Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2024 – 03:48 am GMT

PDB ID	:	6G46
Title	:	Red kidney bean purple acid phosphatase in complex with 2-(Naphthalen-1-yl)thiazole-4-carboxylic acid
Authors	:	Feder, D.F.
Deposited on	:	2018-03-26
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 (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:

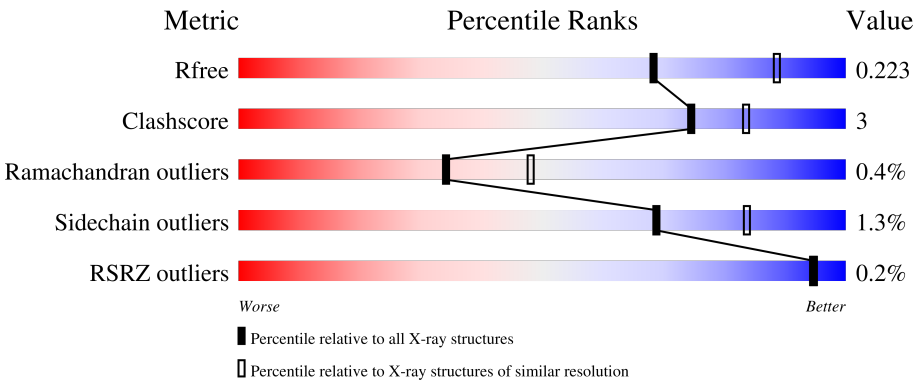
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 <=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	426	88% 11% •
1	B	426	92% 7%
1	C	426	90% 9%
1	D	426	92% 7% •
2	E	3	67% 33%

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Mol	Chain	Length	Quality of chain
2	F	3	100%
2	G	3	100%
2	I	3	67% 33%
2	J	3	67% 33%
2	M	3	67% 33%
3	H	2	100%
3	K	2	50% 50%
3	L	2	50% 50%

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	SO4	D	512	-	-	X	-

2 Entry composition (i)

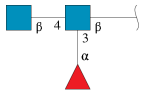
There are 13 unique types of molecules in this entry. The entry contains 15764 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Fe(3+)-Zn(2+) purple acid phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	424	3502	2248	610	634	10	0	1	0
1	B	425	3524	2260	612	641	11	9	3	0
1	D	423	3493	2245	606	632	10	0	1	0
1	C	424	3497	2246	608	633	10	0	0	0

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[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	E	3	38	22	2	14	0	0	0
2	F	3	38	22	2	14	0	0	0
2	G	3	38	22	2	14	0	0	0
2	I	3	38	22	2	14	0	0	0
2	J	3	38	22	2	14	0	0	0
2	M	3	38	22	2	14	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	H	2	24	14	1	9	0	0	0
3	K	2	24	14	1	9	0	0	0
3	L	2	24	14	1	9	0	0	0

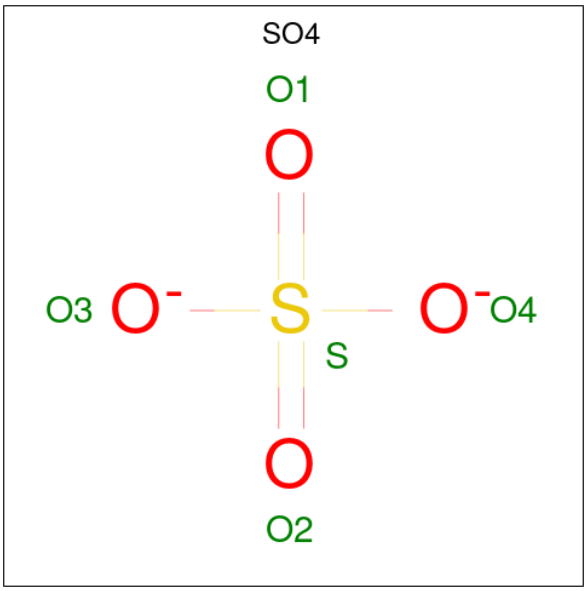
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	A	1	1	1	0	0
4	B	1	1	1	0	0
4	D	1	1	1	0	0
4	C	1	1	1	0	0

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe).

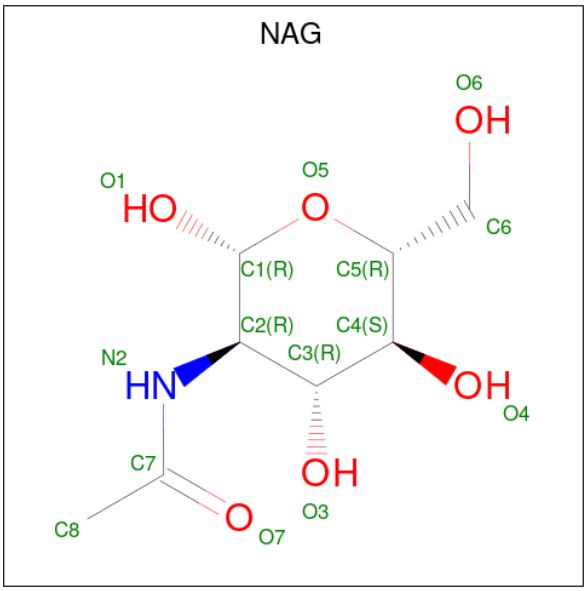
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
5	A	1	1	1	0	0
5	B	1	1	1	0	0
5	D	1	1	1	0	0
5	C	1	1	1	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



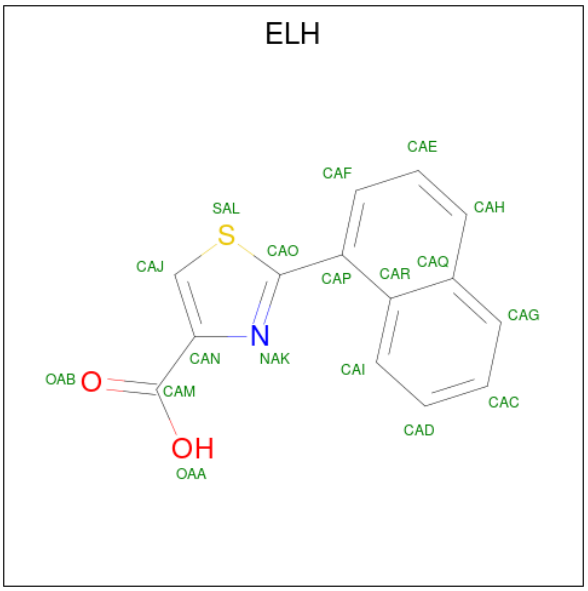
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



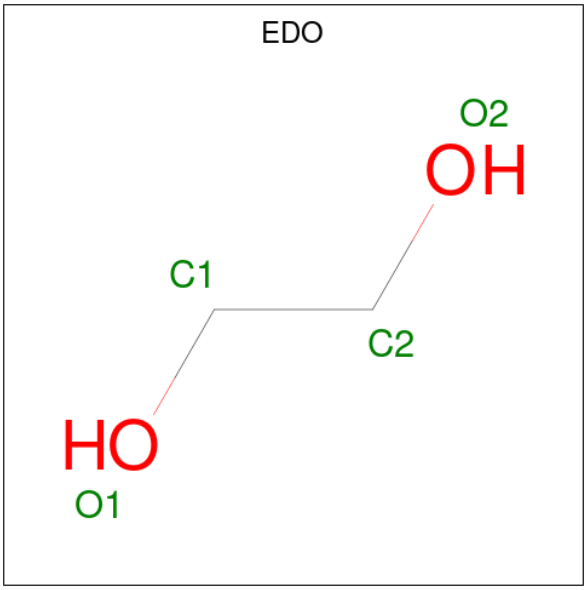
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	14	8	1	5	0	0
			Total	C	N	O		
7	B	1	14	8	1	5	0	0
			Total	C	N	O		
7	B	1	14	8	1	5	0	0
			Total	C	N	O		
7	D	1	14	8	1	5	0	0
			Total	C	N	O		
7	D	1	14	8	1	5	0	0
			Total	C	N	O		
7	C	1	14	8	1	5	0	0
			Total	C	N	O		
7	C	1	14	8	1	5	0	0

- Molecule 8 is 2-naphthalen-1-yl-1,3-thiazole-4-carboxylic acid (three-letter code: ELH) (formula: $C_{14}H_9NO_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
8	A	1	18	14	1	2	1	0	0
			Total	C	N	O	S		
8	B	1	18	14	1	2	1	0	0

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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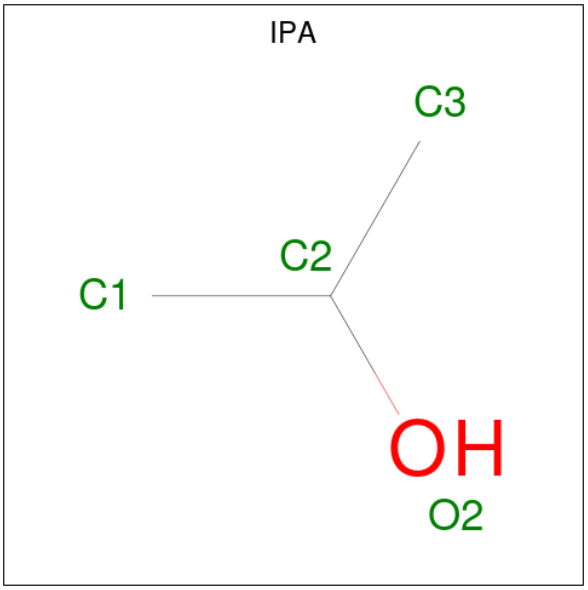
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	D	1	Total C O 4 2 2	0	0
9	D	1	Total C O 4 2 2	0	0
9	C	1	Total C O 4 2 2	0	0

- Molecule 10 is SODIUM ION (three-letter code: NA) (formula: Na).

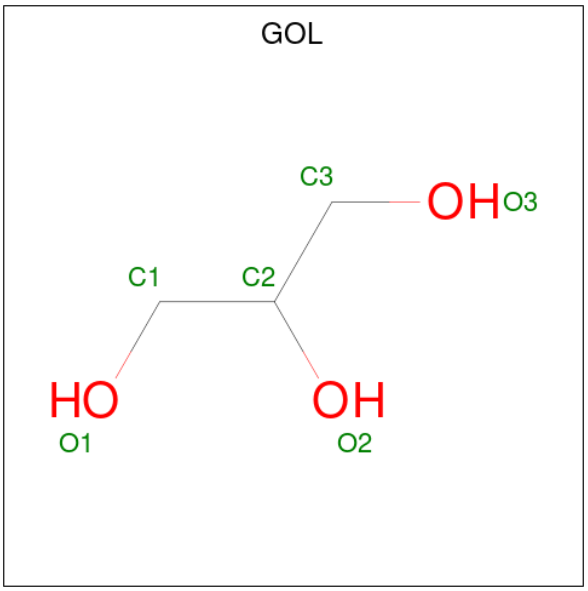
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	2	Total Na 2 2	0	0
10	D	1	Total Na 1 1	0	0

- Molecule 11 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total C O 4 3 1	0	0

- Molecule 12 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
12	C	1	6	3	3	0	0

- Molecule 13 is water.

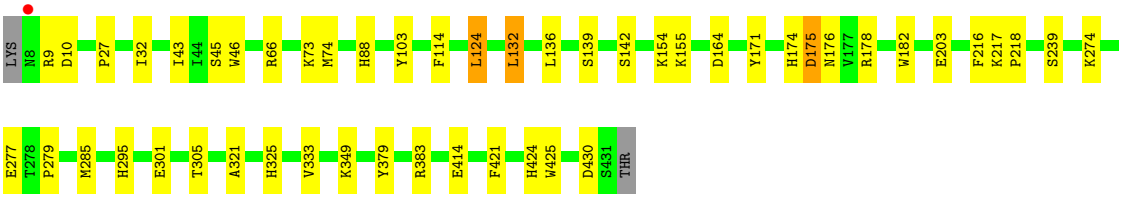
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
13	A	332	332	332	0	0
			Total	O		
13	B	283	283	283	0	0
			Total	O		
13	D	319	319	319	0	0
			Total	O		
13	C	291	291	291	0	0

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.

