Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2022 – 04:52 pm BST

PDB ID	:	7NSK
Title	:	Endoplasmic reticulum aminopeptidase 2 complexed with a hydroxamic ligand
Authors	:	Mpakali, A.; Giastas, P.; Stratikos, E.
Deposited on	:	2021-03-08
Resolution	:	3.10 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 following versions of software and data (see references (i)) were used in the production of this report:

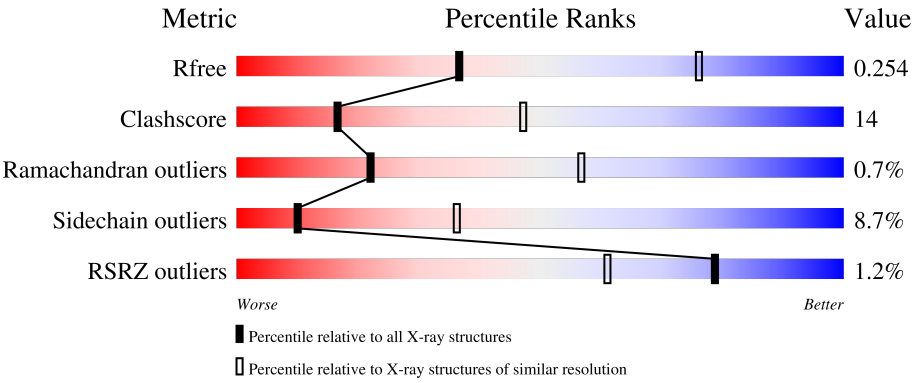
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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.



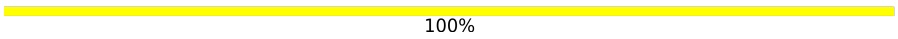
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	963	60% 31% • 5%
1	B	963	2% 55% 31% • 9%
2	C	5	40% 20% 40%
2	H	5	80% 20%
3	D	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	I	2	
3	J	2	
3	K	2	
3	L	2	
4	E	3	
4	F	3	
4	G	3	

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 15016 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

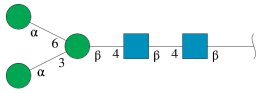
- Molecule 1 is a protein called Endoplasmic reticulum aminopeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	912	Total	C	N	O	S	0	3	0
			7383	4749	1226	1375	33			
1	B	877	Total	C	N	O	S	0	0	0
			6995	4514	1157	1296	28			

There are 8 discrepancies between the modelled and reference sequences:

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

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



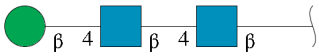
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	H	5	Total	C	N	O	0	0	0
			61	34	2	25			

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

cetamido-2-deoxy-beta-D-glucopyranose.

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

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

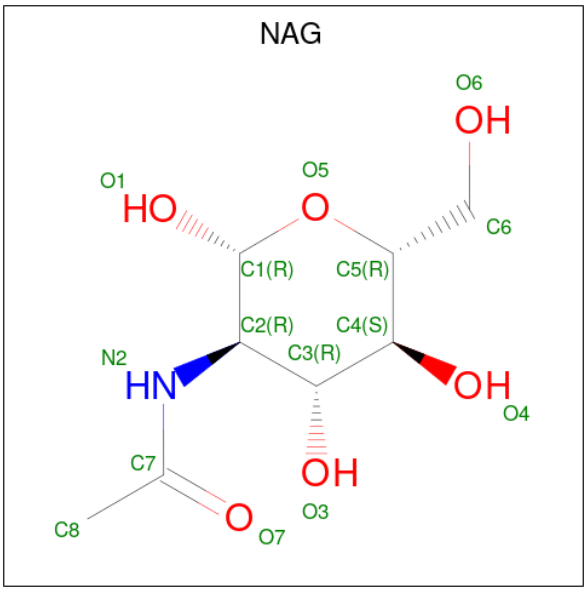


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	E	3	Total C N O 39 22 2 15	0	0	0
4	F	3	Total C N O 39 22 2 15	0	0	0
4	G	3	Total C N O 39 22 2 15	0	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

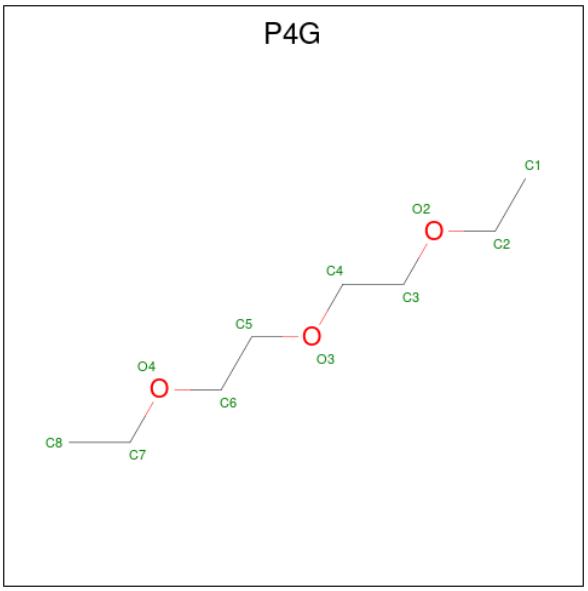
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Zn 1 1	0	0
5	B	1	Total Zn 1 1	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



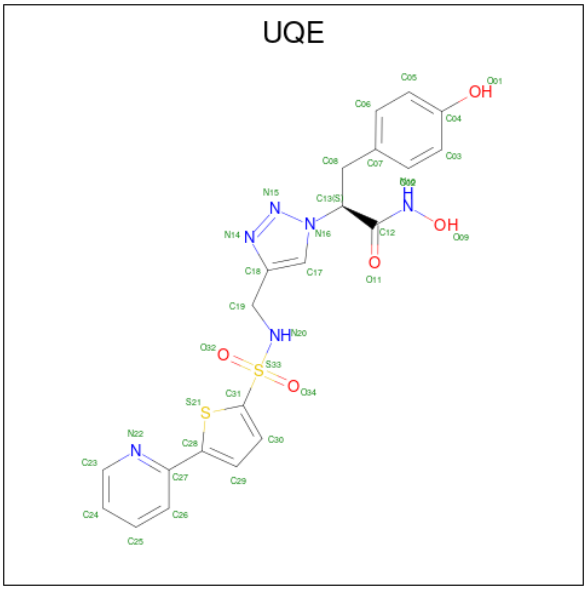
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	B	1	Total C N O 14 8 1 5	0	0
6	B	1	Total C N O 14 8 1 5	0	0

- Molecule 7 is 1-ETHOXY-2-(2-ETHOXYETHOXY)ETHANE (three-letter code: P4G) (formula: $C_8H_{18}O_3$).



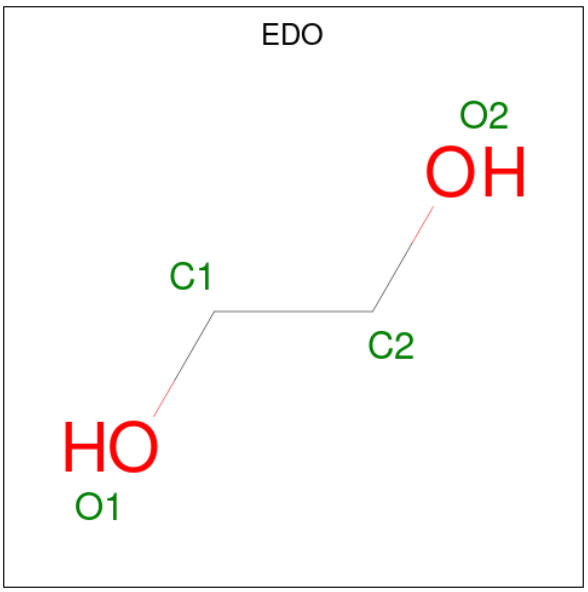
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 11 8 3	0	0

- Molecule 8 is (2 {S})-3-(4-hydroxyphenyl)- {N}-oxidanyl-2-[4-[[(5-pyridin-2-ylthiophen-2-yl)sulfonylamino]methyl]-1,2,3-triazol-1-yl]propanamide (three-letter code: UQE) (formula: $C_{21}H_{20}N_6O_5S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O S 68 42 12 10 4	0	1
8	B	1	Total C N O S 34 21 6 5 2	0	0

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



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

- Molecule 10 is water.

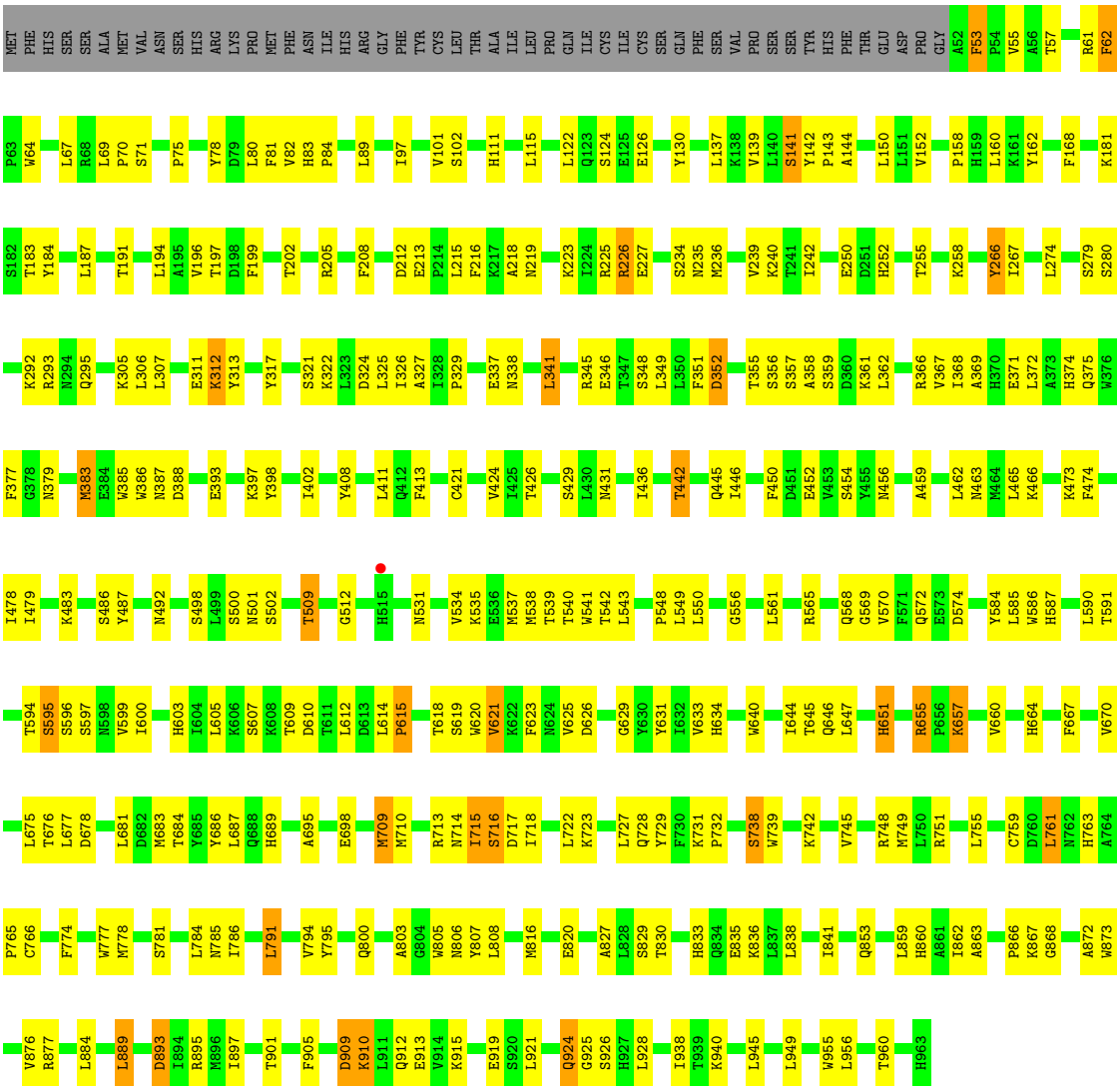
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	29	Total O 29 29	0	0
10	B	11	Total O 11 11	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

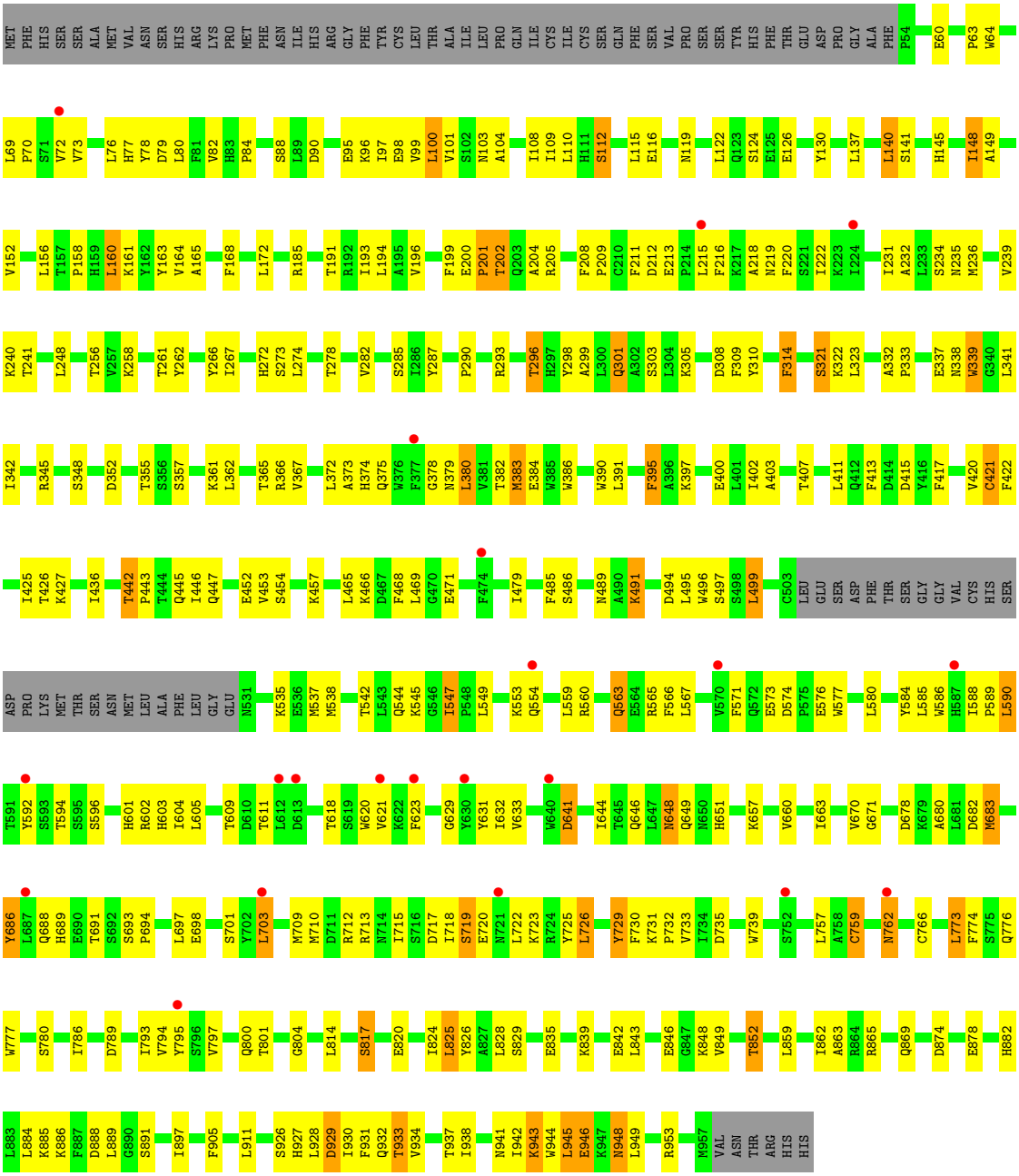
• Molecule 1: Endoplasmic reticulum aminopeptidase 2

Chain A:

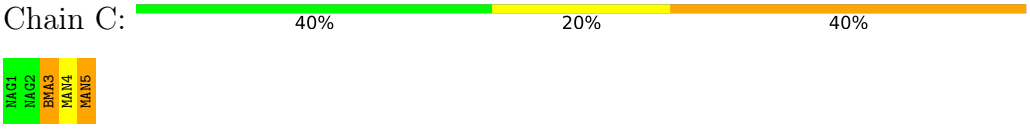


• Molecule 1: Endoplasmic reticulum aminopeptidase 2

Chain B:

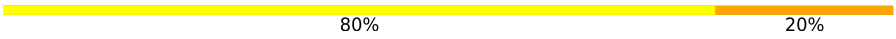


• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



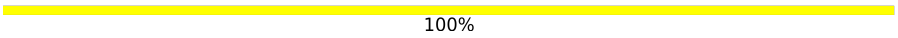
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



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

Chain D:



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

Chain I:

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

Chain J:

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

Chain K:

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

Chain L:

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

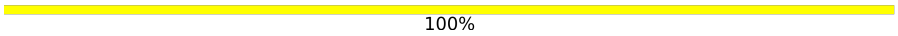
Chain E:

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

Chain F:

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

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.56Å 134.57Å 128.64Å 90.00° 90.20° 90.00°	Depositor
Resolution (Å)	75.56 – 3.10 75.56 – 3.10	Depositor EDS
% Data completeness (in resolution range)	88.7 (75.56-3.10) 88.7 (75.56-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.187 , 0.254 0.187 , 0.254	Depositor DCC
R_{free} test set	2102 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	79.5	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.024 for -h,-l,-k 0.008 for -h,l,k 0.035 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	15016	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P4G, BMA, UQE, NAG, EDO, ZN, MAN

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	0.52	0/7578	0.66	4/10283 (0.0%)
1	B	0.44	0/7172	0.62	3/9748 (0.0%)
All	All	0.48	0/14750	0.64	7/20031 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	421	CYS	CA-CB-SG	-6.91	101.56	114.00
1	A	543	LEU	CA-CB-CG	-6.07	101.34	115.30
1	B	580	LEU	CA-CB-CG	5.85	128.76	115.30
1	B	100	LEU	CA-CB-CG	5.80	128.64	115.30
1	A	859	LEU	CB-CG-CD2	-5.47	101.70	111.00
1	A	859	LEU	CA-CB-CG	-5.23	103.27	115.30
1	A	341	LEU	CA-CB-CG	-5.02	103.75	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7383	0	7235	206	0
1	B	6995	0	6791	210	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	61	0	52	5	0
2	H	61	0	52	1	0
3	D	28	0	25	0	0
3	I	28	0	25	0	0
3	J	28	0	25	1	0
3	K	28	0	25	1	0
3	L	28	0	25	0	0
4	E	39	0	34	0	0
4	F	39	0	34	0	0
4	G	39	0	34	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	56	0	52	0	0
6	B	28	0	26	0	0
7	A	11	0	18	0	0
8	A	68	0	0	1	0
8	B	34	0	0	0	0
9	A	20	0	30	2	0
10	A	29	0	0	0	0
10	B	11	0	0	0	0
All	All	15016	0	14483	417	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 14.

