAG-CAF	-2.10	104.21	107.66
7	B	1003[A]	J2G	OAY-CAV-CAN	-2.10	115.87	121.45
7	A	1003[A]	J2G	OAP-SAG-CAF	-2.05	104.30	107.66
7	A	1003[A]	J2G	CBD-CBE-CBB	-2.04	104.90	111.18
8	A	1009	LYS	OXT-C-CA	2.02	120.25	113.38
6	B	1002	MES	C7-N4-C5	2.01	116.38	111.23

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1002	MES	C7-C8-S-O2S
6	A	1002	MES	C7-C8-S-O3S
7	A	1003[A]	J2G	CAE-CAF-SAG-NAH
7	A	1003[A]	J2G	CAE-CAF-SAG-OAC
7	A	1003[A]	J2G	CAE-CAF-SAG-OAP
7	A	1003[B]	J2G	CAF-CAE-OAB-CAA
7	A	1003[B]	J2G	CAE-CAF-SAG-NAH
7	A	1003[B]	J2G	CAE-CAF-SAG-OAP
7	A	1003[B]	J2G	CAI-NAH-SAG-CAF
7	B	1003[A]	J2G	CAE-CAF-SAG-NAH
7	B	1003[A]	J2G	CAE-CAF-SAG-OAC
7	B	1003[A]	J2G	CAE-CAF-SAG-OAP
7	B	1003[B]	J2G	CAF-CAE-OAB-CAA
7	B	1003[B]	J2G	CAE-CAF-SAG-NAH
7	B	1003[B]	J2G	CAE-CAF-SAG-OAP
7	A	1003[A]	J2G	CAO-CAN-CAV-OAW
7	A	1003[B]	J2G	CAM-CAN-CAV-OAW

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Mol	Chain	Res	Type	Atoms
7	A	1003[B]	J2G	CAO-CAN-CAV-OAW
7	B	1003[A]	J2G	CAO-CAN-CAV-OAW
7	B	1003[B]	J2G	CAM-CAN-CAV-OAW
7	B	1003[B]	J2G	CAO-CAN-CAV-OAW
7	A	1003[A]	J2G	CAM-CAN-CAV-OAY
7	A	1003[A]	J2G	CAO-CAN-CAV-OAY
7	A	1003[B]	J2G	CAM-CAN-CAV-OAY
7	A	1003[B]	J2G	CAO-CAN-CAV-OAY
7	B	1003[A]	J2G	CAO-CAN-CAV-OAY
7	B	1003[B]	J2G	CAM-CAN-CAV-OAY
7	B	1003[B]	J2G	CAO-CAN-CAV-OAY
7	A	1003[A]	J2G	CAM-CAN-CAV-OAW
7	B	1003[A]	J2G	CAM-CAN-CAV-OAW
7	B	1003[A]	J2G	CAM-CAN-CAV-OAY
7	A	1003[A]	J2G	CAI-NAH-SAG-CAF
7	A	1003[A]	J2G	CAI-NAH-SAG-OAC
7	A	1003[B]	J2G	CAI-NAH-SAG-OAP
7	B	1003[A]	J2G	CAI-NAH-SAG-CAF
7	B	1003[A]	J2G	CAI-NAH-SAG-OAC
7	B	1003[B]	J2G	CAI-NAH-SAG-CAF
7	B	1003[B]	J2G	CAI-NAH-SAG-OAP
9	A	1006	NAG	O5-C5-C6-O6
7	A	1003[B]	J2G	CAO-CAF-SAG-OAP
7	B	1003[B]	J2G	CAO-CAF-SAG-OAP
9	A	1005	NAG	O5-C5-C6-O6
9	A	1006	NAG	C4-C5-C6-O6
11	A	1011	PGE	O2-C3-C4-O3
8	A	1004	LYS	OXT-C-CA-N
8	B	1004	LYS	OXT-C-CA-N
9	B	1007	NAG	C8-C7-N2-C2
9	B	1007	NAG	O7-C7-N2-C2
7	A	1003[B]	J2G	CAO-CAF-SAG-NAH
7	B	1003[B]	J2G	CAO-CAF-SAG-NAH
9	B	1005	NAG	C4-C5-C6-O6
7	A	1003[B]	J2G	CAD-CAE-OAB-CAA
9	B	1006	NAG	O5-C5-C6-O6
7	B	1003[A]	J2G	CAF-CAE-OAB-CAA
7	B	1003[B]	J2G	CAD-CAE-OAB-CAA
9	A	1005	NAG	C4-C5-C6-O6
7	B	1003[A]	J2G	CAO-CAF-SAG-OAC
7	A	1003[A]	J2G	CAO-CAF-SAG-OAP
7	B	1003[A]	J2G	CAO-CAF-SAG-OAP

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Mol	Chain	Res	Type	Atoms
7	A	1003[A]	J2G	CAF-CAE-OAB-CAA
7	A	1003[A]	J2G	CAO-CAF-SAG-OAC
8	A	1004	LYS	O-C-CA-CB
8	A	1004	LYS	OXT-C-CA-CB
8	B	1004	LYS	O-C-CA-CB
8	B	1004	LYS	OXT-C-CA-CB
9	B	1005	NAG	O5-C5-C6-O6
7	A	1003[B]	J2G	CAE-CAF-SAG-OAC
7	B	1003[B]	J2G	CAE-CAF-SAG-OAC
7	B	1003[A]	J2G	CAO-CAF-SAG-NAH
7	A	1003[A]	J2G	CAR-CAQ-NAZ-CBC
7	B	1003[A]	J2G	CAR-CAQ-NAZ-CBC
9	B	1007	NAG	C4-C5-C6-O6
7	A	1003[A]	J2G	CAO-CAF-SAG-NAH
7	A	1003[A]	J2G	CAR-CAQ-NAZ-CBA
7	B	1003[A]	J2G	CAR-CAQ-NAZ-CBA
8	A	1004	LYS	O-C-CA-N
8	B	1004	LYS	O-C-CA-N
11	A	1011	PGE	C1-C2-O2-C3
7	B	1003[A]	J2G	CAD-CAE-OAB-CAA
7	A	1003[A]	J2G	CAD-CAE-OAB-CAA
8	A	1009	LYS	OXT-C-CA-CB
6	A	1002	MES	C7-C8-S-O1S
8	B	1010	LYS	O-C-CA-CB
8	B	1010	LYS	OXT-C-CA-CB
9	A	1007	NAG	C4-C5-C6-O6
8	A	1009	LYS	O-C-CA-CB
9	B	1007	NAG	O5-C5-C6-O6
7	A	1003[A]	J2G	CAI-CAQ-NAZ-CBC
7	B	1003[A]	J2G	CAI-CAQ-NAZ-CBC
7	A	1003[A]	J2G	CAI-CAQ-NAZ-CBA
7	B	1003[A]	J2G	CAI-CAQ-NAZ-CBA
11	A	1011	PGE	C3-C4-O3-C5

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1004	LYS	2	0
7	A	1003[B]	J2G	1	0
6	A	1002	MES	3	0
11	A	1011	PGE	2	0

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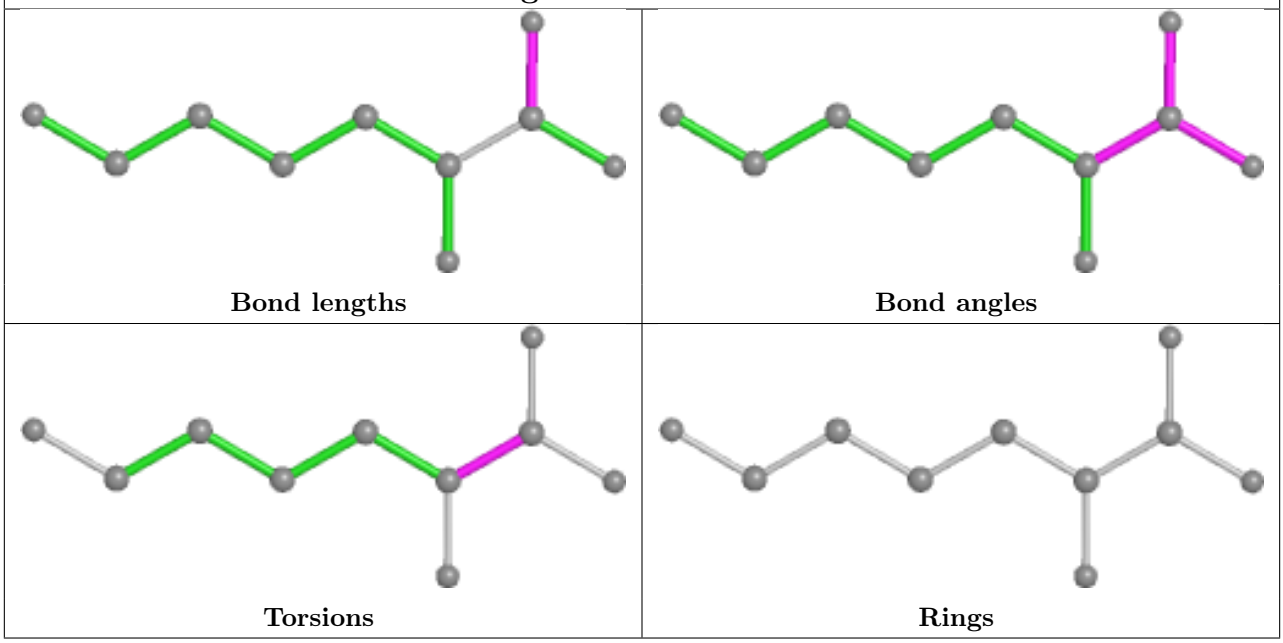
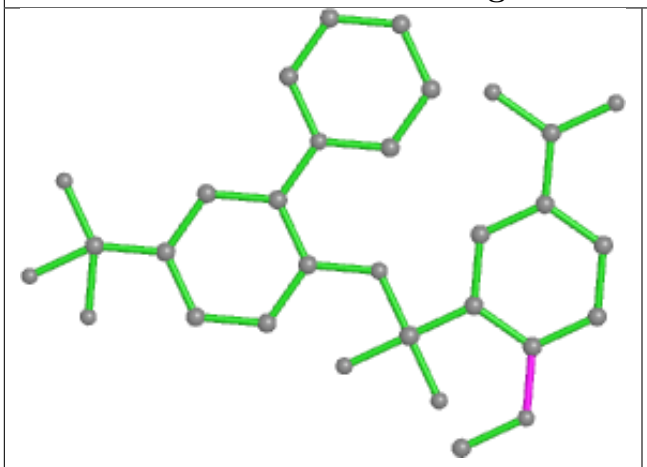
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1002	MES	2	0
10	B	1008	IMD	2	0
8	A	1009	LYS	1	0
8	A	1004	LYS	1	0

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 then 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.