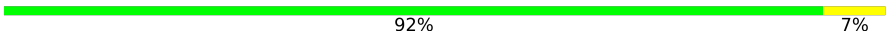
• Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase

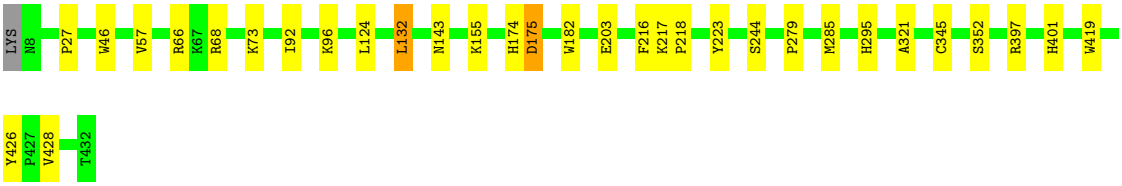
Chain A:



• Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase

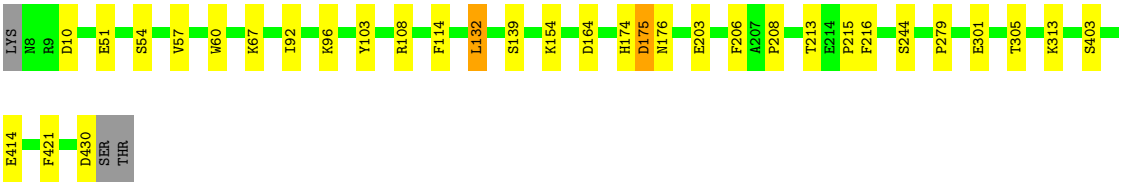
Chain B:





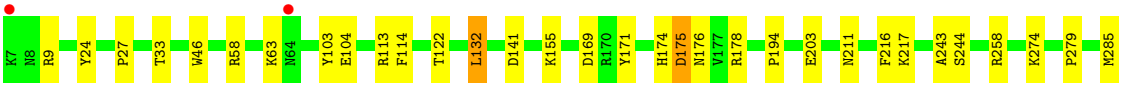
• Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase

Chain D:



• Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase

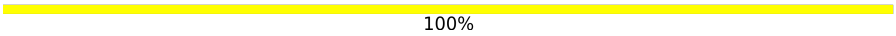
Chain C:



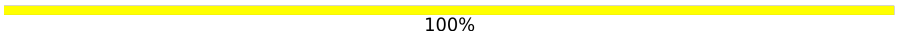
• Molecule 2: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

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

Chain F: 

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

Chain G: 

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

Chain I:

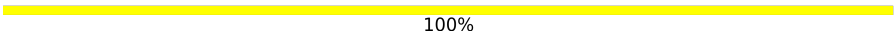
• Molecule 2: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

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

Chain M:

• Molecule 3: alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 

- Molecule 3: alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

- Molecule 3: alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	126.21Å 126.21Å 297.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.26 – 2.40 43.26 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (43.26-2.40) 98.8 (43.26-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.99 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.172 , 0.223 0.172 , 0.223	Depositor DCC
R_{free} test set	5324 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	33.9	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 27.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.146 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15764	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: GOL, NAG, FE, ZN, IPA, ELH, NA, FUC, EDO, SO4

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	0.45	0/3624	0.60	1/4927 (0.0%)
1	B	0.44	0/3643	0.57	1/4953 (0.0%)
1	C	0.46	0/3616	0.59	1/4916 (0.0%)
1	D	0.44	0/3615	0.60	1/4916 (0.0%)
All	All	0.45	0/14498	0.59	4/19712 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	132	LEU	CA-CB-CG	-7.33	98.43	115.30
1	A	132	LEU	CA-CB-CG	-6.50	100.35	115.30
1	D	132	LEU	CA-CB-CG	-6.42	100.55	115.30
1	B	132	LEU	CA-CB-CG	-5.95	101.61	115.30

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	3502	0	3321	24	0
1	B	3524	0	3334	20	0
1	C	3497	0	3316	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3493	0	3314	17	0
2	E	38	0	34	0	0
2	F	38	0	34	0	0
2	G	38	0	34	0	0
2	I	38	0	34	0	0
2	J	38	0	34	0	0
2	M	38	0	34	0	0
3	H	24	0	22	0	0
3	K	24	0	22	1	0
3	L	24	0	22	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	10	0	0	0	0
6	B	10	0	0	0	0
6	C	10	0	0	1	0
6	D	10	0	0	2	0
7	A	14	0	13	0	0
7	B	28	0	26	1	0
7	C	28	0	26	0	0
7	D	28	0	26	0	0
8	A	18	0	0	4	0
8	B	18	0	0	3	0
9	A	4	0	6	0	0
9	B	12	0	18	1	0
9	C	4	0	6	1	0
9	D	8	0	12	2	0
10	B	2	0	0	0	0
10	D	1	0	0	0	0
11	B	4	0	8	0	0
12	C	6	0	8	0	0
13	A	332	0	0	2	0
13	B	283	0	0	1	0
13	C	291	0	0	2	0
13	D	319	0	0	1	0
All	All	15764	0	13704	90	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 3.

All (90) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:ARG:N	6:C:511:SO4:O2	2.19	0.76
1:B:143:ASN:HD22	7:B:507:NAG:H83	1.54	0.72
1:B:244:SER:HB2	1:B:279:PRO:HD2	1.79	0.65
1:C:169:ASP:OD2	13:C:601:HOH:O	2.14	0.64
1:B:124:LEU:HD12	1:B:279:PRO:HG3	1.83	0.60
1:D:244:SER:HB2	1:D:279:PRO:HD2	1.84	0.58
1:C:113:ARG:HH12	9:C:512:EDO:H11	1.67	0.57
1:C:244:SER:HB2	1:C:279:PRO:HD2	1.86	0.57
1:B:203:GLU:O	1:B:216:PHE:HA	2.05	0.55
1:B:27:PRO:HB3	1:B:46:TRP:CD1	2.42	0.54
1:B:66:ARG:HH11	1:B:68:ARG:HE	1.56	0.54
1:A:295:HIS:NE2	8:A:515:ELH:CAF	2.72	0.53
1:D:51:GLU:OE1	1:D:108:ARG:NH2	2.41	0.52
1:C:9:ARG:NH2	1:C:141:ASP:OD2	2.42	0.52
1:D:203:GLU:O	1:D:216:PHE:HA	2.10	0.52
1:D:313:LYS:NZ	13:D:609:HOH:O	2.38	0.52
1:C:285:MET:O	1:C:321:ALA:HA	2.11	0.51
1:C:203:GLU:O	1:C:216:PHE:HA	2.09	0.51
1:D:54:SER:HB2	1:D:108:ARG:HG3	1.93	0.51
1:A:325:HIS:CE1	8:A:515:ELH:CAJ	2.94	0.51
1:A:301:GLU:O	1:A:305:THR:HG23	2.12	0.50
1:B:397:ARG:HD2	9:B:517:EDO:O1	2.11	0.50
1:A:414:GLU:HG2	13:A:882:HOH:O	2.11	0.50
8:A:515:ELH:NAK	8:A:515:ELH:CAI	2.72	0.50
1:C:103:TYR:CZ	1:C:114:PHE:HB2	2.46	0.50
1:C:27:PRO:HB3	1:C:46:TRP:CD1	2.47	0.49
1:D:60:TRP:HB3	1:D:67:LYS:HA	1.94	0.48
8:B:512:ELH:CAG	1:C:258:ARG:HH22	2.26	0.48
6:D:512:SO4:O4	9:D:514:EDO:H21	2.14	0.48
1:B:155:LYS:HD3	13:B:673:HOH:O	2.13	0.47
8:B:512:ELH:CAI	8:B:512:ELH:NAK	2.76	0.47
1:A:45:SER:HA	1:A:88:HIS:O	2.15	0.47
1:A:9:ARG:HB3	1:A:9:ARG:NH1	2.29	0.47
1:A:136:LEU:HD23	1:A:182:TRP:CZ2	2.50	0.47
1:D:421:PHE:CD2	1:D:430:ASP:HB3	2.50	0.46
1:C:24:TYR:CD2	3:L:1:NAG:H82	2.51	0.46
1:A:421:PHE:CD2	1:A:430:ASP:HB3	2.51	0.45
1:C:217:LYS:NZ	13:C:622:HOH:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:LYS:HB3	1:A:218:PRO:HD3	1.98	0.45
1:A:285:MET:O	1:A:321:ALA:HA	2.16	0.45
1:A:203:GLU:O	1:A:216:PHE:HA	2.17	0.45
1:D:213:THR:O	1:D:215:PRO:HD3	2.16	0.45
1:C:58:ARG:HD2	1:C:104:GLU:OE1	2.16	0.45
1:B:124:LEU:HD12	1:B:124:LEU:HA	1.83	0.45
1:B:426:TYR:O	1:B:428:VAL:N	2.50	0.44
6:D:512:SO4:S	9:D:514:EDO:H21	2.56	0.44
1:C:9:ARG:NH2	1:C:9:ARG:HB3	2.32	0.44
1:D:301:GLU:O	1:D:305:THR:HG23	2.17	0.44
1:A:274:LYS:HA	1:A:274:LYS:HD3	1.71	0.44
1:A:171:TYR:CE1	1:A:178:ARG:HG3	2.53	0.44
1:D:57:VAL:HG11	1:D:92[A]:ILE:HD11	2.00	0.44
1:A:10:ASP:HA	1:A:139:SER:HA	2.00	0.43
1:A:73:LYS:HG3	1:A:74:MET:N	2.32	0.43
1:C:155:LYS:HA	1:C:155:LYS:HD3	1.83	0.43
1:B:401:HIS:HB2	1:B:419:TRP:CZ3	2.54	0.43
1:C:33:THR:HA	1:C:194:PRO:HB3	2.00	0.43
1:A:32:ILE:HA	1:A:43:ILE:O	2.17	0.43
1:B:217:LYS:HB3	1:B:218:PRO:HD3	2.01	0.43
1:A:424:HIS:HD2	1:A:425:TRP:CD1	2.36	0.43
1:D:174:HIS:O	1:D:175:ASP:C	2.57	0.43
1:B:295:HIS:NE2	8:B:512:ELH:CAF	2.82	0.42
1:D:10:ASP:HA	1:D:139:SER:HA	2.01	0.42
1:A:277:GLU:OE1	13:A:601:HOH:O	2.21	0.42
1:D:154:LYS:NZ	1:D:414:GLU:OE2	2.21	0.42
1:B:285:MET:O	1:B:321:ALA:HA	2.20	0.42
1:D:103:TYR:CZ	1:D:114:PHE:HB2	2.55	0.42
1:A:27:PRO:HB3	1:A:46:TRP:CD1	2.54	0.42
1:C:171:TYR:CE1	1:C:178:ARG:HG3	2.54	0.42
1:B:174:HIS:O	1:B:175:ASP:C	2.57	0.42
1:C:274:LYS:HA	1:C:274:LYS:HD2	1.74	0.42
1:A:103:TYR:CE1	1:A:114:PHE:HB2	2.55	0.41
1:A:174:HIS:O	1:A:175:ASP:C	2.58	0.41
1:C:63:LYS:HA	1:C:63:LYS:HD3	1.70	0.41
1:C:103:TYR:CE1	1:C:114:PHE:HB2	2.55	0.41
1:B:57:VAL:HG11	1:B:92:ILE:HD11	2.02	0.41
1:D:96:LYS:HD3	1:D:96:LYS:HA	1.76	0.41
1:A:124:LEU:O	1:A:279:PRO:HG3	2.20	0.41
1:B:96:LYS:HA	1:B:96:LYS:HD3	1.93	0.41
1:C:325:HIS:HA	1:C:360:GLY:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:HIS:HE1	8:A:515:ELH:CAJ	2.34	0.41
1:B:182:TRP:HZ3	1:B:223:TYR:HH	1.64	0.41
1:D:154:LYS:HE3	1:D:403:SER:OG	2.20	0.41
3:K:1:NAG:O4	3:K:2:FUC:H5	2.21	0.41
1:A:333:VAL:HG21	1:A:379:TYR:HB2	2.03	0.40
1:B:66:ARG:NH1	1:B:68:ARG:HE	2.18	0.40
1:C:122:THR:HA	1:C:243:ALA:O	2.21	0.40
1:C:364:ASN:OD1	1:C:365:TYR:N	2.52	0.40
1:D:206:PHE:CE2	1:D:208:PRO:HG3	2.56	0.40
1:B:345:CYS:HB2	1:C:338:TYR:CE1	2.57	0.40
1:C:174:HIS:O	1:C:175:ASP:C	2.60	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	423/426 (99%)	402 (95%)	18 (4%)	3 (1%)	22 32
1	B	426/426 (100%)	404 (95%)	21 (5%)	1 (0%)	47 62
1	C	422/426 (99%)	400 (95%)	21 (5%)	1 (0%)	47 62
1	D	422/426 (99%)	403 (96%)	17 (4%)	2 (0%)	29 41
All	All	1693/1704 (99%)	1609 (95%)	77 (4%)	7 (0%)	34 48

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	ASP
1	B	175	ASP
1	D	175	ASP
1	C	175	ASP

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Mol	Chain	Res	Type
1	A	164	ASP
1	D	164	ASP
1	A	155	LYS

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	374/375 (100%)	365 (98%)	9 (2%)	49	68
1	B	377/375 (100%)	374 (99%)	3 (1%)	81	91
1	C	373/375 (100%)	368 (99%)	5 (1%)	69	84
1	D	373/375 (100%)	371 (100%)	2 (0%)	88	95
All	All	1497/1500 (100%)	1478 (99%)	19 (1%)	69	84

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	A	124	LEU
1	A	132	LEU
1	A	142	SER
1	A	154	LYS
1	A	176	ASN
1	A	239	SER
1	A	349	LYS
1	A	383	ARG
1	B	73	LYS
1	B	132	LEU
1	B	352	SER
1	D	132	LEU
1	D	176	ASN
1	C	132	LEU
1	C	176	ASN
1	C	211	ASN
1	C	391	MET