All (417) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:THR:HG22	1:B:445:GLN:H	1.40	0.86
1:A:348:SER:HB3	1:A:367:VAL:HG21	1.59	0.82
1:B:239:VAL:HG23	1:B:240:LYS:H	1.43	0.81
1:A:436:ILE:HD12	1:A:436:ILE:H	1.50	0.77
1:A:540:THR:HG21	1:A:586:TRP:HA	1.68	0.75
1:A:905:PHE:HB2	1:A:938:ILE:HD13	1.69	0.74
1:B:911:LEU:HD12	1:B:938:ILE:HG23	1.68	0.74
1:B:549:LEU:HB2	1:B:566:PHE:HD2	1.52	0.74
1:B:623:PHE:HB2	1:B:633:VAL:HG21	1.70	0.74
1:A:205:ARG:HH21	1:A:212:ASP:HB3	1.53	0.73
1:A:355:THR:HG21	1:A:820:GLU:HB2	1.69	0.73
1:B:72:VAL:HG13	1:B:103:ASN:HB2	1.71	0.72
1:B:829:SER:HB2	1:B:862:ILE:HG22	1.70	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:620:TRP:HE1	1:B:646:GLN:HG3	1.56	0.71
1:B:682:ASP:O	1:B:683:MET:HB2	1.88	0.71
1:A:827:ALA:O	1:A:830:THR:HG22	1.91	0.71
1:B:152:VAL:HG21	1:B:156:LEU:HD11	1.72	0.70
1:B:565:ARG:HD2	1:B:584:TYR:HD1	1.55	0.70
1:A:429:SER:HB3	1:A:568:GLN:HB2	1.75	0.69
1:B:852:THR:HG21	1:B:886:LYS:HE2	1.74	0.69
1:B:378:GLY:O	1:B:382:THR:HB	1.94	0.68
1:A:122:LEU:HD11	1:A:162:TYR:HB3	1.76	0.68
1:B:938:ILE:HA	1:B:941:ASN:HB2	1.76	0.68
1:A:295:GLN:HG2	1:A:352:ASP:HB2	1.75	0.68
1:B:594:THR:HA	1:B:621:VAL:HG22	1.74	0.68
1:B:76:LEU:HD11	1:B:100:LEU:HG	1.76	0.68
1:B:882:HIS:HA	1:B:885:LYS:HE2	1.74	0.68
1:B:417:PHE:O	1:B:420:VAL:HG12	1.93	0.67
1:B:122:LEU:HB2	1:B:137:LEU:HD11	1.76	0.67
1:A:137:LEU:HD23	1:A:150:LEU:HB3	1.77	0.67
1:A:479:ILE:HG22	1:A:483:LYS:HD2	1.77	0.66
1:A:126:GLU:HB3	1:A:160:LEU:HD22	1.77	0.66
1:A:763:HIS:CD2	1:A:765:PRO:HD2	2.31	0.66
1:B:497:SER:HA	1:B:535:LYS:HE3	1.76	0.66
1:A:226:ARG:HG3	1:A:227:GLU:O	1.95	0.65
1:B:348:SER:HB3	1:B:367:VAL:HG11	1.78	0.65
1:A:873:TRP:CZ2	1:A:877:ARG:HD3	2.31	0.65
1:B:342:ILE:HD11	1:B:375:GLN:HE22	1.60	0.65
1:B:703:LEU:HD13	1:B:726:LEU:HD23	1.79	0.64
1:A:800:GLN:NE2	1:A:830:THR:HG23	2.13	0.64
1:B:298:TYR:OH	1:B:365:THR:HB	1.98	0.63
1:B:236:MET:SD	1:B:256:THR:HA	2.38	0.63
1:A:945:LEU:HD22	1:A:949:LEU:HD12	1.79	0.63
1:A:53:PHE:HZ	1:A:61:ARG:HE	1.45	0.63
1:A:605:LEU:HD22	1:A:607:SER:H	1.64	0.62
1:B:160:LEU:HG	1:B:161:LYS:HD2	1.81	0.62
1:A:777:TRP:HB2	1:A:786:ILE:HD11	1.82	0.62
1:B:73:VAL:HG12	1:B:99:VAL:HG21	1.80	0.61
1:B:442:THR:HG22	1:B:445:GLN:HG2	1.82	0.61
1:B:299:ALA:O	1:B:303:SER:OG	2.08	0.61
1:B:101:VAL:HG23	1:B:158:PRO:HA	1.83	0.61
1:B:342:ILE:HD11	1:B:375:GLN:NE2	2.16	0.61
1:A:398:TYR:CE2	1:A:402:ILE:HD11	2.36	0.61
1:B:239:VAL:HG23	1:B:240:LYS:N	2.15	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:VAL:HG12	1:A:240:LYS:HB2	1.84	0.60
1:A:841:ILE:HD11	1:A:862:ILE:HD12	1.83	0.60
1:A:634:HIS:CD2	1:A:640:TRP:HE1	2.20	0.60
1:B:200:GLU:HG3	1:B:262:TYR:CD1	2.36	0.60
1:B:697:LEU:O	1:B:701:SER:N	2.32	0.60
1:B:795:TYR:CD2	1:B:824:ILE:HG12	2.37	0.60
1:A:337:GLU:HB3	1:A:371:GLU:OE2	2.02	0.59
1:B:549:LEU:HB2	1:B:566:PHE:CD2	2.36	0.59
1:A:184:TYR:HB3	1:A:329:PRO:HG2	1.83	0.59
1:A:640:TRP:CD1	1:A:675:LEU:HD11	2.38	0.59
1:B:720:GLU:HA	1:B:723:LYS:HE2	1.83	0.59
1:A:436:ILE:HD13	1:A:542:THR:HA	1.85	0.59
1:B:839:LYS:HA	1:B:842:GLU:HG2	1.84	0.59
1:A:75:PRO:HD2	1:A:216:PHE:HD1	1.68	0.58
1:B:332:ALA:O	1:B:345:ARG:NH1	2.36	0.58
1:A:431:ASN:HA	1:A:565:ARG:HH22	1.68	0.58
1:A:833:HIS:ND1	1:A:836:LYS:HE2	2.19	0.58
1:A:386:TRP:CD1	1:A:446:ILE:HD13	2.39	0.58
1:B:592:TYR:CZ	1:B:601:HIS:HB2	2.39	0.57
1:B:69:LEU:HD22	1:B:109:ILE:HG22	1.86	0.57
1:A:791:LEU:HD11	1:A:795:TYR:CZ	2.40	0.57
1:B:930:ILE:HA	1:B:933:THR:CG2	2.34	0.57
1:A:292:LYS:NZ	1:A:346:GLU:OE1	2.38	0.57
1:B:926:SER:O	1:B:931:PHE:HE2	1.88	0.57
1:A:312:LYS:HG3	1:A:313:TYR:N	2.20	0.57
1:A:759:CYS:SG	1:A:766[B]:CYS:HB3	2.45	0.56
1:A:800:GLN:HE22	1:A:830:THR:HG23	1.69	0.56
1:A:345:ARG:HD3	1:A:853:GLN:NE2	2.21	0.56
1:B:565:ARG:HD2	1:B:584:TYR:CD1	2.40	0.56
1:A:223:LYS:HD2	1:A:252:HIS:CE1	2.40	0.56
1:A:538:MET:O	1:A:542:THR:HG23	2.06	0.56
1:A:398:TYR:CE1	1:A:463:ASN:HB2	2.41	0.56
1:A:739:TRP:CE2	1:A:755:LEU:HD13	2.41	0.56
1:B:220:PHE:HZ	1:B:261:THR:HG22	1.71	0.56
1:B:465:LEU:HG	1:B:469:LEU:HD13	1.88	0.56
1:A:565:ARG:HD2	1:A:584:TYR:CD2	2.41	0.55
1:B:215:LEU:HD13	1:B:384:GLU:HG3	1.88	0.55
1:A:234:SER:O	1:A:322:LYS:NZ	2.40	0.55
1:A:431:ASN:HA	1:A:565:ARG:NH2	2.21	0.55
1:A:568:GLN:HG2	1:A:940:LYS:NZ	2.21	0.55
1:B:213:GLU:HB2	1:B:216:PHE:HD1	1.72	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:ARG:HD2	1:A:413:PHE:CE1	2.41	0.55
1:B:77:HIS:HD1	1:B:219:ASN:HB2	1.71	0.55
1:A:713:ARG:HB2	1:A:715:ILE:HG13	1.89	0.55
1:B:202:THR:O	1:B:202:THR:OG1	2.18	0.55
1:B:397:LYS:HA	1:B:400:GLU:HG3	1.88	0.55
1:B:403:ALA:O	1:B:407:THR:OG1	2.20	0.55
1:B:352:ASP:HB3	1:B:355:THR:HG22	1.89	0.55
1:B:366:ARG:HD2	1:B:413:PHE:CE1	2.42	0.54
1:B:443:PRO:O	1:B:447:GLN:HG3	2.07	0.54
1:B:79:ASP:HB2	1:B:96:LYS:HG2	1.89	0.54
1:A:62:PHE:CD1	1:A:142:TYR:HB2	2.41	0.54
1:A:111:HIS:HD2	1:A:212:ASP:H	1.55	0.54
1:A:677:LEU:HG	1:A:681:LEU:HD13	1.90	0.54
1:B:537:MET:HE1	1:B:589:PRO:HB3	1.90	0.54
1:A:124:SER:N	1:A:130:TYR:O	2.41	0.54
1:A:450:PHE:O	1:A:895:ARG:NH2	2.40	0.53
1:B:590:LEU:HD11	1:B:605:LEU:HB2	1.90	0.53
1:B:620:TRP:NE1	1:B:646:GLN:HG3	2.22	0.53
1:B:846:GLU:HG3	1:B:848:LYS:H	1.74	0.53
1:B:774:PHE:HB2	1:B:794:VAL:HG12	1.91	0.53
1:A:681:LEU:HB3	1:A:955:TRP:CE2	2.44	0.53
1:B:759:CYS:HB3	1:B:766:CYS:SG	2.49	0.52
1:A:387:ASN:OD1	1:A:387:ASN:N	2.42	0.52
1:A:383:MET:O	1:A:383:MET:HG2	2.08	0.52
1:A:362:LEU:O	1:A:366:ARG:HG3	2.10	0.52
1:A:647:LEU:O	1:A:651:HIS:HB3	2.08	0.52
1:A:956:LEU:O	1:A:960:THR:HG23	2.10	0.52
1:A:540:THR:CG2	1:A:586:TRP:HA	2.39	0.52
1:B:641:ASP:HA	1:B:644:ILE:HD12	1.92	0.52
1:B:78:TYR:CD2	1:B:97:ILE:HG12	2.45	0.52
1:B:660:VAL:O	1:B:663:ILE:HG22	2.10	0.52
1:A:486:SER:HB3	1:A:487:TYR:CD1	2.44	0.52
1:B:874:ASP:O	1:B:878:GLU:HB2	2.10	0.52
1:A:676:THR:OG1	1:A:678:ASP:OD1	2.16	0.52
1:B:731:LYS:HE2	1:B:735:ASP:OD2	2.10	0.52
1:A:374:HIS:HA	1:A:377:PHE:O	2.10	0.51
1:B:361:LYS:O	1:B:365:THR:HG22	2.10	0.51
1:B:930:ILE:O	1:B:934:VAL:HG12	2.09	0.51
1:B:678:ASP:OD1	1:B:678:ASP:N	2.43	0.51
1:A:234:SER:OG	1:A:235:ASN:N	2.43	0.51
1:A:345:ARG:HD3	1:A:853:GLN:HE22	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:688:GLN:HB2	1:B:729:TYR:HE2	1.74	0.51
1:A:591:THR:HB	1:A:625:VAL:HG12	1.93	0.51
1:B:273:SER:HB3	1:B:287:TYR:CD2	2.46	0.51
1:A:82:VAL:HG12	1:A:84:PRO:HD3	1.93	0.51
1:A:393:GLU:OE1	8:A:1007[A]:UQE:O09	2.28	0.51
1:B:442:THR:HG22	1:B:445:GLN:N	2.20	0.51
1:B:563:GLN:HE22	1:B:585:LEU:HB2	1.76	0.51
1:B:590:LEU:HD12	1:B:603:HIS:O	2.11	0.51
1:B:862:ILE:HG13	1:B:863:ALA:N	2.25	0.50
1:B:442:THR:CG2	1:B:445:GLN:HG2	2.41	0.50
1:B:383:MET:SD	1:B:383:MET:N	2.84	0.50
1:A:436:ILE:H	1:A:436:ILE:CD1	2.22	0.50
1:A:731:LYS:N	1:A:732:PRO:HD2	2.26	0.50
1:A:311:GLU:HG2	1:A:317:TYR:HA	1.93	0.50
1:A:714:ASN:O	1:A:716:SER:N	2.44	0.50
1:A:778:MET:HG3	1:A:807:TYR:CE2	2.46	0.50
1:A:833:HIS:HB2	1:A:836:LYS:HG3	1.94	0.50
1:A:436:ILE:HD12	1:A:436:ILE:N	2.25	0.49
1:B:82:VAL:HG12	1:B:84:PRO:HD3	1.93	0.49
1:B:293:ARG:HH12	2:C:3:BMA:H61	1.76	0.49
1:B:468:PHE:CD1	1:B:469:LEU:HD12	2.47	0.49
1:B:795:TYR:HD2	1:B:824:ILE:HG12	1.75	0.49
3:J:2:NAG:H83	3:J:2:NAG:H3	1.94	0.49
1:A:421:CYS:O	1:A:424:VAL:HG12	2.13	0.49
1:A:565:ARG:HD2	1:A:584:TYR:CE2	2.47	0.49
1:A:274:LEU:HD21	1:A:293:ARG:HD3	1.92	0.49
1:A:280:SER:HB2	1:A:311:GLU:OE1	2.11	0.49
1:B:199:PHE:CD1	1:B:204:ALA:HA	2.47	0.49
1:B:338:ASN:HB2	1:B:341:LEU:O	2.11	0.49
1:B:95:GLU:OE1	1:B:209:PRO:HD2	2.11	0.49
1:A:168:PHE:CE2	1:A:208:PHE:HA	2.47	0.49
1:B:234:SER:OG	1:B:235:ASN:N	2.43	0.49
1:B:859:LEU:HD13	1:B:897:ILE:HG23	1.93	0.49
1:A:681:LEU:HD23	1:A:955:TRP:CE3	2.48	0.49
1:B:96:LYS:HA	1:B:165:ALA:HA	1.93	0.49
1:A:89:LEU:HD22	1:A:181:LYS:HE2	1.95	0.49
1:A:362:LEU:HD12	1:A:411:LEU:HD13	1.95	0.49
1:A:774:PHE:HB2	1:A:794:VAL:HG13	1.95	0.49
1:A:742:LYS:O	1:A:751:ARG:NH2	2.36	0.48
1:B:678:ASP:HB3	1:B:949:LEU:HD12	1.94	0.48
1:B:843:LEU:O	1:B:846:GLU:HG2	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:888:ASP:O	1:B:891:SER:HB3	2.13	0.48
1:A:351:PHE:HE2	1:A:361:LYS:HB2	1.78	0.48
1:A:872:ALA:O	1:A:876:VAL:HG23	2.14	0.48
1:B:273:SER:H	2:C:5:MAN:H62	1.78	0.48
1:B:889:LEU:HG	1:B:928:LEU:HD21	1.95	0.48
1:A:62:PHE:CE1	1:A:142:TYR:HB2	2.48	0.48
1:A:196:VAL:HG23	1:A:267:ILE:HG12	1.95	0.48
1:B:603:HIS:CD2	1:B:604:ILE:H	2.30	0.48
1:B:905:PHE:O	1:B:938:ILE:HG13	2.14	0.48
1:A:218:ALA:O	1:A:258:LYS:HA	2.12	0.48
1:A:910:LYS:HA	1:A:913:GLU:HG3	1.94	0.48
1:B:88:SER:HB2	1:B:90:ASP:OD1	2.13	0.48
1:B:731:LYS:N	1:B:732:PRO:HD2	2.29	0.48
1:A:623:PHE:HB2	1:A:633:VAL:HG21	1.96	0.48
1:B:793:ILE:HG13	1:B:794:VAL:N	2.28	0.48
1:A:388:ASP:OD1	1:A:492:ASN:HB2	2.14	0.48
1:B:560:ARG:HA	1:B:611:THR:HG22	1.94	0.48
1:A:398:TYR:OH	1:A:466:LYS:HD3	2.14	0.48
1:A:597:SER:HB3	1:A:599:VAL:HG22	1.96	0.48
1:B:365:THR:HG21	1:B:411:LEU:CD1	2.44	0.48
1:B:386:TRP:CD1	1:B:446:ILE:HD13	2.49	0.48
1:B:453:VAL:O	1:B:457:LYS:HB3	2.13	0.48
2:C:3:BMA:H62	2:C:5:MAN:H2	1.35	0.48
1:A:509:THR:O	1:A:512:GLY:N	2.47	0.47
1:A:596:SER:H	1:A:618:THR:HG21	1.79	0.47
1:A:242:ILE:CG1	1:A:250:GLU:HB3	2.44	0.47
1:A:644:ILE:HG12	1:A:683:MET:HE2	1.94	0.47
1:B:201:PRO:HG2	1:B:202:THR:HG22	1.95	0.47
1:A:83:HIS:ND1	1:A:225:ARG:HD2	2.29	0.47
1:B:301:GLN:O	1:B:305:LYS:HG3	2.13	0.47
1:B:839:LYS:O	1:B:843:LEU:HB2	2.14	0.47
1:A:327:ALA:HB2	1:A:349:LEU:HD23	1.96	0.47
1:A:873:TRP:O	1:A:877:ARG:HG3	2.15	0.47
1:B:468:PHE:O	1:B:602:ARG:NH1	2.48	0.47
1:A:80:LEU:HD11	1:A:208:PHE:CD1	2.49	0.47
1:B:64:TRP:CE3	1:B:70:PRO:HG3	2.50	0.47
1:A:69:LEU:HD23	1:A:69:LEU:HA	1.72	0.47
1:A:306:LEU:HD13	1:A:369:ALA:HA	1.97	0.47
1:A:501:ASN:HA	1:A:531:ASN:ND2	2.30	0.47
1:B:395:PHE:HE1	1:B:495:LEU:HD21	1.80	0.47
1:B:576:GLU:OE1	1:B:576:GLU:N	2.38	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:PHE:CE2	1:B:632:ILE:HD12	2.50	0.47
1:A:305:LYS:HE2	1:A:408:TYR:OH	2.15	0.47
1:B:686:TYR:O	1:B:689:HIS:N	2.47	0.47
1:A:709:MET:HE2	1:A:709:MET:HB2	1.83	0.47
1:B:126:GLU:HB2	1:B:160:LEU:HD23	1.97	0.46
1:B:549:LEU:HD12	1:B:632:ILE:O	2.15	0.46
1:B:826:TYR:OH	1:B:865:ARG:NH2	2.48	0.46
1:A:442:THR:O	1:A:446:ILE:HG13	2.16	0.46
1:A:456:ASN:OD1	1:A:456:ASN:N	2.48	0.46
1:B:215:LEU:HD12	1:B:489:ASN:ND2	2.30	0.46
1:B:670:VAL:HG21	1:B:680:ALA:HB2	1.97	0.46
1:A:548:PRO:HB3	1:A:586:TRP:CE3	2.50	0.46
1:A:678:ASP:OD1	1:A:678:ASP:N	2.49	0.46
1:B:274:LEU:HD13	1:B:296:THR:HB	1.97	0.46
1:B:820:GLU:O	1:B:824:ILE:HG13	2.14	0.46
1:A:80:LEU:HD23	1:A:81:PHE:N	2.30	0.46
1:A:600:ILE:HD12	1:A:625:VAL:HG11	1.98	0.46
1:B:116:GLU:O	1:B:168:PHE:HA	2.16	0.46
1:B:239:VAL:CG2	1:B:240:LYS:H	2.20	0.46
1:B:719:SER:O	1:B:723:LYS:HG3	2.15	0.46
1:A:745:VAL:O	1:A:749:MET:HG3	2.15	0.46
1:A:808:LEU:HD23	1:A:808:LEU:HA	1.66	0.46
1:B:273:SER:H	2:C:5:MAN:C6	2.29	0.46
1:B:73:VAL:HG11	1:B:108:ILE:HG23	1.97	0.46
1:B:648:ASN:N	1:B:648:ASN:OD1	2.48	0.46
1:B:703:LEU:HD23	1:B:703:LEU:HA	1.77	0.46
1:A:102:SER:O	1:A:158:PRO:HB3	2.16	0.46
1:A:349:LEU:HD12	1:A:368:ILE:HD11	1.97	0.46
1:A:738:SER:O	1:A:751:ARG:HD3	2.15	0.46
1:A:915:LYS:HE2	1:A:919:GLU:OE2	2.14	0.46
1:B:495:LEU:O	1:B:499:LEU:HB2	2.16	0.46
1:A:358:ALA:HB2	1:A:748:ARG:CZ	2.46	0.46
1:B:69:LEU:HD13	1:B:211:PHE:HD1	1.81	0.45
1:A:537:MET:HG3	1:A:587:HIS:HB2	1.98	0.45
1:B:355:THR:HG21	1:B:817:SER:CB	2.46	0.45
1:A:213:GLU:HB2	1:A:216:PHE:HD2	1.81	0.45
1:B:485:PHE:CE2	1:B:494:ASP:HB3	2.52	0.45
1:A:778:MET:HG3	1:A:807:TYR:CD2	2.52	0.45
1:A:684:THR:HB	1:A:687:LEU:HD12	1.98	0.45
1:A:717:ASP:OD1	1:A:717:ASP:N	2.50	0.45
1:B:77:HIS:HB3	1:B:98:GLU:HB3	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ARG:HH22	1:B:814:LEU:HG	1.81	0.45
1:B:337:GLU:HG3	1:B:374:HIS:HB3	1.97	0.45
1:B:948:ASN:O	1:B:949:LEU:HD23	2.17	0.45
1:A:727:LEU:HD22	1:A:763:HIS:ND1	2.31	0.45
1:B:333:PRO:O	1:B:345:ARG:HD2	2.17	0.45
1:B:693:SER:O	1:B:697:LEU:HD12	2.16	0.45
1:B:825:LEU:HA	1:B:828:LEU:HD12	1.98	0.45
1:B:272:HIS:HD2	1:B:290:PRO:HB3	1.82	0.45
1:B:927:HIS:O	1:B:928:LEU:HD23	2.16	0.45
1:B:314:PHE:HA	1:B:479:ILE:HG12	1.99	0.45
1:B:390:TRP:CE2	1:B:391:LEU:HD12	2.52	0.45
1:B:421:CYS:O	1:B:425:ILE:HG13	2.16	0.45
1:A:620:TRP:HE1	1:A:646:GLN:HE21	1.65	0.45
1:A:664:HIS:HB2	1:A:698:GLU:OE2	2.16	0.45
1:B:545:LYS:NZ	3:K:1:NAG:H62	2.32	0.45
1:B:436:ILE:HG22	1:B:542:THR:HA	1.99	0.44
1:B:496:TRP:CZ3	1:B:538:MET:HG3	2.52	0.44
1:B:773:LEU:HD22	1:B:786:ILE:HG12	2.00	0.44
1:B:929:ASP:O	1:B:933:THR:HG22	2.17	0.44
1:A:595:SER:HB3	1:A:620:TRP:H	1.82	0.44
1:A:626:ASP:HA	1:A:657:LYS:HB2	2.00	0.44
1:A:909:ASP:OD1	1:A:909:ASP:N	2.51	0.44
1:A:569:GLY:O	1:A:570:VAL:HG23	2.18	0.44
1:A:723:LYS:HG3	1:A:761:LEU:HG	2.00	0.44
1:B:205:ARG:HH21	1:B:212:ASP:HB3	1.82	0.44
1:B:725:TYR:O	1:B:729:TYR:HB2	2.17	0.44
1:B:801:THR:HG23	1:B:804:GLY:H	1.83	0.44
1:A:728:GLN:HG2	1:A:729:TYR:N	2.33	0.44
1:A:141:SER:O	1:A:143:PRO:HD3	2.17	0.44
1:A:205:ARG:NH2	1:A:212:ASP:HB3	2.28	0.44
1:A:462:LEU:O	1:A:465:LEU:N	2.51	0.44
1:A:629:GLY:HA3	1:A:631:TYR:CE1	2.53	0.44
1:B:96:LYS:HE2	1:B:163:TYR:HD2	1.83	0.43
1:B:547:ILE:HD11	1:B:631:TYR:HA	2.00	0.43
1:A:142:TYR:CE1	1:A:144:ALA:HB3	2.53	0.43
1:A:385:TRP:CG	1:A:386:TRP:N	2.85	0.43
1:A:600:ILE:HG23	1:A:625:VAL:HG11	2.00	0.43
1:A:675:LEU:HD23	1:A:675:LEU:HA	1.71	0.43
1:B:934:VAL:HA	1:B:937:THR:OG1	2.18	0.43
1:A:805:TRP:CZ2	1:A:836:LYS:HB3	2.53	0.43
1:A:584:TYR:O	1:A:585:LEU:HD13	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:LEU:HA	1:A:615:PRO:HD3	1.90	0.43
1:B:60:GLU:HB2	1:B:140:LEU:HD21	2.00	0.43
1:B:109:ILE:HD13	1:B:149:ALA:HA	2.01	0.43
1:A:267:ILE:HD13	1:A:326:ILE:HD13	2.00	0.43
1:A:473:LYS:HG2	1:A:502:SER:OG	2.19	0.43
1:B:309:PHE:HZ	1:B:402:ILE:HG22	1.83	0.43
1:B:422:PHE:O	1:B:426:THR:HG23	2.18	0.43
1:A:429:SER:CB	1:A:568:GLN:HB2	2.46	0.43
1:A:594:THR:HG22	1:A:621:VAL:HG12	2.00	0.43
1:A:667:PHE:O	1:A:670:VAL:HG22	2.18	0.43
1:B:168:PHE:CE2	1:B:208:PHE:HA	2.53	0.43
1:B:248:LEU:HD22	2:H:1:NAG:H83	2.01	0.43
1:A:64:TRP:CD2	1:A:70:PRO:HG3	2.54	0.43
1:A:538:MET:O	1:A:541:TRP:N	2.52	0.43
1:A:618:THR:OG1	1:A:619:SER:N	2.49	0.43
1:A:629:GLY:HA3	1:A:631:TYR:HE1	1.84	0.43
1:A:893:ASP:O	1:A:897:ILE:HG13	2.19	0.43
1:B:355:THR:OG1	1:B:820:GLU:HB2	2.18	0.43
1:A:411:LEU:HA	1:A:411:LEU:HD23	1.53	0.43
1:B:172:LEU:HD23	1:B:172:LEU:HA	1.71	0.43
1:B:380:LEU:HD23	1:B:486:SER:HA	2.01	0.43
1:A:187:LEU:HD13	1:A:816:MET:HG3	2.00	0.43
1:A:219:ASN:OD1	1:A:258:LYS:HE2	2.19	0.43
1:A:242:ILE:HG12	1:A:250:GLU:HB3	2.00	0.43
1:A:250:GLU:HG2	1:A:252:HIS:NE2	2.34	0.43
1:A:924:GLN:O	1:A:926:SER:N	2.51	0.43
1:B:339:TRP:CD2	1:B:379:ASN:HB3	2.54	0.43
1:B:710:MET:SD	1:B:715:ILE:HD11	2.59	0.43
1:A:345:ARG:NH1	1:A:853:GLN:HB2	2.34	0.42
1:A:655:ARG:H	1:A:655:ARG:HG2	1.57	0.42
1:A:660:VAL:HG12	1:A:695:ALA:HA	2.01	0.42
1:A:710:MET:HG3	1:A:718:ILE:HG22	2.00	0.42
1:B:112:SER:HB3	1:B:148:ILE:HD13	2.01	0.42
1:B:310:TYR:OH	1:B:373:ALA:HB2	2.18	0.42
1:B:323:LEU:HD21	1:B:372:LEU:HD21	2.01	0.42
1:B:544:GLN:NE2	1:B:545:LYS:HE3	2.34	0.42
1:B:660:VAL:HA	1:B:663:ILE:HG22	2.01	0.42
1:A:307:LEU:HD12	1:A:307:LEU:HA	1.85	0.42
1:A:452:GLU:H	1:A:452:GLU:CD	2.21	0.42
1:A:500:SER:HB3	1:A:534:VAL:HG23	2.01	0.42
1:A:860:HIS:HD1	9:A:1009:EDO:H11	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:866:PRO:C	1:A:868:GLY:H	2.22	0.42
1:B:762:ASN:OD1	1:B:762:ASN:N	2.51	0.42
1:A:351:PHE:CD1	1:A:351:PHE:C	2.93	0.42
1:A:352:ASP:OD2	1:A:355:THR:HB	2.19	0.42
1:B:248:LEU:HD23	1:B:248:LEU:HA	1.79	0.42
1:A:325:LEU:N	1:A:325:LEU:HD12	2.34	0.42
1:A:568:GLN:HG2	1:A:940:LYS:HZ3	1.84	0.42
1:B:427:LYS:HE3	1:B:452:GLU:OE1	2.19	0.42
1:B:730:PHE:HB3	1:B:733:VAL:HG12	2.00	0.42
1:B:943:LYS:O	1:B:946:GLU:HB3	2.20	0.42
1:A:372:LEU:O	1:A:375:GLN:HG2	2.19	0.42
1:A:324:ASP:HB2	1:A:341:LEU:HD12	2.02	0.42
1:A:375:GLN:HA	1:A:379:ASN:HD22	1.85	0.42
1:B:231:ILE:HG13	1:B:232:ALA:H	1.84	0.42
1:B:554:GLN:OE1	1:B:559:LEU:HD21	2.20	0.42
1:B:603:HIS:CG	1:B:604:ILE:N	2.87	0.42
1:B:817:SER:HG	1:B:820:GLU:H	1.62	0.42
1:B:80:LEU:O	1:B:222:ILE:HA	2.20	0.42
1:A:250:GLU:HG2	1:A:252:HIS:CD2	2.55	0.42
1:A:442:THR:HG23	1:A:445:GLN:H	1.84	0.42
1:A:884:LEU:HD23	1:A:884:LEU:HA	1.65	0.42
1:B:124:SER:N	1:B:130:TYR:O	2.53	0.42
1:B:586:TRP:HB2	1:B:588:ILE:HD11	2.02	0.42
1:B:718:ILE:H	1:B:718:ILE:HG13	1.59	0.42
1:B:293:ARG:NH1	2:C:3:BMA:H61	2.33	0.41
1:A:603:HIS:CG	1:A:612:LEU:HD21	2.54	0.41
1:B:196:VAL:HG23	1:B:267:ILE:HD11	2.01	0.41
1:B:213:GLU:HB2	1:B:216:PHE:CD1	2.53	0.41
1:A:377:PHE:HZ	1:A:478:ILE:HG23	1.84	0.41
1:A:398:TYR:HE1	1:A:463:ASN:HB2	1.84	0.41
1:B:200:GLU:HA	1:B:201:PRO:HA	1.81	0.41
1:B:218:ALA:HA	1:B:258:LYS:HE2	2.02	0.41
1:B:282:VAL:HA	1:B:321:SER:O	2.20	0.41
1:B:384:GLU:OE1	1:B:491:LYS:HE3	2.20	0.41
1:B:739:TRP:N	1:B:739:TRP:CD1	2.88	0.41
1:B:776:GLN:O	1:B:780:SER:N	2.54	0.41
1:A:366:ARG:HE	1:A:366:ARG:HB3	1.66	0.41
1:B:77:HIS:ND1	1:B:219:ASN:HB2	2.35	0.41
1:A:197:THR:HG23	1:A:266:TYR:O	2.20	0.41
1:B:651:HIS:CE1	1:B:691:THR:HG22	2.56	0.41
1:B:709:MET:O	1:B:713:ARG:HG2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:PHE:CE2	1:A:361:LYS:HB2	2.55	0.41
1:A:921:LEU:O	1:A:926:SER:HB2	2.20	0.41
1:B:104:ALA:HB2	1:B:158:PRO:HG3	2.02	0.41
1:B:278:THR:HG22	1:B:282:VAL:O	2.20	0.41
1:B:688:GLN:HB2	1:B:729:TYR:CE2	2.53	0.41
1:A:359:SER:HB2	1:A:749:MET:CE	2.51	0.41
1:A:835:GLU:H	1:A:835:GLU:HG3	1.64	0.41
1:B:64:TRP:CD2	1:B:70:PRO:HG3	2.56	0.41
1:B:415:ASP:HB3	1:B:694:PRO:HG3	2.02	0.41
1:B:553:LYS:O	1:B:559:LEU:HA	2.21	0.41
1:B:629:GLY:O	1:B:631:TYR:N	2.52	0.41
1:B:651:HIS:NE2	1:B:689:HIS:O	2.54	0.41
1:A:78:TYR:CD1	1:A:97:ILE:HG12	2.56	0.41
1:A:474:PHE:O	1:A:478:ILE:HG13	2.21	0.41
1:A:111:HIS:HD2	1:A:212:ASP:N	2.19	0.40
1:A:561:LEU:HB2	1:A:610:ASP:O	2.21	0.40
1:A:805:TRP:CD2	1:A:836:LYS:HD3	2.56	0.40
1:A:889:LEU:HG	1:A:928:LEU:HD21	2.02	0.40
1:B:272:HIS:CD2	1:B:290:PRO:HB3	2.57	0.40
1:B:415:ASP:HB3	1:B:694:PRO:CG	2.51	0.40
1:B:942:ILE:HA	1:B:945:LEU:HD22	2.03	0.40
1:A:191:THR:H	1:B:191:THR:HB	1.86	0.40
1:A:197:THR:HB	1:A:199:PHE:CE1	2.56	0.40
1:A:397:LYS:HB3	1:A:459:ALA:HB2	2.03	0.40
1:A:398:TYR:CZ	1:A:402:ILE:HD11	2.56	0.40
1:A:722:LEU:HD23	1:A:722:LEU:HA	1.94	0.40
1:A:785:ASN:HA	9:A:1010:EDO:H11	2.03	0.40
1:A:863:ALA:HB2	1:A:901:THR:HG22	2.03	0.40
1:A:338:ASN:HB2	1:A:341:LEU:O	2.21	0.40
1:A:590:LEU:N	1:A:603:HIS:O	2.46	0.40
1:B:96:LYS:HA	1:B:164:VAL:O	2.22	0.40
1:B:466:LYS:HE2	1:B:471:GLU:HB3	2.03	0.40
1:B:592:TYR:CE1	1:B:601:HIS:HB2	2.56	0.40
1:B:671:GLY:HA2	1:B:944:TRP:HD1	1.87	0.40
1:B:777:TRP:HA	1:B:780:SER:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	913/963 (95%)	833 (91%)	73 (8%)	7 (1%)	19	54
1	B	873/963 (91%)	813 (93%)	55 (6%)	5 (1%)	25	59
All	All	1786/1926 (93%)	1646 (92%)	128 (7%)	12 (1%)	22	57

