Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 09:05 AM EDT

PDB ID	:	5A0C
Title	:	Crystal Structure of human neutrophil elastase in complex with a dihydropyrimidone inhibitor
Authors	:	vonNussbaum, F.; Li, V.M.-J.; Allerheiligen, S.; Anlauf, S.; Baerfacker, L.; Bechem, M.; Delbeck, M.; Fitzgerald, M.F.; Gerisch, M.; Gielen-Haertwig, H.; Haning, H.; Karthaus, D.; Lang, D.; Lustig, K.; Meibom, D.; Mittendorf, J.; Rosentreter, U.; Schaefer, M.; Schaefer, S.; Schamberger, J.; Telan, L.A.; Tersteegen, A.
Deposited on	:	2015-04-17
Resolution	:	2.10 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:

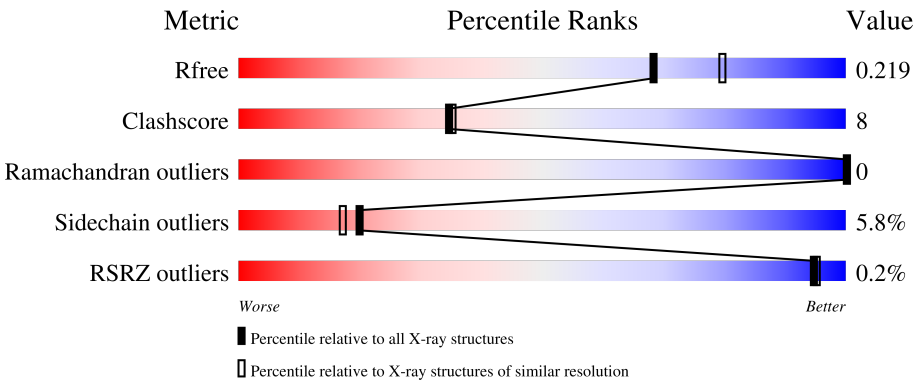
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	218	88% 11% •
1	B	218	80% 14% • •
2	C	3	67% 33%

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Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

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Mol	Chain	Length	Quality of chain
2	E	3	67% 33%
3	D	2	100%
3	F	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	XPE	A	1003	-	X	-	-

2 Entry composition (i)

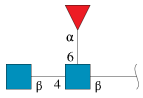
There are 7 unique types of molecules in this entry. The entry contains 3848 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NEUTROPHIL ELASTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	218	1636	1026	316	283	11	0	0	0
1	B	218	1636	1026	316	283	11	0	0	0

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



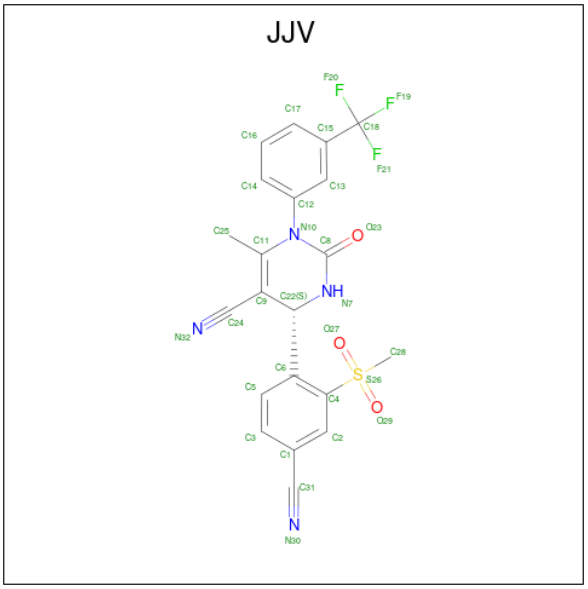
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	3	38	22	2	14	0	0	0
2	E	3	38	22	2	14	0	0	0

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	2	24	14	1	9	0	0	0
3	F	2	24	14	1	9	0	0	0

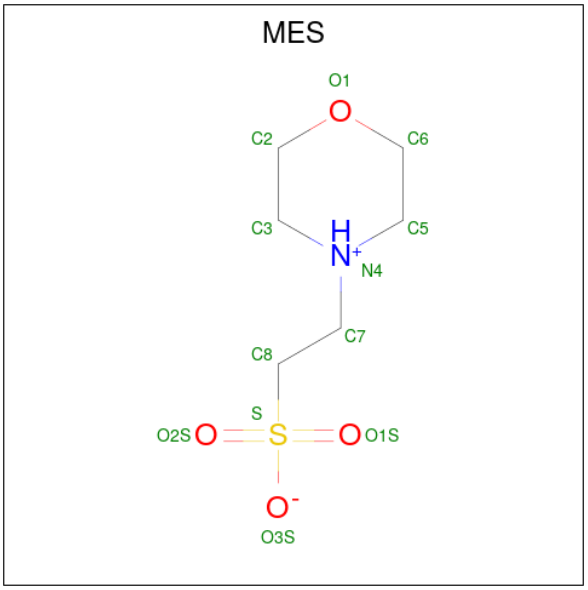
- Molecule 4 is (6S)-6-(4-cyano-2-methylsulfonyl-phenyl)-4-methyl-2-oxidanylidene-3-[3-(trifl

uoromethyl)phenyl]-1,6-dihydropyrimidine-5-carbonitrile (three-letter code: JJV) (formula: $C_{21}H_{15}F_3N_4O_3S$).



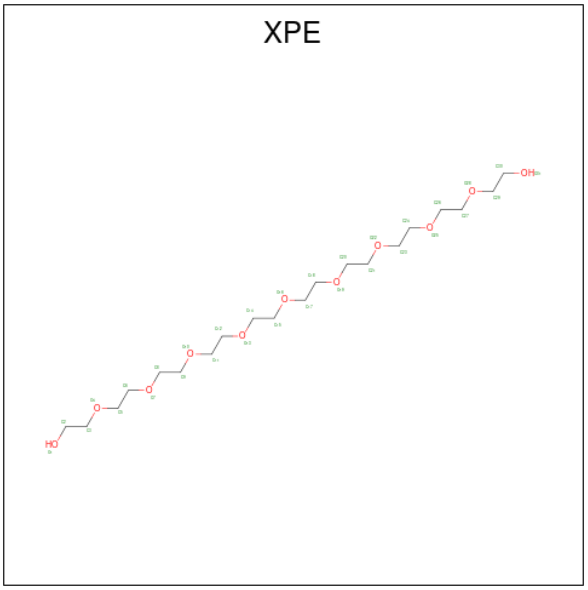
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	S		
4	A	1	32	21	3	4	3	1	0	0
			Total	C	F	N	O	S		
4	B	1	32	21	3	4	3	1	0	0

- Molecule 5 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		
5	A	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
5	B	1	12	6	1	4	1	0	0

- Molecule 6 is 3,6,9,12,15,18,21,24,27-NONAOXANONACOSANE-1,29-DIOL (three-letter code: XPE) (formula: $C_{20}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	30	20	10	0	0

- Molecule 7 is water.

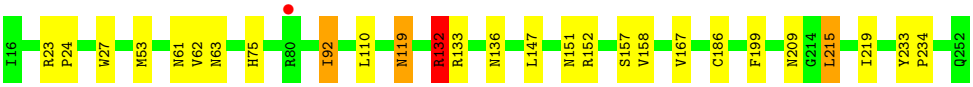
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	173	173	173	0	0
			Total	O		
7	B	161	161	161	0	0

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.

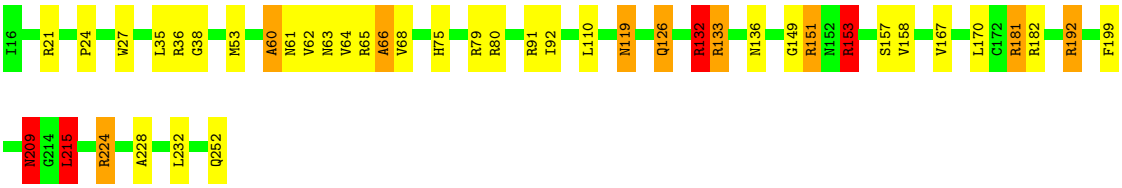
• Molecule 1: NEUTROPHIL ELASTASE

Chain A:



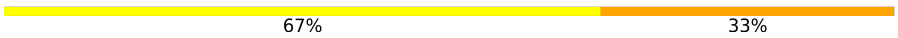
• Molecule 1: NEUTROPHIL ELASTASE

Chain B:



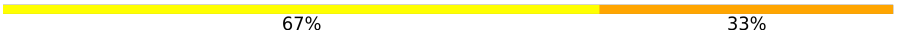
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



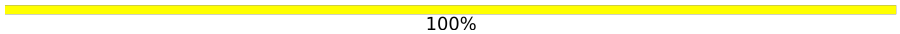
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



• Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 100%

NAG1
FUC2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	71.52Å 71.52Å 97.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.29 – 2.10 38.28 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.29-2.10) 99.8 (38.28-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.30 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.163 , 0.213 0.172 , 0.219	Depositor DCC
R_{free} test set	1641 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	23.5	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 34.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l 0.488 for h,-h-k,-l 0.026 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3848	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.64% 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: MES, FUC, XPE, NAG, JJV