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Mol	Chain	Res	Type
1	C	417	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	E	1	1,2	14,14,15	0.57	0	17,19,21	0.52	0
2	FUC	E	2	2	10,10,11	1.15	1 (10%)	14,14,16	1.29	2 (14%)
2	NAG	E	3	2	14,14,15	0.38	0	17,19,21	0.49	0
2	NAG	F	1	1,2	14,14,15	0.55	0	17,19,21	0.72	1 (5%)
2	FUC	F	2	2	10,10,11	0.77	0	14,14,16	1.17	2 (14%)
2	NAG	F	3	2	14,14,15	0.59	0	17,19,21	0.64	1 (5%)
2	NAG	G	1	1,2	14,14,15	0.53	0	17,19,21	0.71	1 (5%)
2	FUC	G	2	2	10,10,11	1.08	0	14,14,16	1.05	1 (7%)
2	NAG	G	3	2	14,14,15	0.74	1 (7%)	17,19,21	0.72	1 (5%)
3	NAG	H	1	1,3	14,14,15	0.68	0	17,19,21	0.83	1 (5%)
3	FUC	H	2	3	10,10,11	0.92	0	14,14,16	1.00	1 (7%)
2	NAG	I	1	1,2	14,14,15	0.59	0	17,19,21	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FUC	I	2	2	10,10,11	0.94	1 (10%)	14,14,16	1.01	1 (7%)
2	NAG	I	3	2	14,14,15	0.47	0	17,19,21	0.63	0
2	NAG	J	1	1,2	14,14,15	0.48	0	17,19,21	0.50	0
2	FUC	J	2	2	10,10,11	1.12	1 (10%)	14,14,16	1.21	1 (7%)
2	NAG	J	3	2	14,14,15	0.36	0	17,19,21	0.49	0
3	NAG	K	1	1,3	14,14,15	0.52	0	17,19,21	0.72	0
3	FUC	K	2	3	10,10,11	1.34	2 (20%)	14,14,16	0.93	0
3	NAG	L	1	1,3	14,14,15	0.46	0	17,19,21	0.73	0
3	FUC	L	2	3	10,10,11	0.91	0	14,14,16	0.84	0
2	NAG	M	1	1,2	14,14,15	0.63	1 (7%)	17,19,21	0.48	0
2	FUC	M	2	2	10,10,11	0.90	0	14,14,16	0.85	0
2	NAG	M	3	2	14,14,15	0.48	0	17,19,21	0.40	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	E	1	1,2	-	0/6/23/26	0/1/1/1
2	FUC	E	2	2	-	-	0/1/1/1
2	NAG	E	3	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	FUC	F	2	2	-	-	0/1/1/1
2	NAG	F	3	2	-	4/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	FUC	G	2	2	-	-	0/1/1/1
2	NAG	G	3	2	-	0/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	FUC	H	2	3	-	-	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	FUC	I	2	2	-	-	0/1/1/1
2	NAG	I	3	2	-	1/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	FUC	J	2	2	-	-	0/1/1/1
2	NAG	J	3	2	-	2/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	0/6/23/26	0/1/1/1
3	FUC	K	2	3	-	-	0/1/1/1
3	NAG	L	1	1,3	-	0/6/23/26	0/1/1/1
3	FUC	L	2	3	-	-	0/1/1/1
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FUC	M	2	2	-	-	0/1/1/1
2	NAG	M	3	2	-	2/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	2	FUC	C2-C3	2.35	1.56	1.52
2	G	3	NAG	O5-C1	-2.26	1.40	1.43
3	K	2	FUC	O5-C5	2.25	1.48	1.43
2	I	2	FUC	O5-C5	2.13	1.48	1.43
3	K	2	FUC	C4-C3	2.10	1.57	1.52
2	M	1	NAG	O5-C1	-2.06	1.40	1.43
2	E	2	FUC	O5-C5	2.05	1.47	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	2	FUC	C1-O5-C5	3.16	119.94	112.78
3	H	1	NAG	C1-O5-C5	2.94	116.17	112.19
2	E	2	FUC	O2-C2-C1	2.66	114.59	109.15
2	F	2	FUC	C1-O5-C5	2.49	118.42	112.78
3	H	2	FUC	C1-O5-C5	2.40	118.22	112.78
2	E	2	FUC	O5-C5-C4	2.39	113.80	109.52
2	G	2	FUC	C1-O5-C5	2.31	118.01	112.78
2	G	1	NAG	C1-O5-C5	2.31	115.32	112.19
2	G	3	NAG	C1-O5-C5	2.28	115.29	112.19
2	F	1	NAG	C1-O5-C5	2.22	115.20	112.19
2	F	2	FUC	C2-C3-C4	-2.09	107.28	110.89
2	I	2	FUC	C1-O5-C5	2.03	117.39	112.78
2	F	3	NAG	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	3	NAG	O5-C5-C6-O6
2	F	3	NAG	O5-C5-C6-O6
2	E	3	NAG	C4-C5-C6-O6
2	F	3	NAG	C4-C5-C6-O6
2	J	3	NAG	C4-C5-C6-O6
2	M	3	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	F	3	NAG	C8-C7-N2-C2
2	F	3	NAG	O7-C7-N2-C2
2	E	3	NAG	O5-C5-C6-O6
2	M	3	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
2	I	3	NAG	O5-C5-C6-O6

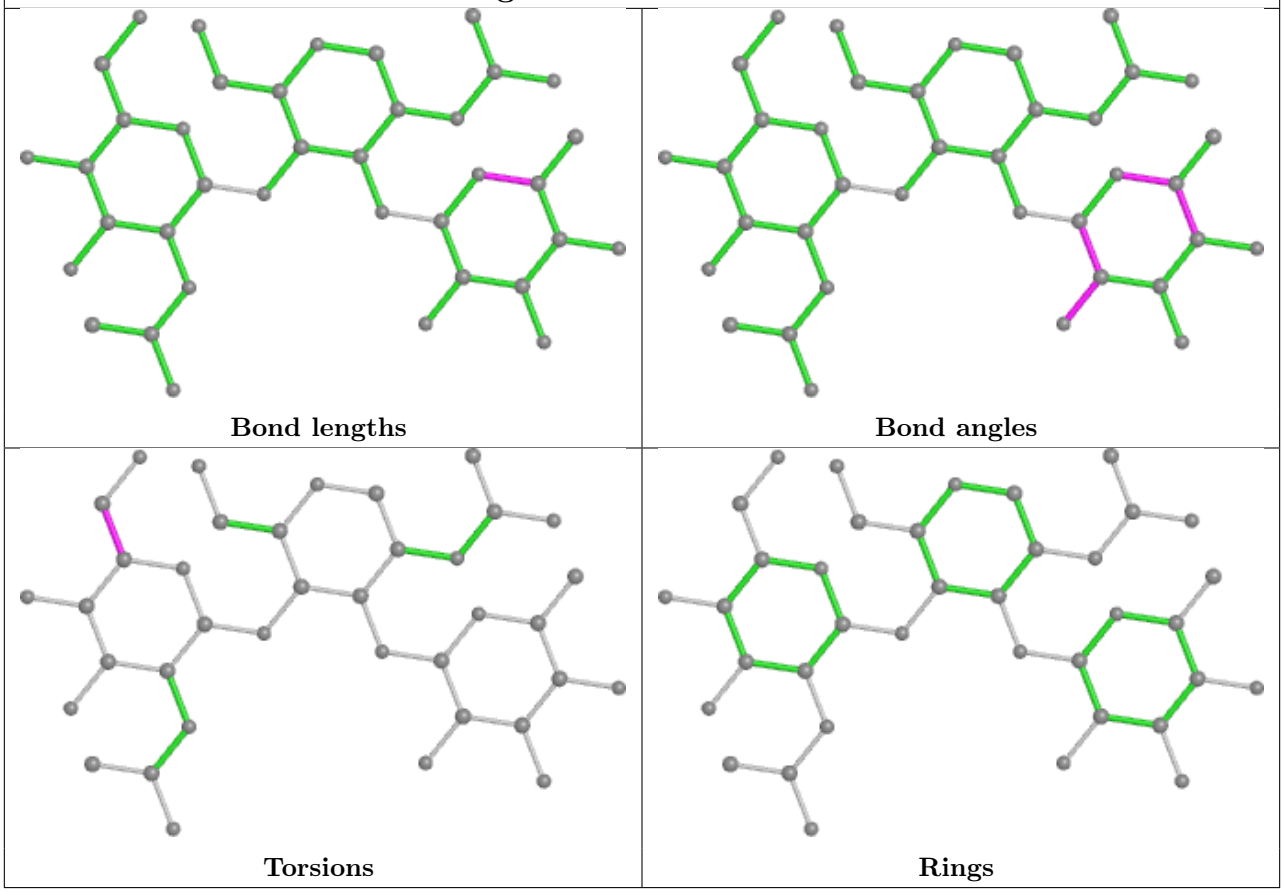
There are no ring outliers.

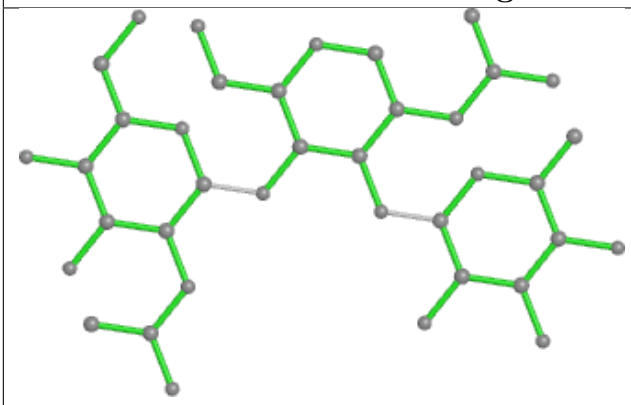
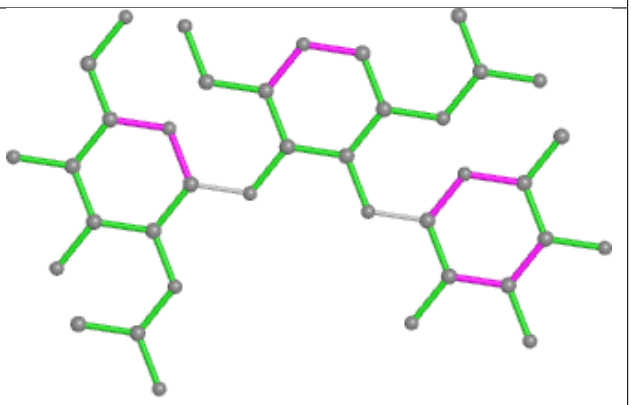
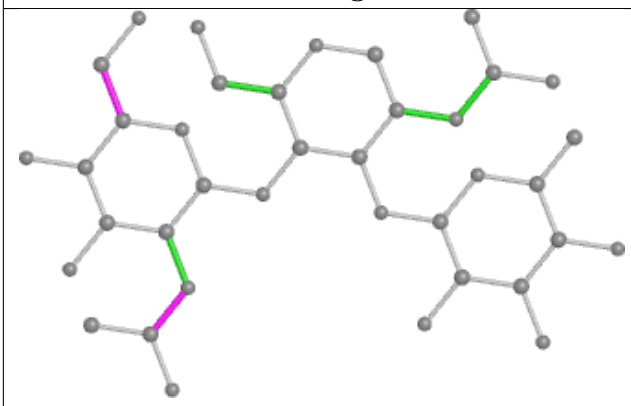
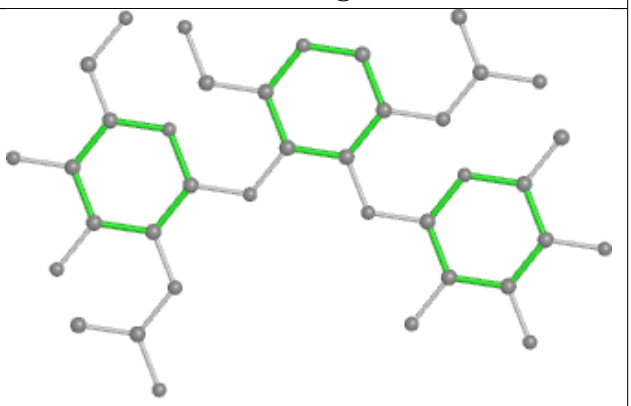
3 monomers are involved in 2 short contacts:

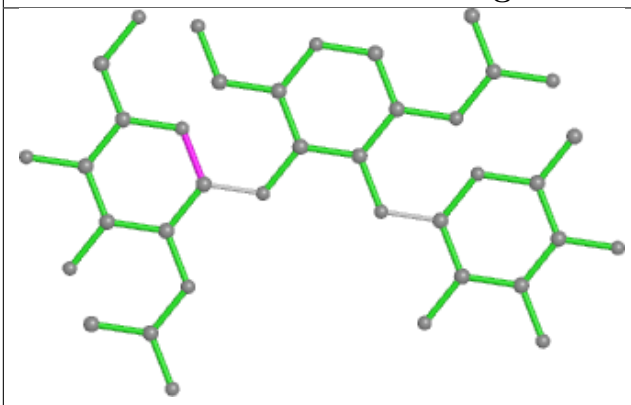
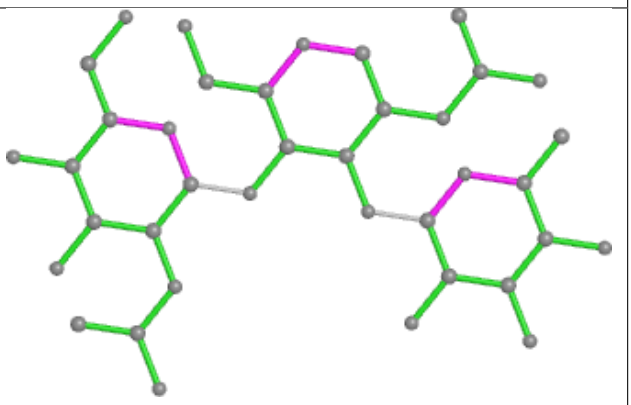
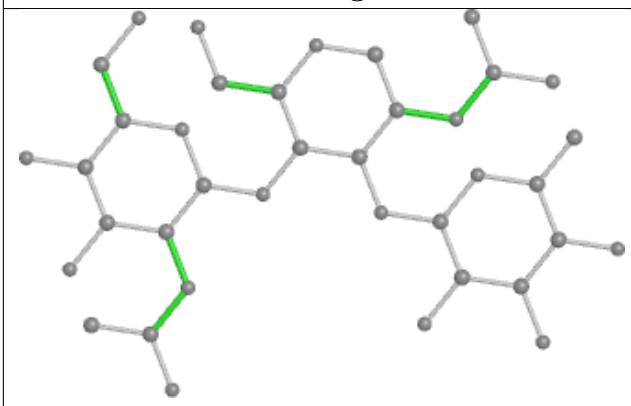
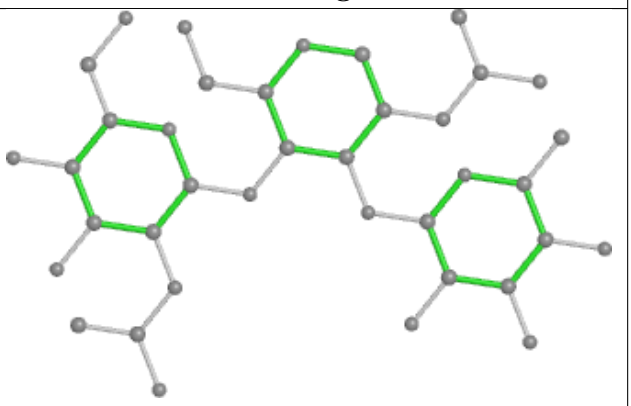
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	2	FUC	1	0
3	L	1	NAG	1	0
3	K	1	NAG	1	0