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	556	GLY
1	A	215	LEU
1	A	803	ALA
1	B	762	ASN
1	A	867	LYS
1	B	683	MET
1	A	615	PRO
1	B	649	GLN
1	A	925	GLY
1	B	63	PRO
1	A	715	ILE
1	B	201	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	810/866 (94%)	749 (92%)	61 (8%)	13	42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	749/866 (86%)	674 (90%)	75 (10%)	7 28
All	All	1559/1732 (90%)	1423 (91%)	136 (9%)	10 36

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	PHE
1	A	55	VAL
1	A	57	THR
1	A	62	PHE
1	A	67	LEU
1	A	71	SER
1	A	101	VAL
1	A	115	LEU
1	A	139	VAL
1	A	141	SER
1	A	152	VAL
1	A	183	THR
1	A	194	LEU
1	A	202	THR
1	A	226	ARG
1	A	236	MET
1	A	255	THR
1	A	266	TYR
1	A	279	SER
1	A	312	LYS
1	A	321	SER
1	A	352	ASP
1	A	356	SER
1	A	357	SER
1	A	383	MET
1	A	426	THR
1	A	442	THR
1	A	454	SER
1	A	498	SER
1	A	509	THR
1	A	535	LYS
1	A	539	THR
1	A	549	LEU
1	A	550	LEU
1	A	572	GLN
1	A	574	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	595	SER
1	A	609	THR
1	A	621	VAL
1	A	645	THR
1	A	651	HIS
1	A	655	ARG
1	A	657	LYS
1	A	686	TYR
1	A	689	HIS
1	A	709	MET
1	A	716	SER
1	A	738	SER
1	A	761	LEU
1	A	781	SER
1	A	784	LEU
1	A	791	LEU
1	A	806	ASN
1	A	829	SER
1	A	838	LEU
1	A	889	LEU
1	A	893	ASP
1	A	909	ASP
1	A	910	LYS
1	A	912	GLN
1	A	924	GLN
1	B	110	LEU
1	B	112	SER
1	B	115	LEU
1	B	119	ASN
1	B	140	LEU
1	B	141	SER
1	B	145	HIS
1	B	148	ILE
1	B	160	LEU
1	B	193	ILE
1	B	194	LEU
1	B	202	THR
1	B	241	THR
1	B	266	TYR
1	B	285	SER
1	B	296	THR
1	B	301	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	308	ASP
1	B	314	PHE
1	B	321	SER
1	B	322	LYS
1	B	339	TRP
1	B	357	SER
1	B	362	LEU
1	B	380	LEU
1	B	383	MET
1	B	395	PHE
1	B	442	THR
1	B	454	SER
1	B	491	LYS
1	B	499	LEU
1	B	547	ILE
1	B	563	GLN
1	B	567	LEU
1	B	571	PHE
1	B	573	GLU
1	B	574	ASP
1	B	577	TRP
1	B	590	LEU
1	B	596	SER
1	B	609	THR
1	B	618	THR
1	B	641	ASP
1	B	648	ASN
1	B	657	LYS
1	B	686	TYR
1	B	698	GLU
1	B	703	LEU
1	B	712	ARG
1	B	717	ASP
1	B	719	SER
1	B	722	LEU
1	B	726	LEU
1	B	729	TYR
1	B	757	LEU
1	B	759	CYS
1	B	773	LEU
1	B	789	ASP
1	B	797	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	800	GLN
1	B	817	SER
1	B	825	LEU
1	B	835	GLU
1	B	849	VAL
1	B	852	THR
1	B	869	GLN
1	B	884	LEU
1	B	929	ASP
1	B	932	GLN
1	B	933	THR
1	B	943	LYS
1	B	945	LEU
1	B	946	GLU
1	B	948	ASN
1	B	953	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	HIS
1	A	295	GLN
1	A	392	ASN
1	A	531	ASN
1	A	603	HIS
1	A	634	HIS
1	A	646	GLN
1	A	721	ASN
1	B	272	HIS
1	B	603	HIS
1	B	668	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)