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	1.26	2/1666 (0.1%)	1.17	7/2263 (0.3%)
1	B	1.42	11/1665 (0.7%)	1.44	22/2260 (1.0%)
All	All	1.34	13/3331 (0.4%)	1.31	29/4523 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	ALA	C-N	18.43	1.76	1.34
1	B	209	ASN	C-N	12.81	1.56	1.33
1	B	192	ARG	C-N	11.30	1.60	1.34
1	B	228	ALA	C-N	7.31	1.50	1.34
1	B	170	LEU	C-N	6.82	1.49	1.34
1	B	151	ARG	CD-NE	-6.57	1.35	1.46
1	B	149	GLY	C-N	6.48	1.49	1.34
1	B	132	ARG	CD-NE	6.12	1.56	1.46
1	B	149	GLY	N-CA	-5.83	1.37	1.46
1	B	91	ARG	CZ-NH1	5.47	1.40	1.33
1	A	132	ARG	CD-NE	5.24	1.55	1.46
1	A	233	TYR	CZ-OH	-5.21	1.28	1.37
1	B	60	ALA	C-O	5.10	1.33	1.23

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	66	ALA	O-C-N	-20.28	90.25	122.70
1	B	151	ARG	NE-CZ-NH1	-17.91	111.34	120.30
1	A	133	ARG	NE-CZ-NH1	9.90	125.25	120.30
1	B	153	ARG	NE-CZ-NH1	9.81	125.20	120.30
1	B	224	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	B	151	ARG	NE-CZ-NH2	9.62	125.11	120.30
1	B	192	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	B	151	ARG	CD-NE-CZ	9.01	136.21	123.60
1	B	181	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	B	132	ARG	NE-CZ-NH2	8.53	124.57	120.30
1	A	23	ARG	NE-CZ-NH1	8.27	124.44	120.30
1	B	215	LEU	CB-CG-CD1	8.04	124.66	111.00
1	A	215	LEU	CB-CG-CD1	8.03	124.65	111.00
1	B	151	ARG	CG-CD-NE	-8.02	94.97	111.80
1	B	153	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	B	21	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	B	132	ARG	CB-CG-CD	6.07	127.39	111.60
1	A	53	MET	CG-SD-CE	-6.06	90.51	100.20
1	A	132	ARG	CB-CG-CD	6.03	127.27	111.60
1	B	224	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	B	182	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	B	133	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	A	133	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	B	79	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	132	ARG	NE-CZ-NH2	5.67	123.14	120.30
1	B	181	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	53	MET	CG-SD-CE	-5.26	91.79	100.20
1	B	182	ARG	CA-CB-CG	-5.22	101.92	113.40
1	B	133	ARG	NE-CZ-NH1	5.10	122.85	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	151	ARG	Sidechain
1	B	192	ARG	Mainchain
1	B	209	ASN	Mainchain

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	1636	0	1650	20	0
1	B	1636	0	1648	26	0
2	C	38	0	34	1	0
2	E	38	0	34	1	0
3	D	24	0	22	0	0
3	F	24	0	22	0	0
4	A	32	0	15	5	0
4	B	32	0	15	6	0
5	A	12	0	13	0	0
5	B	12	0	13	0	0
6	A	30	0	39	8	0
7	A	173	0	0	5	0
7	B	161	0	0	6	0
All	All	3848	0	3505	58	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 8.

All (58) 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)
6:A:1003:XPE:C6	6:A:1003:XPE:O7	1.63	1.43
1:B:66:ALA:C	1:B:68:VAL:N	1.76	1.36
6:A:1003:XPE:O22	6:A:1003:XPE:C21	1.71	1.36
1:B:36:ARG:C	1:B:38:GLY:N	2.21	0.94
1:B:252:GLN:HG2	7:B:2155:HOH:O	1.66	0.94
1:B:66:ALA:O	1:B:68:VAL:N	2.15	0.78
6:A:1003:XPE:H231	7:A:2145:HOH:O	1.83	0.78
1:B:63:ASN:HB3	7:B:2031:HOH:O	1.95	0.66
4:A:1001:JJV:C28	4:A:1001:JJV:H22	2.25	0.66
6:A:1003:XPE:C21	6:A:1003:XPE:C23	2.75	0.64
1:B:132:ARG:HH21	1:B:209:ASN:HD22	1.46	0.62
4:B:1001:JJV:C28	4:B:1001:JJV:H22	2.30	0.61
6:A:1003:XPE:C6	6:A:1003:XPE:C8	2.77	0.59
1:A:63:ASN:HB2	1:B:63:ASN:HB2	1.84	0.58
1:B:126:GLN:HB3	1:B:215:LEU:HD12	1.86	0.58
1:B:92:ILE:HG22	1:B:110:LEU:HD22	1.86	0.56
1:B:75:HIS:CE1	1:B:158:VAL:HG13	2.41	0.56
6:A:1003:XPE:C21	6:A:1003:XPE:C24	2.84	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ASN:CB	7:B:2031:HOH:O	2.54	0.55
1:A:24:PRO:HA	1:A:75:HIS:CD2	2.42	0.55
1:A:151:ASN:HD21	1:B:181:ARG:HH21	1.57	0.52
4:A:1001:JJV:H281	4:A:1001:JJV:C22	2.41	0.51
4:A:1001:JJV:H22	4:A:1001:JJV:H283	1.92	0.51
1:A:75:HIS:CE1	1:A:158:VAL:HG13	2.46	0.51
1:A:61:ASN:HB3	1:B:35:LEU:HD12	1.94	0.49
1:B:132:ARG:NH2	1:B:209:ASN:HD22	2.10	0.49
1:A:132:ARG:HH21	1:A:209:ASN:HD22	1.60	0.49
1:B:27:TRP:CH2	2:E:3:FUC:H61	2.48	0.48
1:B:153:ARG:NH2	7:B:2105:HOH:O	2.45	0.48
1:A:186:CYS:HB3	1:A:234:PRO:HB2	1.95	0.48
4:A:1001:JJV:C28	4:A:1001:JJV:C22	2.91	0.48
1:A:92:ILE:HG22	1:A:110:LEU:CD2	2.44	0.47
6:A:1003:XPE:O7	6:A:1003:XPE:C5	2.48	0.47
1:A:147:LEU:HD11	4:B:1001:JJV:H282	1.96	0.47
1:A:199:PHE:CG	4:B:1001:JJV:H283	2.48	0.47
1:B:92:ILE:HG22	1:B:110:LEU:CD2	2.45	0.46
1:B:119:ASN:C	1:B:119:ASN:HD22	2.18	0.46
1:B:136:ASN:ND2	1:B:167:VAL:HA	2.30	0.45
4:A:1001:JJV:H283	1:B:199:PHE:CG	2.51	0.45
4:B:1001:JJV:H22	4:B:1001:JJV:H283	1.97	0.45
1:A:27:TRP:CH2	2:C:3:FUC:H61	2.53	0.44
1:A:151:ASN:ND2	1:B:181:ARG:HH21	2.15	0.44
4:B:1001:JJV:C28	4:B:1001:JJV:C22	2.96	0.44
1:A:136:ASN:ND2	1:A:167:VAL:HA	2.33	0.44
1:B:24:PRO:HA	1:B:75:HIS:CD2	2.53	0.44
1:A:136:ASN:ND2	7:A:2104:HOH:O	2.51	0.43
6:A:1003:XPE:H241	6:A:1003:XPE:H212	1.99	0.43
1:B:60:ALA:O	1:B:61:ASN:HB2	2.20	0.42
1:A:63:ASN:HB3	7:A:2042:HOH:O	2.19	0.42
1:B:66:ALA:CA	1:B:68:VAL:N	2.75	0.42
1:B:136:ASN:ND2	7:B:2090:HOH:O	2.46	0.41
1:A:119:ASN:C	1:A:119:ASN:HD22	2.24	0.41
1:A:132:ARG:NH2	1:A:209:ASN:HD22	2.17	0.41
4:B:1001:JJV:C22	4:B:1001:JJV:H281	2.51	0.41
1:A:63:ASN:CB	7:A:2042:HOH:O	2.69	0.41
1:A:92:ILE:HD13	7:A:2060:HOH:O	2.21	0.41
1:A:219:ILE:HG21	1:A:219:ILE:HD13	1.91	0.40
1:B:132:ARG:NH1	7:B:2076:HOH:O	2.52	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	216/218 (99%)	207 (96%)	9 (4%)	0	100	100
1	B	214/218 (98%)	204 (95%)	10 (5%)	0	100	100
All	All	430/436 (99%)	411 (96%)	19 (4%)	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	172/172 (100%)	165 (96%)	7 (4%)	30	31
1	B	172/172 (100%)	159 (92%)	13 (8%)	13	10
All	All	344/344 (100%)	324 (94%)	20 (6%)	20	17

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	VAL
1	A	92	ILE
1	A	119	ASN
1	A	132	ARG
1	A	152	ARG
1	A	157	SER
1	A	215	LEU
1	B	62	VAL