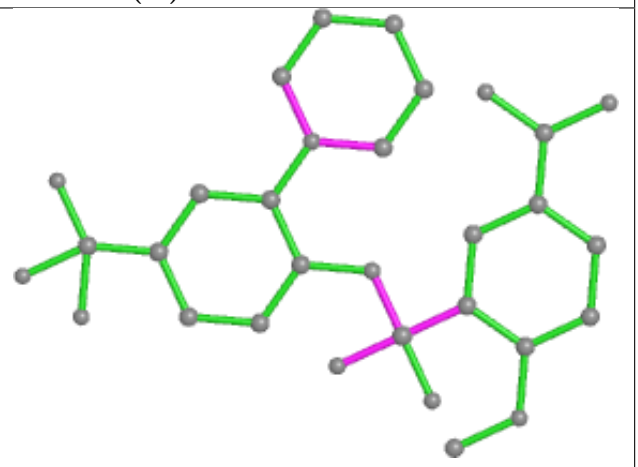
Ligand LYS B 1004



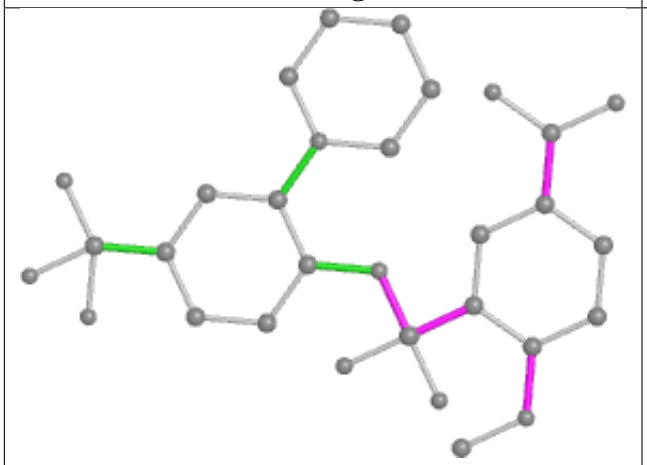
Ligand J2G A 1003 (B)



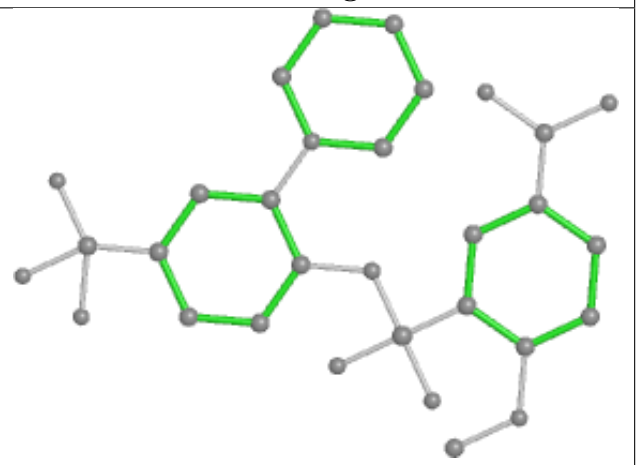
Bond lengths



Bond angles

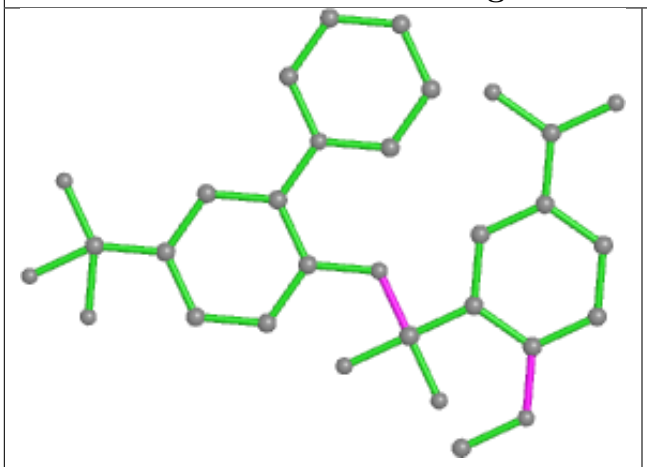


Torsions

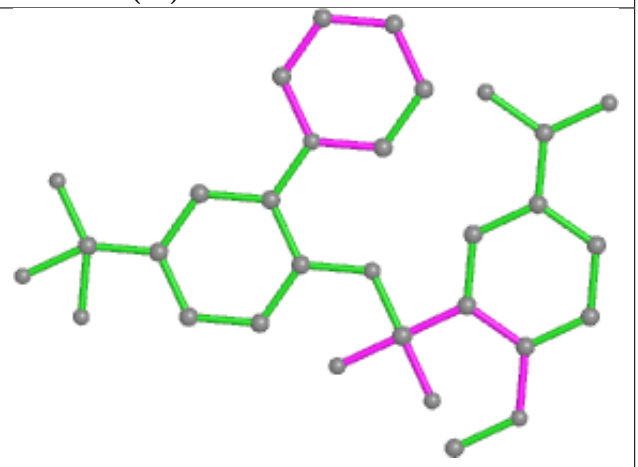


Rings

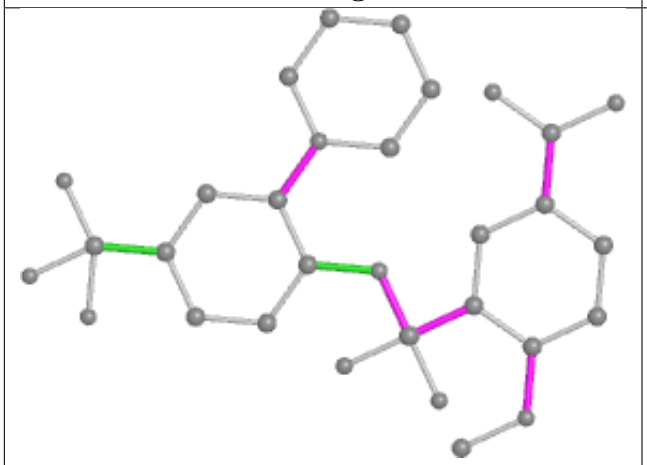
Ligand J2G A 1003 (A)



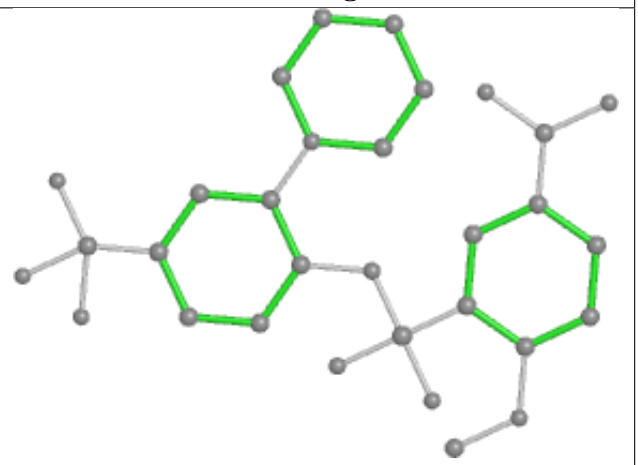
Bond lengths



Bond angles

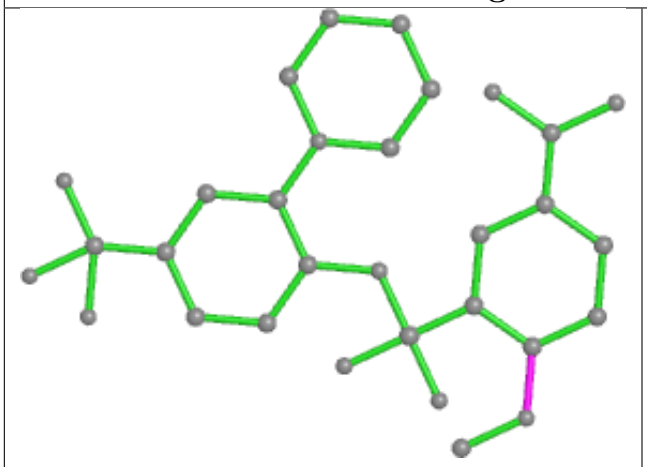


Torsions

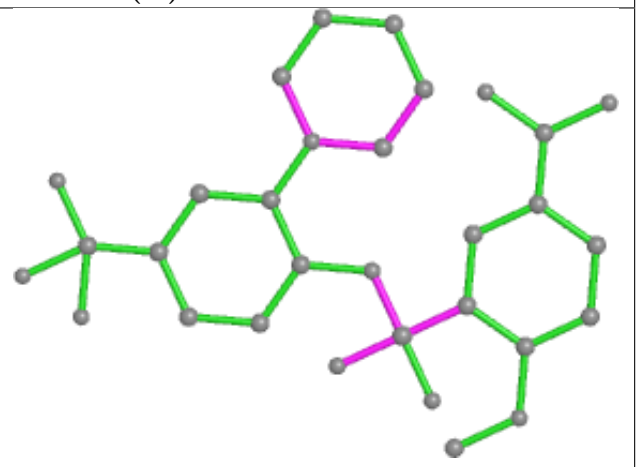


Rings

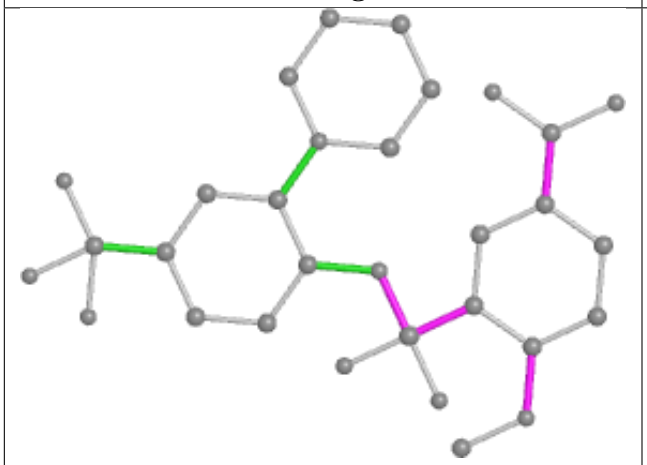
Ligand J2G B 1003 (B)