29 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	C	1	2,1	14,14,15	0.60	0	17,19,21	0.53	0
2	NAG	C	2	2	14,14,15	0.48	0	17,19,21	0.73	0
2	BMA	C	3	2	11,11,12	1.25	1 (9%)	15,15,17	1.42	1 (6%)
2	MAN	C	4	2	11,11,12	3.05	8 (72%)	15,15,17	1.66	3 (20%)
2	MAN	C	5	2	11,11,12	2.33	6 (54%)	15,15,17	2.33	3 (20%)
3	NAG	D	1	1,3	14,14,15	0.66	1 (7%)	17,19,21	0.60	0
3	NAG	D	2	3	14,14,15	0.47	0	17,19,21	0.75	1 (5%)
4	NAG	E	1	4,1	14,14,15	0.29	0	17,19,21	0.51	0
4	NAG	E	2	4	14,14,15	0.53	0	17,19,21	0.69	0
4	BMA	E	3	4	11,11,12	1.97	3 (27%)	15,15,17	1.61	2 (13%)
4	NAG	F	1	4,1	14,14,15	0.32	0	17,19,21	0.61	0
4	NAG	F	2	4	14,14,15	0.49	0	17,19,21	0.66	0
4	BMA	F	3	4	11,11,12	1.17	0	15,15,17	1.18	1 (6%)
4	NAG	G	1	4,1	14,14,15	0.61	0	17,19,21	1.06	1 (5%)
4	NAG	G	2	4	14,14,15	0.86	1 (7%)	17,19,21	0.66	0
4	BMA	G	3	4	11,11,12	1.98	4 (36%)	15,15,17	1.39	3 (20%)
2	NAG	H	1	2,1	14,14,15	0.76	1 (7%)	17,19,21	0.60	0
2	NAG	H	2	2	14,14,15	0.89	1 (7%)	17,19,21	0.85	0
2	BMA	H	3	2	11,11,12	1.55	3 (27%)	15,15,17	1.22	2 (13%)
2	MAN	H	4	2	11,11,12	1.83	3 (27%)	15,15,17	1.06	2 (13%)
2	MAN	H	5	2	11,11,12	1.74	3 (27%)	15,15,17	1.22	2 (13%)
3	NAG	I	1	1,3	14,14,15	0.33	0	17,19,21	0.52	0
3	NAG	I	2	3	14,14,15	1.07	2 (14%)	17,19,21	0.61	0
3	NAG	J	1	1,3	14,14,15	0.65	1 (7%)	17,19,21	0.91	1 (5%)
3	NAG	J	2	3	14,14,15	0.63	0	17,19,21	1.25	1 (5%)
3	NAG	K	1	1,3	14,14,15	0.87	1 (7%)	17,19,21	0.61	0
3	NAG	K	2	3	14,14,15	1.34	2 (14%)	17,19,21	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	L	1	1,3	14,14,15	0.47	0	17,19,21	0.45	0
3	NAG	L	2	3	14,14,15	0.92	1 (7%)	17,19,21	0.90	1 (5%)

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

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

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4	MAN	C2-C3	5.83	1.61	1.52
4	E	3	BMA	O5-C1	4.20	1.50	1.43
3	K	2	NAG	O5-C1	4.03	1.50	1.43
2	C	5	MAN	O5-C5	4.00	1.51	1.43
2	C	4	MAN	C4-C3	3.95	1.62	1.52
2	C	4	MAN	O5-C5	3.70	1.50	1.43
2	C	5	MAN	C1-C2	3.69	1.60	1.52
2	C	4	MAN	C1-C2	3.57	1.60	1.52
2	H	4	MAN	C2-C3	3.54	1.57	1.52
2	H	5	MAN	C4-C3	3.50	1.61	1.52
4	G	3	BMA	C2-C3	3.46	1.57	1.52
4	G	3	BMA	C1-C2	3.37	1.59	1.52
2	H	3	BMA	C2-C3	3.35	1.57	1.52
2	H	5	MAN	C4-C5	3.35	1.60	1.53
3	I	2	NAG	O5-C1	3.16	1.48	1.43
3	L	2	NAG	O5-C1	2.92	1.48	1.43
3	K	1	NAG	O5-C1	2.79	1.48	1.43
4	G	2	NAG	O5-C1	2.76	1.48	1.43
2	H	2	NAG	O5-C1	-2.76	1.39	1.43
2	H	4	MAN	C1-C2	2.73	1.58	1.52
2	H	1	NAG	O5-C1	-2.73	1.39	1.43
2	C	5	MAN	O5-C1	2.72	1.48	1.43
2	C	5	MAN	C4-C5	2.66	1.58	1.53
3	K	2	NAG	C1-C2	2.62	1.56	1.52
2	C	3	BMA	C1-C2	2.61	1.58	1.52
2	C	4	MAN	O5-C1	2.58	1.47	1.43
4	E	3	BMA	O5-C5	2.57	1.48	1.43
4	E	3	BMA	C1-C2	2.51	1.57	1.52
2	H	3	BMA	C4-C5	2.42	1.58	1.53
2	C	4	MAN	C4-C5	2.38	1.58	1.53
2	C	4	MAN	O2-C2	2.37	1.48	1.43
3	I	2	NAG	C1-C2	2.29	1.55	1.52
2	C	5	MAN	C4-C3	2.28	1.58	1.52
3	J	1	NAG	O5-C1	2.28	1.47	1.43
2	C	5	MAN	O2-C2	2.27	1.48	1.43
2	H	4	MAN	O2-C2	2.25	1.48	1.43
4	G	3	BMA	O5-C5	2.20	1.47	1.43
3	D	1	NAG	C1-C2	2.19	1.55	1.52
4	G	3	BMA	O5-C1	2.16	1.47	1.43
2	H	3	BMA	C1-C2	2.13	1.57	1.52
2	C	4	MAN	O3-C3	2.05	1.47	1.43
2	H	5	MAN	O2-C2	2.04	1.47	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	5	MAN	C1-O5-C5	7.06	121.76	112.19
4	E	3	BMA	C1-O5-C5	5.14	119.15	112.19
3	J	2	NAG	C2-N2-C7	4.32	129.05	122.90
2	C	3	BMA	C1-O5-C5	4.05	117.68	112.19
2	C	4	MAN	C1-O5-C5	3.97	117.57	112.19
2	C	5	MAN	O5-C1-C2	3.69	116.46	110.77
4	G	1	NAG	C1-O5-C5	3.61	117.08	112.19
3	L	2	NAG	C1-O5-C5	3.33	116.70	112.19
3	J	1	NAG	C1-O5-C5	3.02	116.28	112.19
4	G	3	BMA	O5-C5-C6	2.90	111.75	107.20
4	F	3	BMA	C1-O5-C5	2.89	116.10	112.19
3	D	2	NAG	C1-O5-C5	2.74	115.90	112.19
2	H	5	MAN	O2-C2-C1	2.70	114.68	109.15
2	C	5	MAN	O2-C2-C1	2.64	114.56	109.15
4	G	3	BMA	C1-O5-C5	2.37	115.40	112.19
2	H	3	BMA	C2-C3-C4	2.29	114.86	110.89
4	E	3	BMA	O5-C1-C2	2.13	114.06	110.77
2	H	4	MAN	O2-C2-C1	2.11	113.48	109.15
2	H	3	BMA	C3-C4-C5	2.11	114.01	110.24
2	H	4	MAN	O3-C3-C2	2.10	114.02	109.99
2	C	4	MAN	C1-C2-C3	2.06	112.20	109.67
2	H	5	MAN	C6-C5-C4	2.02	117.75	113.00
4	G	3	BMA	O2-C2-C1	2.02	113.29	109.15
2	C	4	MAN	O2-C2-C1	2.01	113.27	109.15

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	2	NAG	C4-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	C	4	MAN	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
2	H	3	BMA	C4-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	C	5	MAN	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	L	2	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
4	E	3	BMA	O5-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6
3	J	2	NAG	C8-C7-N2-C2
3	J	2	NAG	O7-C7-N2-C2
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
2	H	3	BMA	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
2	C	5	MAN	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
2	H	5	MAN	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
4	E	3	BMA	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
4	F	3	BMA	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	G	3	BMA	O5-C5-C6-O6
2	H	5	MAN	C4-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
3	J	2	NAG	C3-C2-N2-C7
2	C	1	NAG	O5-C5-C6-O6
3	J	2	NAG	C1-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	5	MAN	3	0
2	H	1	NAG	1	0

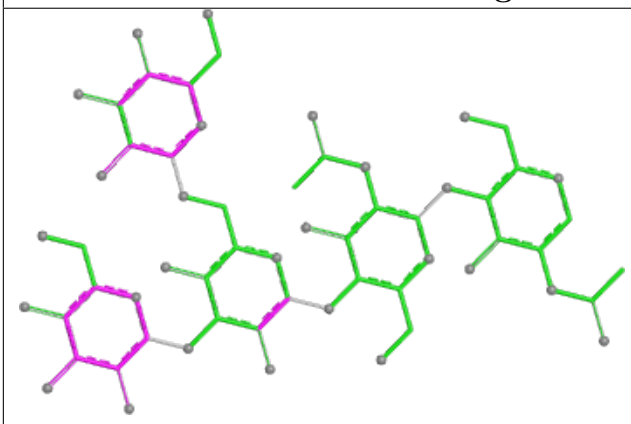
Continued on next page...

Continued from previous page...

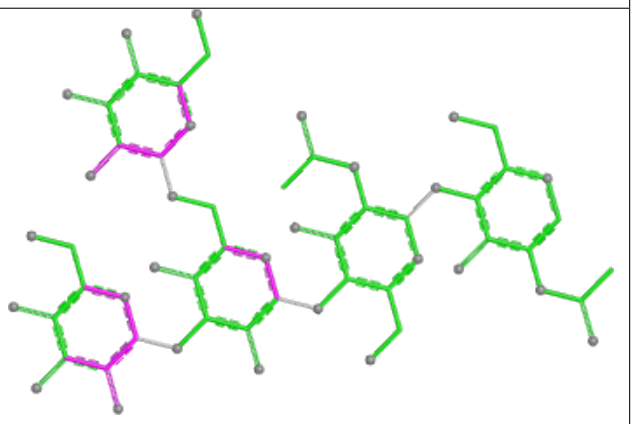
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	BMA	3	0
3	J	2	NAG	1	0
3	K	1	NAG	1	0