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

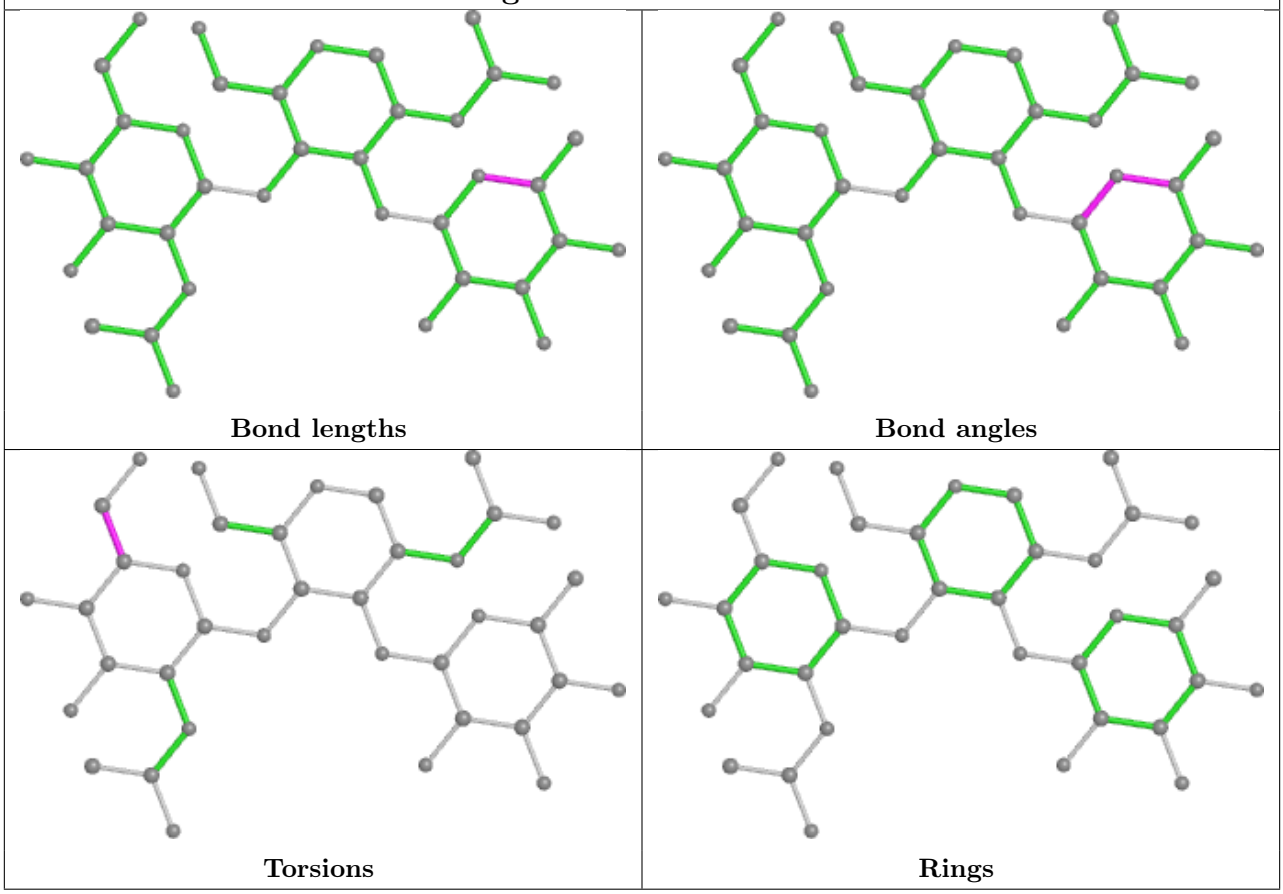
Oligosaccharide Chain E

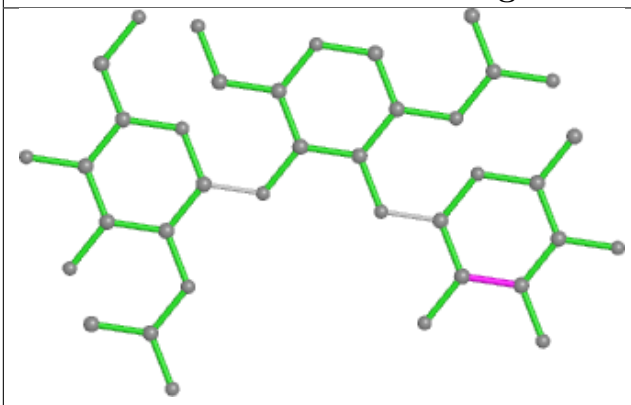
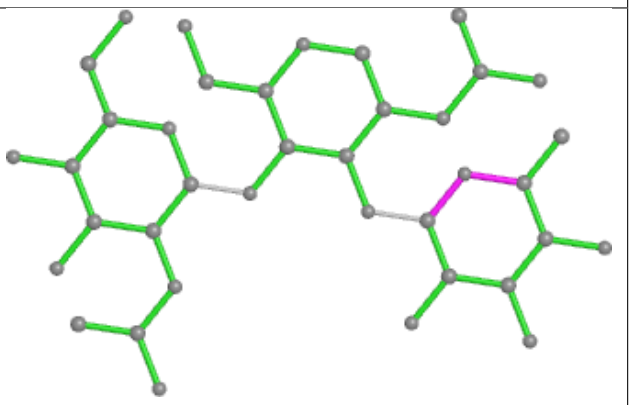
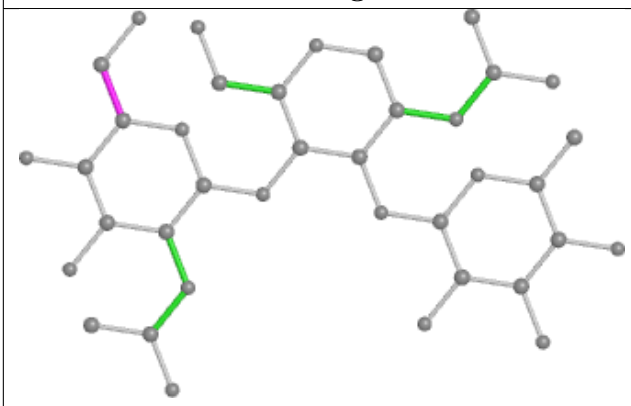
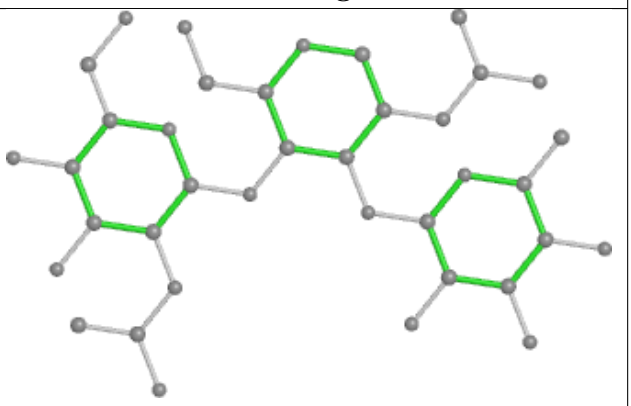


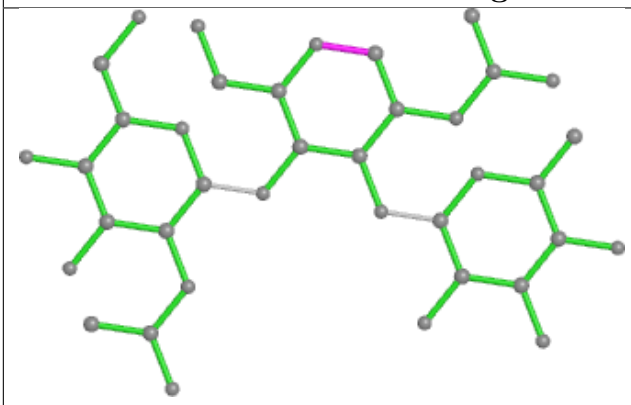
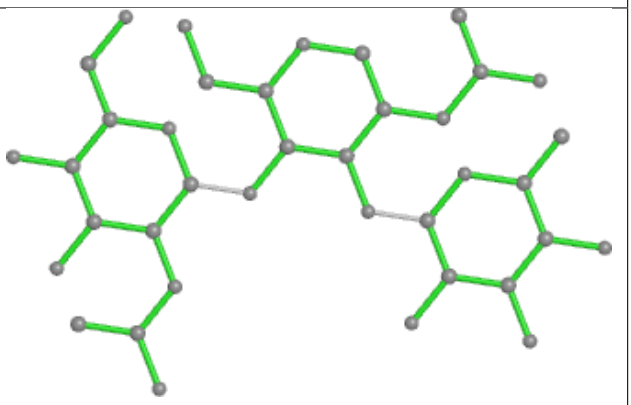
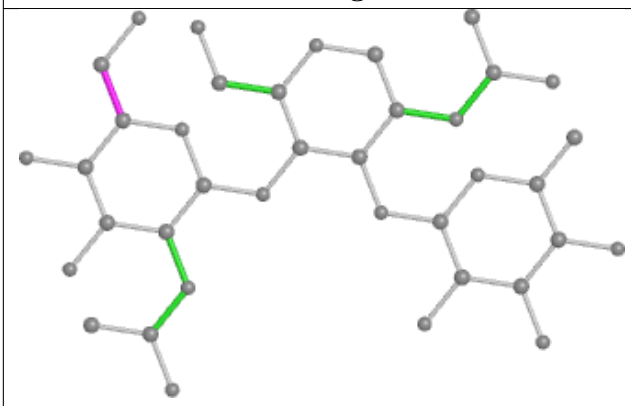
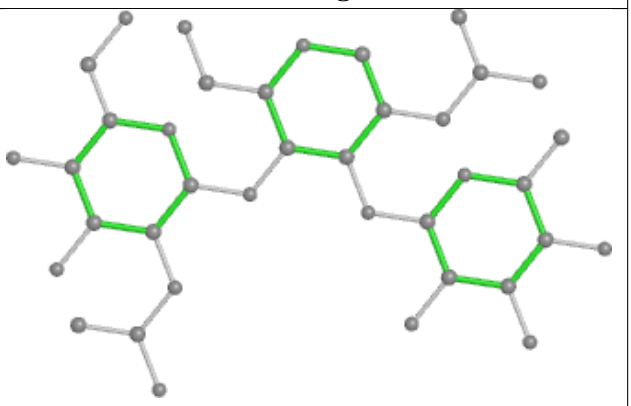
Oligosaccharide Chain F	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain G	
 Bond lengths	 Bond angles
 Torsions	 Rings

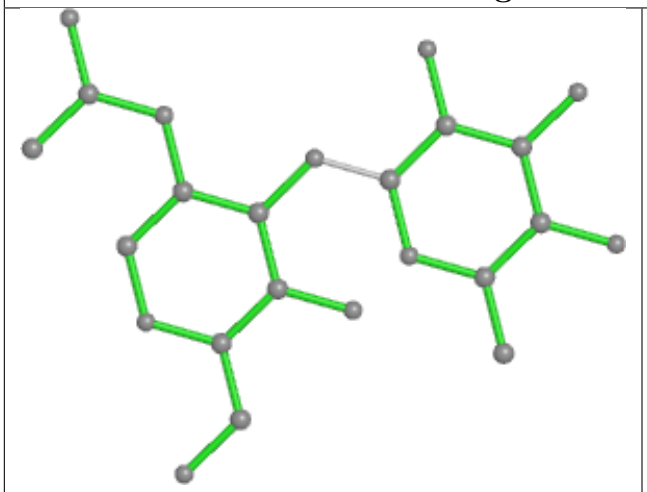
Oligosaccharide Chain I



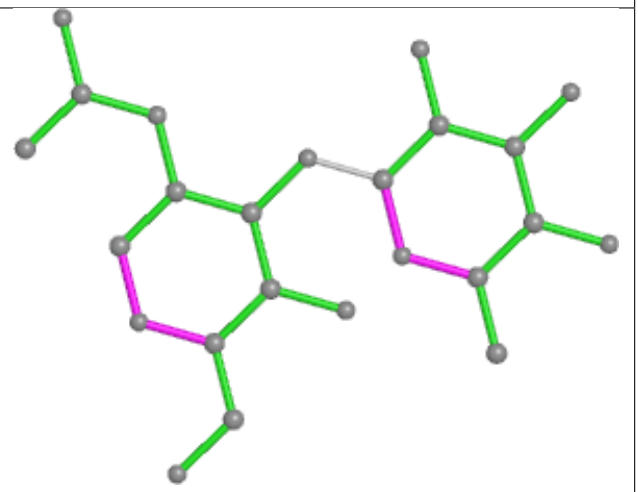
Oligosaccharide Chain J	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain M	
 Bond lengths	 Bond angles
 Torsions	 Rings