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Mol	Chain	Res	Type
1	B	64	VAL
1	B	65	ARG
1	B	80	ARG
1	B	119	ASN
1	B	126	GLN
1	B	132	ARG
1	B	133	ARG
1	B	153	ARG
1	B	157	SER
1	B	215	LEU
1	B	224	ARG
1	B	232	LEU

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

Mol	Chain	Res	Type
1	A	75	HIS
1	A	96	ASN
1	A	119	ASN
1	A	121	ASN
1	A	123	GLN
1	A	136	ASN
1	A	151	ASN
1	A	209	ASN
1	A	217	HIS
1	A	242	GLN
1	B	75	HIS
1	B	96	ASN
1	B	119	ASN
1	B	121	ASN
1	B	136	ASN
1	B	139	GLN
1	B	209	ASN
1	B	242	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)

10 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	1,2	14,14,15	0.97	1 (7%)	17,19,21	1.28	1 (5%)
2	NAG	C	2	2	14,14,15	1.31	2 (14%)	17,19,21	1.75	4 (23%)
2	FUC	C	3	2	10,10,11	0.91	0	14,14,16	1.34	2 (14%)
3	NAG	D	1	1,3	14,14,15	1.24	2 (14%)	17,19,21	2.76	7 (41%)
3	FUC	D	2	3	10,10,11	0.68	0	14,14,16	2.42	7 (50%)
2	NAG	E	1	1,2	14,14,15	1.14	1 (7%)	17,19,21	1.61	2 (11%)
2	NAG	E	2	2	14,14,15	1.47	2 (14%)	17,19,21	2.61	7 (41%)
2	FUC	E	3	2	10,10,11	0.96	0	14,14,16	1.75	4 (28%)
3	NAG	F	1	1,3	14,14,15	1.40	1 (7%)	17,19,21	2.64	9 (52%)
3	FUC	F	2	3	10,10,11	0.83	0	14,14,16	1.89	4 (28%)

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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
2	FUC	C	3	2	-	-	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	FUC	D	2	3	-	-	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1

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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	NAG	O4-C4	3.35	1.50	1.43
2	E	2	NAG	O4-C4	3.35	1.50	1.43
2	E	2	NAG	O5-C5	3.24	1.50	1.43
2	C	1	NAG	O5-C1	-2.59	1.39	1.43
2	C	2	NAG	O5-C5	2.53	1.48	1.43
3	D	1	NAG	C2-N2	-2.22	1.42	1.46
2	E	1	NAG	O5-C1	-2.18	1.40	1.43
3	F	1	NAG	O4-C4	2.13	1.48	1.43
3	D	1	NAG	C4-C5	2.07	1.57	1.53

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2	NAG	C1-O5-C5	5.93	120.22	112.19
2	E	1	NAG	C1-O5-C5	5.36	119.45	112.19
3	F	1	NAG	C8-C7-N2	5.32	125.11	116.10
3	D	1	NAG	O7-C7-N2	-5.00	112.75	121.95
3	D	1	NAG	C1-C2-N2	-4.67	102.52	110.49
3	D	1	NAG	C8-C7-N2	4.66	124.00	116.10
2	E	2	NAG	O5-C5-C4	4.64	122.12	110.83
3	F	1	NAG	O7-C7-N2	-4.60	113.50	121.95
3	D	2	FUC	O3-C3-C2	-4.48	101.42	109.99
3	D	1	NAG	C3-C4-C5	-4.40	102.39	110.24
3	F	1	NAG	C1-C2-N2	-4.00	103.66	110.49
2	C	1	NAG	C1-O5-C5	3.89	117.46	112.19
2	E	3	FUC	O3-C3-C2	-3.73	102.85	109.99
2	C	2	NAG	O4-C4-C5	3.70	118.47	109.30
3	F	1	NAG	C3-C4-C5	-3.57	103.86	110.24
3	D	1	NAG	O3-C3-C4	3.55	118.55	110.35
3	F	1	NAG	O4-C4-C3	3.53	118.50	110.35
2	E	2	NAG	O4-C4-C5	3.39	117.72	109.30
3	F	2	FUC	O3-C3-C4	3.37	118.13	110.35
3	F	2	FUC	C2-C3-C4	-3.34	105.11	110.89
2	E	3	FUC	O3-C3-C4	3.29	117.96	110.35
3	D	2	FUC	C1-C2-C3	3.27	113.68	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2	NAG	C6-C5-C4	-3.13	105.68	113.00
3	D	1	NAG	O4-C4-C3	3.08	117.46	110.35
3	D	2	FUC	O4-C4-C5	-3.07	102.86	109.67
3	F	2	FUC	O4-C4-C5	-3.00	103.02	109.67
2	C	2	NAG	C6-C5-C4	-3.00	105.98	113.00
2	E	2	NAG	O6-C6-C5	-2.94	101.21	111.29
2	E	2	NAG	O3-C3-C4	-2.88	103.69	110.35
3	D	2	FUC	O2-C2-C3	-2.73	104.67	110.14
2	C	2	NAG	C8-C7-N2	2.71	120.69	116.10
3	F	1	NAG	O6-C6-C5	-2.64	102.22	111.29
3	D	2	FUC	O5-C1-C2	2.57	114.74	110.77
3	F	1	NAG	C2-N2-C7	2.54	126.52	122.90
2	E	3	FUC	O2-C2-C3	-2.50	105.12	110.14
2	C	2	NAG	C1-C2-N2	2.44	114.66	110.49
2	E	1	NAG	O5-C1-C2	2.41	115.09	111.29
3	D	2	FUC	O3-C3-C4	2.36	115.81	110.35
3	D	1	NAG	O5-C1-C2	-2.33	107.62	111.29
2	E	2	NAG	O5-C5-C6	-2.32	103.57	107.20
2	C	3	FUC	O2-C2-C3	-2.28	105.58	110.14
3	D	2	FUC	O2-C2-C1	2.22	113.69	109.15
3	F	1	NAG	O3-C3-C4	2.21	115.45	110.35
2	E	3	FUC	O2-C2-C1	2.09	113.42	109.15
3	F	1	NAG	O5-C1-C2	-2.05	108.06	111.29
3	F	2	FUC	C1-C2-C3	-2.04	107.16	109.67
2	C	3	FUC	C6-C5-C4	2.02	116.81	113.07

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
2	C	2	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	FUC	1	0

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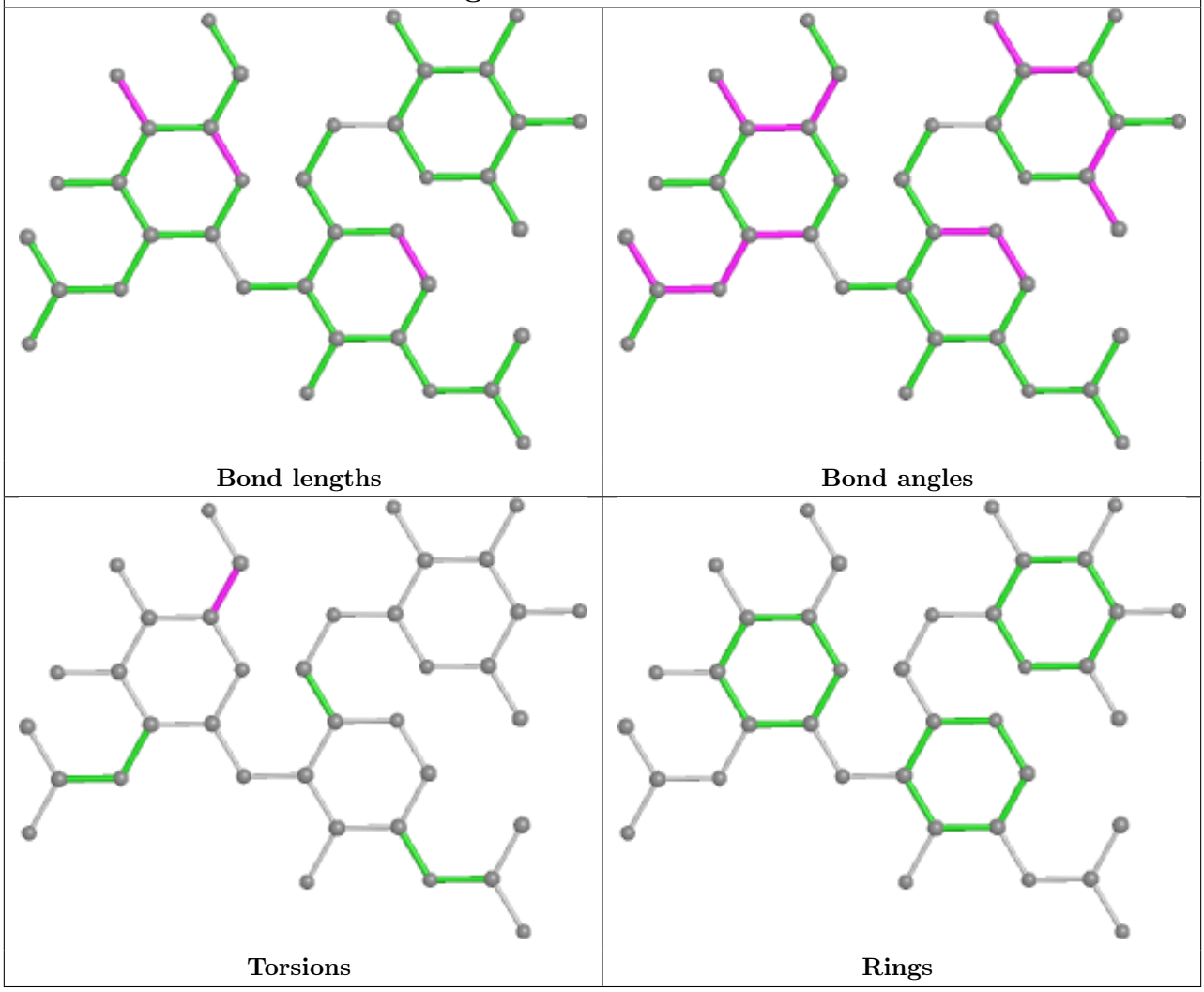
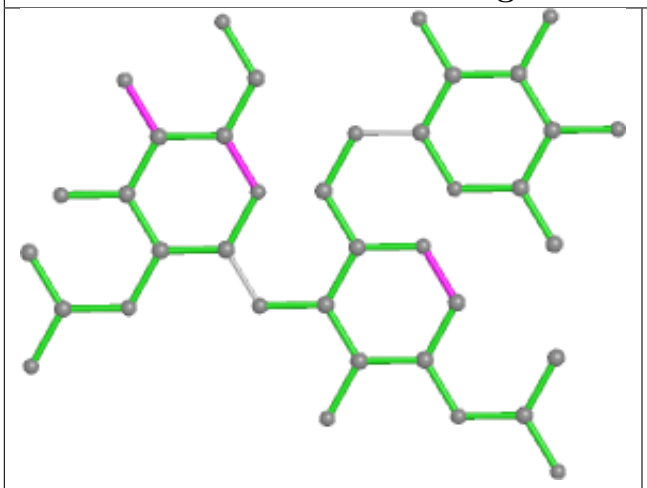
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	3	FUC	1	0