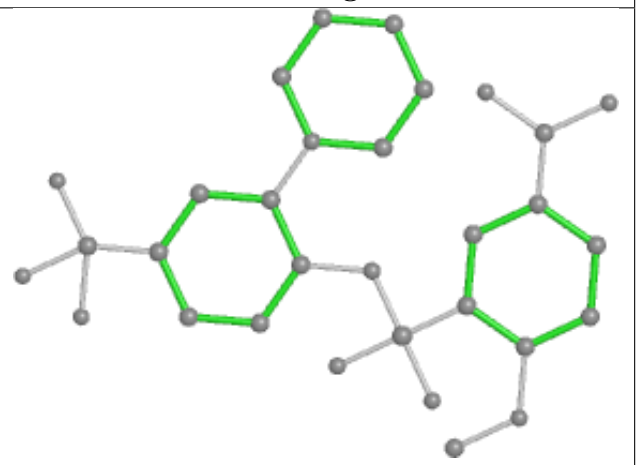
Bond lengths



Bond angles

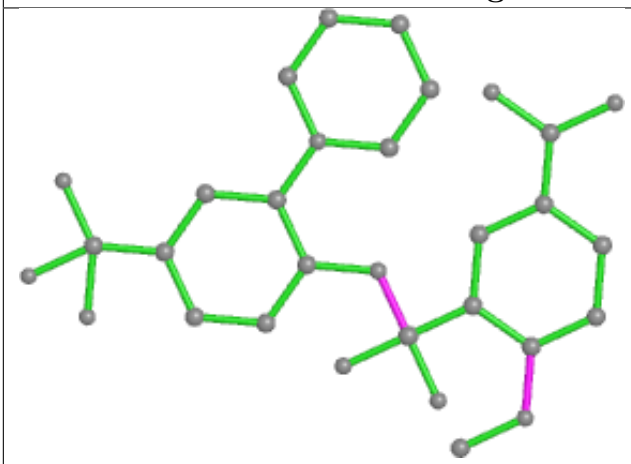


Torsions

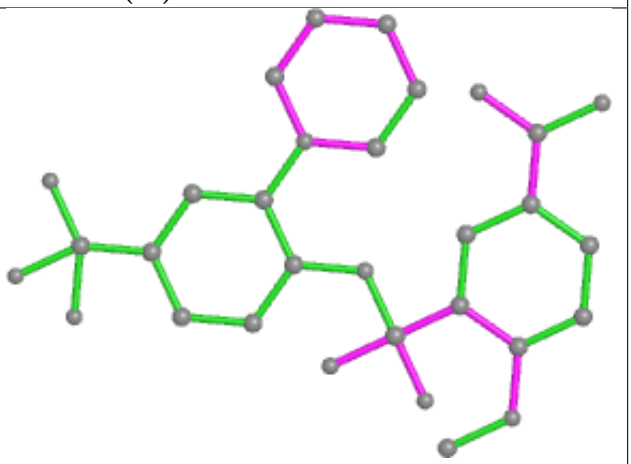


Rings

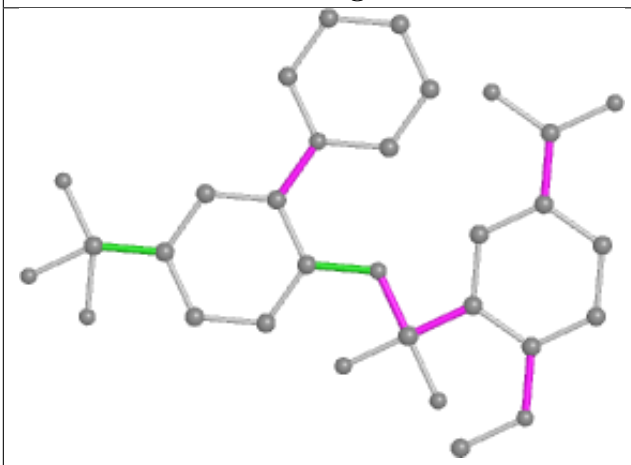
Ligand J2G B 1003 (A)