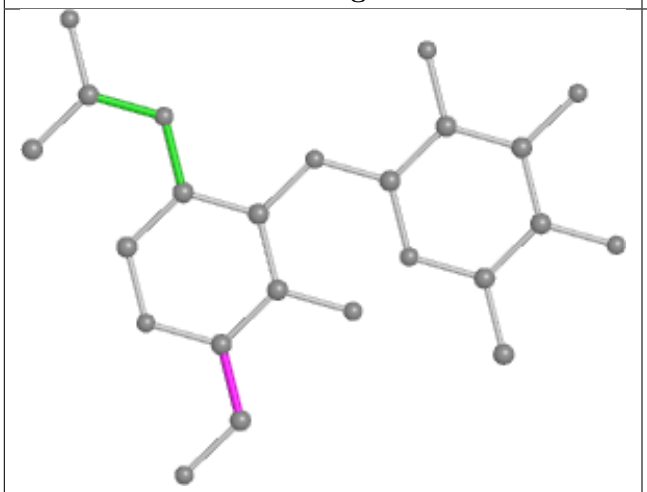
Oligosaccharide Chain H



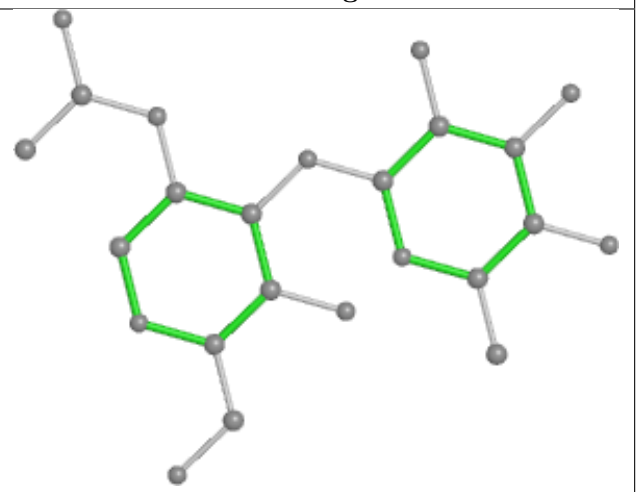
Bond lengths



Bond angles

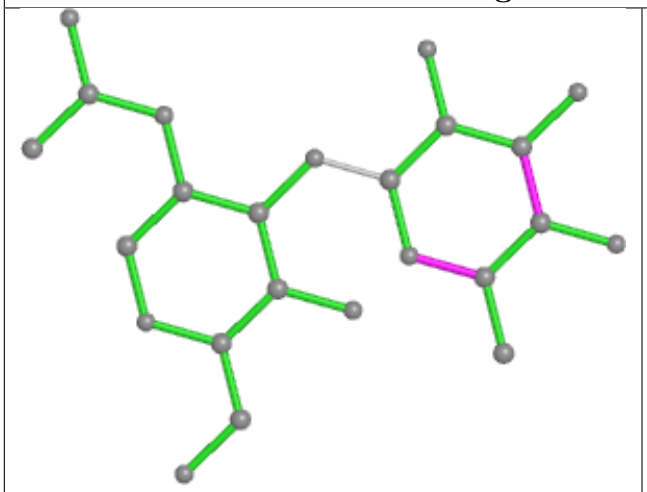


Torsions

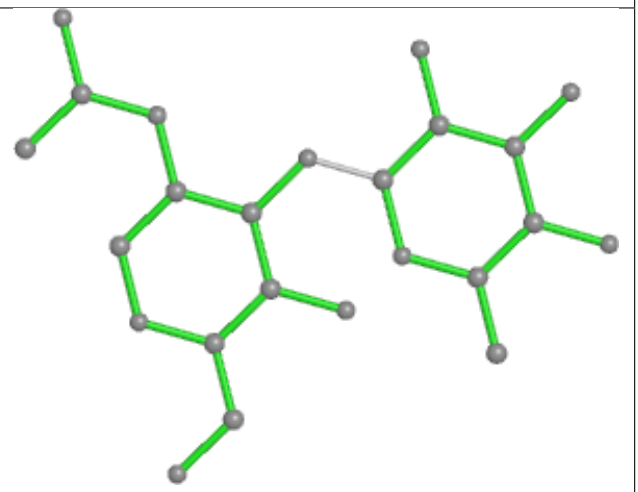


Rings

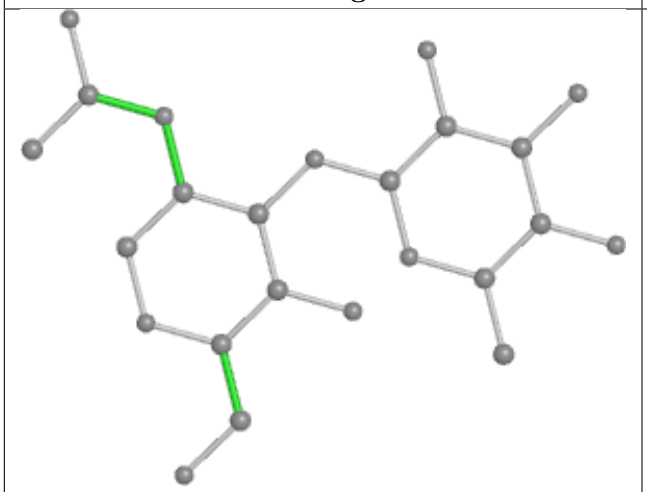
Oligosaccharide Chain K



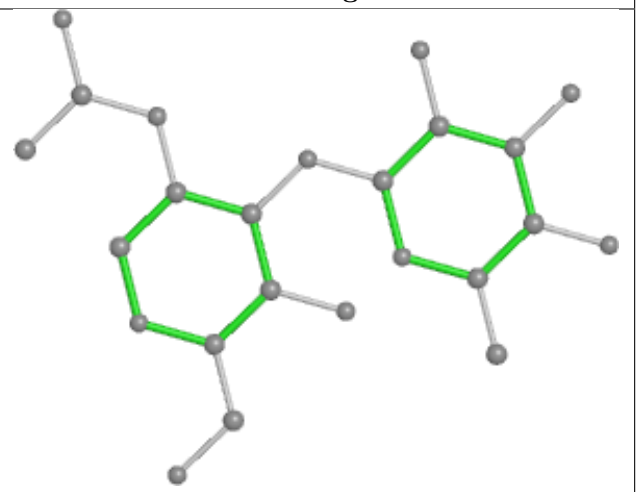
Bond lengths



Bond angles

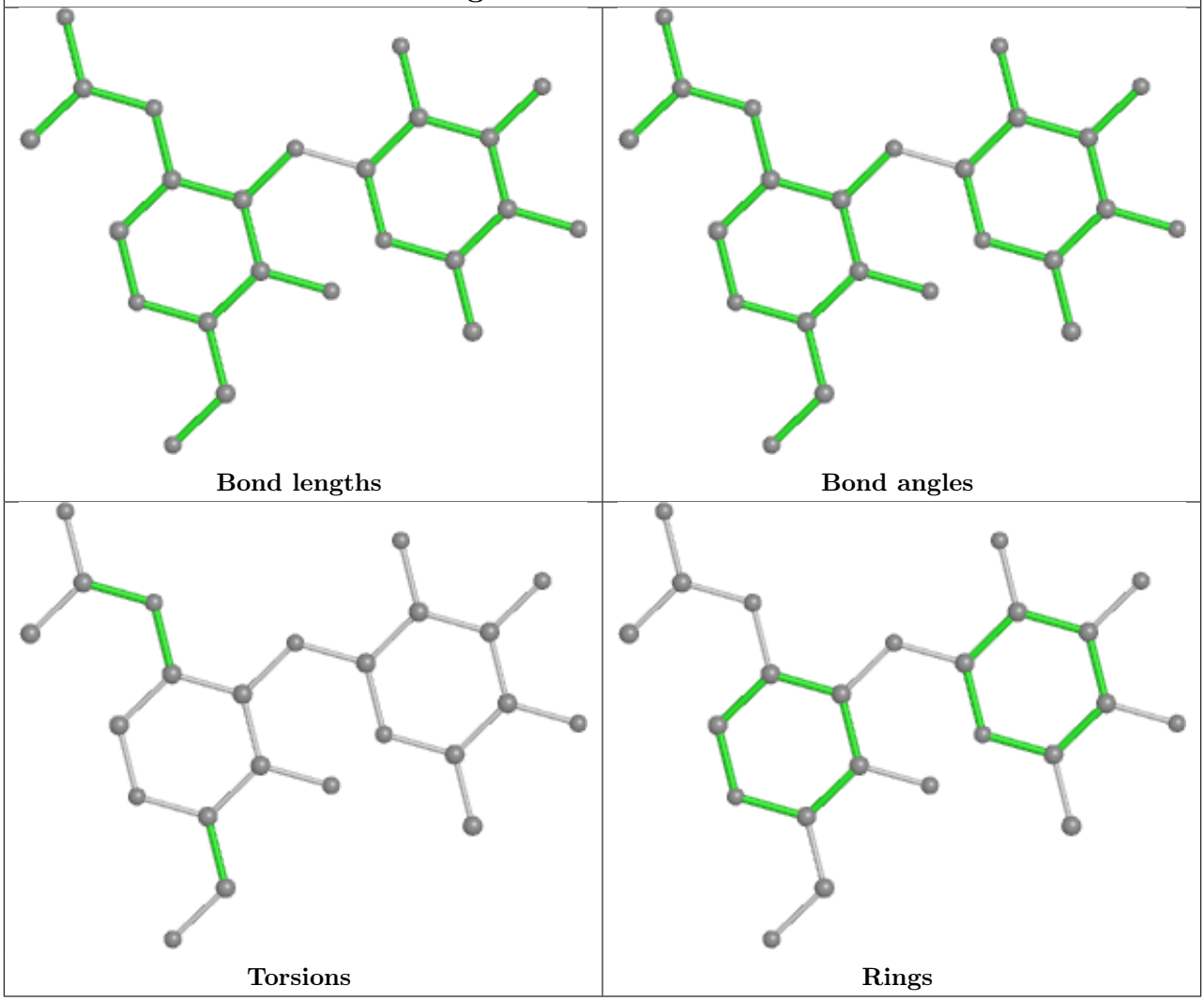


Torsions



Rings

Oligosaccharide Chain L



5.6 Ligand geometry (i)

Of 37 ligands modelled in this entry, 11 are monoatomic - leaving 26 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	$\#\|Z\| > 2$
9	EDO	C	512	-	3,3,3	0.52	0	2,2,2	0.33	0
6	SO4	B	505	-	4,4,4	0.18	0	6,6,6	0.14	0
6	SO4	B	511	-	4,4,4	0.19	0	6,6,6	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	SO4	C	511	10	4,4,4	0.32	0	6,6,6	0.34	0
6	SO4	A	504	-	4,4,4	0.17	0	6,6,6	0.21	0
8	ELH	B	512	4,5	18,20,20	3.74	3 (16%)	20,28,28	2.52	9 (45%)
9	EDO	D	514	-	3,3,3	0.54	0	2,2,2	0.16	0
9	EDO	B	516	-	3,3,3	0.49	0	2,2,2	0.43	0
9	EDO	B	518	-	3,3,3	0.57	0	2,2,2	0.18	0
7	NAG	C	505	1	14,14,15	0.63	0	17,19,21	0.79	1 (5%)
9	EDO	B	517	-	3,3,3	0.47	0	2,2,2	0.40	0
7	NAG	B	506	1	14,14,15	0.97	2 (14%)	17,19,21	0.81	1 (5%)
6	SO4	D	503	-	4,4,4	0.15	0	6,6,6	0.19	0
7	NAG	D	511	1	14,14,15	1.07	2 (14%)	17,19,21	0.86	1 (5%)
12	GOL	C	513	-	5,5,5	1.21	1 (20%)	5,5,5	1.07	1 (20%)
9	EDO	A	516	-	3,3,3	0.58	0	2,2,2	0.27	0
7	NAG	A	505	1	14,14,15	0.38	0	17,19,21	0.65	0
7	NAG	B	507	1	14,14,15	0.49	0	17,19,21	0.60	0
8	ELH	A	515	4,5	18,20,20	7.41	6 (33%)	20,28,28	1.92	3 (15%)
7	NAG	C	509	1	14,14,15	0.46	0	17,19,21	0.54	0
6	SO4	D	512	4,5	4,4,4	0.13	0	6,6,6	0.21	0
9	EDO	D	505	-	3,3,3	0.55	0	2,2,2	0.15	0
11	IPA	B	515	-	3,3,3	0.44	0	3,3,3	0.32	0
7	NAG	D	504	1	14,14,15	0.40	0	17,19,21	0.41	0
6	SO4	A	503	-	4,4,4	0.20	0	6,6,6	0.37	0
6	SO4	C	510	4,5	4,4,4	0.15	0	6,6,6	0.37	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
9	EDO	B	518	-	-	0/1/1/1	-
7	NAG	C	505	1	-	0/6/23/26	0/1/1/1
8	ELH	B	512	4,5	-	2/4/8/8	0/3/3/3
9	EDO	D	514	-	-	1/1/1/1	-
9	EDO	C	512	-	-	0/1/1/1	-
7	NAG	B	507	1	-	4/6/23/26	0/1/1/1
9	EDO	B	517	-	-	0/1/1/1	-
7	NAG	B	506	1	-	1/6/23/26	0/1/1/1
8	ELH	A	515	4,5	-	2/4/8/8	0/3/3/3
7	NAG	C	509	1	-	0/6/23/26	0/1/1/1
7	NAG	D	511	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	GOL	C	513	-	-	1/4/4/4	-
9	EDO	B	516	-	-	0/1/1/1	-
7	NAG	D	504	1	-	2/6/23/26	0/1/1/1
9	EDO	A	516	-	-	0/1/1/1	-
7	NAG	A	505	1	-	2/6/23/26	0/1/1/1
9	EDO	D	505	-	-	0/1/1/1	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	515	ELH	CAO-SAL	-25.43	1.38	1.73
8	A	515	ELH	CAN-CAM	-15.69	1.28	1.50
8	B	512	ELH	CAN-CAM	-11.70	1.34	1.50
8	B	512	ELH	CAO-SAL	-9.37	1.60	1.73
8	A	515	ELH	CAJ-SAL	-7.57	1.58	1.70
8	B	512	ELH	CAJ-SAL	-3.41	1.65	1.70
7	D	511	NAG	O5-C1	3.23	1.48	1.43
8	A	515	ELH	CAR-CAQ	-3.14	1.37	1.43
7	B	506	NAG	C1-C2	2.74	1.56	1.52
8	A	515	ELH	CAP-CAR	-2.45	1.37	1.42
12	C	513	GOL	C3-C2	2.24	1.60	1.51
8	A	515	ELH	OAA-CAM	-2.23	1.23	1.30
7	B	506	NAG	O5-C1	2.22	1.47	1.43
7	D	511	NAG	C1-C2	2.17	1.55	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	515	ELH	CAN-CAJ-SAL	-5.56	104.96	111.79
8	B	512	ELH	CAO-CAP-CAR	-5.24	117.33	123.46
8	B	512	ELH	CAN-CAJ-SAL	-4.92	105.75	111.79
8	A	515	ELH	CAO-CAP-CAR	-4.49	118.20	123.46
8	B	512	ELH	CAH-CAE-CAF	-4.13	114.41	120.99
8	B	512	ELH	OAA-CAM-CAN	4.08	123.97	114.69
8	B	512	ELH	CAI-CAR-CAQ	2.94	121.69	117.89
7	D	511	NAG	C1-O5-C5	2.59	115.70	112.19
8	A	515	ELH	OAA-CAM-CAN	2.53	120.44	114.69
7	B	506	NAG	C1-O5-C5	2.42	115.47	112.19
7	C	505	NAG	C1-O5-C5	2.32	115.34	112.19
8	B	512	ELH	CAD-CAI-CAR	-2.32	117.67	120.89
12	C	513	GOL	C3-C2-C1	-2.16	103.32	111.70
8	B	512	ELH	OAA-CAM-OAB	-2.09	118.72	123.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	512	ELH	OAB-CAM-CAN	-2.03	117.13	121.24
8	B	512	ELH	CAJ-CAN-CAM	-2.02	122.48	128.42

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	515	ELH	NAK-CAO-CAP-CAF
8	A	515	ELH	SAL-CAO-CAP-CAF
8	B	512	ELH	NAK-CAO-CAP-CAF
8	B	512	ELH	SAL-CAO-CAP-CAF
7	B	507	NAG	O5-C5-C6-O6
7	B	507	NAG	C4-C5-C6-O6
7	B	507	NAG	C8-C7-N2-C2
7	B	507	NAG	O7-C7-N2-C2
9	D	514	EDO	O1-C1-C2-O2
7	D	504	NAG	C4-C5-C6-O6
7	D	504	NAG	O5-C5-C6-O6
7	B	506	NAG	O5-C5-C6-O6
7	A	505	NAG	C4-C5-C6-O6
7	A	505	NAG	O5-C5-C6-O6
12	C	513	GOL	C1-C2-C3-O3

There are no ring outliers.