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

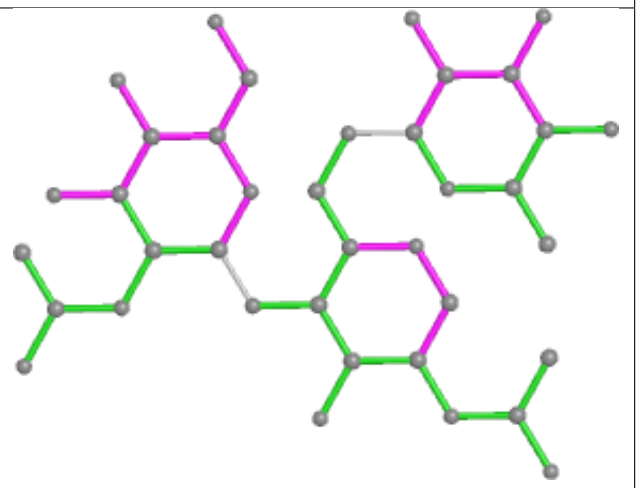
Oligosaccharide Chain C



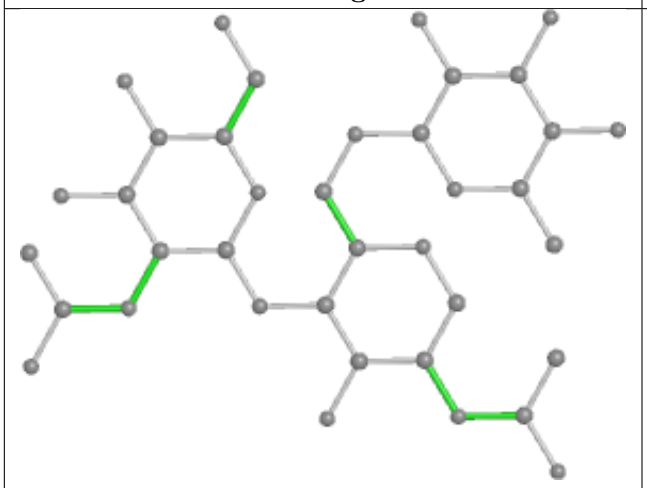
Oligosaccharide Chain E



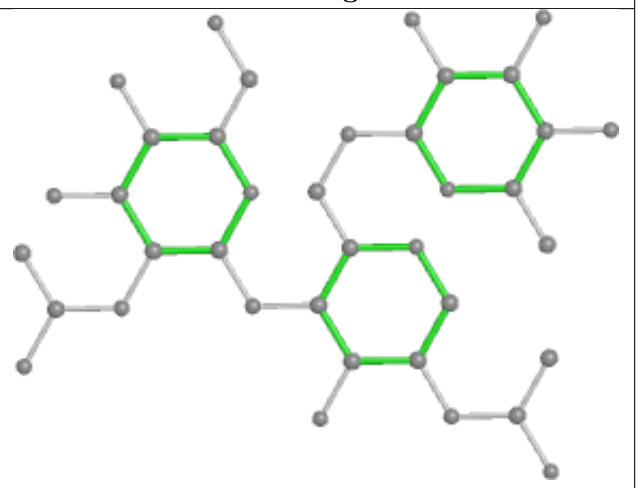
Bond lengths



Bond angles

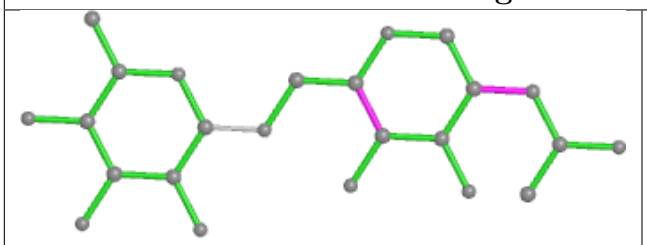


Torsions

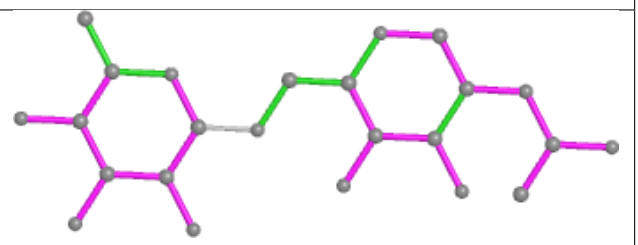


Rings

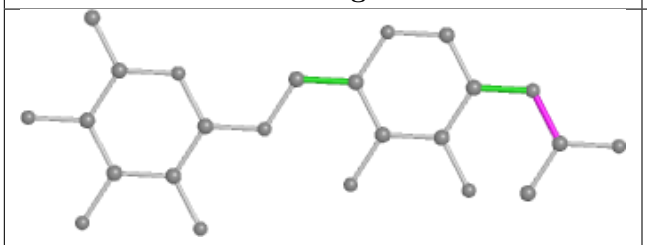
Oligosaccharide Chain D



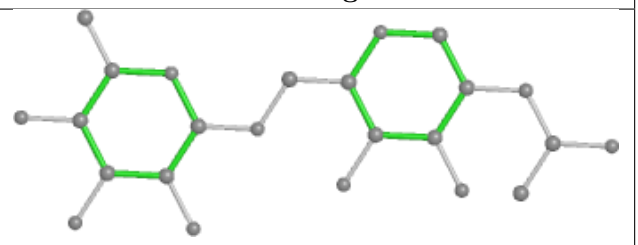
Bond lengths



Bond angles

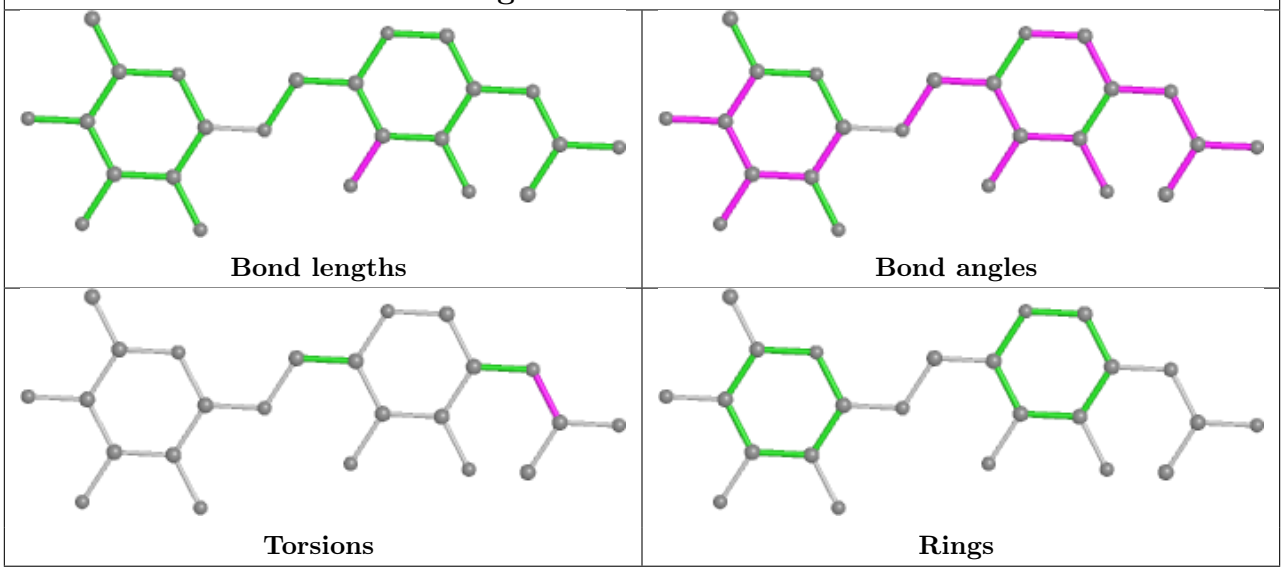


Torsions



Rings

Oligosaccharide Chain F



5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	JJV	A	1001	-	34,34,34	2.05	10 (29%)	49,52,52	3.60	20 (40%)
5	MES	A	1002	-	12,12,12	1.82	1 (8%)	14,16,16	1.66	4 (28%)
5	MES	B	1002	-	12,12,12	1.84	3 (25%)	14,16,16	2.39	3 (21%)
4	JJV	B	1001	-	34,34,34	2.09	8 (23%)	49,52,52	3.55	17 (34%)
6	XPE	A	1003	-	29,29,30	2.58	10 (34%)	28,28,29	2.37	7 (25%)