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

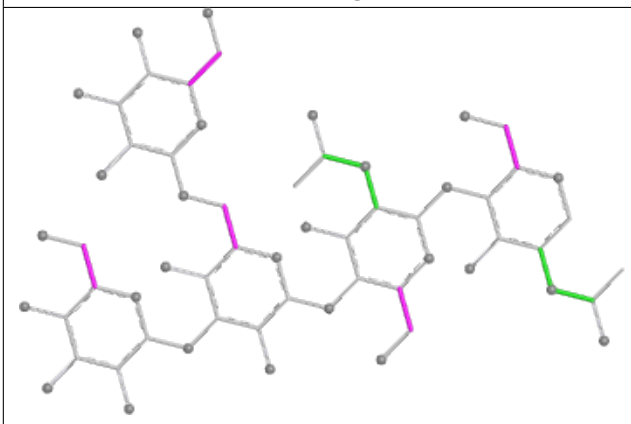
Oligosaccharide Chain C



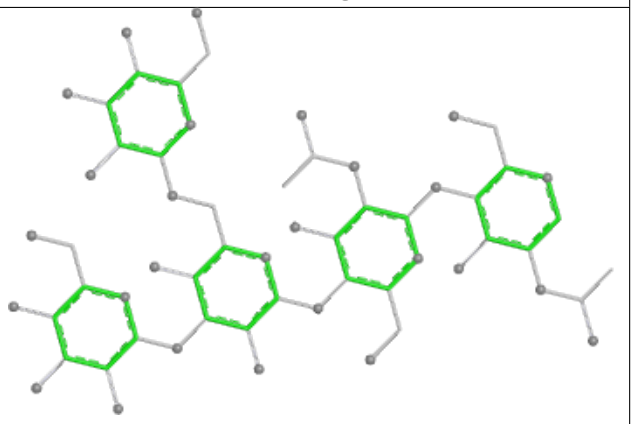
Bond lengths



Bond angles

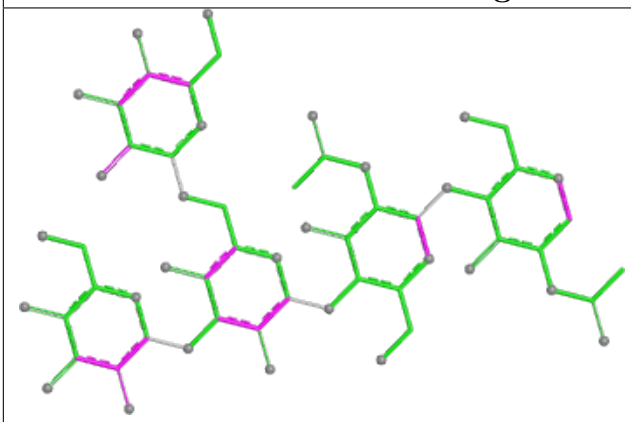


Torsions

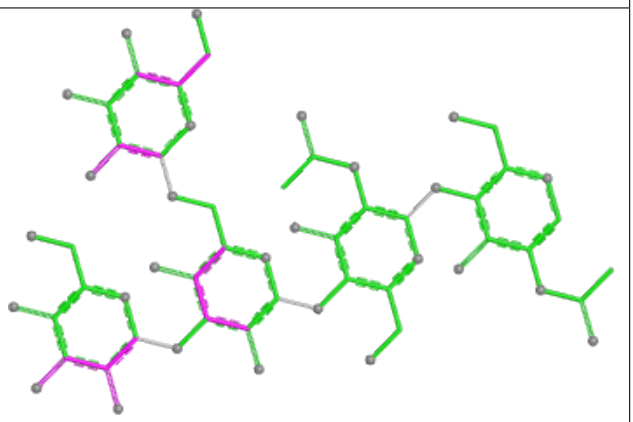


Rings

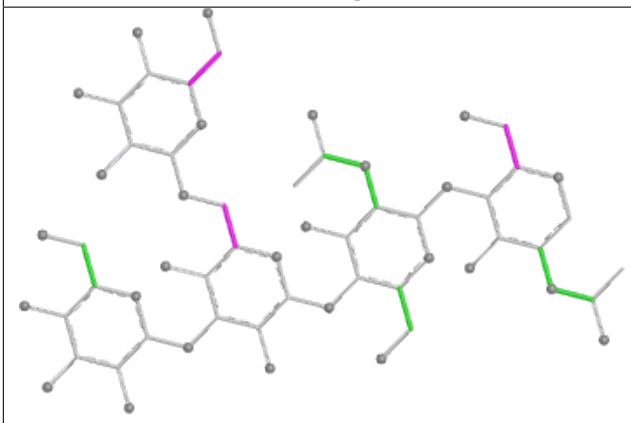
Oligosaccharide Chain H



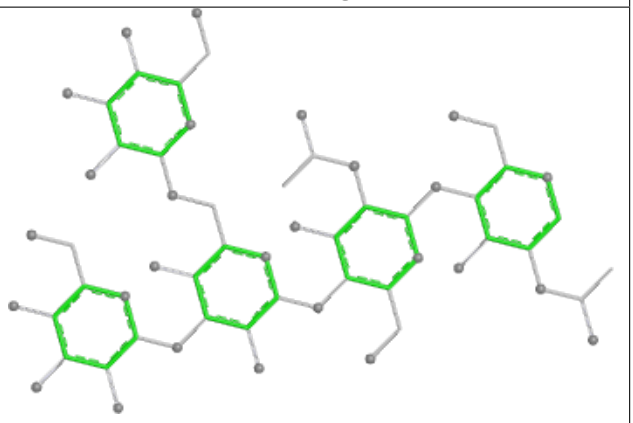
Bond lengths



Bond angles

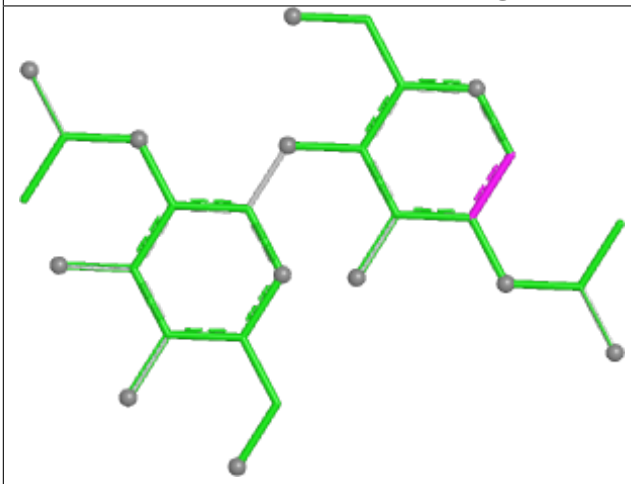


Torsions

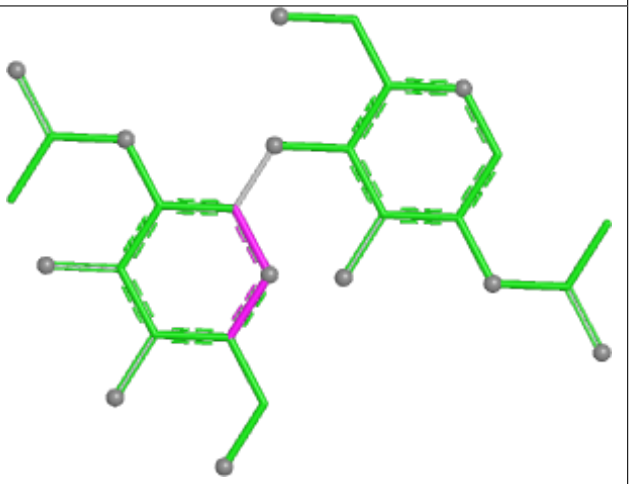


Rings

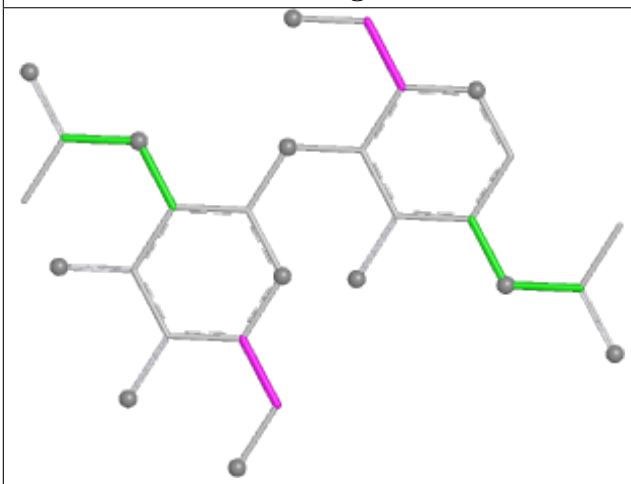
Oligosaccharide Chain D



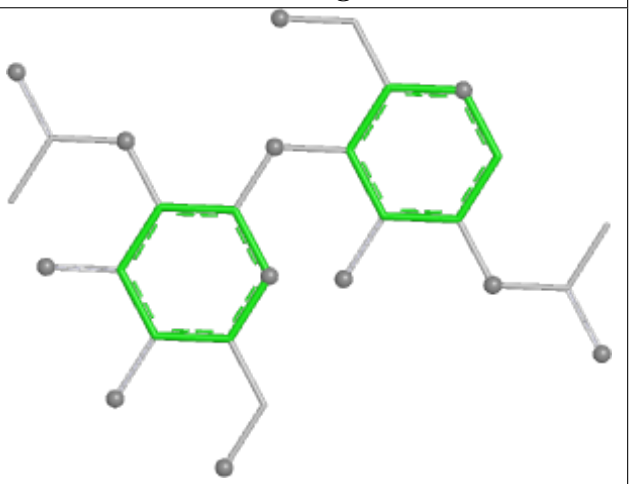
Bond lengths



Bond angles

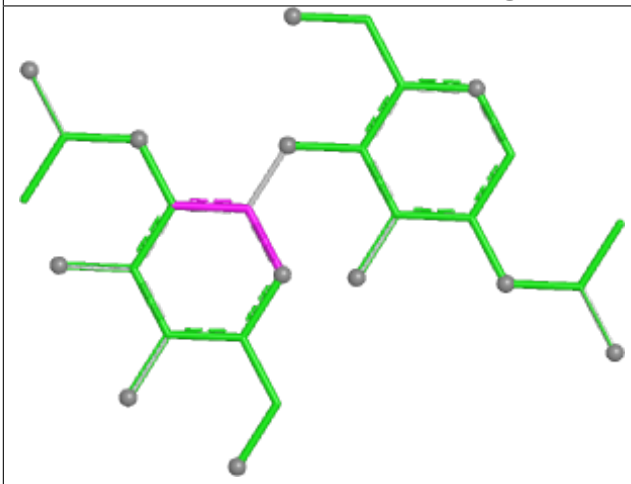


Torsions

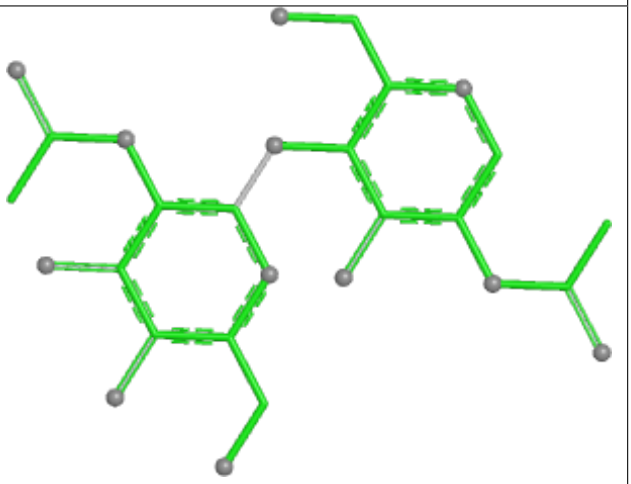


Rings

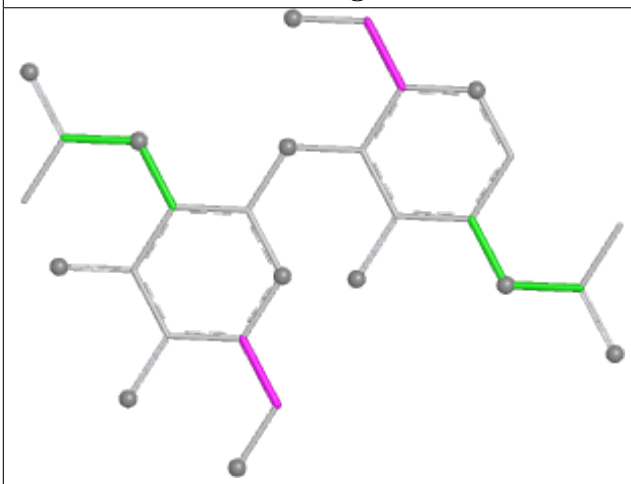
Oligosaccharide Chain I



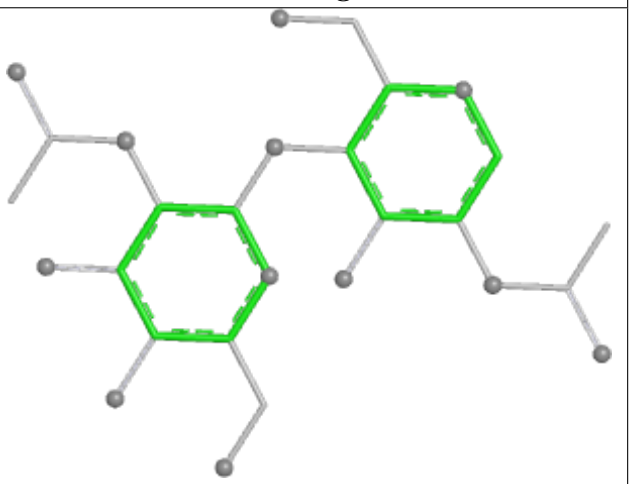
Bond lengths



Bond angles

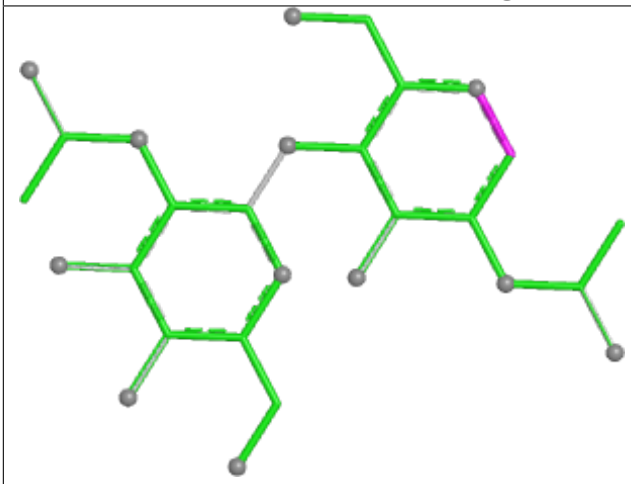


Torsions

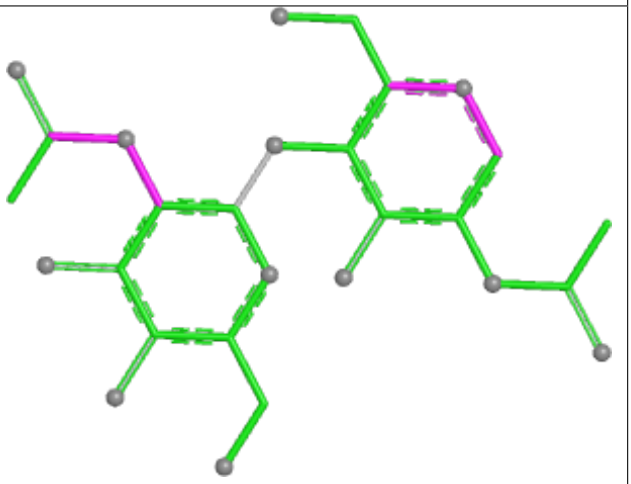


Rings

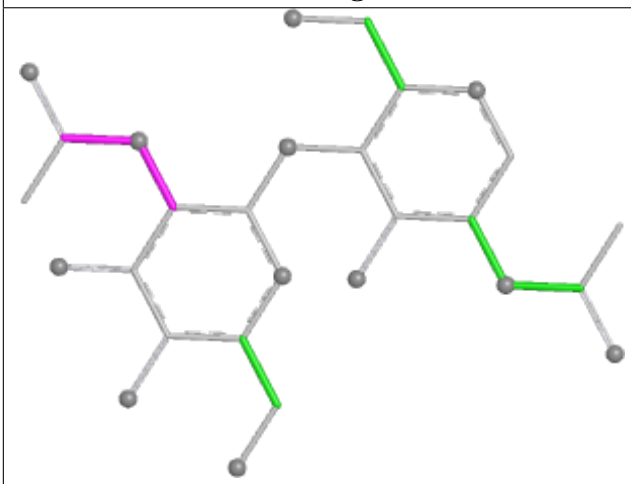
Oligosaccharide Chain J



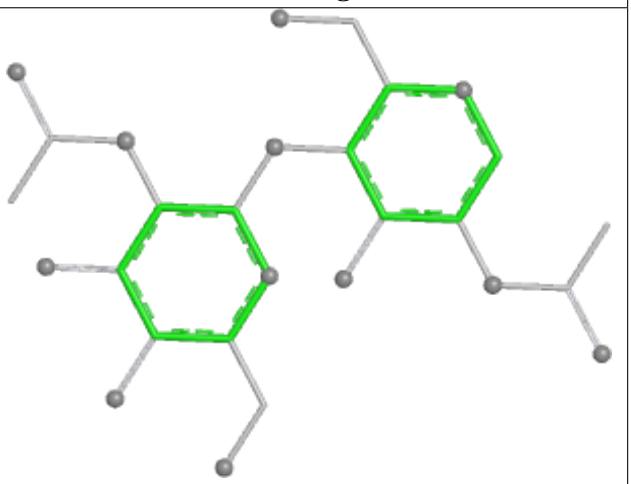
Bond lengths



Bond angles

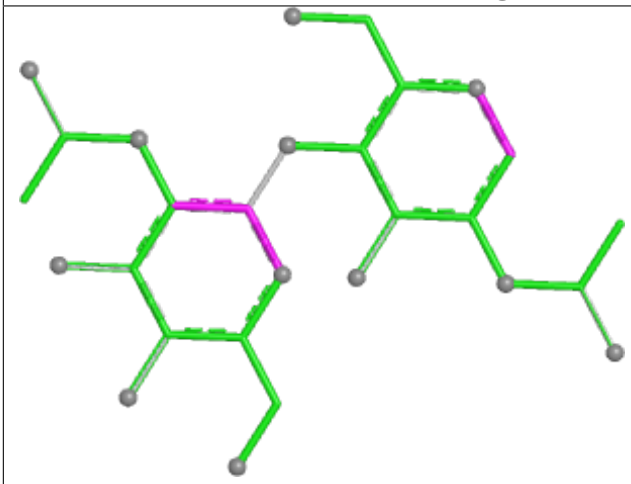


Torsions

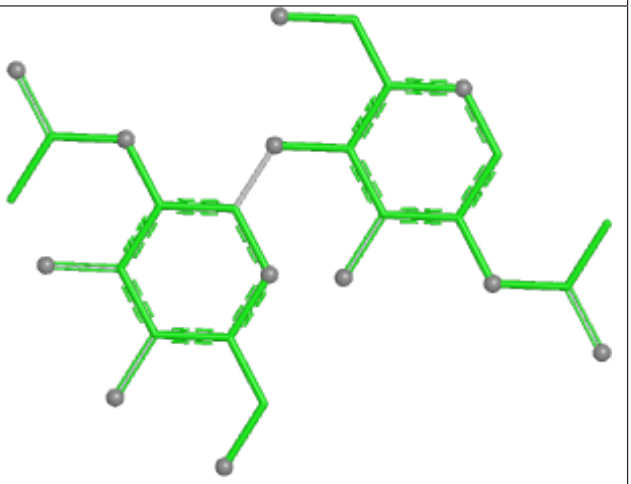


Rings

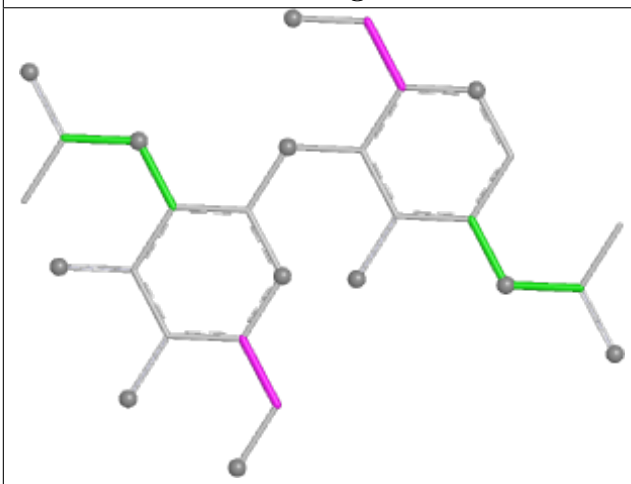
Oligosaccharide Chain K



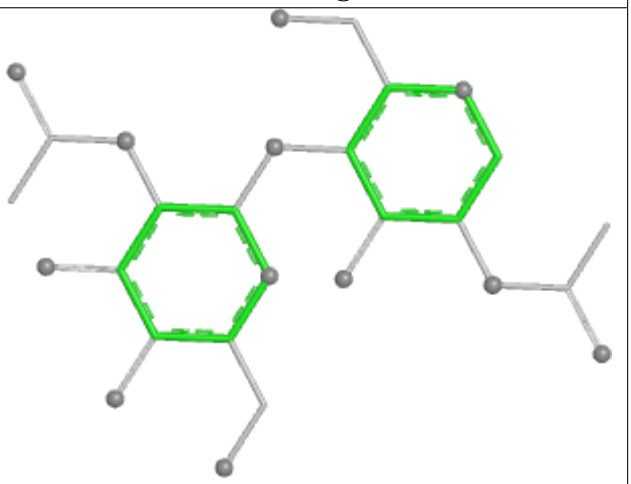
Bond lengths



Bond angles

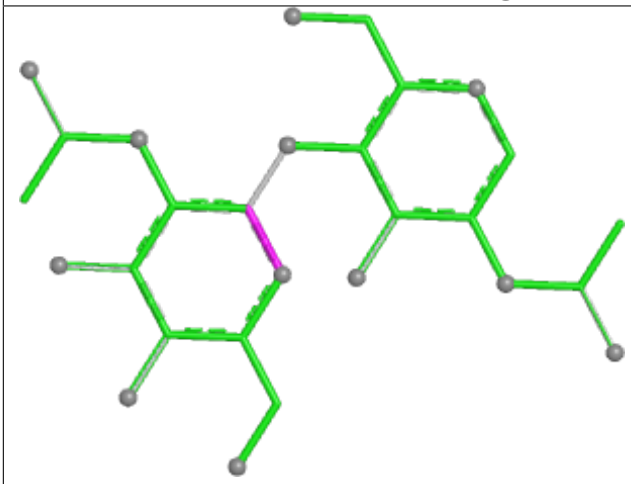


Torsions

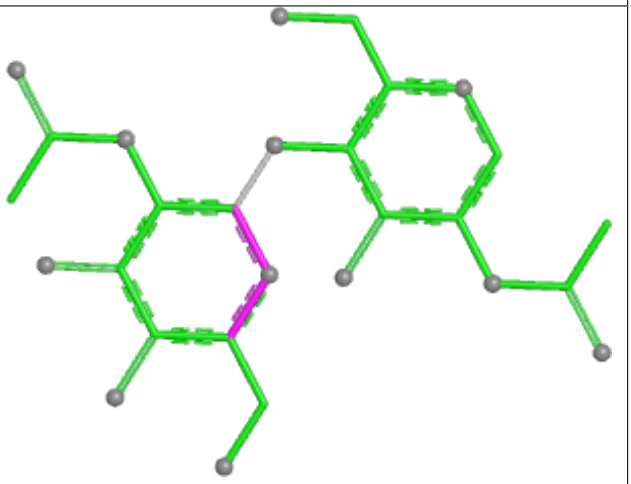


Rings

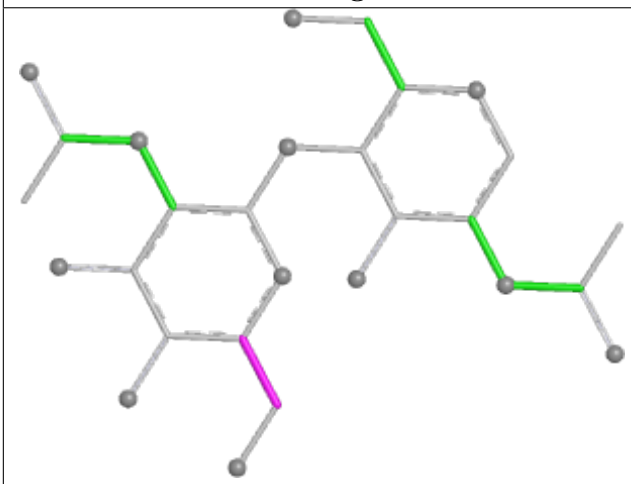
Oligosaccharide Chain L



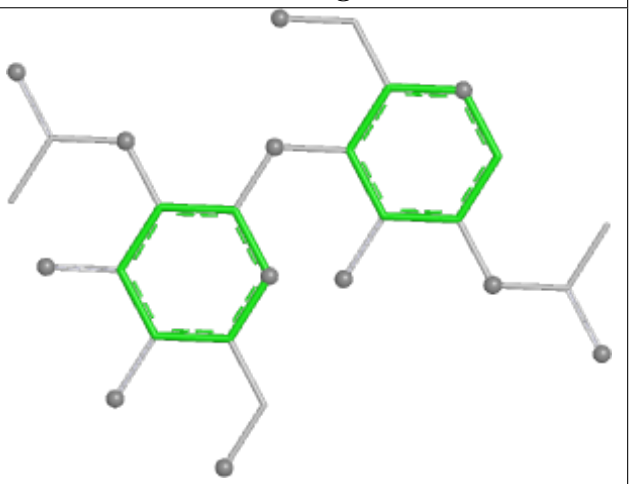
Bond lengths



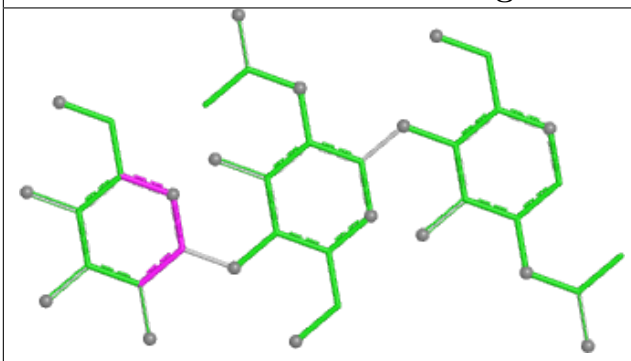
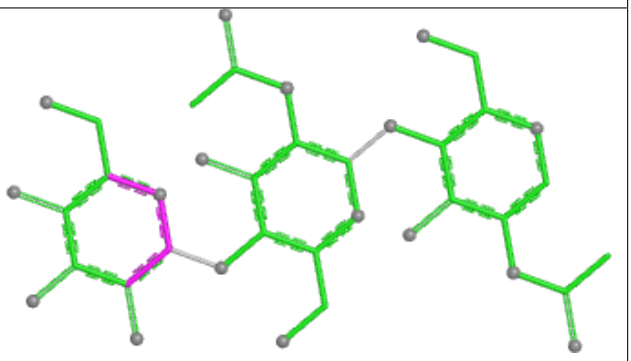
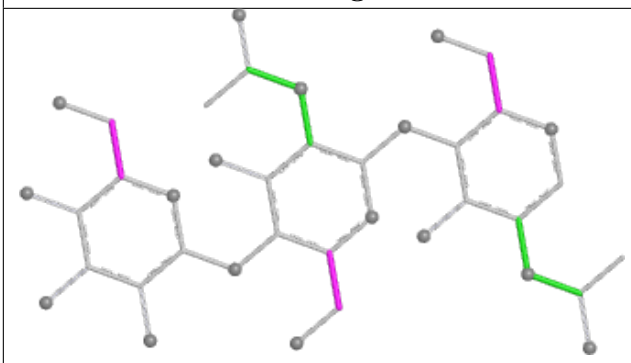
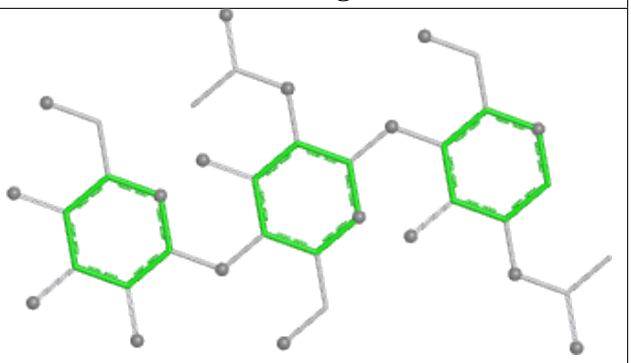
Bond angles