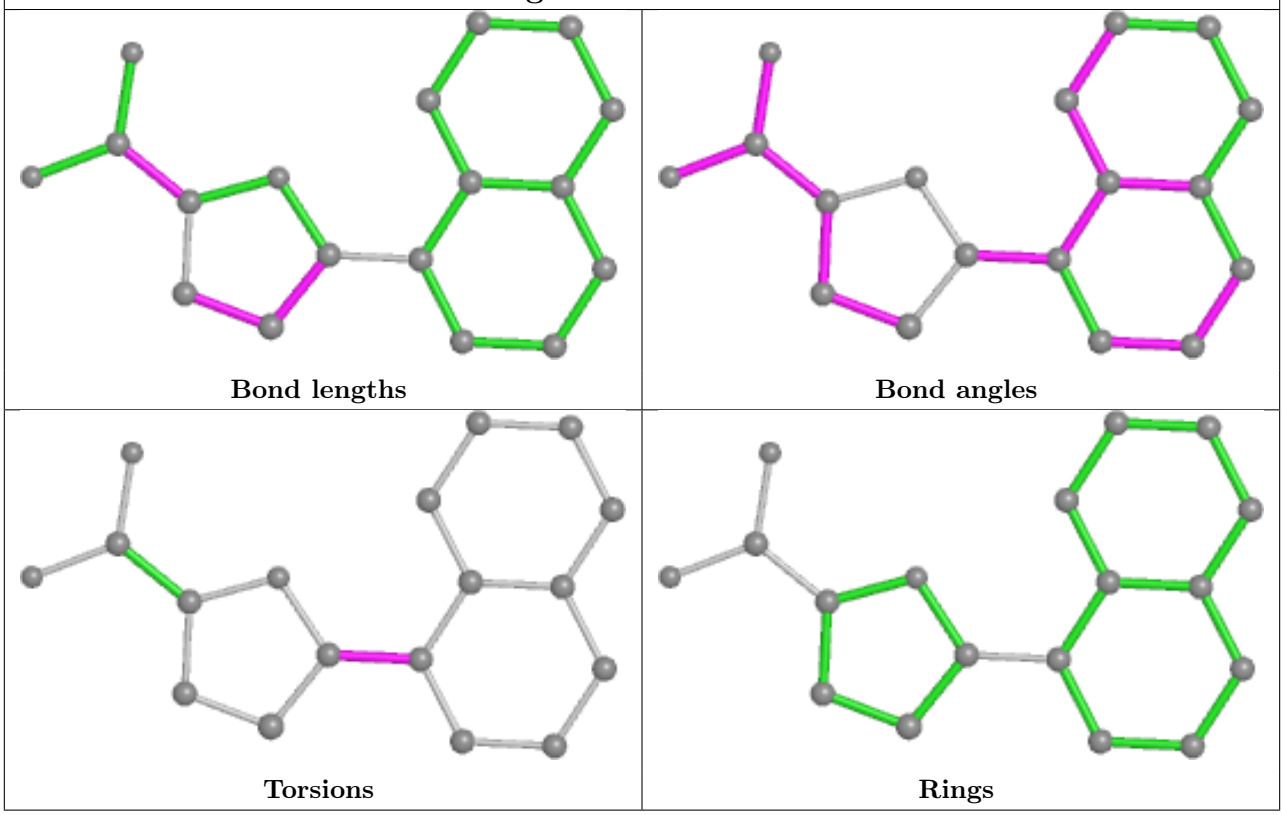
8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	512	EDO	1	0
6	C	511	SO4	1	0
8	B	512	ELH	3	0
9	D	514	EDO	2	0
9	B	517	EDO	1	0
7	B	507	NAG	1	0
8	A	515	ELH	4	0
6	D	512	SO4	2	0

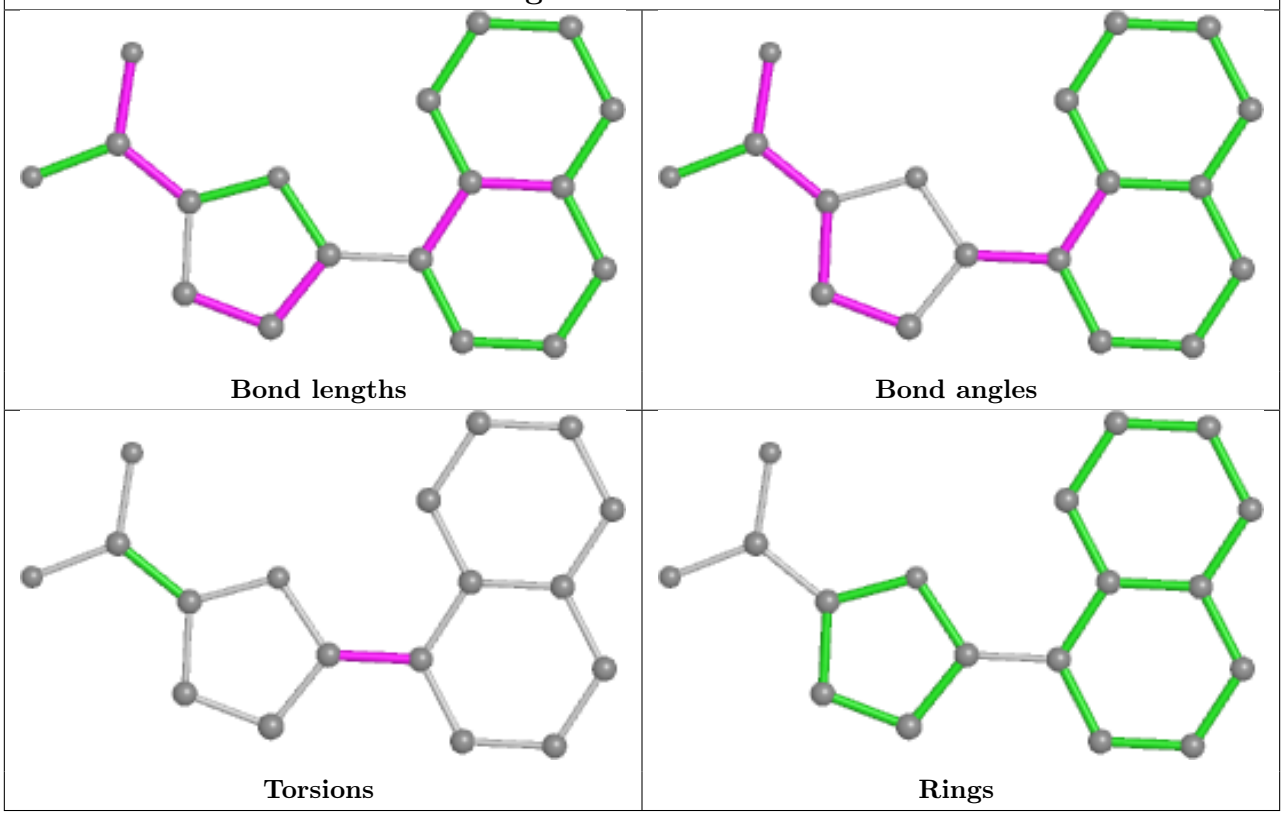
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 ELH B 512



Ligand ELH A 515



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	424/426 (99%)	-0.70	1 (0%) 95 94	23, 30, 41, 61	0
1	B	425/426 (99%)	-0.70	0 100 100	23, 32, 44, 72	0
1	C	424/426 (99%)	-0.67	2 (0%) 91 89	23, 32, 45, 81	0
1	D	423/426 (99%)	-0.71	0 100 100	23, 31, 44, 72	0
All	All	1696/1704 (99%)	-0.69	3 (0%) 95 94	23, 31, 44, 81	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	7	LYS	3.4
1	C	64	ASN	2.7
1	A	8	ASN	2.5

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
3	NAG	H	1	14/15	0.89	0.14	41,56,64,67	0
3	FUC	L	2	10/11	0.89	0.19	55,59,62,64	0
3	NAG	K	1	14/15	0.90	0.13	47,51,59,60	0
3	FUC	K	2	10/11	0.90	0.23	57,67,70,74	0

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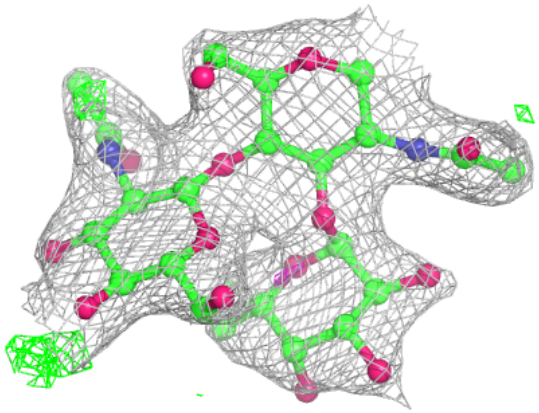
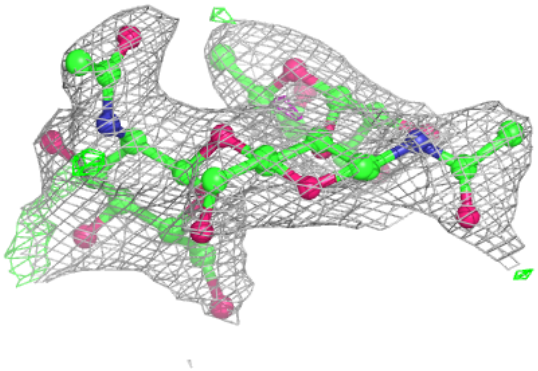
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FUC	J	2	10/11	0.90	0.14	44,54,58,59	0
2	NAG	F	3	14/15	0.91	0.20	65,73,77,77	0
3	NAG	L	1	14/15	0.91	0.14	35,52,61,61	0
2	NAG	E	3	14/15	0.91	0.15	40,59,63,64	0
2	FUC	E	2	10/11	0.93	0.20	55,62,69,75	0
3	FUC	H	2	10/11	0.93	0.16	61,67,69,74	0
2	NAG	F	1	14/15	0.93	0.11	36,54,68,75	0
2	NAG	I	3	14/15	0.94	0.13	35,41,48,51	0
2	FUC	F	2	10/11	0.94	0.15	65,73,73,74	0
2	FUC	M	2	10/11	0.94	0.08	53,55,62,62	0
2	NAG	M	3	14/15	0.94	0.13	36,47,62,62	0
2	NAG	G	3	14/15	0.94	0.12	28,37,42,42	0
2	NAG	J	3	14/15	0.95	0.12	36,55,63,68	0
2	NAG	E	1	14/15	0.96	0.14	37,49,55,58	0
2	NAG	J	1	14/15	0.97	0.10	37,41,46,53	0
2	NAG	M	1	14/15	0.97	0.11	35,40,46,53	0
2	NAG	G	1	14/15	0.98	0.12	30,36,43,43	0
2	NAG	I	1	14/15	0.98	0.11	25,35,41,42	0
2	FUC	I	2	10/11	0.98	0.11	37,39,49,57	0
2	FUC	G	2	10/11	0.98	0.10	35,38,45,47	0

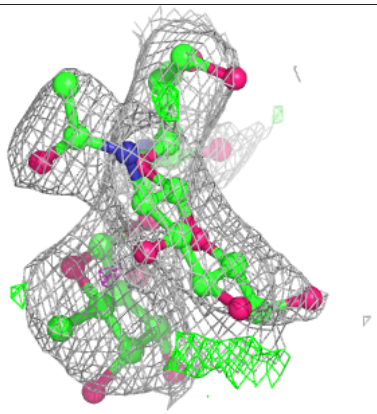
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