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
4	JJV	A	1001	-	-	4/22/44/44	0/3/3/3
5	MES	A	1002	-	-	1/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MES	B	1002	-	-	0/6/14/14	0/1/1/1
4	JJV	B	1001	-	-	4/22/44/44	0/3/3/3
6	XPE	A	1003	-	-	18/27/27/28	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1003	XPE	O22-C21	6.84	1.71	1.42
4	B	1001	JJV	O29-S26	6.18	1.61	1.44
4	B	1001	JJV	C28-S26	-5.47	1.53	1.75
5	A	1002	MES	C8-S	4.96	1.84	1.77
6	A	1003	XPE	O7-C6	4.95	1.63	1.42
5	B	1002	MES	C8-S	4.71	1.84	1.77
4	A	1001	JJV	O29-S26	4.62	1.57	1.44
4	A	1001	JJV	C28-S26	-4.50	1.57	1.75
6	A	1003	XPE	C9-C8	4.34	1.71	1.49
6	A	1003	XPE	O19-C20	4.27	1.60	1.42
6	A	1003	XPE	O25-C24	4.14	1.60	1.42
4	A	1001	JJV	C25-C11	4.05	1.55	1.49
6	A	1003	XPE	O28-C27	3.88	1.58	1.42
4	A	1001	JJV	C12-N10	-3.86	1.38	1.44
4	B	1001	JJV	C6-C22	3.67	1.59	1.52
4	A	1001	JJV	C6-C22	3.58	1.58	1.52
4	B	1001	JJV	C2-C4	3.51	1.44	1.39
4	A	1001	JJV	C11-N10	-3.28	1.35	1.40
4	A	1001	JJV	C22-N7	3.06	1.50	1.47
4	B	1001	JJV	C4-S26	2.98	1.82	1.77
5	B	1002	MES	O2S-S	2.90	1.53	1.45
4	A	1001	JJV	C24-C9	-2.89	1.38	1.42
6	A	1003	XPE	O31-C30	2.72	1.56	1.42
4	B	1001	JJV	C12-N10	-2.66	1.40	1.44
4	A	1001	JJV	O27-S26	2.63	1.51	1.44
4	B	1001	JJV	C22-N7	2.60	1.49	1.47
6	A	1003	XPE	O10-C9	2.59	1.53	1.42
5	B	1002	MES	C5-C6	2.38	1.59	1.50
6	A	1003	XPE	O16-C17	2.31	1.52	1.42
6	A	1003	XPE	C18-C17	2.14	1.60	1.49
4	B	1001	JJV	C8-N7	2.05	1.37	1.34
4	A	1001	JJV	C16-C17	2.04	1.43	1.38

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1001	JJV	O27-S26-C28	14.97	130.01	108.49
4	B	1001	JJV	O27-S26-C28	13.52	127.92	108.49
4	A	1001	JJV	O29-S26-O27	-12.39	96.58	117.92
4	B	1001	JJV	O29-S26-O27	-12.06	97.16	117.92
4	B	1001	JJV	C6-C22-N7	-8.42	99.87	110.35
5	B	1002	MES	O1S-S-C8	-7.73	97.61	106.92
4	A	1001	JJV	C6-C22-N7	-6.95	101.69	110.35
4	A	1001	JJV	C24-C9-C11	6.71	125.05	119.76
6	A	1003	XPE	O19-C20-C21	6.36	139.07	110.39
4	B	1001	JJV	C28-S26-C4	5.78	113.68	105.11
6	A	1003	XPE	O19-C18-C17	5.32	134.38	110.39
4	B	1001	JJV	C14-C12-N10	4.89	125.50	119.64
4	B	1001	JJV	C24-C9-C11	4.81	123.55	119.76
6	A	1003	XPE	O28-C29-C30	4.70	130.71	110.07
6	A	1003	XPE	C20-O19-C18	4.30	131.90	113.29
4	B	1001	JJV	O29-S26-C4	-4.20	103.38	108.27
4	A	1001	JJV	C14-C12-N10	4.07	124.52	119.64
4	A	1001	JJV	C25-C11-C9	-3.82	119.22	124.95
4	B	1001	JJV	O27-S26-C4	-3.75	103.90	108.27
4	A	1001	JJV	O29-S26-C4	-3.75	103.91	108.27
4	B	1001	JJV	C12-C13-C15	3.40	124.57	120.44
4	B	1001	JJV	C25-C11-C9	-3.25	120.08	124.95
4	A	1001	JJV	C9-C22-N7	3.21	111.65	109.09
4	A	1001	JJV	C12-N10-C8	-3.20	113.64	117.83
4	B	1001	JJV	C12-N10-C11	3.17	122.66	119.23
4	B	1001	JJV	C9-C22-N7	3.09	111.56	109.09
6	A	1003	XPE	C8-O7-C6	3.04	126.47	113.29
4	B	1001	JJV	N7-C8-N10	3.03	120.72	116.17
4	A	1001	JJV	C25-C11-N10	3.03	119.84	115.69
4	A	1001	JJV	C16-C17-C15	-2.68	117.94	120.76
5	A	1002	MES	O3S-S-C8	2.67	110.08	105.77
5	A	1002	MES	O1S-S-C8	-2.63	103.75	106.92
4	A	1001	JJV	C28-S26-C4	2.62	109.00	105.11
4	A	1001	JJV	C5-C6-C22	-2.62	116.34	120.89
5	B	1002	MES	C6-C5-N4	-2.62	106.13	110.10
4	B	1001	JJV	C6-C22-C9	2.62	116.79	113.23
4	A	1001	JJV	C2-C1-C31	2.61	123.01	119.54
4	A	1001	JJV	C12-N10-C11	2.44	121.88	119.23
6	A	1003	XPE	O16-C17-C18	-2.41	99.54	110.39
4	B	1001	JJV	F21-C18-C15	-2.37	107.72	112.93
4	A	1001	JJV	C22-C9-C24	-2.31	113.05	118.23
4	A	1001	JJV	O23-C8-N10	-2.30	117.59	121.77
4	A	1001	JJV	C13-C12-N10	-2.29	116.28	119.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1001	JJV	C13-C12-N10	-2.28	116.29	119.12
4	A	1001	JJV	N7-C8-N10	2.21	119.48	116.17
5	B	1002	MES	O2S-S-O1S	2.20	121.55	113.95
6	A	1003	XPE	O13-C12-C11	2.15	120.11	110.39
4	A	1001	JJV	C6-C22-C9	2.11	116.10	113.23
4	B	1001	JJV	C13-C15-C18	2.09	122.40	119.58
5	A	1002	MES	C2-C3-N4	-2.08	106.95	110.10
5	A	1002	MES	O2S-S-O1S	-2.02	106.97	113.95

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	JJV	C2-C4-S26-C28
4	A	1001	JJV	C6-C4-S26-C28
4	A	1001	JJV	C2-C4-S26-O29
4	A	1001	JJV	C6-C4-S26-O29
4	B	1001	JJV	C2-C4-S26-C28
4	B	1001	JJV	C6-C4-S26-C28
4	B	1001	JJV	C6-C4-S26-O29
5	A	1002	MES	C8-C7-N4-C3
6	A	1003	XPE	C23-C24-O25-C26
6	A	1003	XPE	C11-C12-O13-C14
6	A	1003	XPE	C21-C20-O19-C18
6	A	1003	XPE	C5-C6-O7-C8
6	A	1003	XPE	O16-C17-C18-O19
6	A	1003	XPE	C24-C23-O22-C21
6	A	1003	XPE	O25-C26-C27-O28
6	A	1003	XPE	O19-C20-C21-O22
6	A	1003	XPE	O28-C29-C30-O31
6	A	1003	XPE	O7-C8-C9-O10
4	B	1001	JJV	C2-C4-S26-O29
6	A	1003	XPE	C8-C9-O10-C11
6	A	1003	XPE	C17-C18-O19-C20
6	A	1003	XPE	O22-C23-C24-O25
6	A	1003	XPE	C12-C11-O10-C9
6	A	1003	XPE	C20-C21-O22-C23
6	A	1003	XPE	C6-C5-O4-C3
6	A	1003	XPE	C2-C3-O4-C5
6	A	1003	XPE	C14-C15-O16-C17