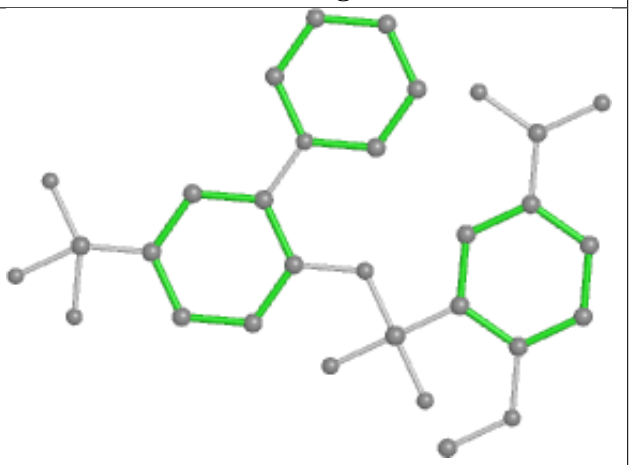
Bond lengths



Bond angles

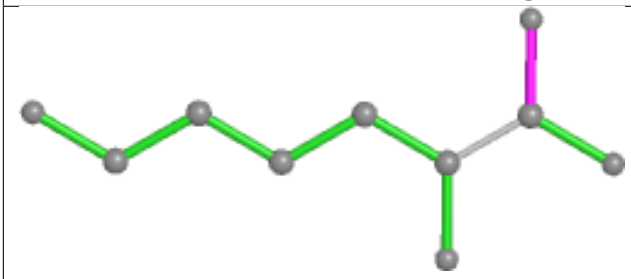


Torsions

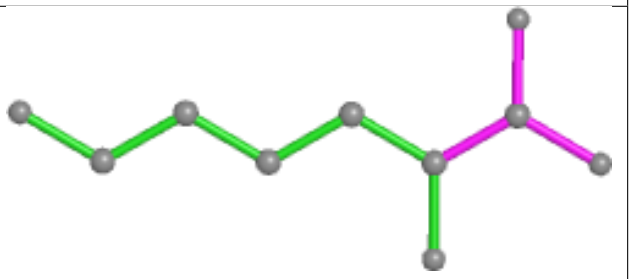


Rings

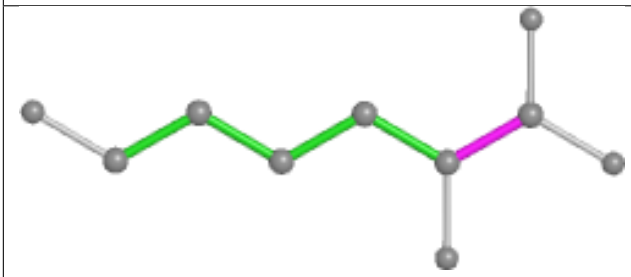
Ligand LYS B 1010



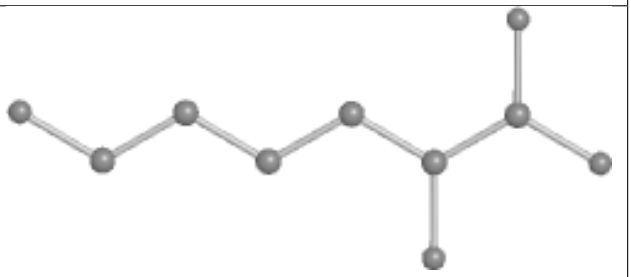
Bond lengths



Bond angles

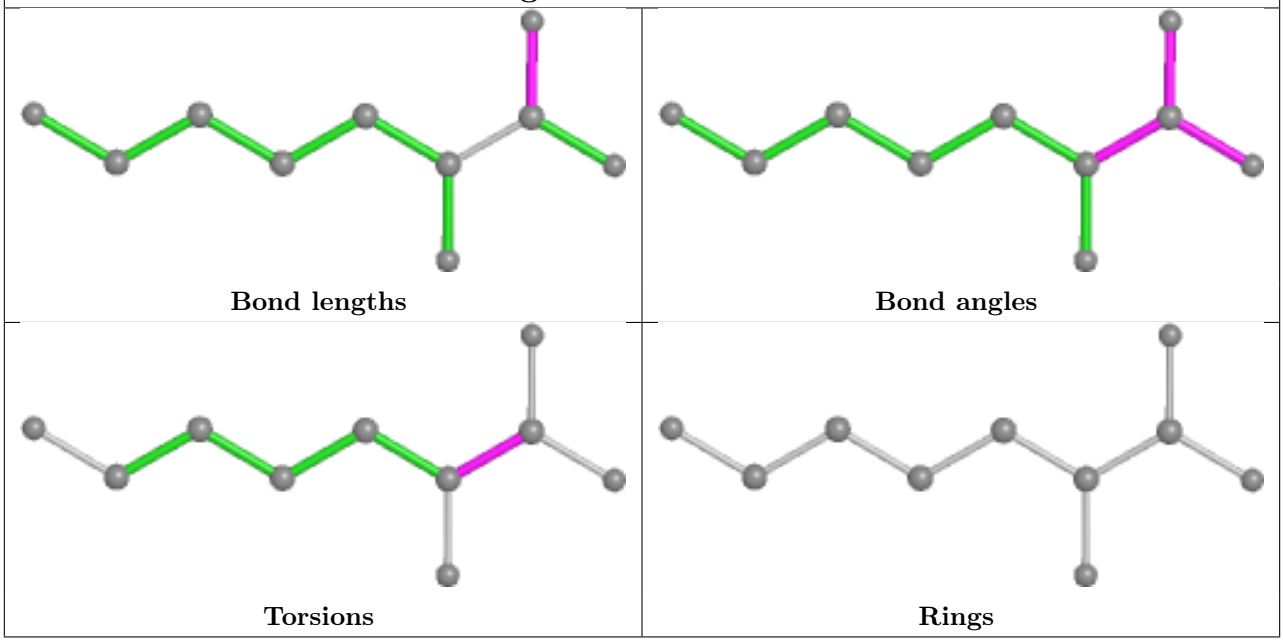


Torsions

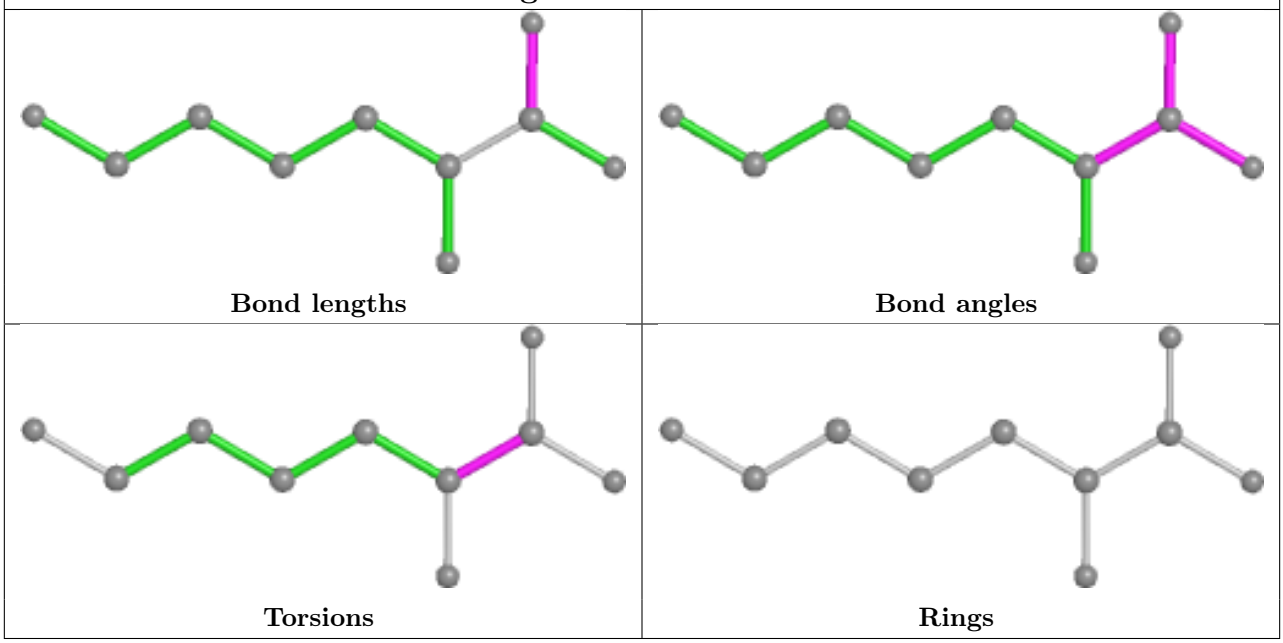


Rings

Ligand LYS A 1009



Ligand LYS A 1004



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	883/911 (96%)	-0.10	22 (2%) 57 53	38, 59, 95, 142	0
1	B	869/911 (95%)	0.63	107 (12%) 4 2	46, 98, 158, 198	0
All	All	1752/1822 (96%)	0.27	129 (7%) 14 11	38, 73, 144, 198	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	556	GLY	6.1
1	B	570	VAL	5.9
1	B	785	ASN	5.9
1	B	105	THR	5.8
1	B	501	ASN	5.8
1	B	781	SER	5.7
1	B	557	CYS	5.7
1	B	607	SER	5.0
1	B	555	ASP	4.9
1	B	592	TYR	4.9
1	B	578	ARG	4.8
1	B	613	ASP	4.8
1	B	500	SER	4.6
1	B	559	LEU	4.6
1	B	580	LEU	4.6
1	B	653	LEU	4.5
1	B	558	SER	4.4
1	B	779	GLU	4.2
1	B	612	LEU	4.1
1	B	620	TRP	4.1
1	B	783	LYS	4.1
1	B	598	ASN	4.1
1	B	623	PHE	4.0
1	A	783	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	784	LEU	3.9
1	B	579	ALA	3.9
1	B	338	ASN	3.9
1	B	264	VAL	3.9
1	B	571	PHE	3.9
1	B	554	GLN	3.9
1	A	785	ASN	3.9
1	A	779	GLU	3.8
1	B	534	VAL	3.7
1	B	577	TRP	3.6
1	A	578[A]	ARG	3.6
1	B	142	TYR	3.5
1	B	635	TYR	3.5
1	B	265	ALA	3.5
1	B	745	VAL	3.5
1	B	106	GLN	3.4
1	B	652	THR	3.4
1	B	107	PHE	3.3
1	B	162	TYR	3.3
1	B	561	LEU	3.2
1	B	591	THR	3.2
1	B	610	ASP	3.1
1	B	140	LEU	3.1
1	B	651	HIS	3.1
1	B	780	SER	3.1
1	B	618	THR	3.1
1	B	632	ILE	3.0
1	B	650	ASN	3.0
1	B	210	CYS	3.0
1	B	153	PRO	3.0
1	B	611	THR	2.9
1	B	631	TYR	2.9
1	B	621	VAL	2.9
1	B	440	ALA	2.9
1	B	472	GLU	2.9
1	A	501	ASN	2.9
1	A	557	CYS	2.8
1	B	742	LYS	2.8
1	B	209	PRO	2.8
1	B	61	ARG	2.8
1	B	583	ARG	2.8
1	B	584	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	67	LEU	2.8
1	B	401	LEU	2.8
1	B	260	SER	2.8
1	A	571	PHE	2.7
1	A	264	VAL	2.7
1	B	573	GLU	2.7
1	A	781	SER	2.7
1	B	57	THR	2.7
1	A	633	VAL	2.6
1	B	548	PRO	2.6
1	A	618	THR	2.6
1	B	56	ALA	2.6
1	B	739	TRP	2.6
1	B	599	VAL	2.6
1	B	476	LYS	2.6
1	B	55	VAL	2.6
1	B	633	VAL	2.5
1	B	778	MET	2.5
1	B	263	LEU	2.5
1	B	261	THR	2.5
1	A	784	LEU	2.5
1	B	619	SER	2.5
1	B	832	LYS	2.5
1	B	266	TYR	2.4
1	A	531	ASN	2.4
1	B	647	LEU	2.4
1	B	602	ARG	2.4
1	B	609	THR	2.4
1	B	564	GLU	2.3
1	A	373	ALA	2.3
1	A	596	SER	2.3
1	B	155	LYS	2.3
1	B	563	GLN	2.3
1	A	614	LEU	2.3
1	B	565	ARG	2.3
1	B	465	LEU	2.3
1	B	141	SER	2.2
1	B	211	PHE	2.2
1	B	867	LYS	2.2
1	A	341	LEU	2.2
1	A	210	CYS	2.2
1	A	265	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	728	GLN	2.2
1	B	774	PHE	2.2
1	A	556	GLY	2.2
1	B	248	LEU	2.2
1	B	624	ASN	2.2
1	A	262	TYR	2.2
1	B	688	GLN	2.2
1	B	768	GLN	2.2
1	B	923	ALA	2.2
1	B	125	GLU	2.1
1	B	341	LEU	2.1
1	B	625	VAL	2.1
1	B	603	HIS	2.1
1	B	131	MET	2.0
1	B	587	HIS	2.0
1	B	945	LEU	2.0
1	B	414	ASP	2.0
1	A	615	PRO	2.0
1	B	375	GLN	2.0
1	B	378	GLY	2.0
1	B	208	PHE	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	D	4	11/12	0.57	0.41	141,143,147,148	0
3	NAG	I	2	14/15	0.66	0.50	135,142,143,143	0
2	MAN	D	5	11/12	0.67	0.37	91,103,112,112	0
3	NAG	F	2	14/15	0.69	0.41	122,136,140,141	0
4	BMA	H	3	11/12	0.70	0.56	136,139,143,143	0
2	BMA	G	3	11/12	0.71	0.29	104,109,118,123	0
2	BMA	C	3	11/12	0.71	0.36	114,117,123,128	0

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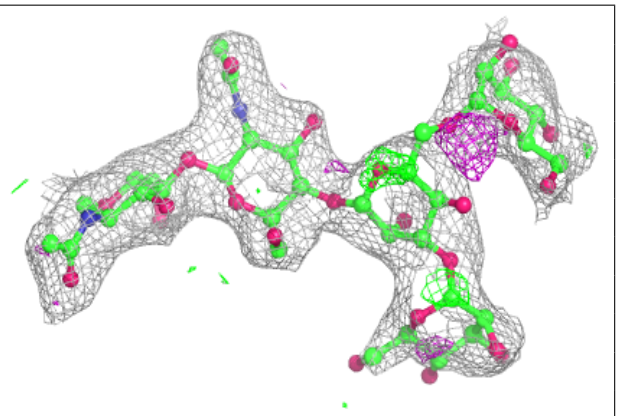
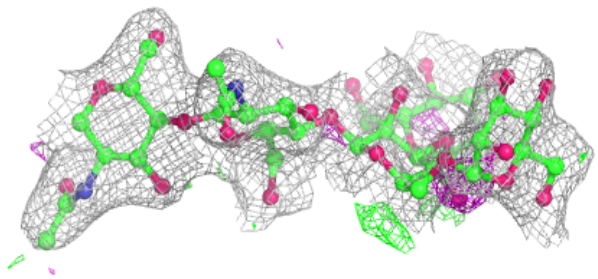
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BMA	D	3	11/12	0.75	0.46	114,120,135,140	0
3	NAG	I	1	14/15	0.76	0.23	112,125,134,139	0
2	MAN	G	4	11/12	0.77	0.47	129,132,135,136	0
2	MAN	G	5	11/12	0.79	0.35	72,96,106,108	0
2	MAN	C	4	11/12	0.81	0.49	124,128,132,134	0
2	MAN	C	5	11/12	0.81	0.41	98,112,119,121	0
3	NAG	E	2	14/15	0.83	0.38	106,117,121,121	0
3	NAG	E	1	14/15	0.84	0.20	71,87,102,111	0
3	NAG	F	1	14/15	0.84	0.29	96,105,123,130	0
4	NAG	H	1	14/15	0.86	0.32	89,100,111,114	0
2	NAG	D	2	14/15	0.86	0.24	65,76,89,108	0
4	NAG	H	2	14/15	0.88	0.39	113,121,126,132	0
2	NAG	C	2	14/15	0.90	0.20	68,86,99,102	0
2	NAG	G	2	14/15	0.92	0.26	63,80,93,100	0
2	NAG	D	1	14/15	0.94	0.13	40,57,62,62	0
2	NAG	G	1	14/15	0.95	0.17	52,63,73,83	0
2	NAG	C	1	14/15	0.95	0.09	53,64,76,78	0

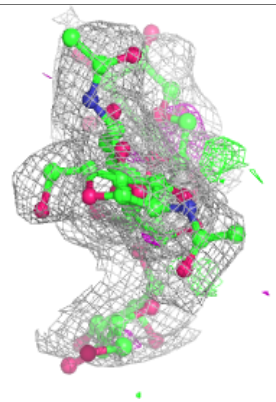
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