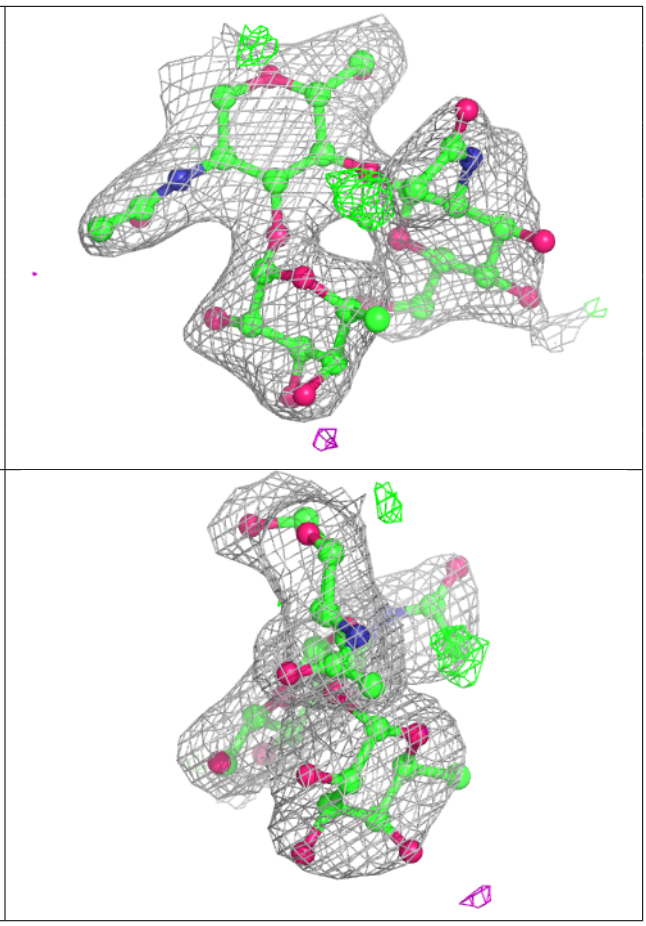






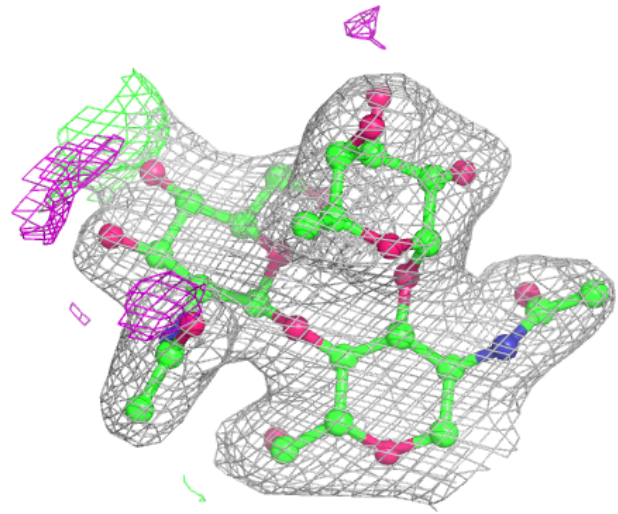
Electron density around Chain F:

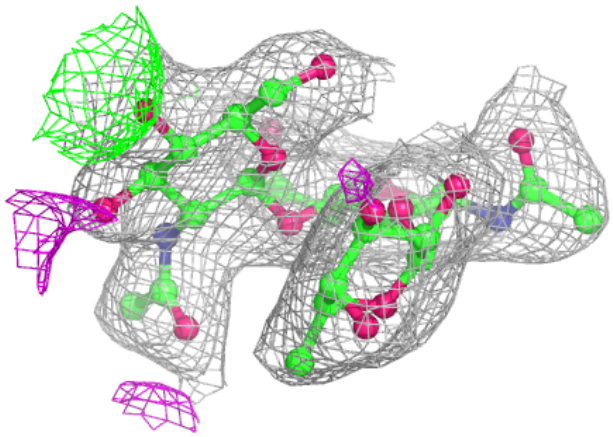
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

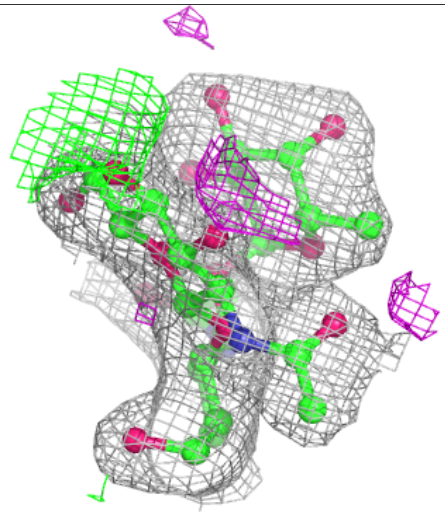


Electron density around Chain G:

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

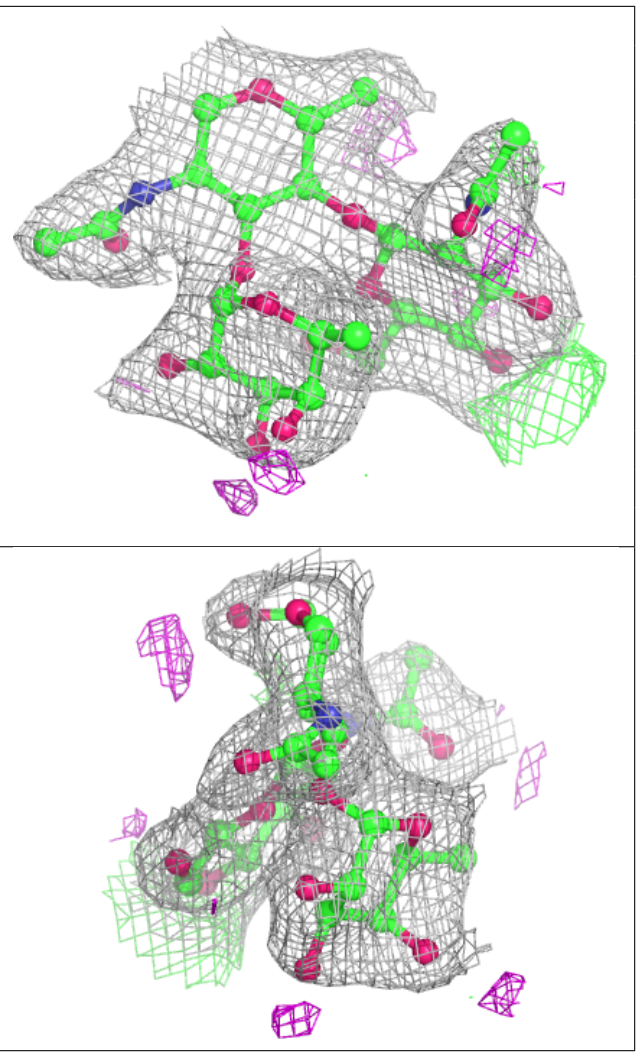






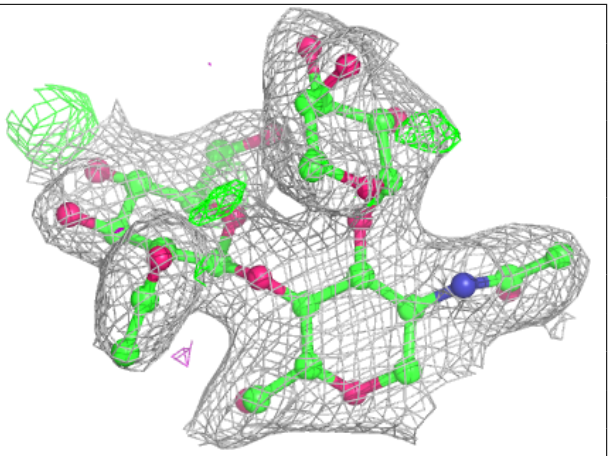
Electron density around Chain I:

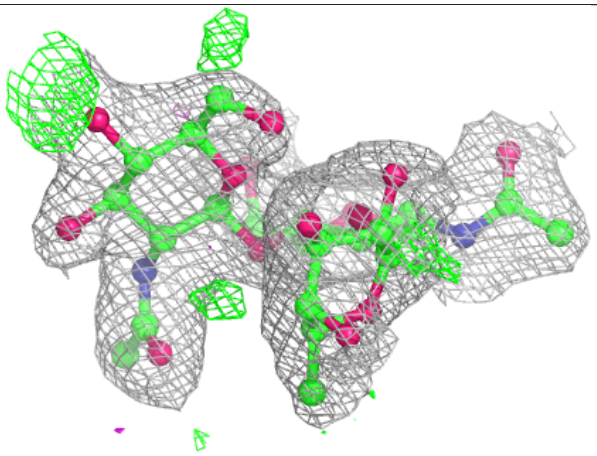
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

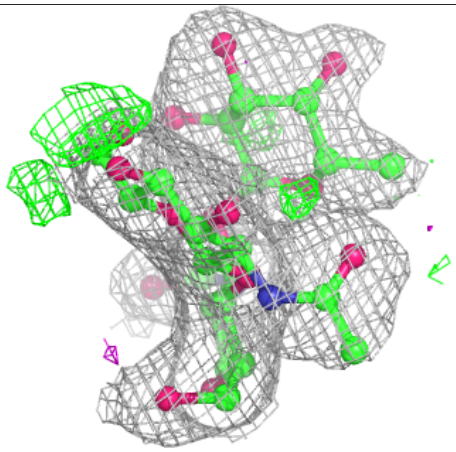


Electron density around Chain J:

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

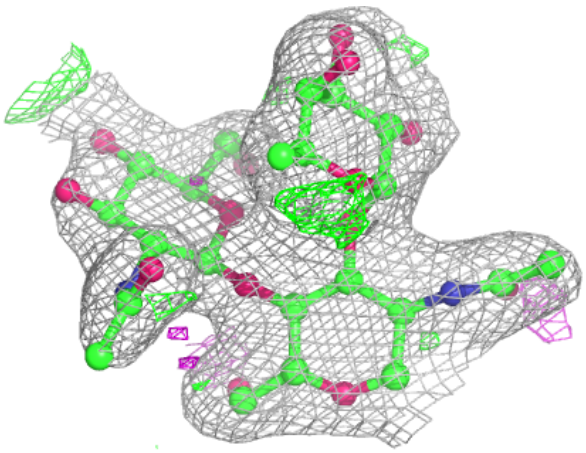


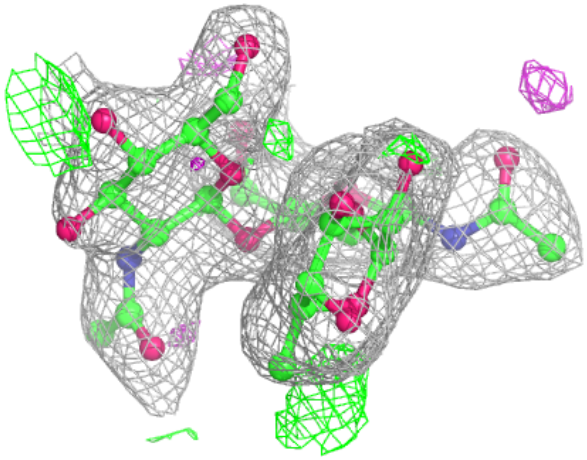


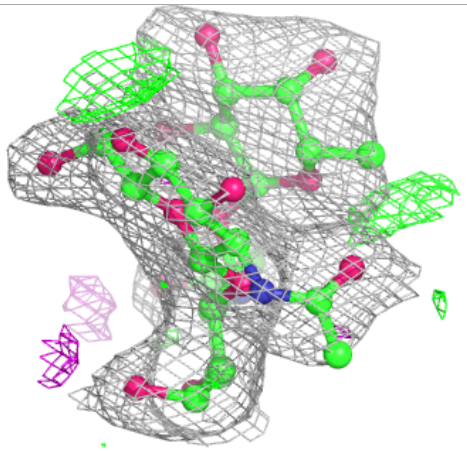


Electron density around Chain M:

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

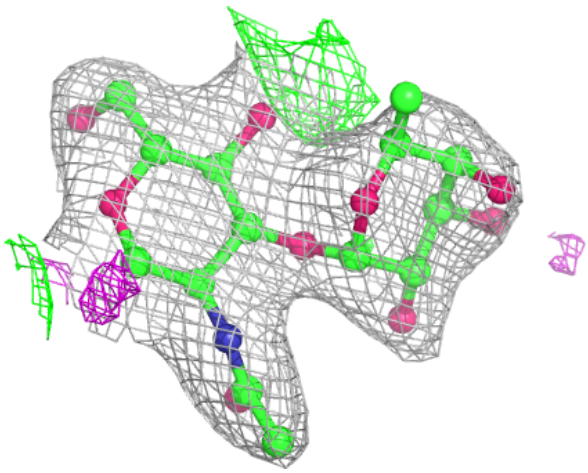


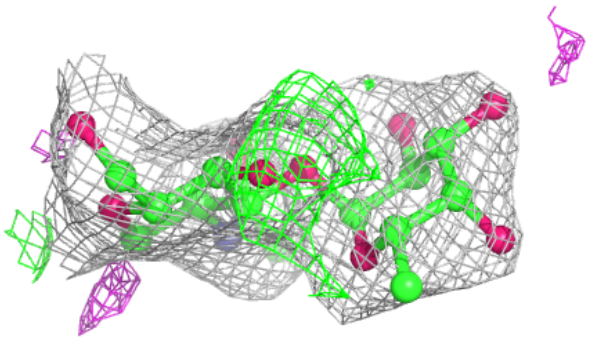


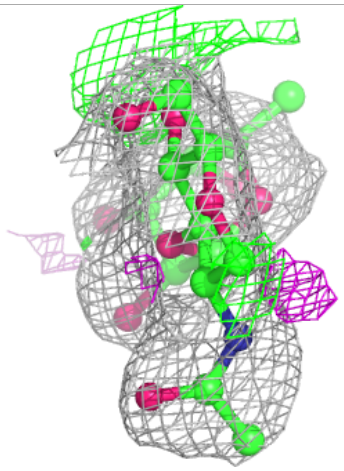


Electron density around Chain H:

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

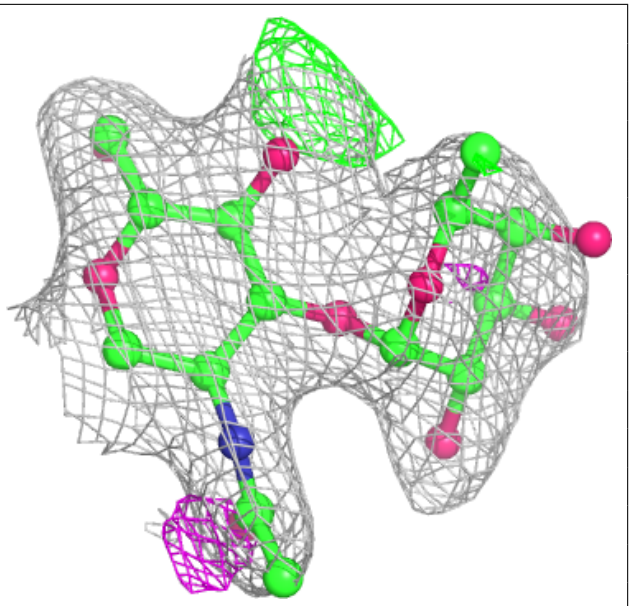


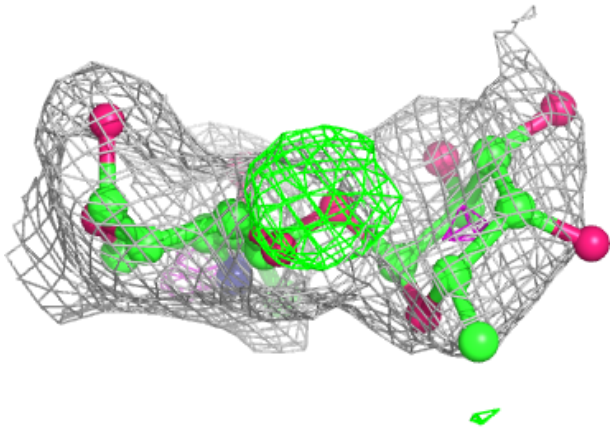


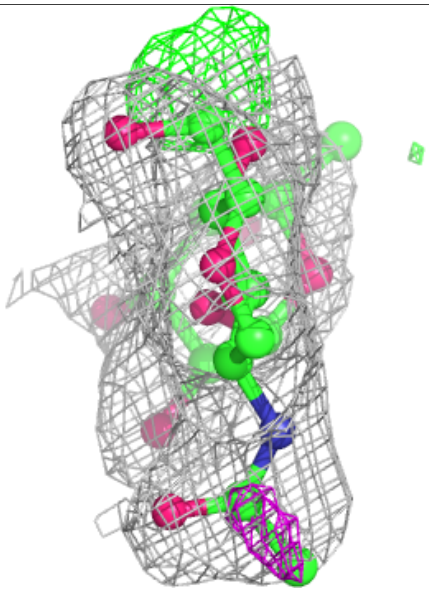


Electron density around Chain K:

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

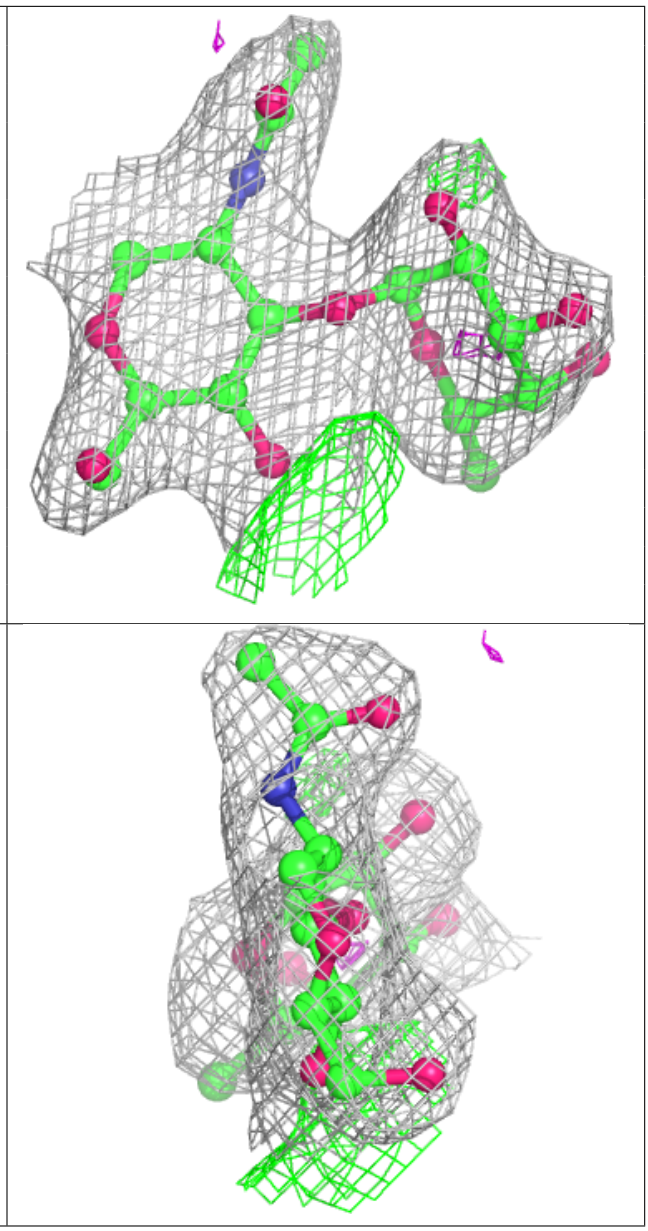






Electron density around Chain L:

$2mF_o$-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	SO4	B	511	5/5	0.81	0.37	50,82,95,100	0
8	ELH	A	515	18/18	0.83	0.28	27,57,70,71	18
9	EDO	B	518	4/4	0.83	0.44	42,42,47,50	0
9	EDO	C	512	4/4	0.83	0.19	51,51,59,60	0

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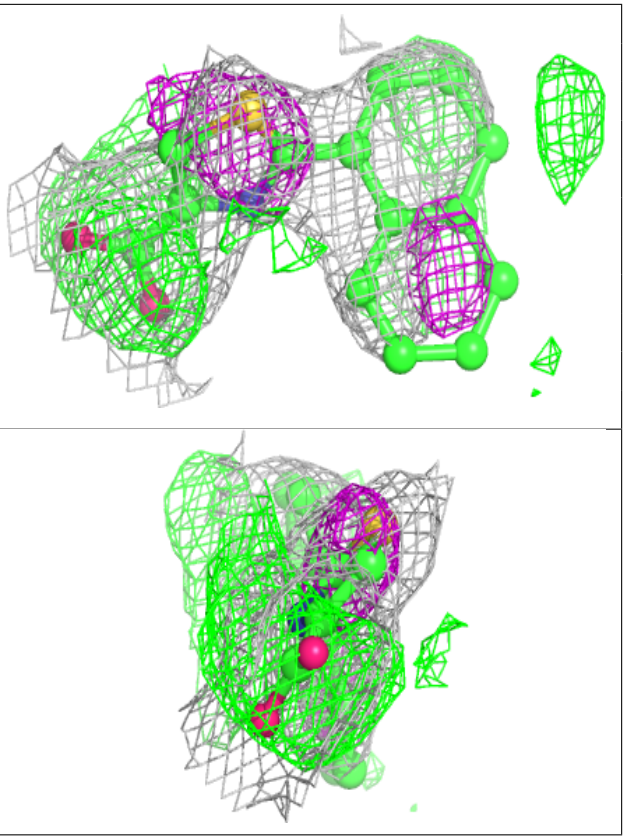
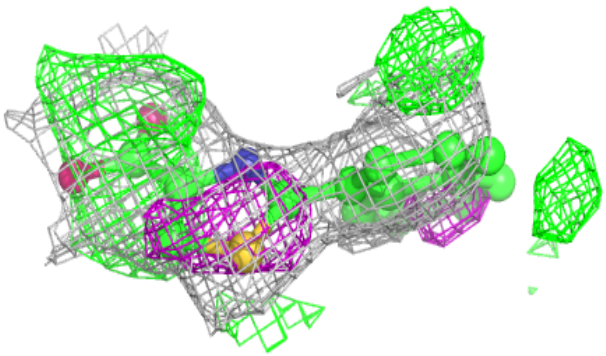
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	EDO	B	517	4/4	0.85	0.33	40,49,50,50	0
6	SO4	A	504	5/5	0.86	0.19	40,42,50,61	5
9	EDO	D	514	4/4	0.87	0.12	45,47,50,54	0
8	ELH	B	512	18/18	0.87	0.27	31,55,67,69	18
7	NAG	D	511	14/15	0.88	0.14	29,48,56,68	0
7	NAG	C	505	14/15	0.89	0.16	38,46,55,56	0
9	EDO	A	516	4/4	0.89	0.10	41,44,48,55	0
7	NAG	B	506	14/15	0.89	0.14	37,46,49,51	0
12	GOL	C	513	6/6	0.89	0.13	37,39,49,51	0
9	EDO	D	505	4/4	0.90	0.22	38,41,47,47	0
6	SO4	B	505	5/5	0.91	0.14	42,49,60,83	3
6	SO4	D	503	5/5	0.92	0.15	39,42,52,57	5
11	IPA	B	515	4/4	0.92	0.22	52,57,64,66	0
9	EDO	B	516	4/4	0.92	0.10	61,62,64,66	0
7	NAG	C	509	14/15	0.95	0.10	27,40,46,46	0
7	NAG	B	507	14/15	0.95	0.12	33,40,48,48	0
7	NAG	A	505	14/15	0.96	0.11	32,34,40,46	0
7	NAG	D	504	14/15	0.97	0.11	31,37,44,47	0
10	NA	B	513	1/1	0.98	0.28	32,32,32,32	0
6	SO4	A	503	5/5	0.98	0.10	43,44,48,51	5
6	SO4	C	510	5/5	0.98	0.12	28,29,35,38	5
6	SO4	C	511	5/5	0.99	0.39	10,28,30,30	5
5	FE	A	502	1/1	0.99	0.12	32,32,32,32	1
5	FE	B	502	1/1	0.99	0.12	30,30,30,30	1
10	NA	D	513	1/1	0.99	0.18	19,19,19,19	0
6	SO4	D	512	5/5	0.99	0.11	28,33,39,40	5
5	FE	D	502	1/1	0.99	0.11	32,32,32,32	1
4	ZN	D	501	1/1	1.00	0.13	32,32,32,32	0
5	FE	C	502	1/1	1.00	0.07	33,33,33,33	1
10	NA	B	514	1/1	1.00	0.17	16,16,16,16	0
4	ZN	C	501	1/1	1.00	0.13	35,35,35,35	0
4	ZN	A	501	1/1	1.00	0.13	34,34,34,34	0
4	ZN	B	501	1/1	1.00	0.13	36,36,36,36	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 ELH A 515:

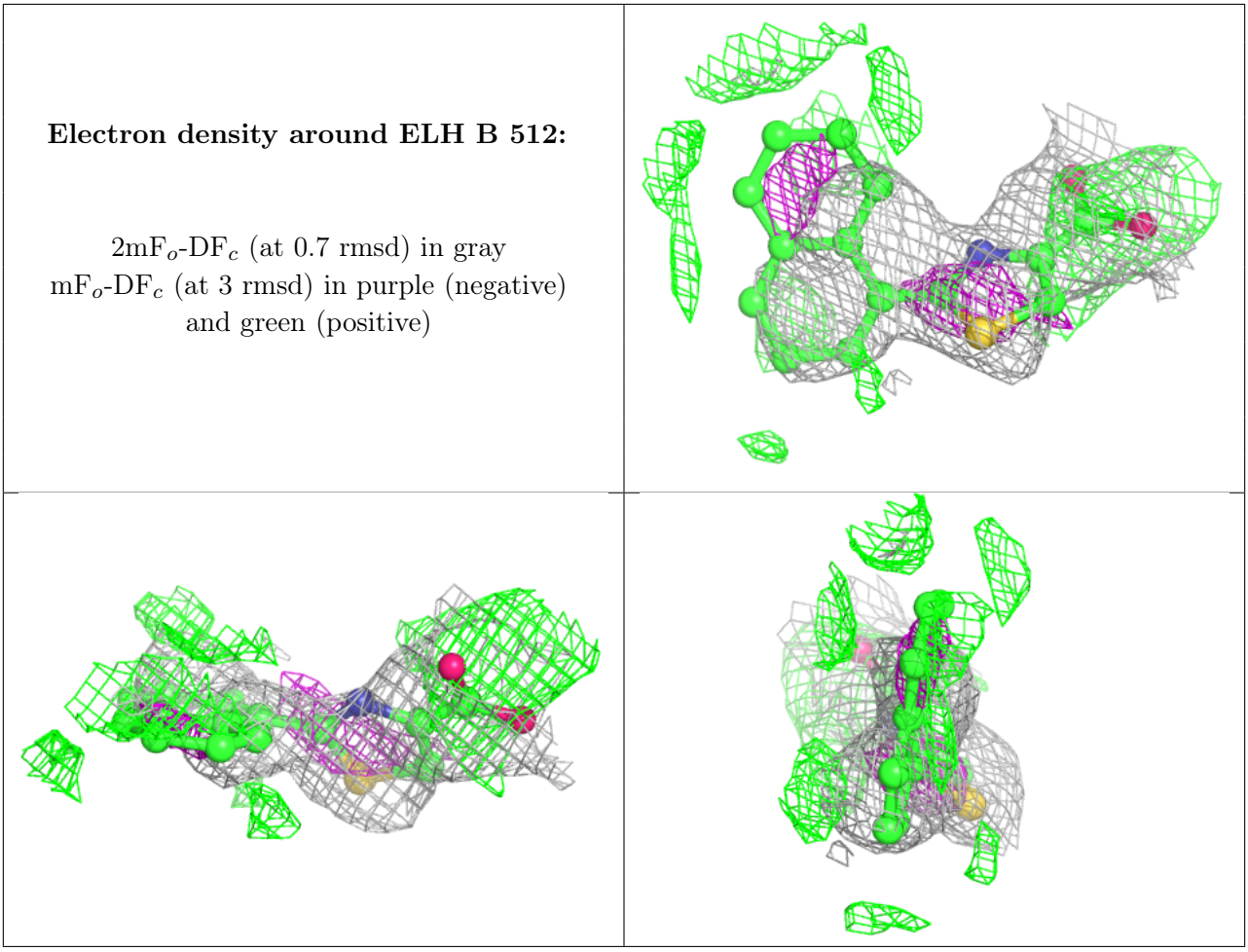
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around ELH B 512:

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.