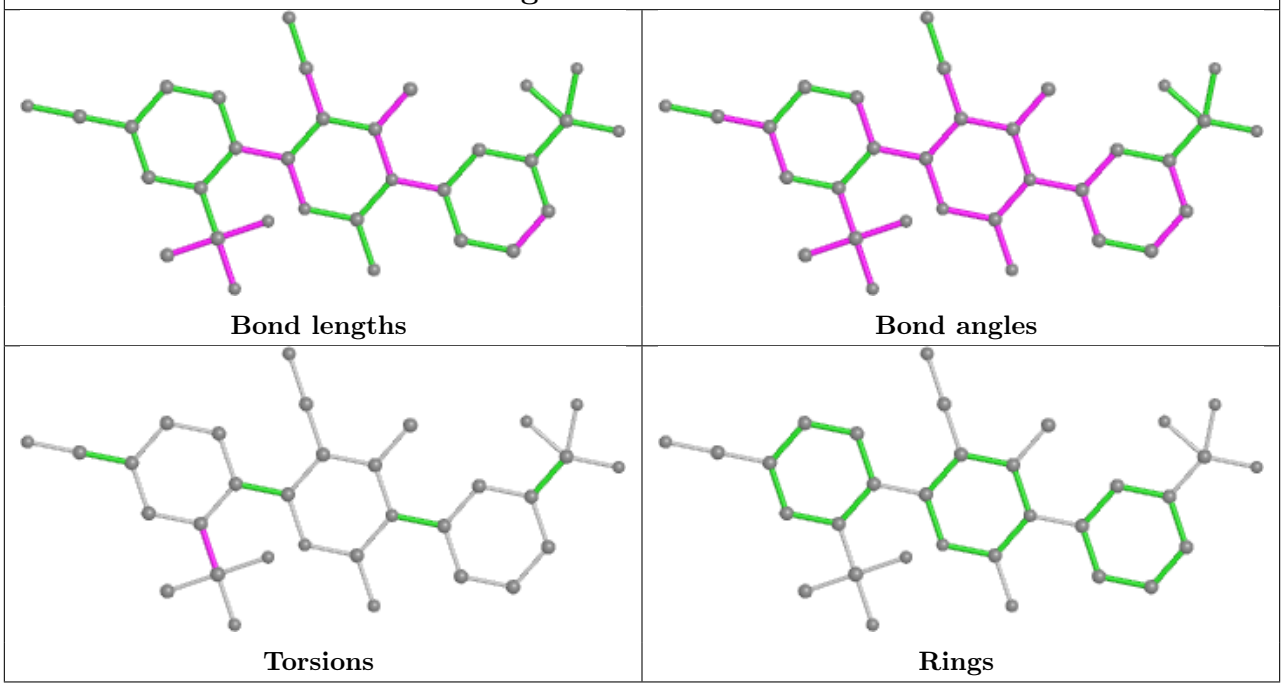
There are no ring outliers.

3 monomers are involved in 19 short contacts:

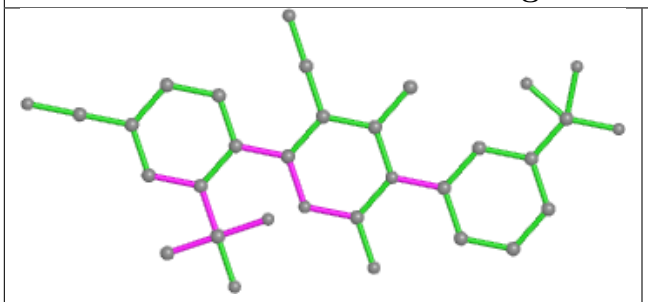
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1001	JJV	5	0
4	B	1001	JJV	6	0
6	A	1003	XPE	8	0

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.

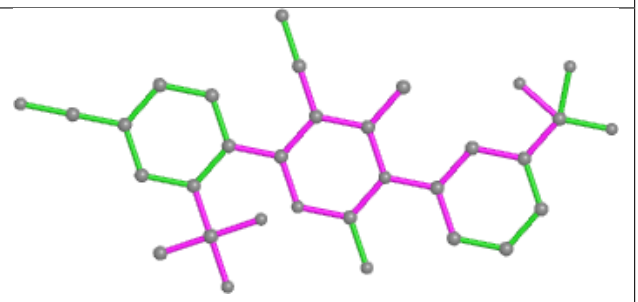
Ligand JJV A 1001



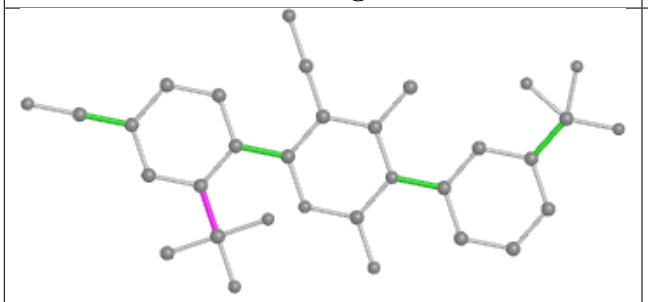
Ligand JJV B 1001



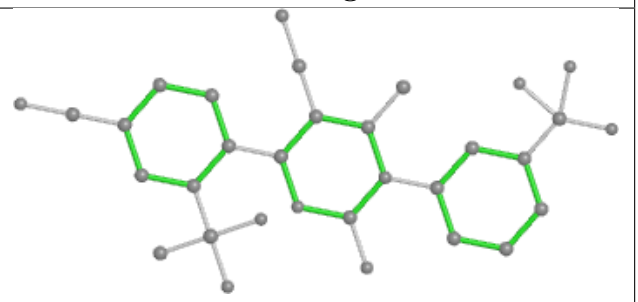
Bond lengths



Bond angles

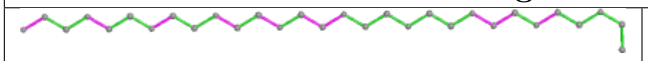


Torsions

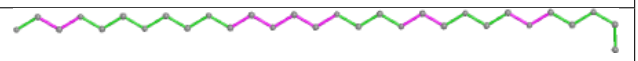


Rings

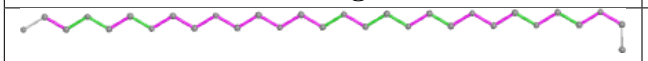
Ligand XPE A 1003



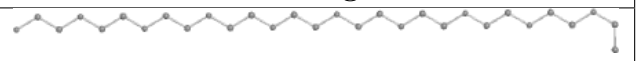
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	36:ARG	C	38:GLY	N	2.21
1	B	66:ALA	C	68:VAL	N	1.76

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	218/218 (100%)	-0.65	1 (0%) 91 92	14, 24, 41, 66	2 (0%)
1	B	218/218 (100%)	-0.71	0 100 100	14, 24, 39, 64	2 (0%)
All	All	436/436 (100%)	-0.68	1 (0%) 95 95	14, 24, 40, 66	4 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	80	ARG	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
3	NAG	D	1	14/15	0.83	0.16	51,57,60,62	0
3	FUC	D	2	10/11	0.84	0.26	57,62,64,68	0
3	FUC	F	2	10/11	0.84	0.19	58,67,70,72	0
3	NAG	F	1	14/15	0.85	0.14	49,55,57,59	0
2	NAG	E	2	14/15	0.88	0.10	37,47,49,53	0
2	NAG	C	2	14/15	0.92	0.12	38,47,54,56	0
2	NAG	C	1	14/15	0.96	0.07	29,33,36,41	0
2	NAG	E	1	14/15	0.97	0.07	27,31,36,39	0

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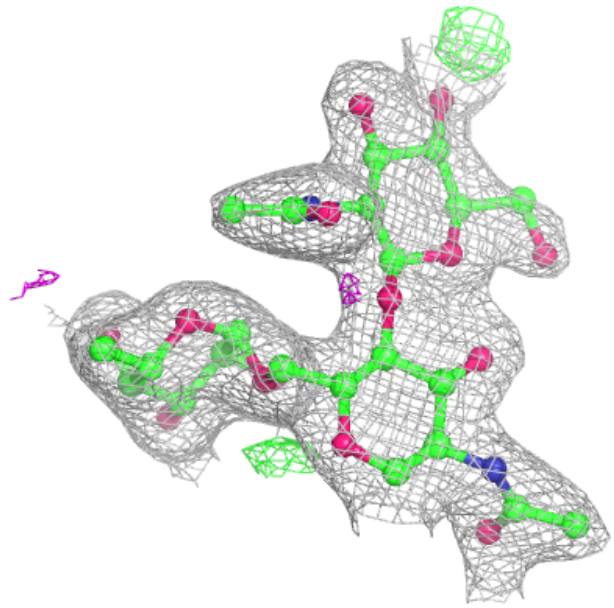
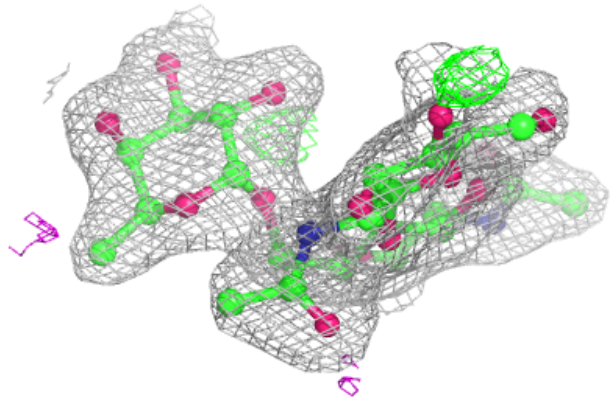
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FUC	C	3	10/11	0.98	0.06	26,28,29,30	0
2	FUC	E	3	10/11	0.98	0.06	24,26,28,29	0