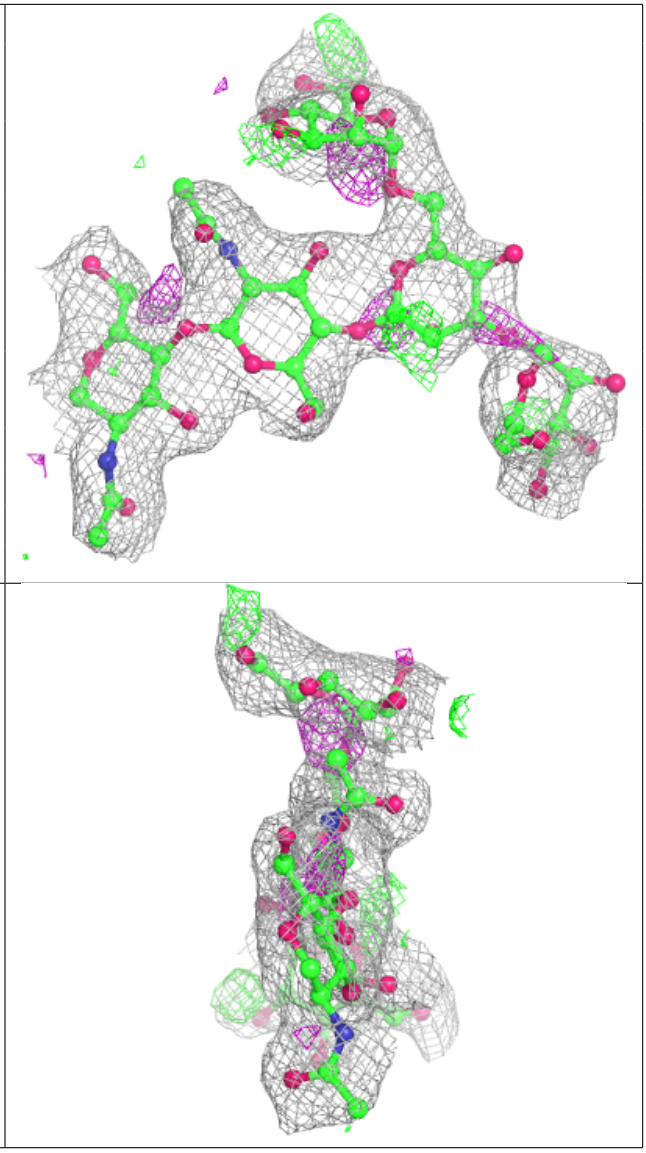






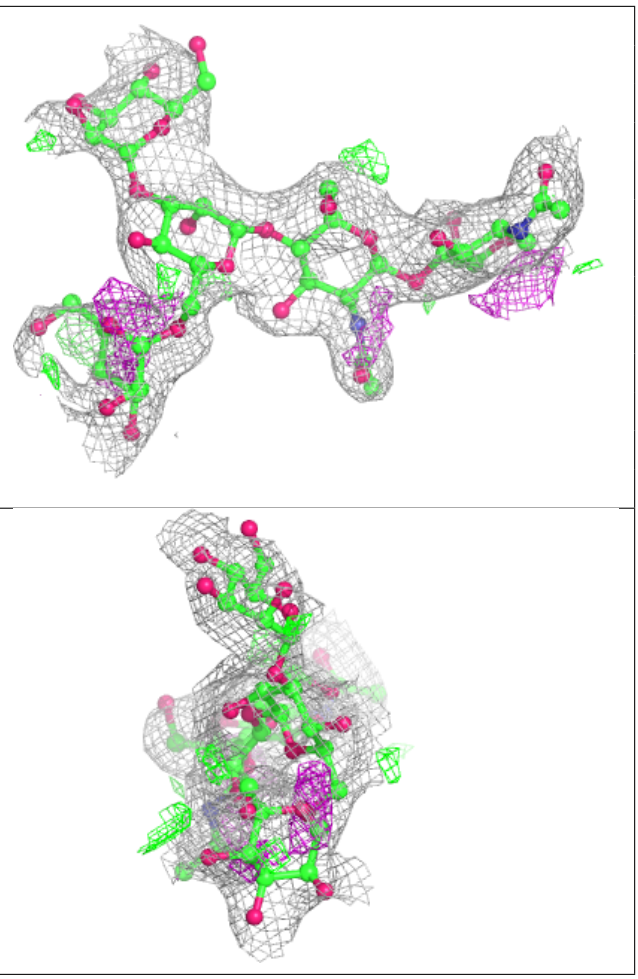
Electron density around Chain D:

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



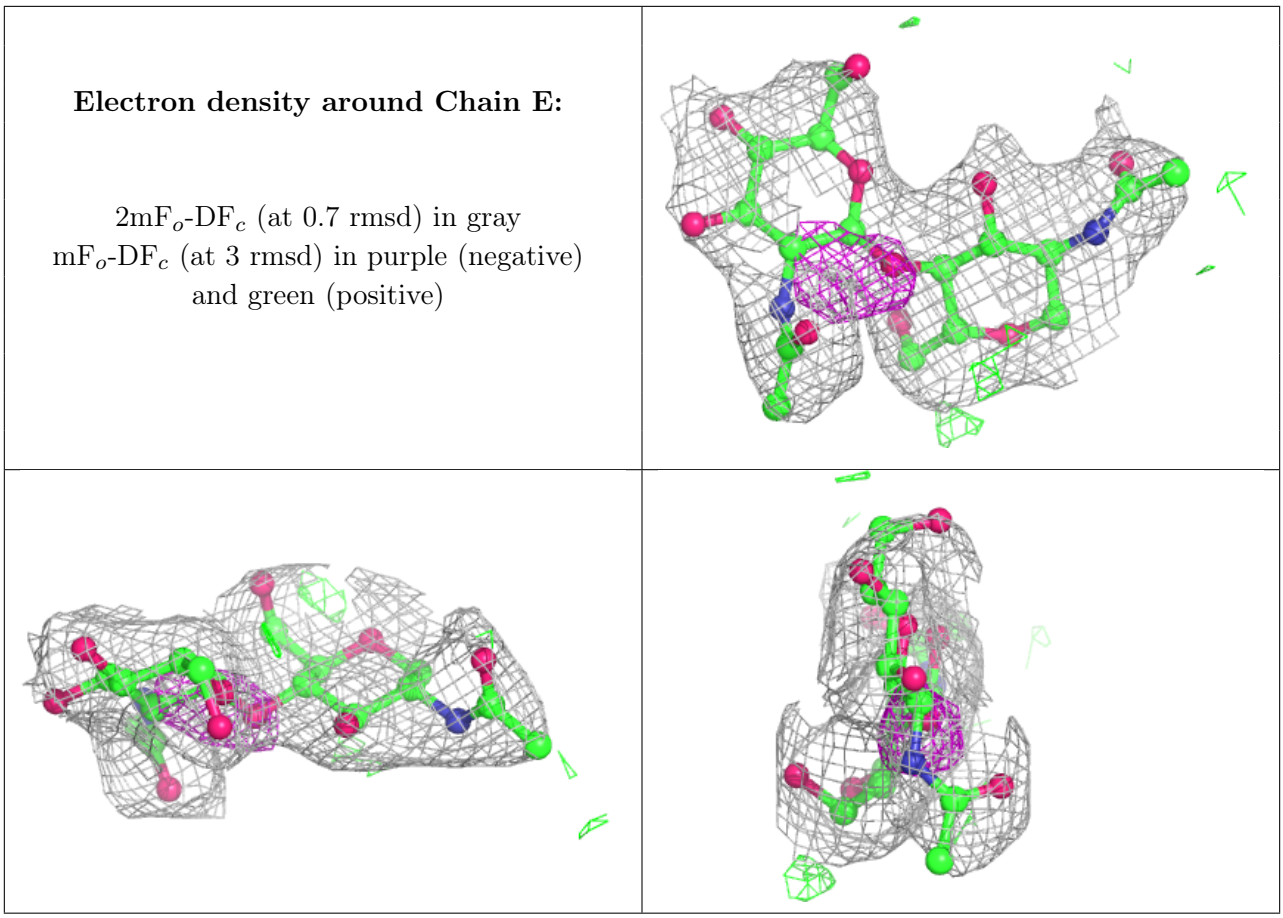
Electron density around Chain G:

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



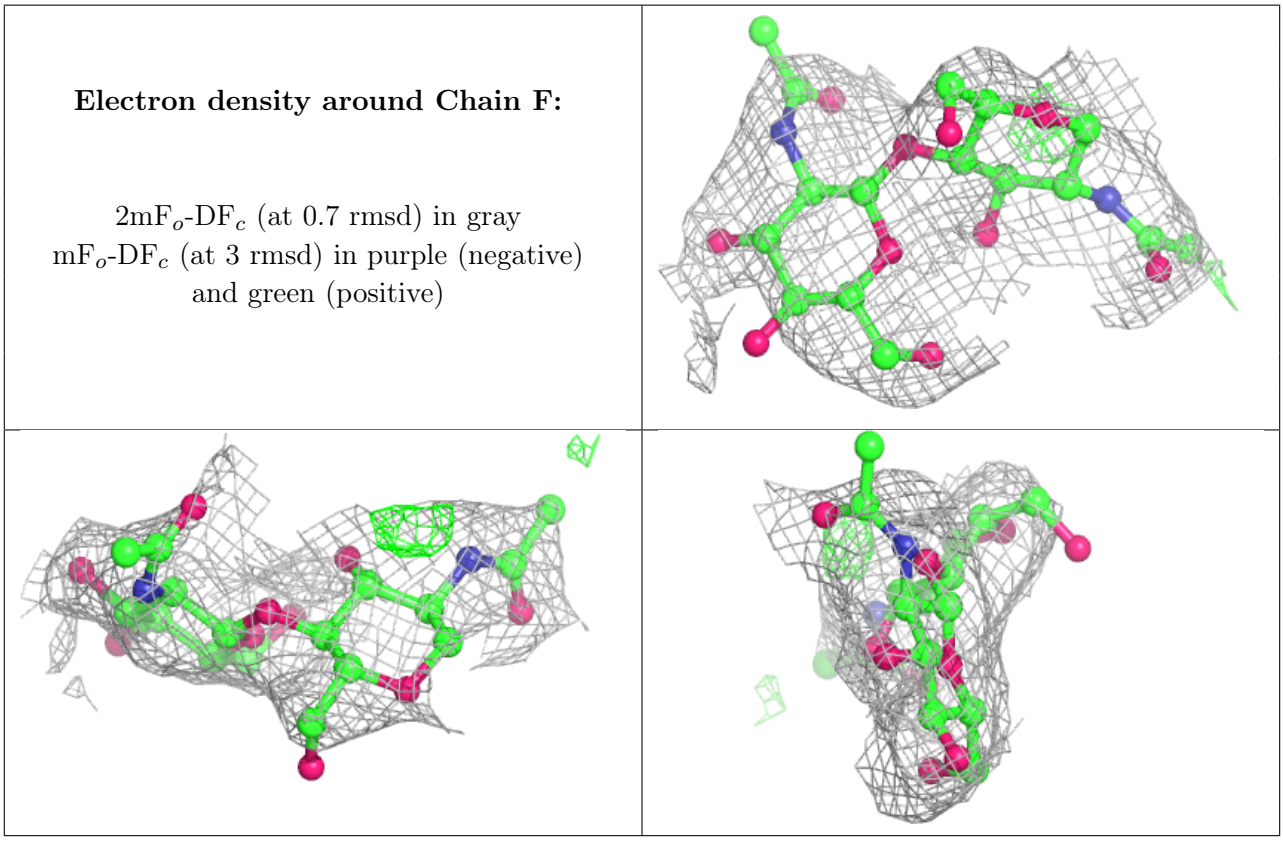
Electron density around Chain E:

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



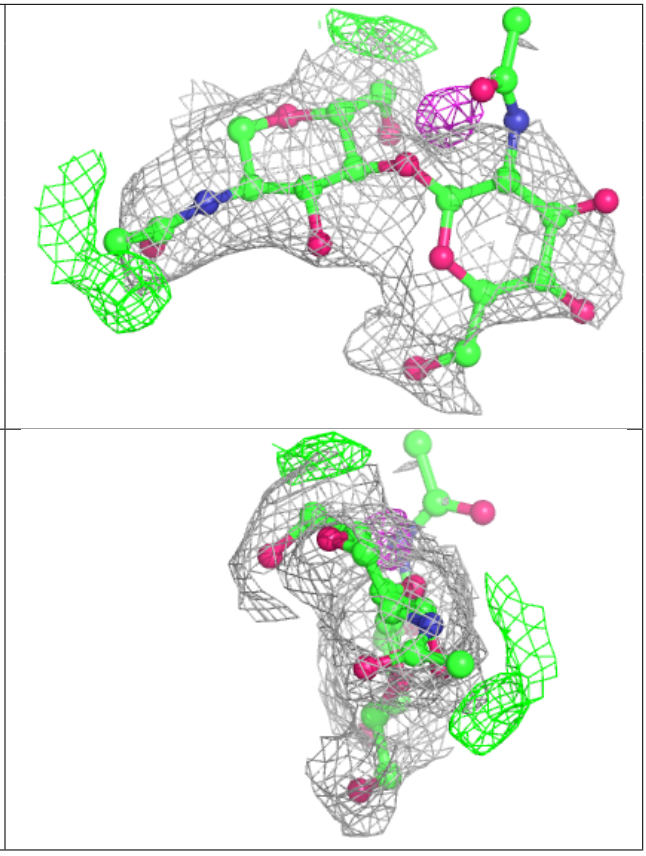
Electron density around Chain F:

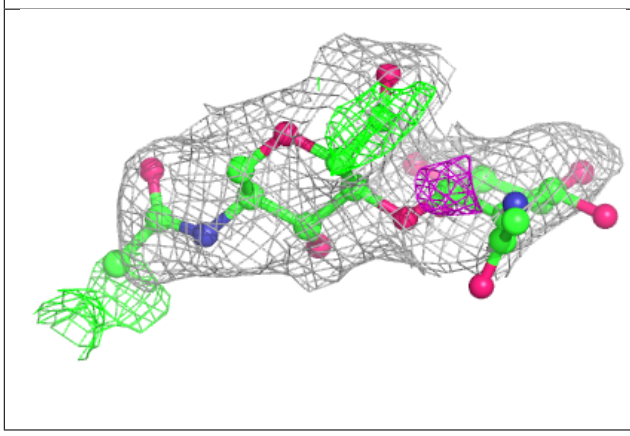
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain I:

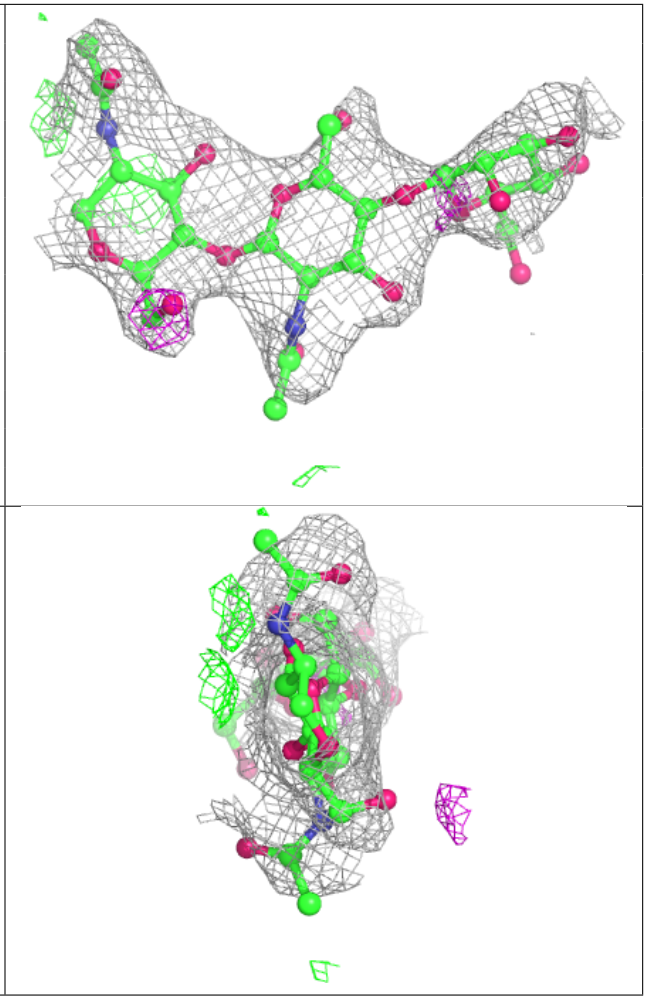
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around Chain H:

$2mF_o$-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
10	IMD	B	1008	5/5	0.54	0.59	95,97,103,111	5
9	NAG	A	1008	14/15	0.62	0.35	107,127,134,144	0
8	LYS	B	1010	10/10	0.63	0.41	83,90,93,93	10
7	J2G	B	1003[A]	31/31	0.63	0.50	81,86,89,89	31
7	J2G	B	1003[B]	31/31	0.63	0.50	81,85,88,90	31
7	J2G	A	1003[B]	31/31	0.69	0.43	50,58,62,63	31
7	J2G	A	1003[A]	31/31	0.69	0.43	50,59,63,64	31
9	NAG	B	1005	14/15	0.71	0.35	143,153,157,157	0
9	NAG	A	1007	14/15	0.72	0.34	118,121,127,131	0
9	NAG	B	1007	14/15	0.80	0.52	188,196,199,200	0

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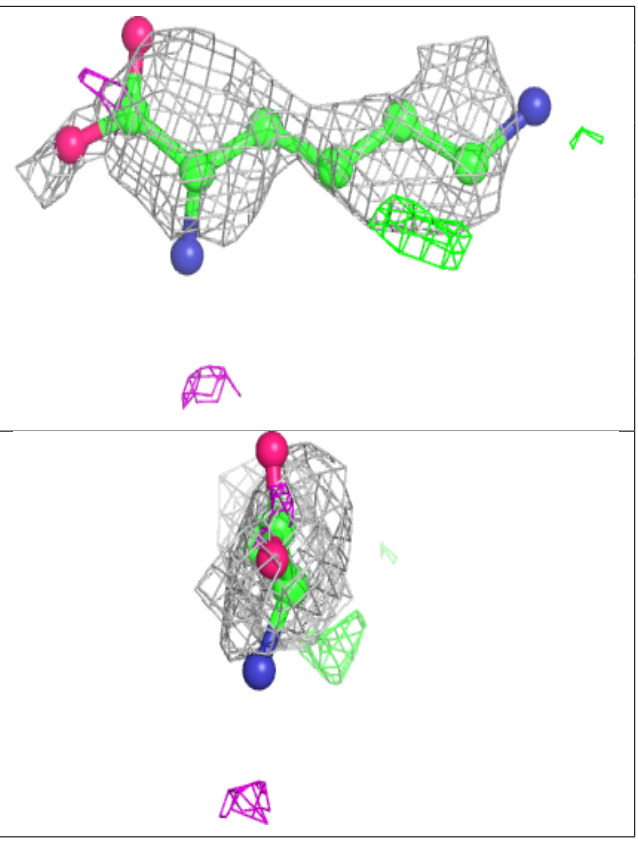
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	NAG	B	1006	14/15	0.81	0.30	169,174,181,182	0
11	PGE	A	1011	10/10	0.81	0.26	55,66,72,82	10
9	NAG	A	1005	14/15	0.82	0.31	119,128,137,141	0
10	IMD	A	1010	5/5	0.83	0.33	54,59,62,64	5
9	NAG	A	1006	14/15	0.83	0.34	89,106,117,118	0
8	LYS	A	1009	10/10	0.83	0.30	63,68,71,72	10
12	EDO	B	1009	4/4	0.83	0.23	98,103,108,112	0
6	MES	B	1002	12/12	0.86	0.23	82,87,88,100	12
8	LYS	B	1004	10/10	0.89	0.27	82,85,88,90	0
6	MES	A	1002	12/12	0.92	0.21	51,58,71,81	12
12	EDO	A	1012	4/4	0.94	0.22	64,67,68,77	0
8	LYS	A	1004	10/10	0.96	0.25	49,51,61,65	0
5	ZN	B	1001	1/1	0.98	0.16	73,73,73,73	0
5	ZN	A	1001	1/1	1.00	0.16	41,41,41,41	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.