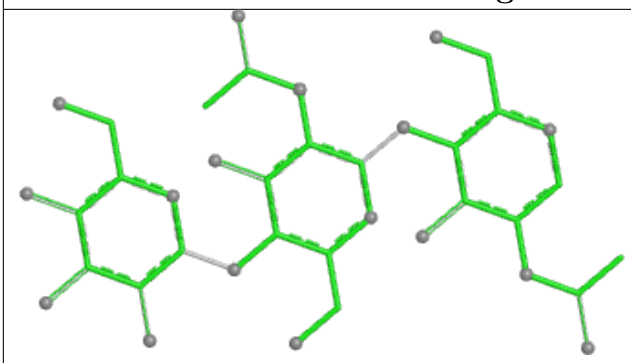
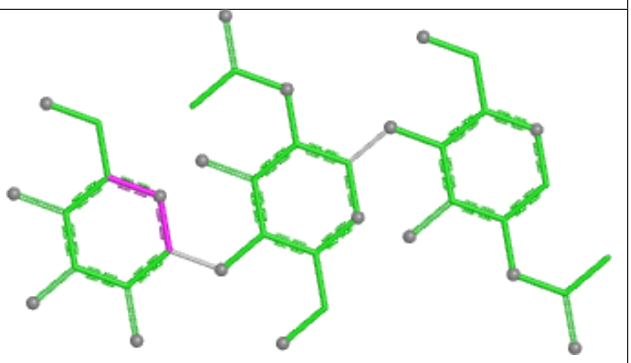
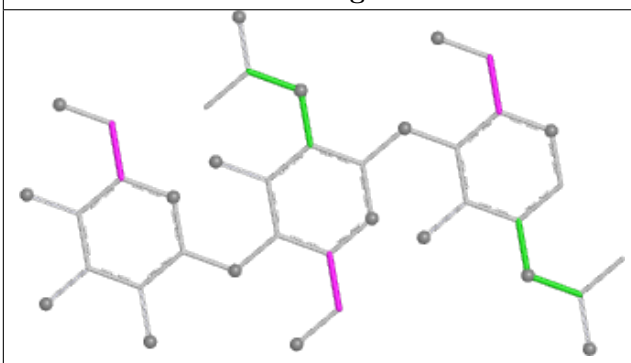
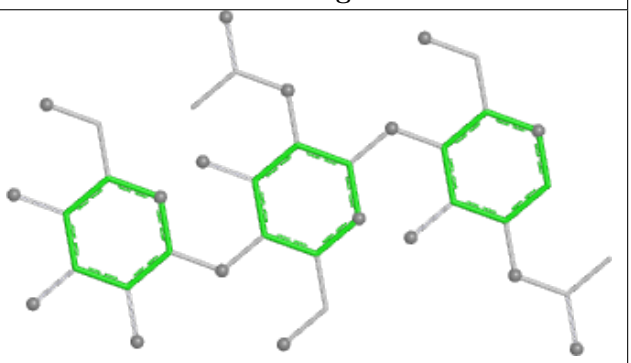


Torsions

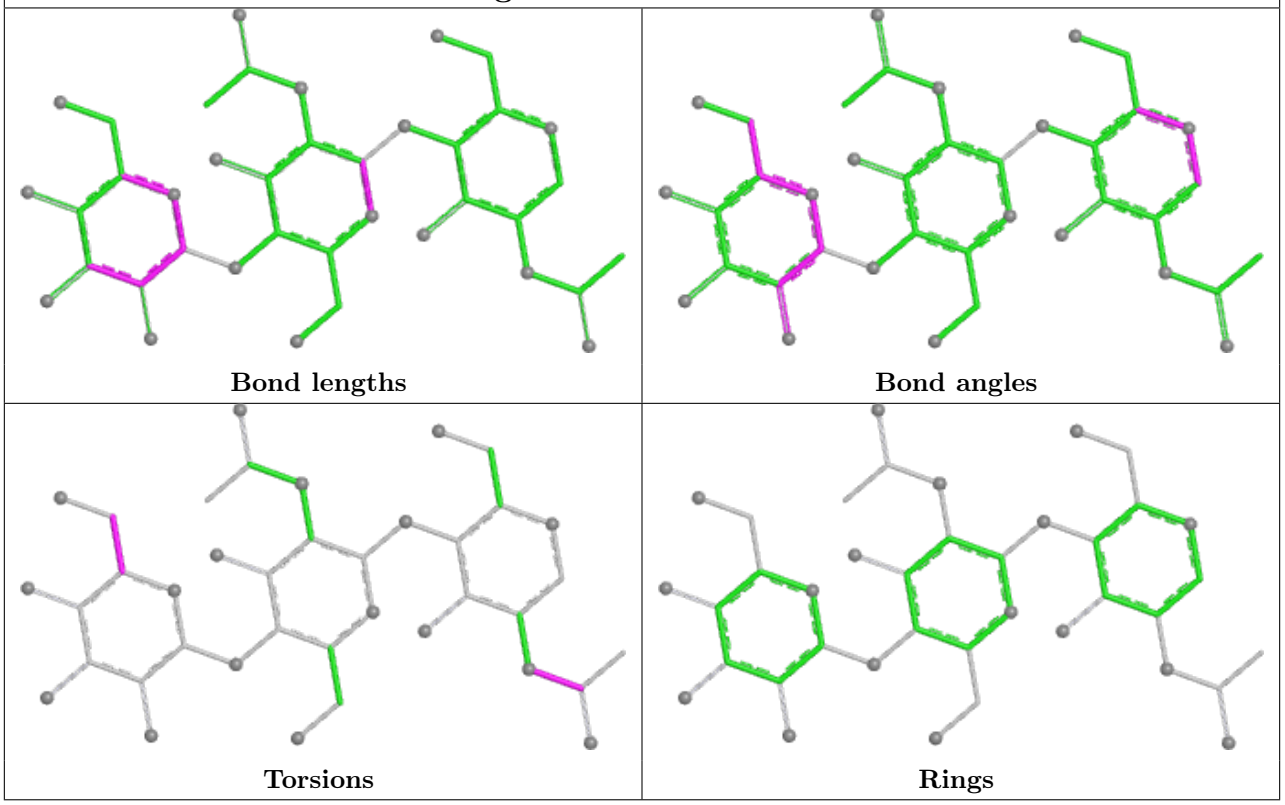


Rings

Oligosaccharide Chain E	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain F	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain G



5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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	$\#\|Z\| > 2$
6	NAG	A	1002	1	14,14,15	0.43	0	17,19,21	0.45	0
9	EDO	A	1012	-	3,3,3	0.55	0	2,2,2	0.19	0
6	NAG	A	1004	1	14,14,15	0.71	1 (7%)	17,19,21	1.11	1 (5%)
7	P4G	A	1006	-	10,10,10	0.61	0	9,9,9	0.43	0
9	EDO	A	1010	-	3,3,3	0.61	0	2,2,2	0.16	0
9	EDO	A	1008	-	3,3,3	0.60	0	2,2,2	0.09	0
6	NAG	A	1005	1	14,14,15	0.36	0	17,19,21	0.54	0
8	UQE	A	1007[A]	5	35,37,37	2.72	10 (28%)	34,52,52	3.46	13 (38%)
9	EDO	A	1009	-	3,3,3	0.58	0	2,2,2	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	A	1003	1	14,14,15	0.94	1 (7%)	17,19,21	0.77	1 (5%)
9	EDO	A	1011	-	3,3,3	0.77	0	2,2,2	0.35	0
6	NAG	B	1003	1	14,14,15	0.48	0	17,19,21	0.52	0
8	UQE	A	1007[B]	5	35,37,37	2.40	7 (20%)	34,52,52	3.76	10 (29%)
8	UQE	B	1004	5	35,37,37	2.87	8 (22%)	34,52,52	3.28	11 (32%)
6	NAG	B	1002	1	14,14,15	0.93	1 (7%)	17,19,21	0.76	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
6	NAG	A	1002	1	-	3/6/23/26	0/1/1/1
9	EDO	A	1012	-	-	0/1/1/1	-
6	NAG	A	1004	1	-	0/6/23/26	0/1/1/1
7	P4G	A	1006	-	-	2/8/8/8	-
9	EDO	A	1010	-	-	0/1/1/1	-
9	EDO	A	1008	-	-	1/1/1/1	-
6	NAG	A	1005	1	-	3/6/23/26	0/1/1/1
8	UQE	A	1007[A]	5	-	2/16/30/30	0/4/4/4
9	EDO	A	1009	-	-	0/1/1/1	-
6	NAG	A	1003	1	-	2/6/23/26	0/1/1/1
9	EDO	A	1011	-	-	0/1/1/1	-
6	NAG	B	1003	1	-	0/6/23/26	0/1/1/1
8	UQE	A	1007[B]	5	-	8/16/30/30	0/4/4/4
8	UQE	B	1004	5	-	3/16/30/30	0/4/4/4
6	NAG	B	1002	1	-	4/6/23/26	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1007[B]	UQE	C12-N10	9.40	1.46	1.33
8	B	1004	UQE	C12-N10	9.32	1.46	1.33
8	A	1007[A]	UQE	C12-N10	8.57	1.45	1.33
8	B	1004	UQE	S33-N20	7.36	1.73	1.61
8	A	1007[A]	UQE	S33-N20	7.07	1.72	1.61
8	B	1004	UQE	C17-C18	7.04	1.46	1.36
8	A	1007[A]	UQE	C17-C18	6.90	1.46	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1004	UQE	C31-S33	5.71	1.85	1.76
8	A	1007[B]	UQE	S33-N20	5.32	1.69	1.61
8	A	1007[B]	UQE	C17-C18	5.02	1.43	1.36
8	A	1007[A]	UQE	C31-S33	4.39	1.83	1.76
8	B	1004	UQE	O34-S33	3.99	1.48	1.43
8	A	1007[A]	UQE	O32-S33	3.94	1.48	1.43
8	B	1004	UQE	O32-S33	3.50	1.47	1.43
8	A	1007[A]	UQE	O34-S33	3.41	1.47	1.43
6	A	1003	NAG	O5-C1	3.08	1.48	1.43
8	A	1007[B]	UQE	C31-S33	3.06	1.81	1.76
8	A	1007[B]	UQE	O34-S33	3.04	1.47	1.43
8	A	1007[A]	UQE	C27-C28	2.97	1.55	1.49
8	B	1004	UQE	C27-C28	2.92	1.55	1.49
8	B	1004	UQE	O11-C12	-2.83	1.17	1.23
6	B	1002	NAG	O5-C1	2.66	1.48	1.43
8	A	1007[A]	UQE	O11-C12	-2.57	1.18	1.23
8	A	1007[B]	UQE	C31-S21	-2.35	1.68	1.72
6	A	1004	NAG	O5-C1	2.31	1.47	1.43
8	A	1007[B]	UQE	O01-C04	2.11	1.41	1.37
8	A	1007[A]	UQE	C31-S21	-2.09	1.68	1.72
8	A	1007[A]	UQE	C19-C18	2.00	1.55	1.51

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1007[B]	UQE	O34-S33-O32	-16.01	99.87	119.55
8	B	1004	UQE	O34-S33-O32	-15.64	100.32	119.55
8	A	1007[A]	UQE	O34-S33-O32	-14.95	101.17	119.55
8	A	1007[B]	UQE	C31-S33-N20	8.34	118.65	107.82
8	A	1007[A]	UQE	C17-N16-C13	5.32	131.50	125.62
8	A	1007[A]	UQE	O32-S33-C31	5.21	116.24	107.66
8	A	1007[A]	UQE	O11-C12-N10	-4.83	117.02	123.27
8	A	1007[B]	UQE	O34-S33-N20	4.71	114.40	107.04
8	A	1007[B]	UQE	O32-S33-C31	-4.71	99.91	107.66
8	A	1007[B]	UQE	C28-C27-N22	4.67	125.04	116.77
8	A	1007[A]	UQE	C23-N22-C27	4.64	123.74	117.23
8	A	1007[B]	UQE	C26-C27-C28	-4.29	113.74	121.27
8	B	1004	UQE	C23-N22-C27	4.26	123.21	117.23
8	A	1007[B]	UQE	O11-C12-N10	-4.18	117.86	123.27
8	A	1007[A]	UQE	C17-C18-N14	-4.16	105.16	111.34
8	B	1004	UQE	O32-S33-C31	4.16	114.50	107.66
8	A	1007[A]	UQE	O32-S33-N20	3.89	113.12	107.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1007[B]	UQE	C18-C19-N20	-3.67	104.77	112.71
8	B	1004	UQE	C17-N16-C13	3.67	129.67	125.62
8	A	1007[B]	UQE	O34-S33-C31	3.58	113.56	107.66
8	B	1004	UQE	O32-S33-N20	3.51	112.52	107.04
8	B	1004	UQE	C19-N20-S33	3.36	126.44	120.00
8	A	1007[B]	UQE	C17-C18-N14	-3.12	106.71	111.34
8	A	1007[A]	UQE	C18-C19-N20	2.91	119.00	112.71
6	A	1004	NAG	C1-O5-C5	2.87	116.08	112.19
8	B	1004	UQE	C17-C18-N14	-2.68	107.35	111.34
8	B	1004	UQE	O34-S33-C31	2.67	112.06	107.66
8	B	1004	UQE	C26-C27-N22	-2.64	118.33	122.26
6	A	1003	NAG	C1-O5-C5	2.56	115.66	112.19
8	A	1007[A]	UQE	C19-C18-C17	2.53	132.83	127.60
8	A	1007[A]	UQE	C26-C27-N22	-2.49	118.56	122.26
8	B	1004	UQE	O11-C12-N10	-2.25	120.36	123.27
8	A	1007[A]	UQE	O34-S33-C31	2.19	111.26	107.66
8	B	1004	UQE	C31-S33-N20	2.16	110.63	107.82
8	A	1007[A]	UQE	C08-C13-C12	2.16	116.29	111.06
8	A	1007[A]	UQE	C31-S33-N20	-2.12	105.07	107.82

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1007[B]	UQE	C13-C12-N10-O09
8	A	1007[B]	UQE	O11-C12-N10-O09
6	B	1002	NAG	C4-C5-C6-O6
6	A	1003	NAG	C4-C5-C6-O6
6	B	1002	NAG	O5-C5-C6-O6
6	A	1003	NAG	O5-C5-C6-O6
7	A	1006	P4G	O3-C5-C6-O4
6	A	1002	NAG	C8-C7-N2-C2
6	A	1002	NAG	O7-C7-N2-C2
6	B	1002	NAG	C8-C7-N2-C2
6	B	1002	NAG	O7-C7-N2-C2
6	A	1005	NAG	O5-C5-C6-O6
6	A	1005	NAG	C4-C5-C6-O6
6	A	1002	NAG	O5-C5-C6-O6
8	A	1007[B]	UQE	C07-C08-C13-C12
8	B	1004	UQE	C06-C07-C08-C13
8	B	1004	UQE	C02-C07-C08-C13
6	A	1005	NAG	C1-C2-N2-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	A	1007[A]	UQE	C06-C07-C08-C13
7	A	1006	P4G	C4-C3-O2-C2
8	A	1007[A]	UQE	C02-C07-C08-C13
8	B	1004	UQE	C26-C27-C28-C29
9	A	1008	EDO	O1-C1-C2-O2
8	A	1007[B]	UQE	O11-C12-C13-C08
8	A	1007[B]	UQE	N10-C12-C13-C08
8	A	1007[B]	UQE	O11-C12-C13-N16
8	A	1007[B]	UQE	N22-C27-C28-C29
8	A	1007[B]	UQE	C07-C08-C13-N16

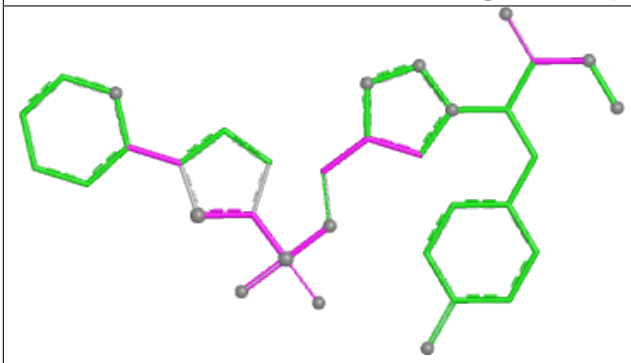
There are no ring outliers.