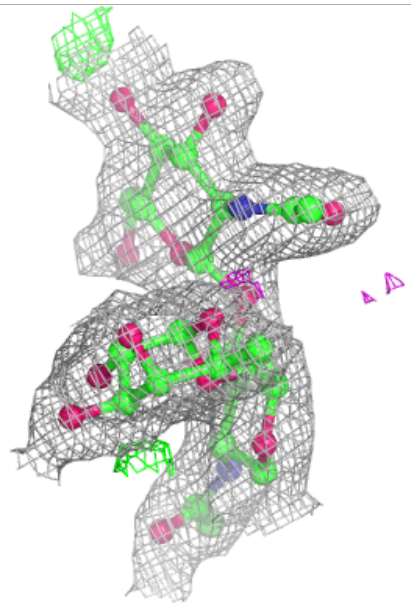
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

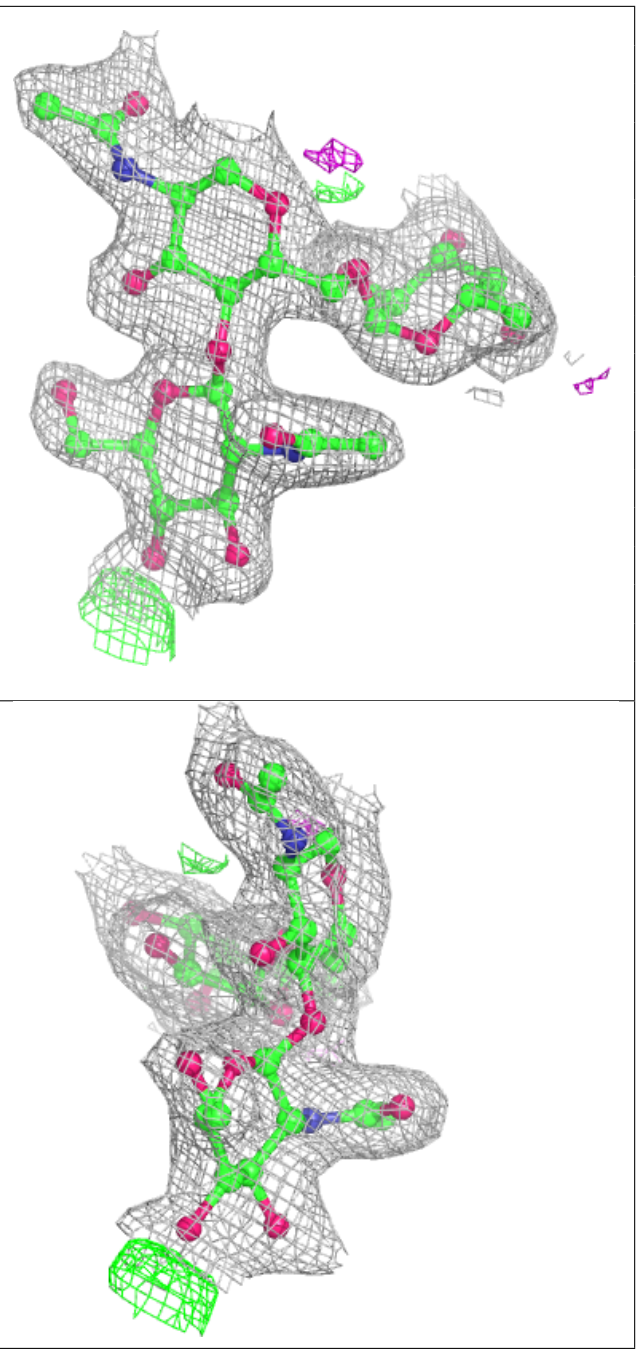






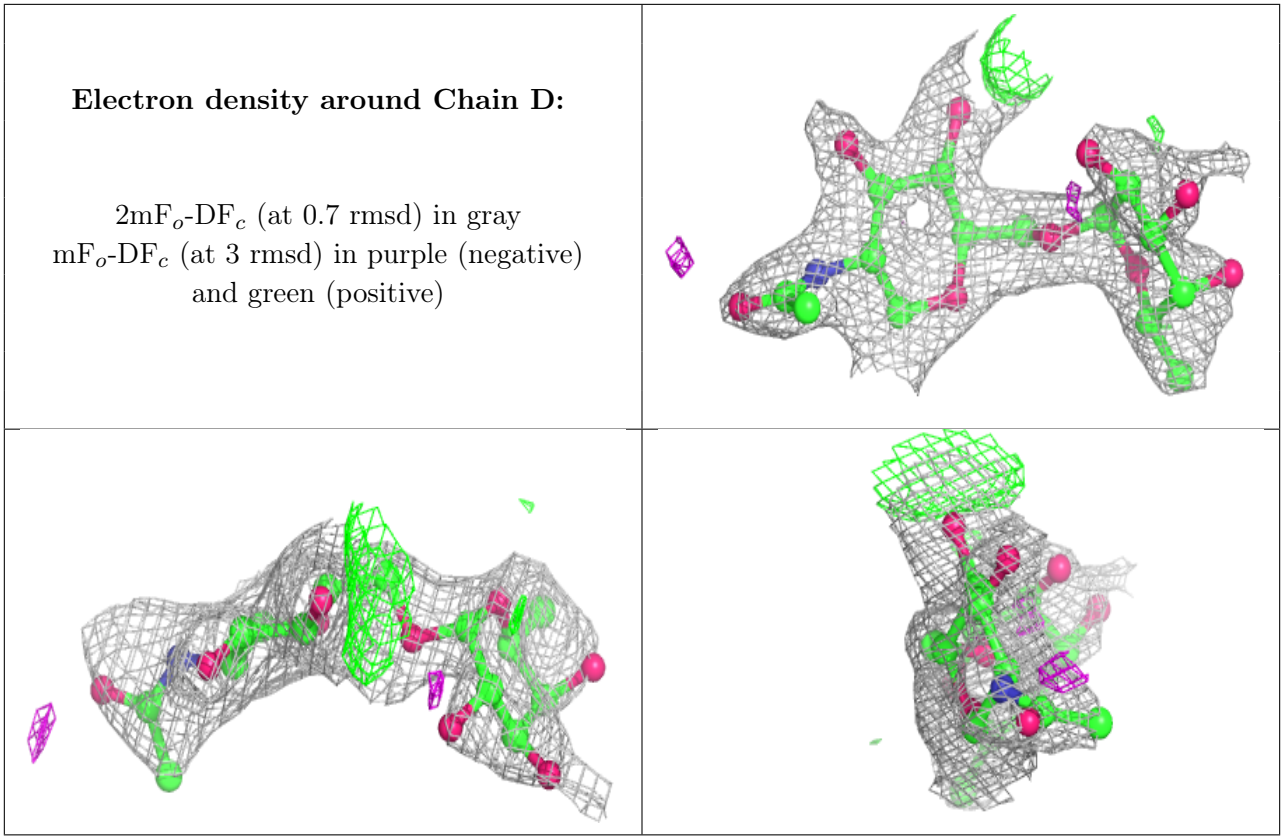
Electron density around Chain E:

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



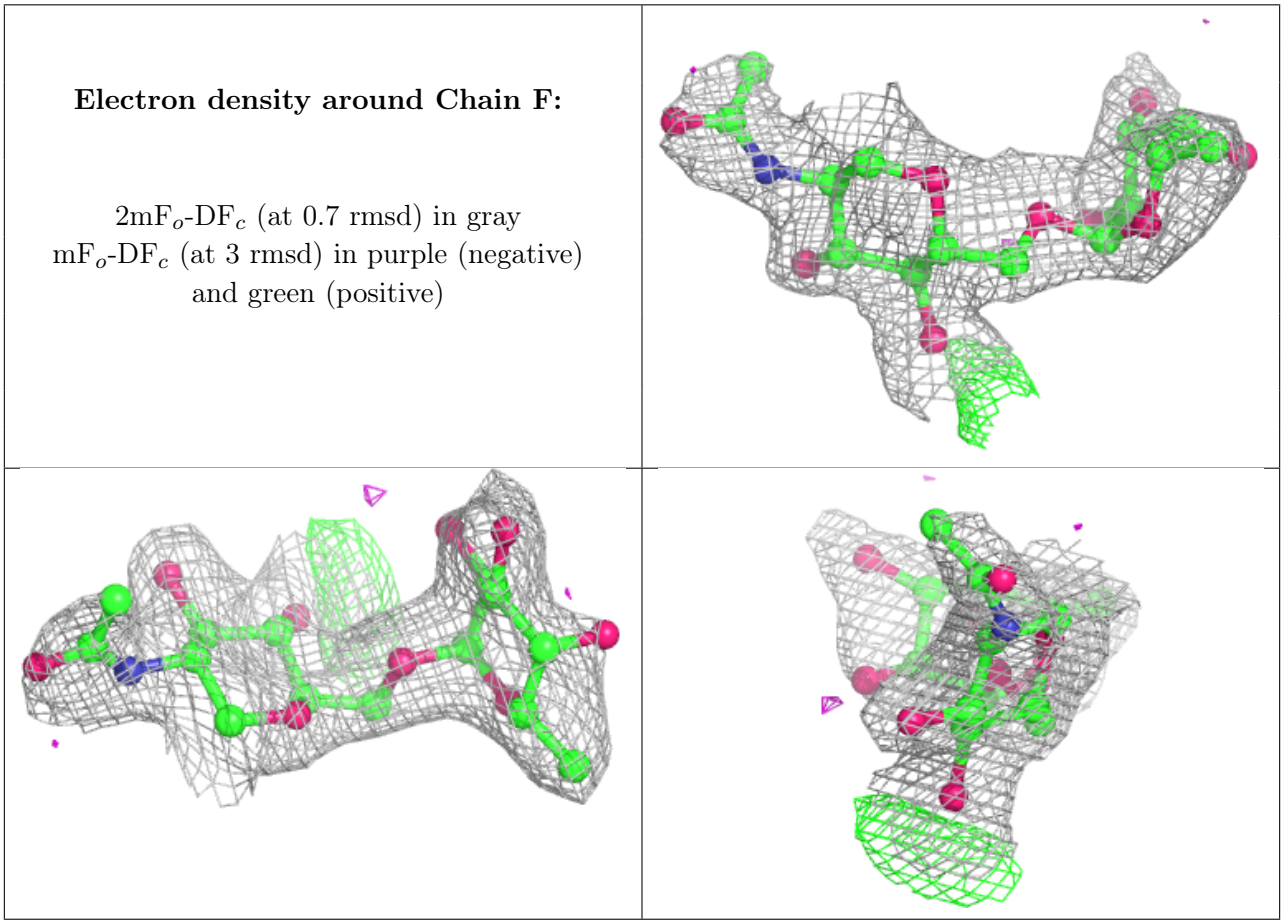
Electron density around Chain D:

$2mF_o$-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 F:

$2mF_o$-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)

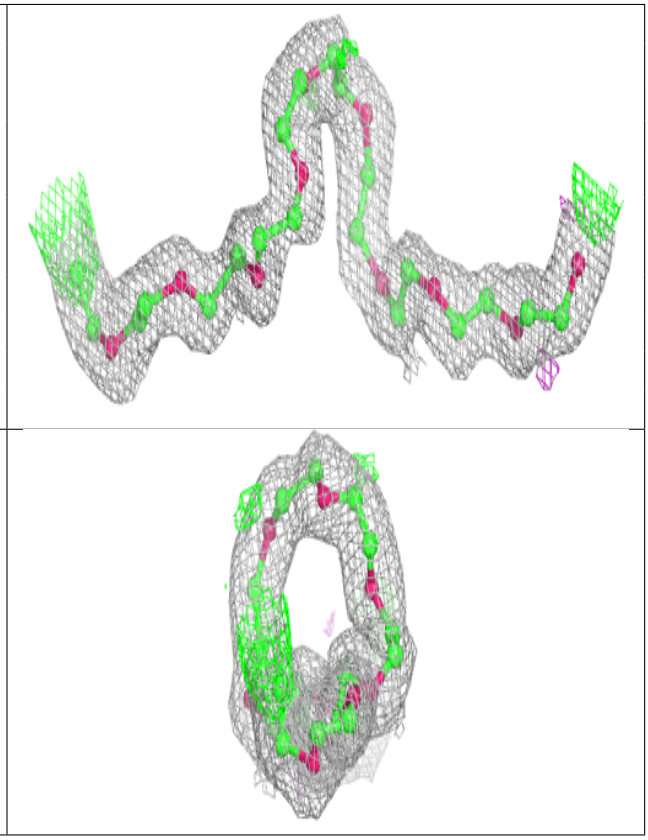
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	XPE	A	1003	30/31	0.94	0.10	20,24,27,29	0
5	MES	B	1002	12/12	0.98	0.09	23,24,25,25	0
5	MES	A	1002	12/12	0.98	0.09	20,22,25,27	0
4	JJV	B	1001	32/32	0.99	0.08	13,15,16,18	0
4	JJV	A	1001	32/32	0.99	0.07	14,15,16,18	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.

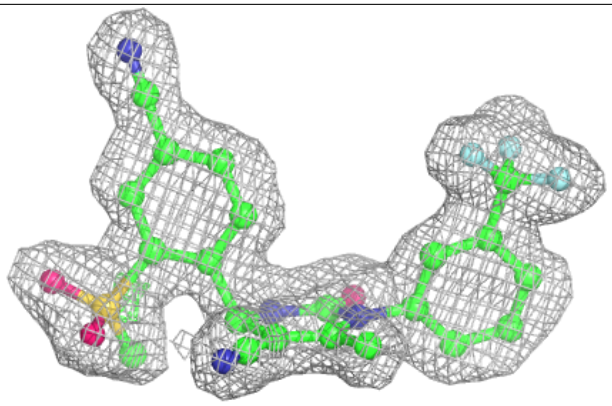
Electron density around XPE A 1003:

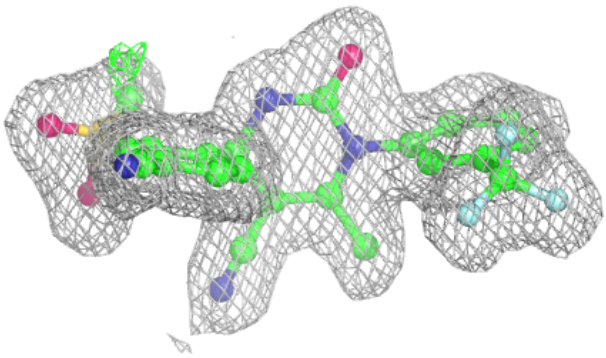
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

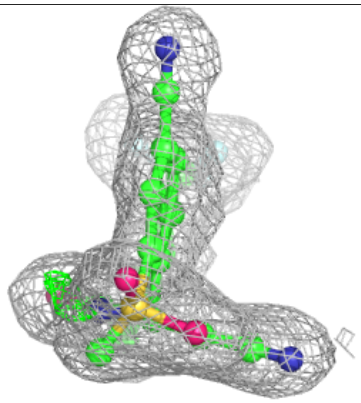


Electron density around JJV B 1001:

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

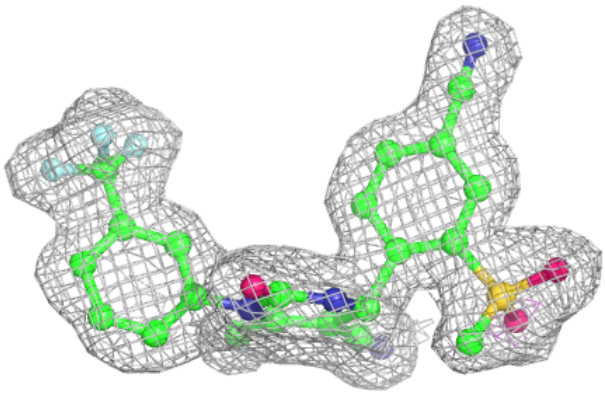


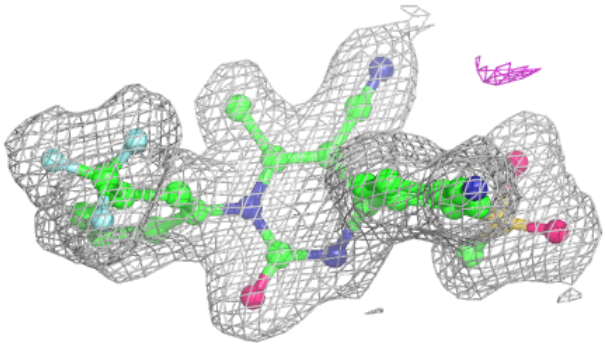


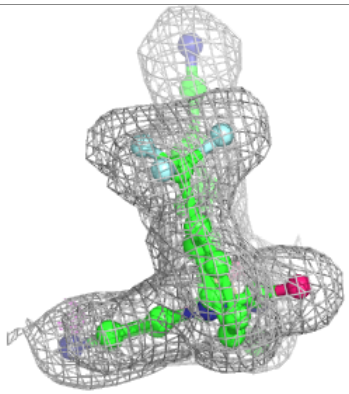


Electron density around JJV A 1001:

$2mF_o$-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.