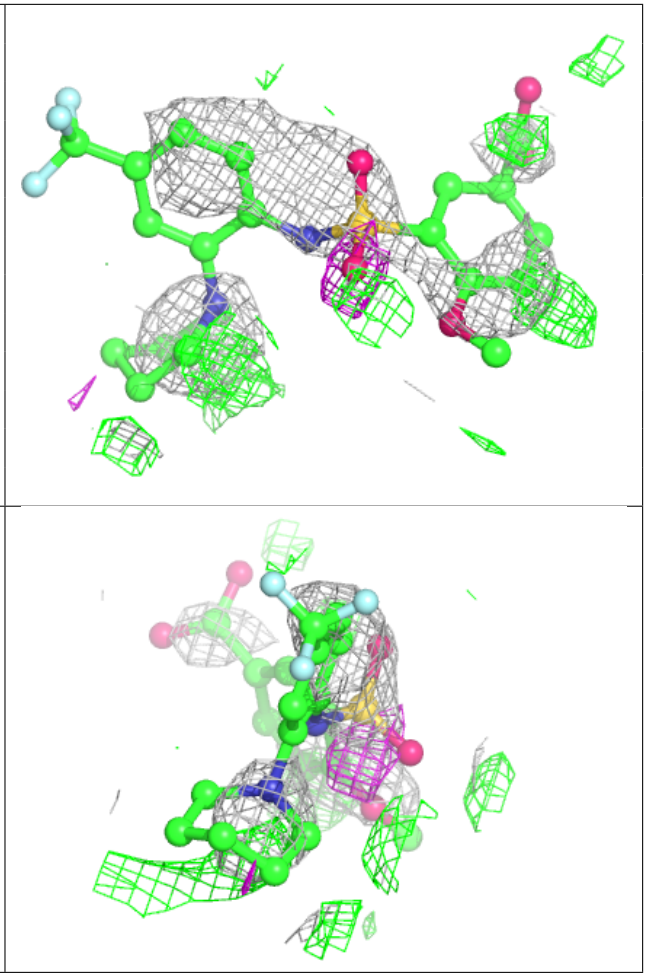
Electron density around LYS B 1010:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



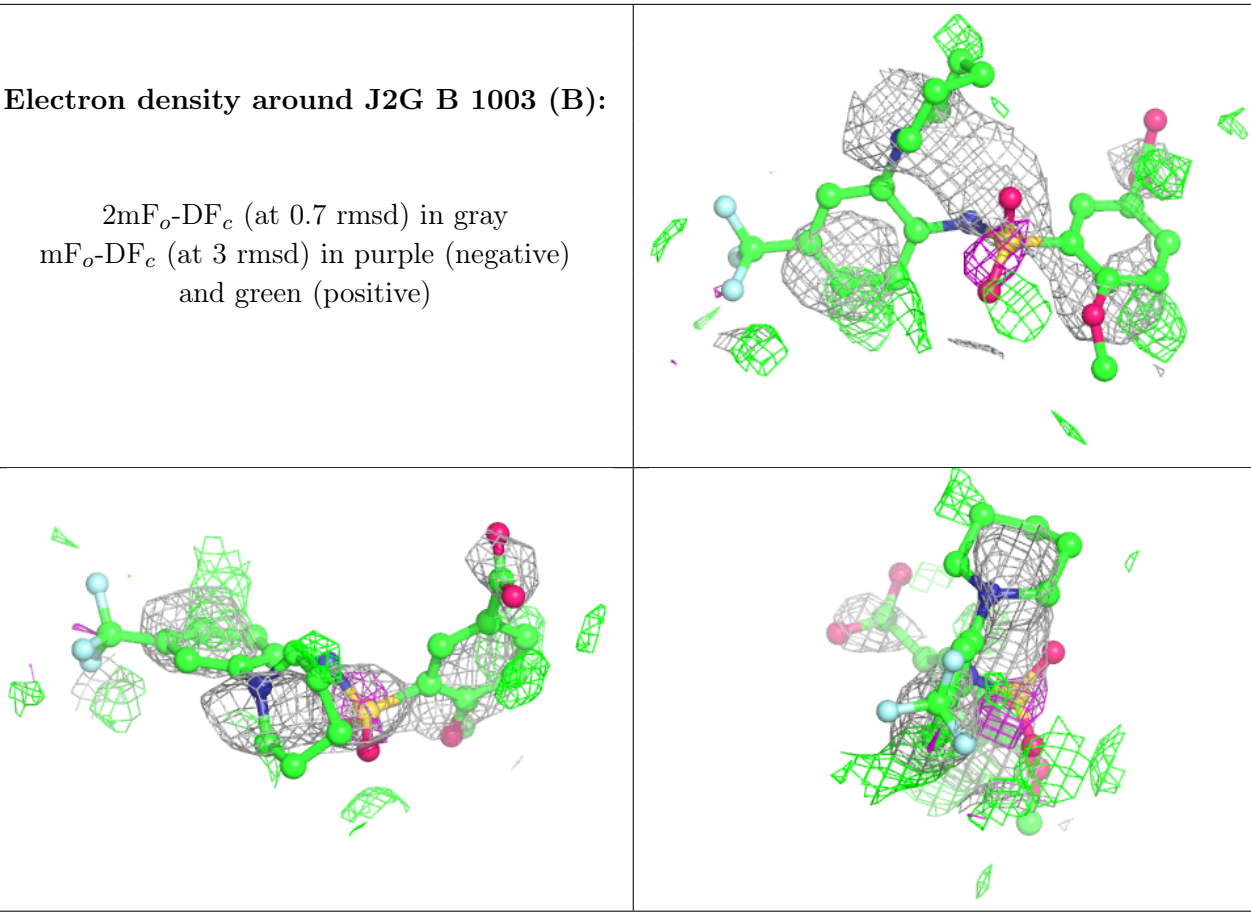
Electron density around J2G B 1003 (A):

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



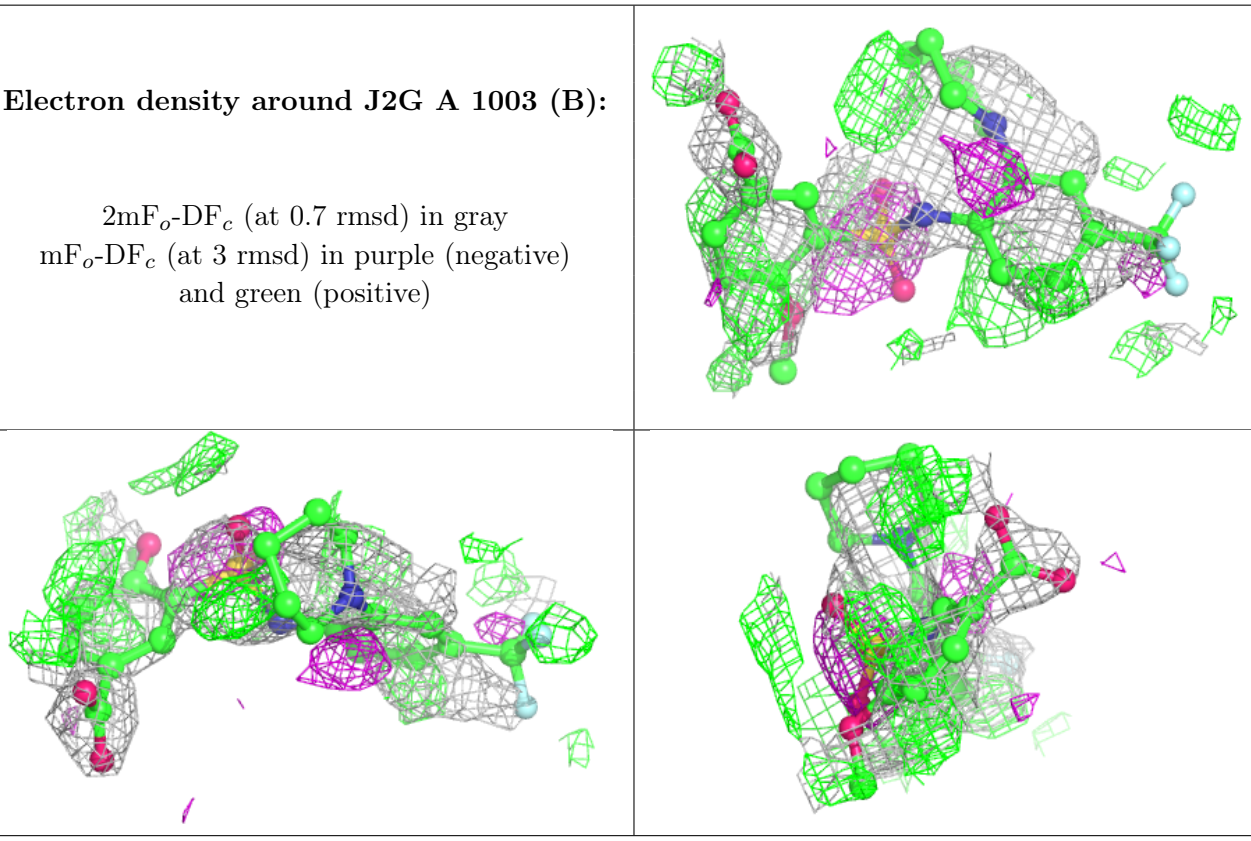
Electron density around J2G B 1003 (B):

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



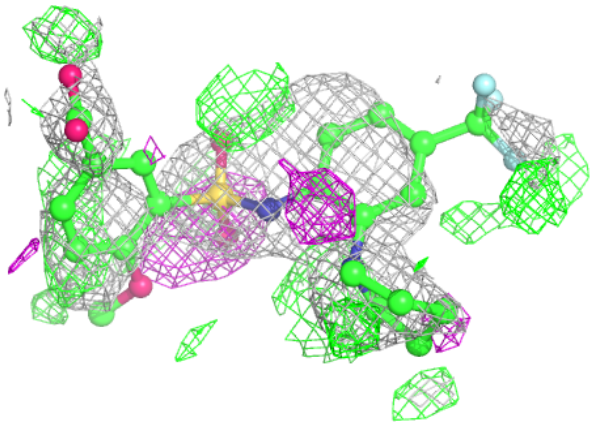
Electron density around J2G A 1003 (B):

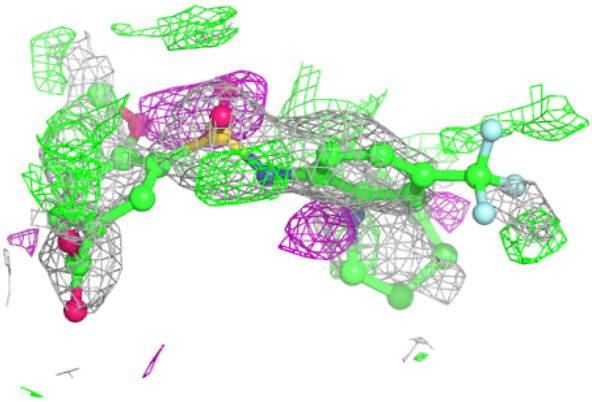
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

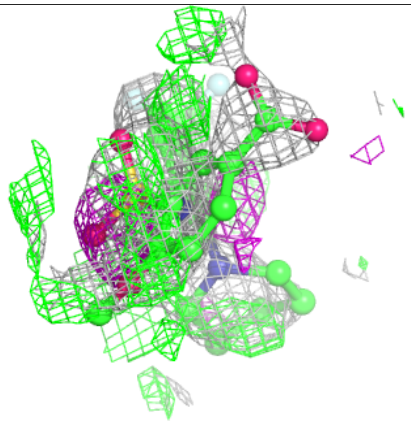


Electron density around J2G A 1003 (A):