3 monomers are involved in 3 short contacts:

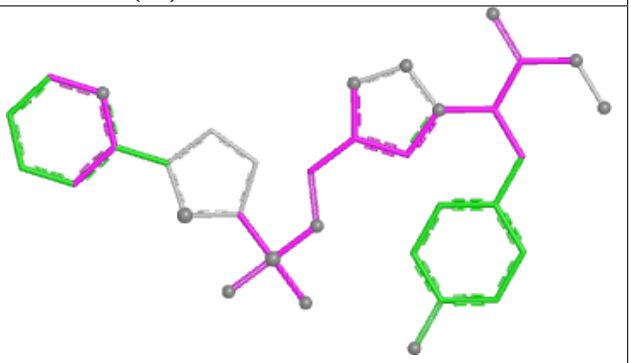
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1010	EDO	1	0
8	A	1007[A]	UQE	1	0
9	A	1009	EDO	1	0

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

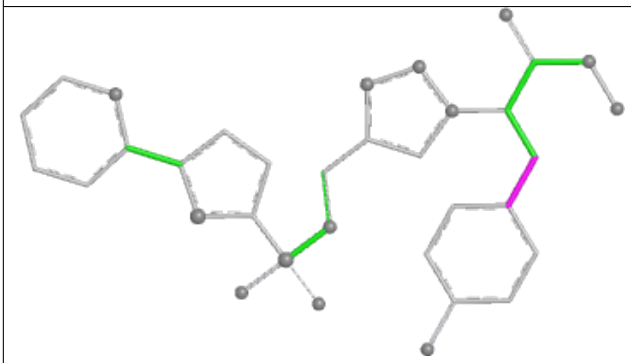
Ligand UQE A 1007 (A)



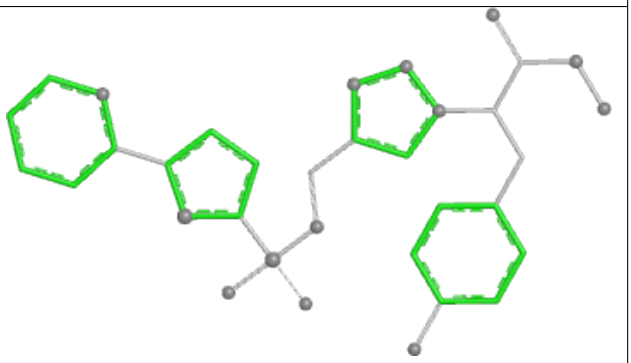
Bond lengths



Bond angles

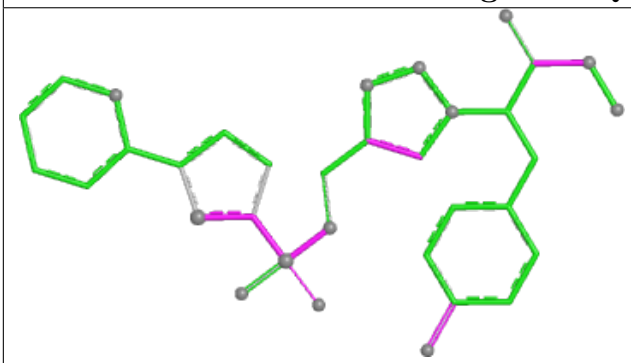


Torsions

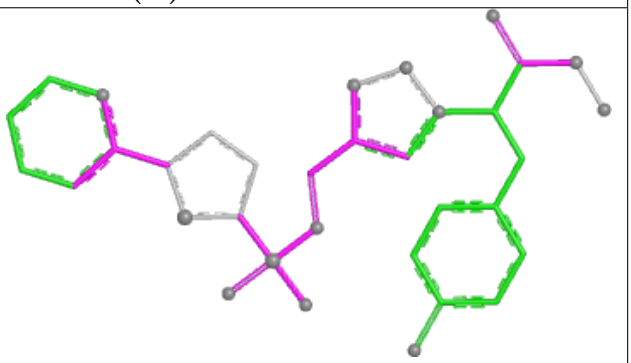


Rings

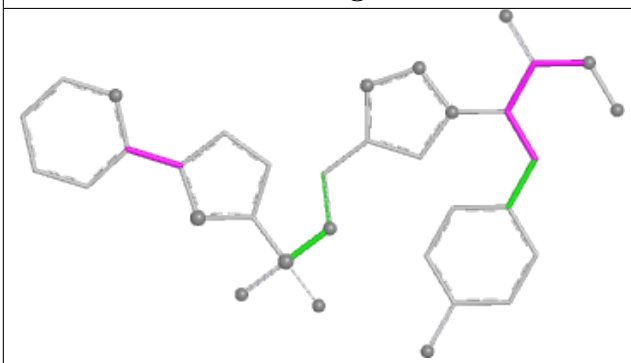
Ligand UQE A 1007 (B)



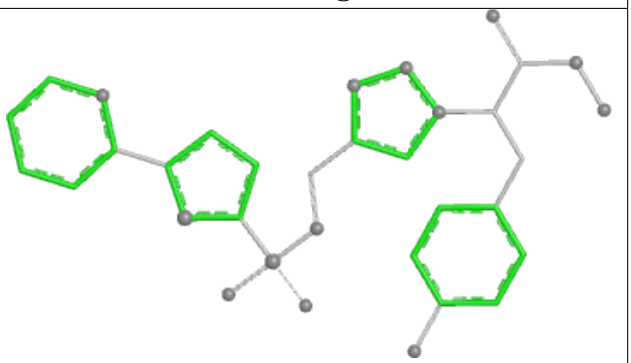
Bond lengths



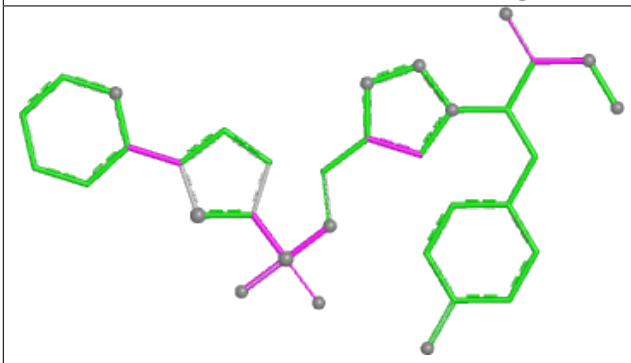
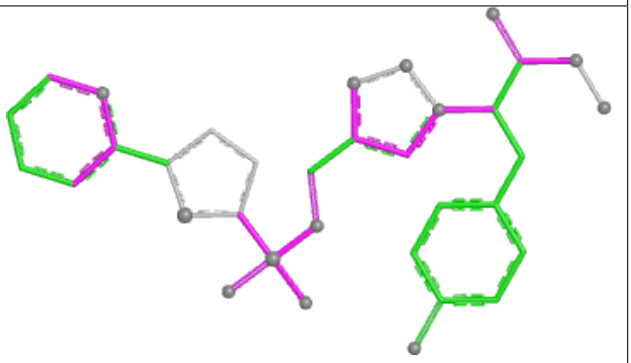
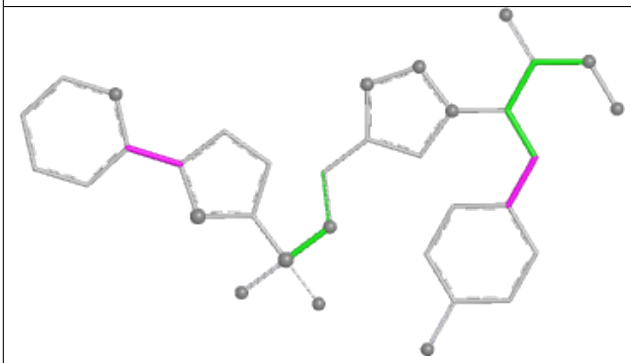
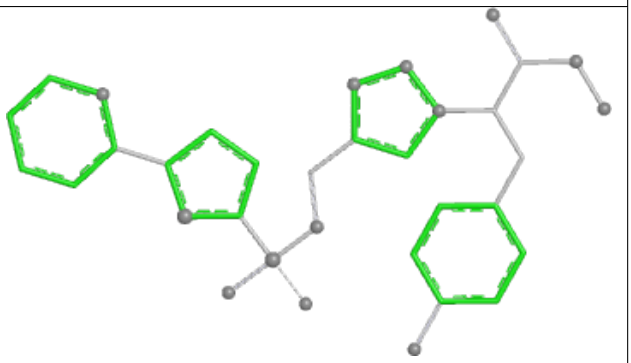
Bond angles



Torsions



Rings

Ligand UQE B 1004	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	912/963 (94%)	-0.15	1 (0%) 95 92	19, 54, 113, 170	0
1	B	877/963 (91%)	0.08	21 (2%) 59 37	29, 94, 150, 207	0
All	All	1789/1926 (92%)	-0.04	22 (1%) 79 61	19, 69, 140, 207	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	762	ASN	4.7
1	B	554	GLN	4.6
1	B	721	ASN	4.1
1	A	515	HIS	3.3
1	B	621	VAL	3.0
1	B	587	HIS	2.9
1	B	474	PHE	2.7
1	B	612	LEU	2.6
1	B	592	TYR	2.6
1	B	623	PHE	2.5
1	B	795	TYR	2.5
1	B	752	SER	2.4
1	B	613	ASP	2.3
1	B	224	ILE	2.3
1	B	630	TYR	2.3
1	B	570	VAL	2.1
1	B	215	LEU	2.1
1	B	377	PHE	2.1
1	B	640	TRP	2.1
1	B	703	LEU	2.0
1	B	687	LEU	2.0
1	B	72	VAL	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)

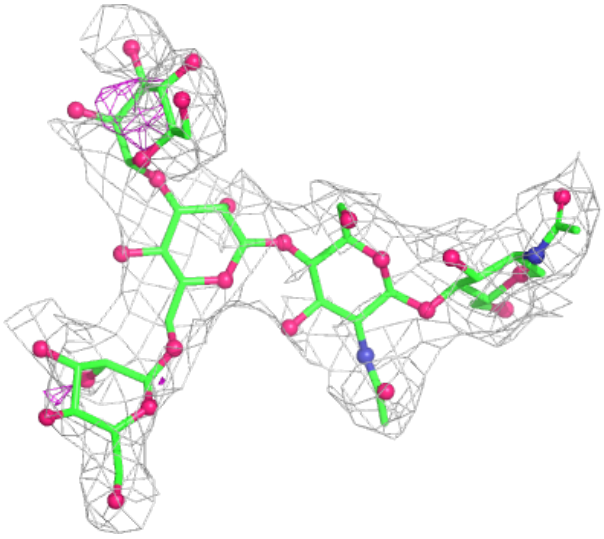
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

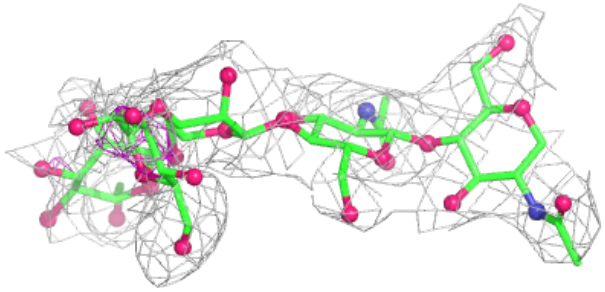
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MAN	C	4	11/12	0.54	0.28	74,100,109,110	0
3	NAG	K	2	14/15	0.72	0.24	94,109,116,123	0
2	MAN	C	5	11/12	0.74	0.27	83,98,104,106	0
4	NAG	G	2	14/15	0.78	0.33	101,106,112,113	0
3	NAG	D	2	14/15	0.80	0.26	97,100,108,113	0
3	NAG	L	2	14/15	0.80	0.28	94,112,117,119	0
3	NAG	I	2	14/15	0.80	0.25	84,93,103,105	0
4	BMA	G	3	11/12	0.81	0.34	94,102,112,112	0
3	NAG	L	1	14/15	0.82	0.21	102,112,122,126	0
3	NAG	J	2	14/15	0.83	0.28	86,102,110,113	0
3	NAG	D	1	14/15	0.83	0.17	91,101,106,107	0
2	MAN	H	4	11/12	0.85	0.18	75,80,95,96	0
4	BMA	E	3	11/12	0.85	0.14	71,86,91,91	0
2	MAN	H	5	11/12	0.86	0.18	65,77,84,87	0
2	BMA	C	3	11/12	0.87	0.14	95,98,103,109	0
3	NAG	K	1	14/15	0.87	0.21	96,103,114,118	0
3	NAG	I	1	14/15	0.88	0.24	71,80,90,92	0
4	NAG	G	1	14/15	0.89	0.16	87,92,101,103	0
4	NAG	F	2	14/15	0.90	0.17	95,105,109,110	0
3	NAG	J	1	14/15	0.90	0.26	78,100,109,112	0
4	BMA	F	3	11/12	0.92	0.14	92,102,106,108	0
2	BMA	H	3	11/12	0.92	0.14	67,75,80,85	0
2	NAG	C	2	14/15	0.93	0.12	68,76,88,91	0
4	NAG	E	2	14/15	0.93	0.13	56,64,76,86	0
2	NAG	C	1	14/15	0.93	0.18	61,70,74,77	0
2	NAG	H	2	14/15	0.93	0.17	56,65,75,75	0
2	NAG	H	1	14/15	0.94	0.18	45,50,54,64	0
4	NAG	F	1	14/15	0.95	0.18	60,72,90,99	0
4	NAG	E	1	14/15	0.96	0.16	42,51,57,59	0

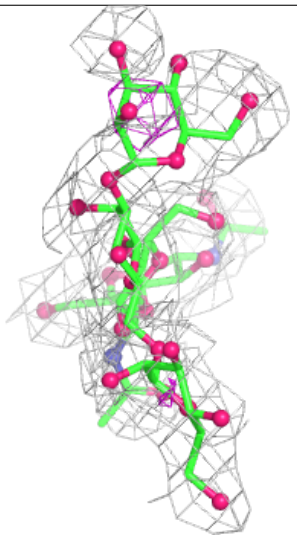
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

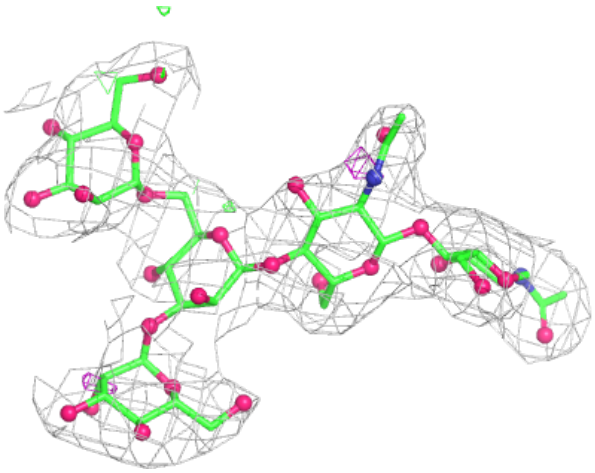


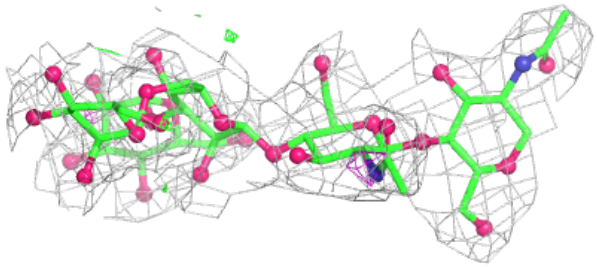


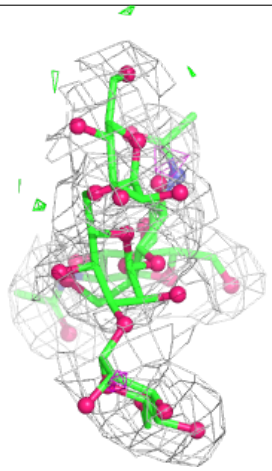


Electron density around Chain H:

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

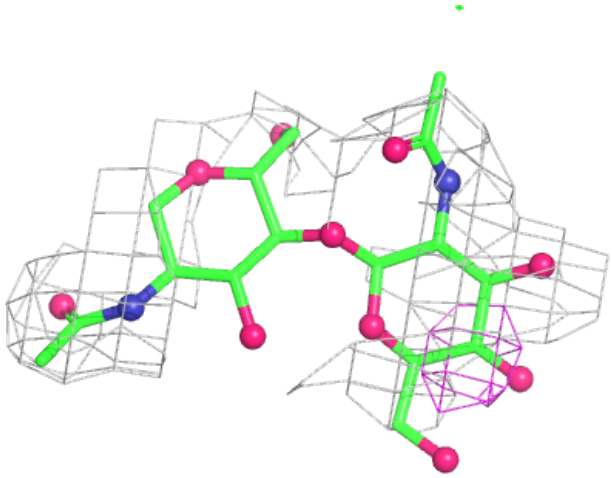


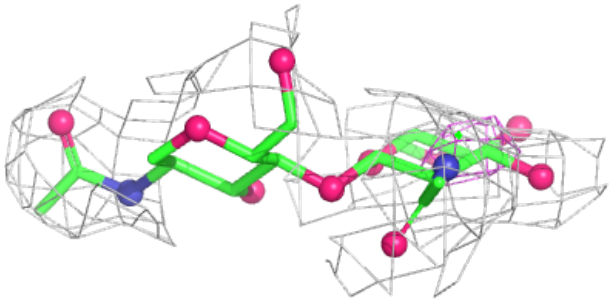


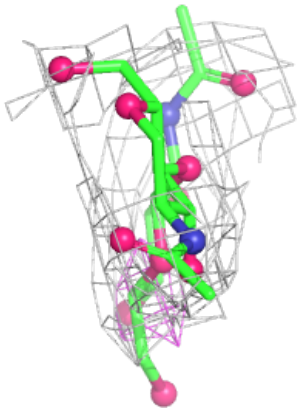


Electron density around Chain D:

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

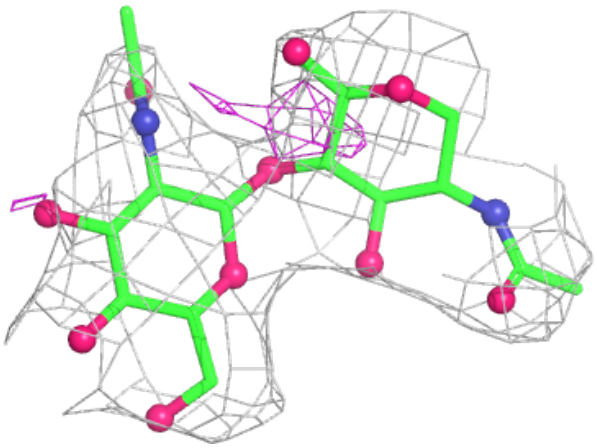


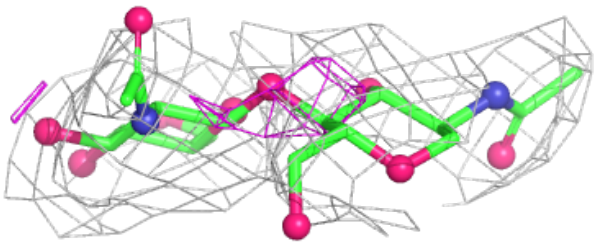


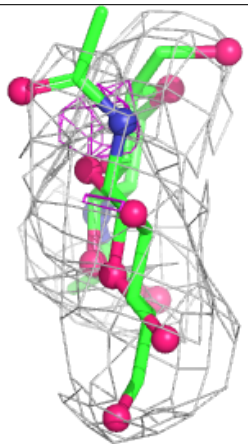


Electron density around Chain I:

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

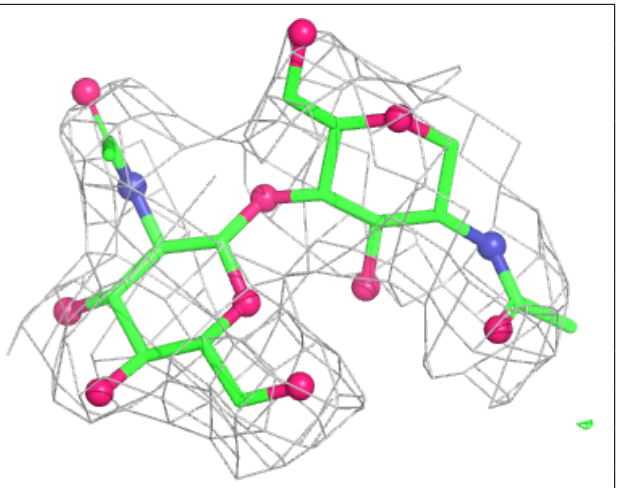


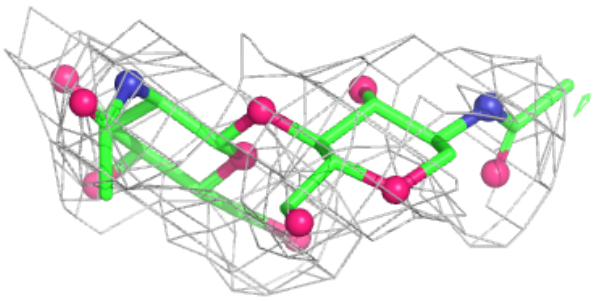


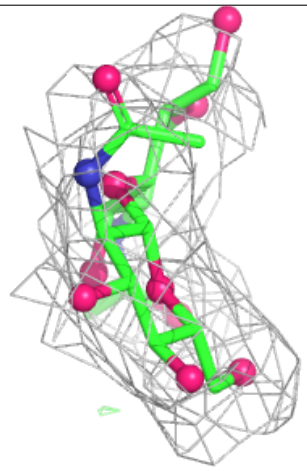


Electron density around Chain J:

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

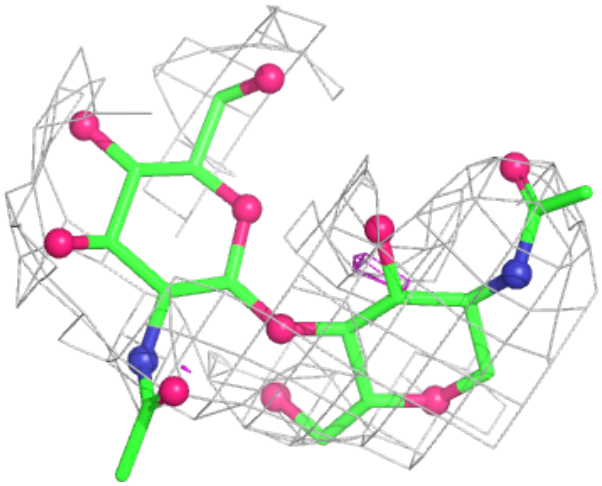


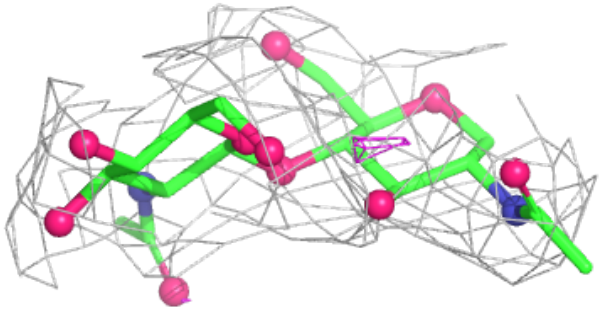


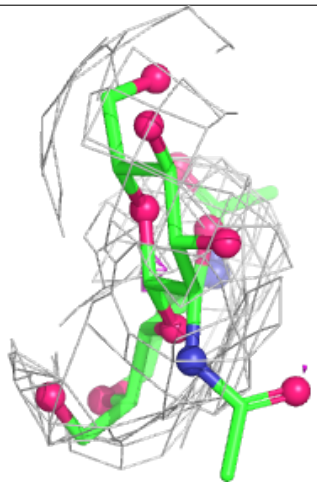


Electron density around Chain K:

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

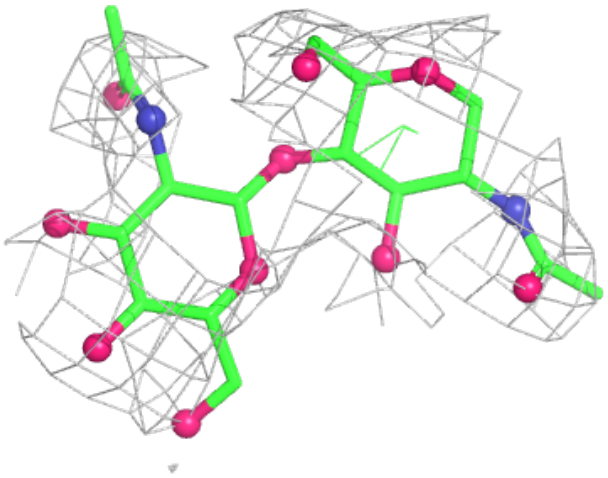


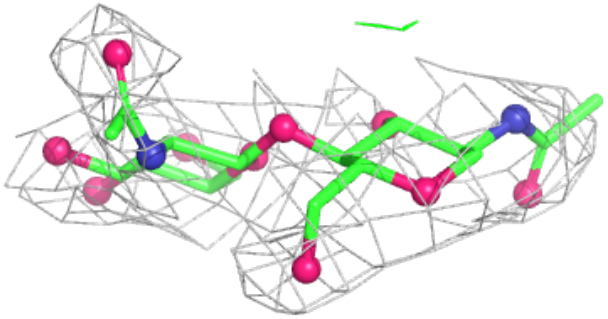


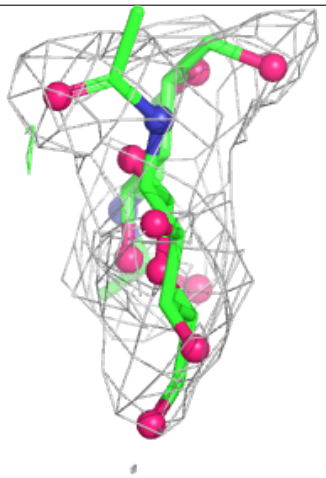


Electron density around Chain L:

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

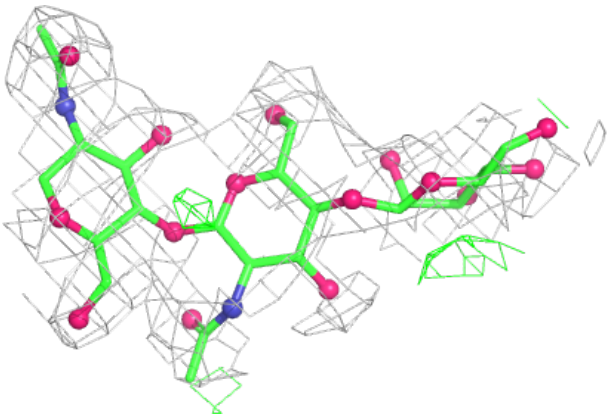


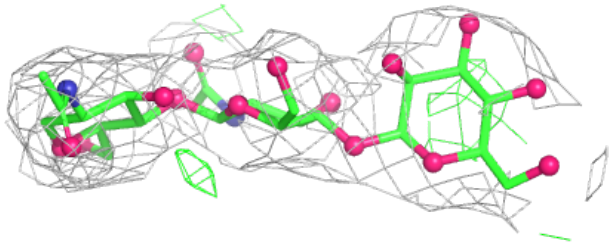


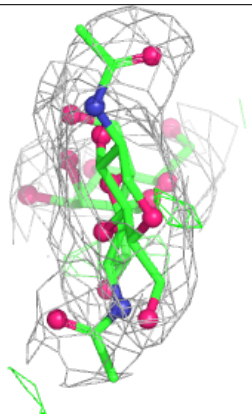


Electron density around Chain E:

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

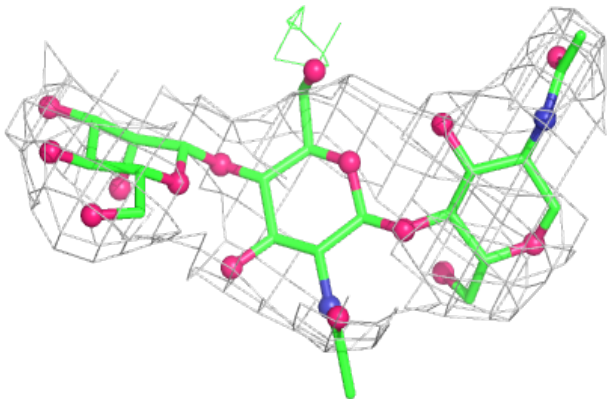


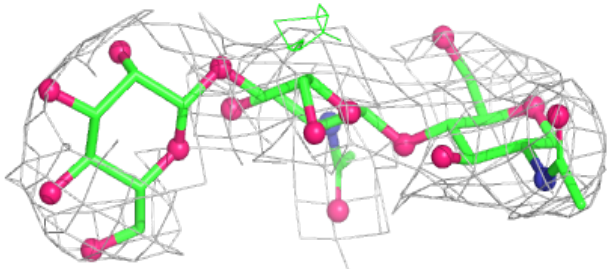


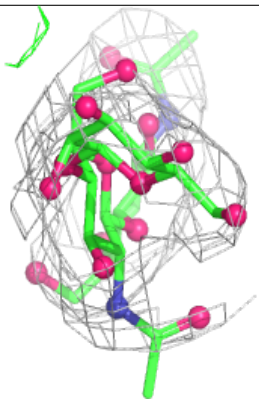


Electron density around Chain F:

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

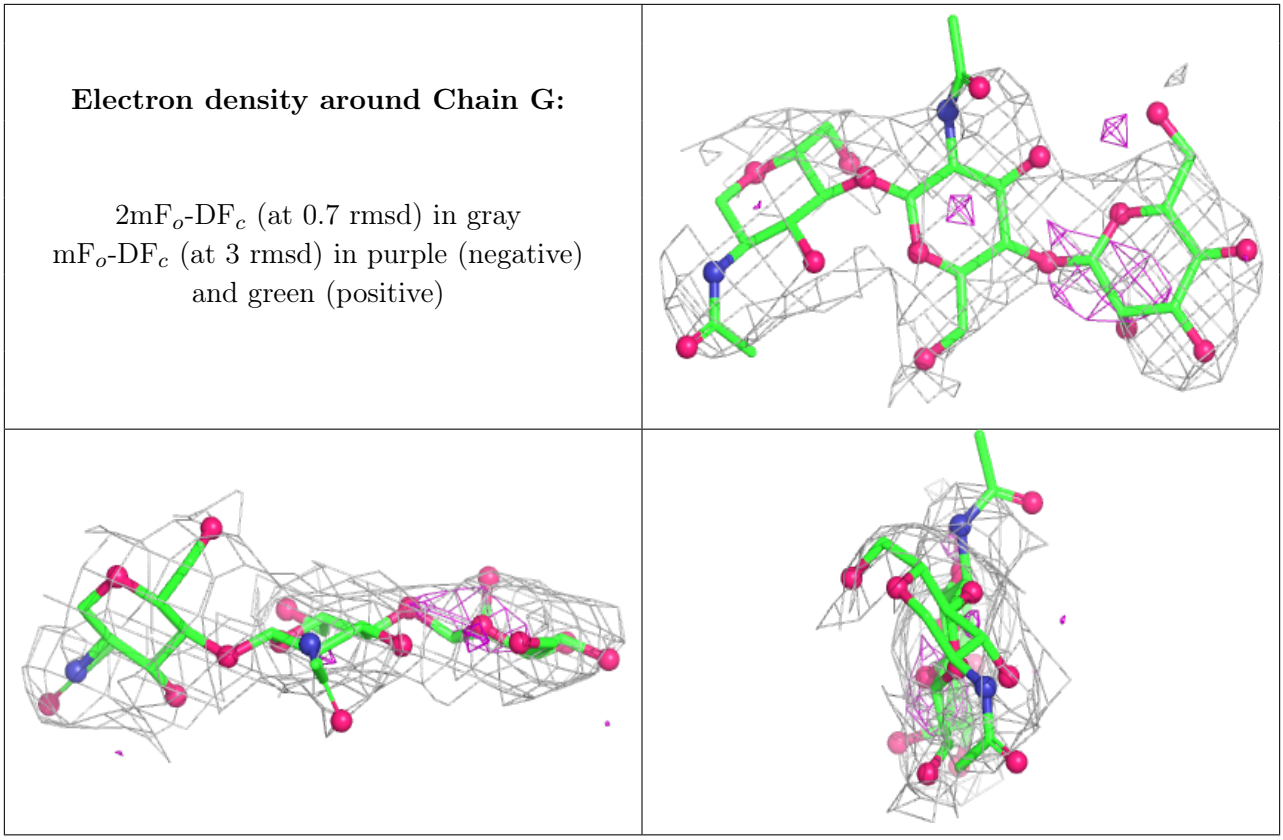






Electron density around Chain G:

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



6.4 Ligands

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, 95^{th} 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	NAG	B	1003	14/15	0.72	0.26	94,104,114,117	0
6	NAG	A	1004	14/15	0.74	0.23	73,90,101,102	0
6	NAG	A	1003	14/15	0.82	0.17	84,97,105,107	0
6	NAG	A	1005	14/15	0.83	0.20	71,91,96,100	0
6	NAG	B	1002	14/15	0.83	0.18	94,102,107,109	0
6	NAG	A	1002	14/15	0.83	0.17	75,91,98,100	0
7	P4G	A	1006	11/11	0.83	0.17	46,74,81,90	0
9	EDO	A	1012	4/4	0.85	0.25	62,70,71,73	0
9	EDO	A	1009	4/4	0.87	0.34	49,50,55,60	0
9	EDO	A	1008	4/4	0.87	0.28	63,67,69,69	0
9	EDO	A	1011	4/4	0.90	0.20	42,47,54,57	0
9	EDO	A	1010	4/4	0.91	0.67	39,54,58,60	0
8	UQE	B	1004	34/34	0.92	0.37	62,78,93,101	0
8	UQE	A	1007[A]	34/34	0.92	0.40	54,63,69,113	34

Continued on next page...

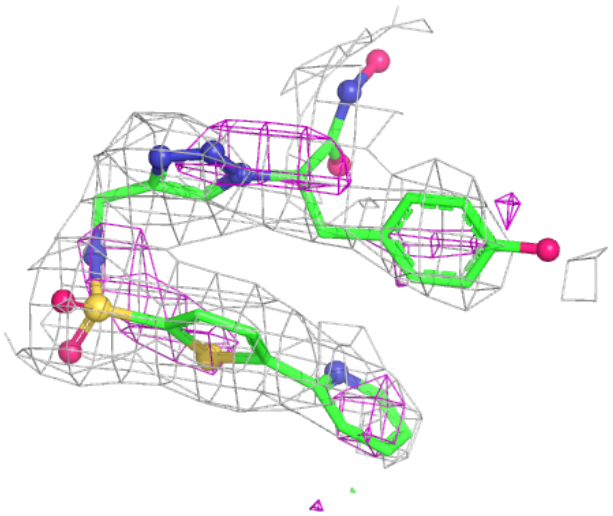
Continued from previous page...

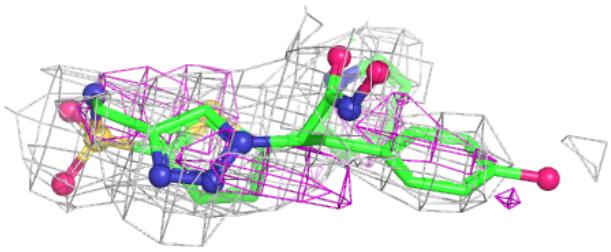
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	UQE	A	1007[B]	34/34	0.92	0.40	53,63,70,109	34
5	ZN	B	1001	1/1	0.99	0.14	51,51,51,51	0
5	ZN	A	1001	1/1	0.99	0.19	30,30,30,30	0

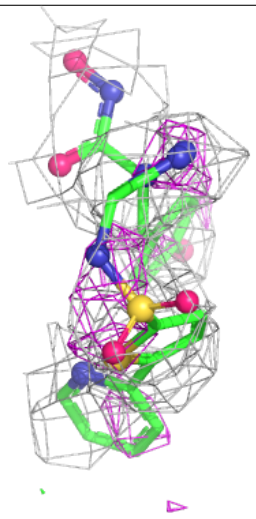
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UQE B 1004:

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

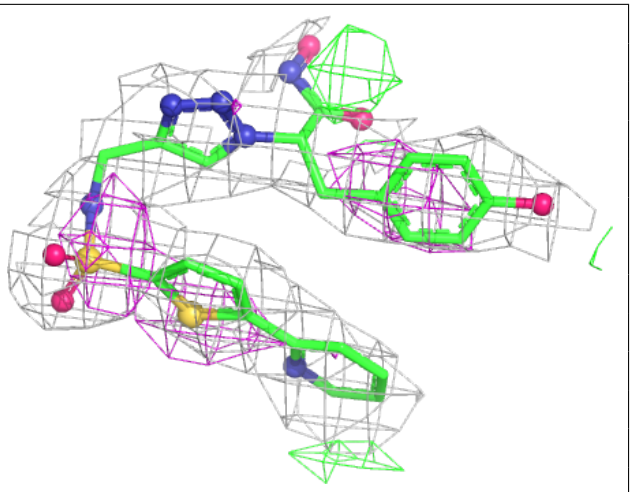


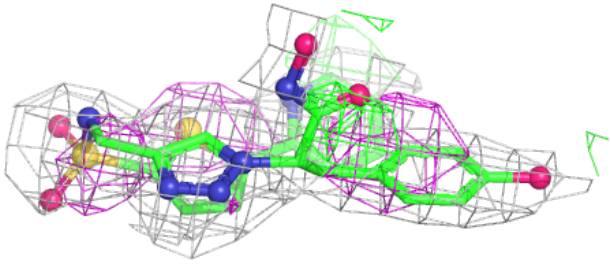


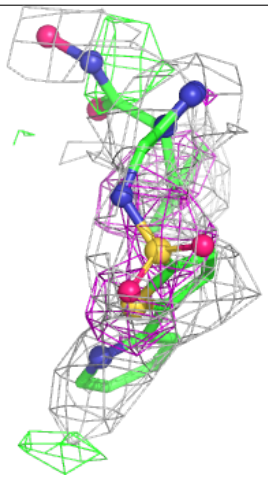


Electron density around UQE A 1007 (A):

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

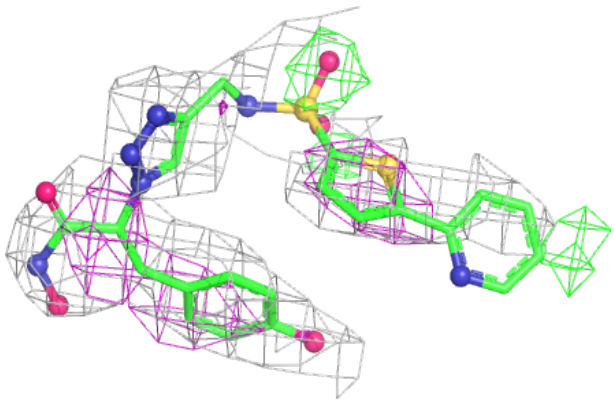


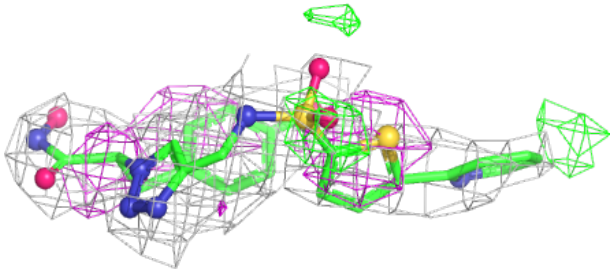


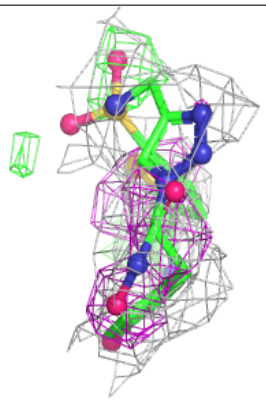


Electron density around UQE A 1007 (B):

$2mF_o$-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

There are no such residues in this entry.