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

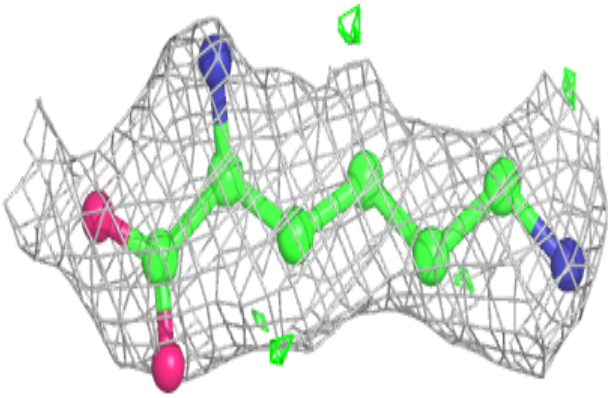


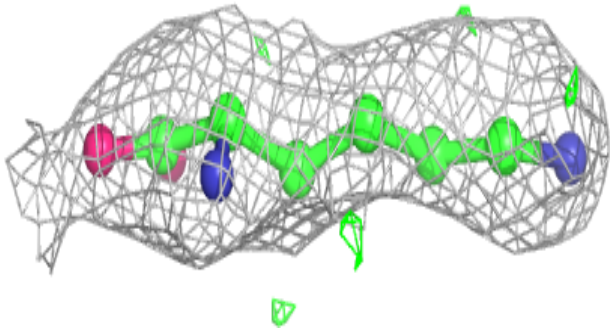


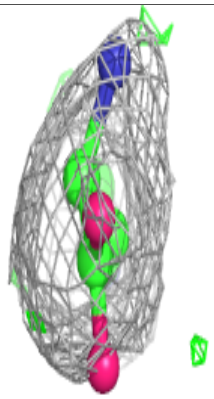


Electron density around LYS A 1009:

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

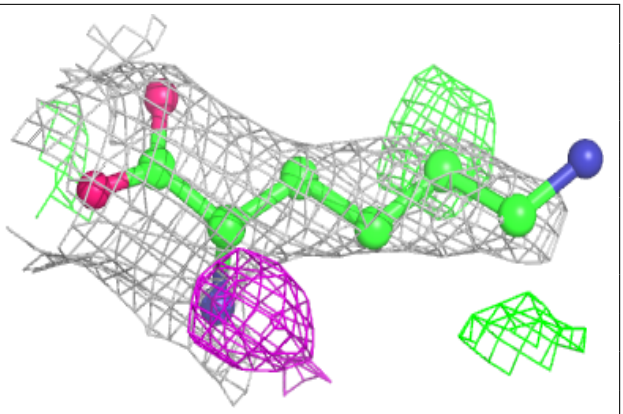


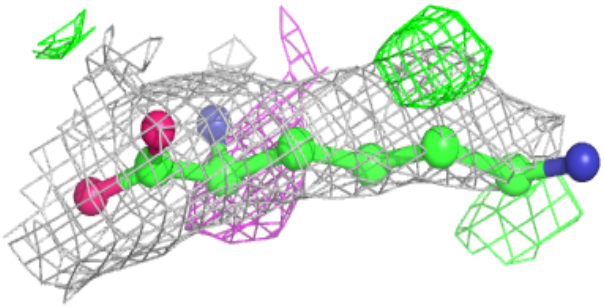


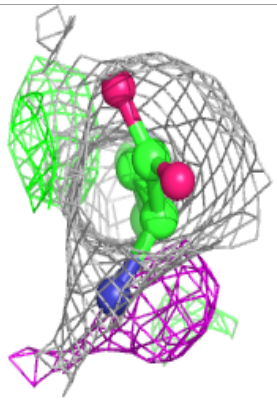


Electron density around LYS B 1004:

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

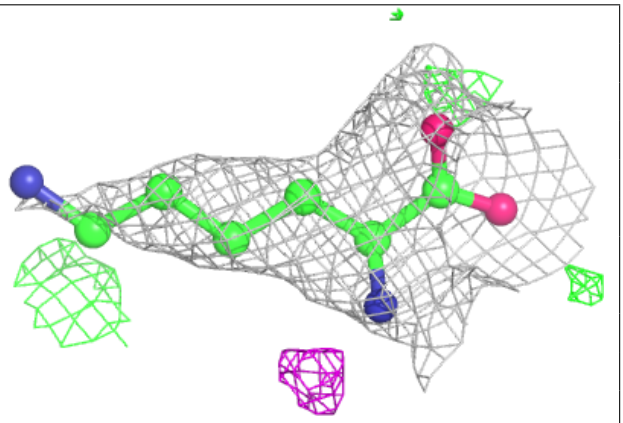


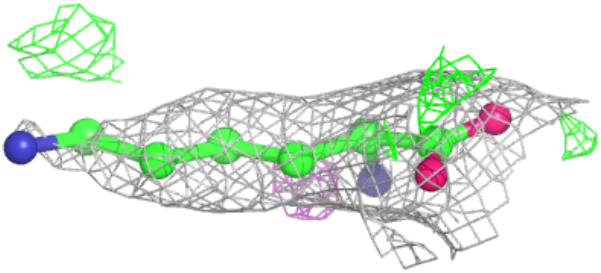


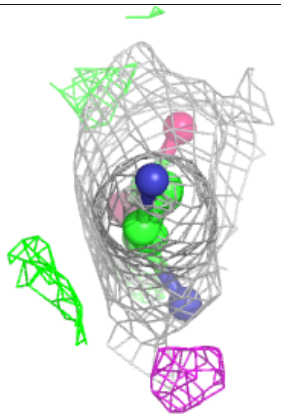


Electron density around LYS A 1004:

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

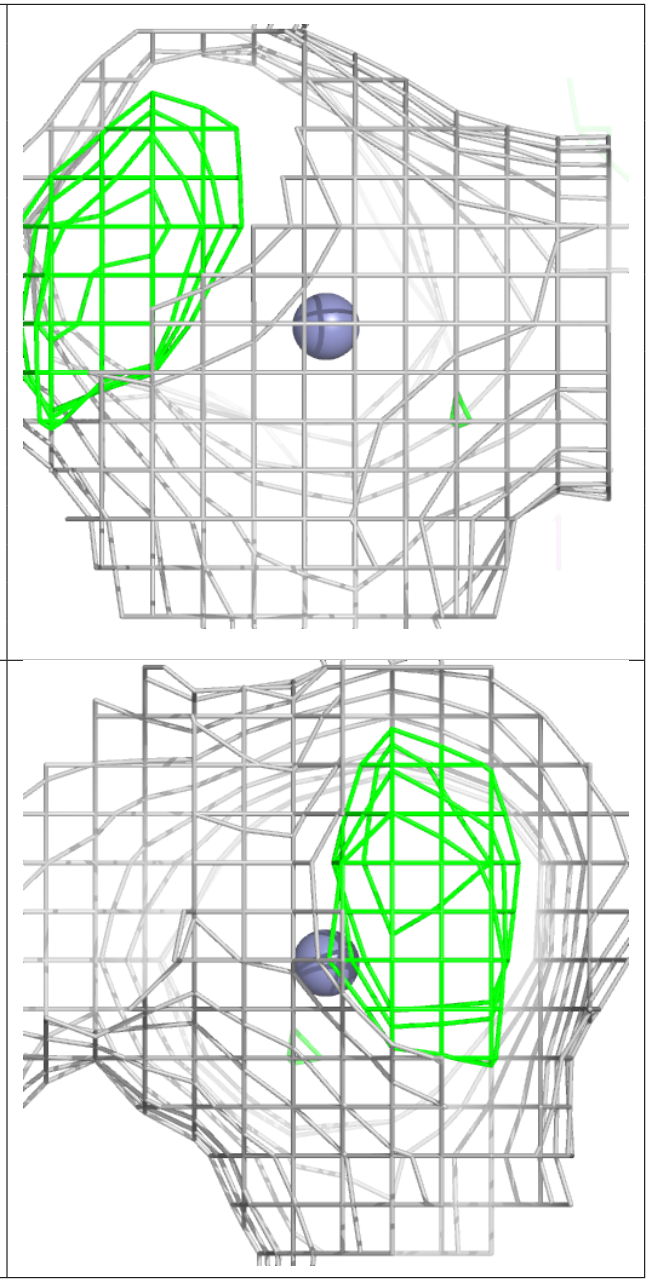






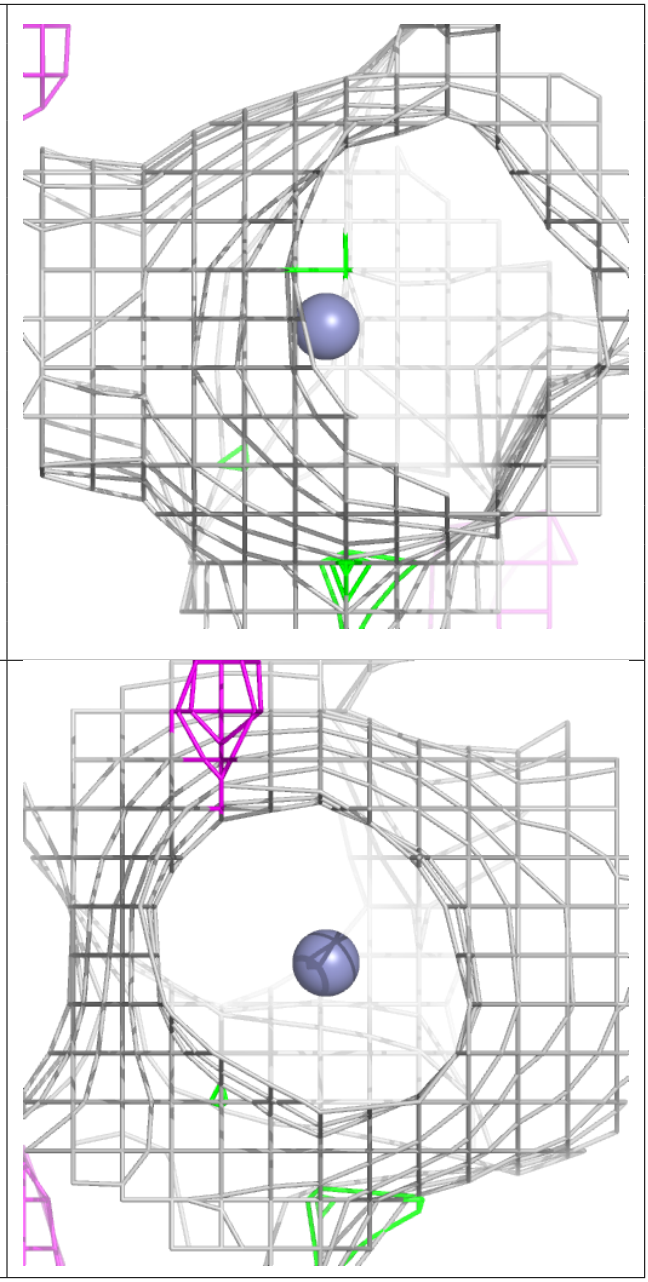
Electron density around ZN B 1001:

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



Electron density around ZN A 1001:

$2mF_o$-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.