Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 12:19 AM BST

PDB ID	:	5WYX
Title	:	Crystal structure of human TLR8 in complex with CU-CPT8m
Authors	:	Tanji, H.; Ohto, U.; Shimizu, T.
Deposited on	:	2017-01-16
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

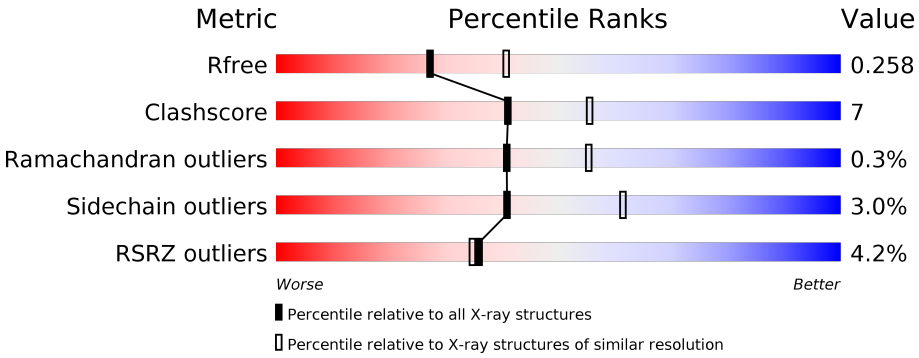
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



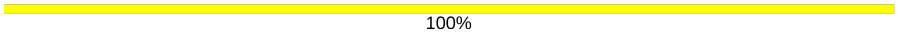
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	811	5% 77% 13% • 8%
1	B	811	3% 81% 9% • 9%
2	C	4	50% 50%
3	D	2	100%
3	G	2	100%
4	E	5	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	F	4	
5	H	4	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12621 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 Toll-like receptor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	750	Total	C	N	O	S	0	0	0
			6038	3861	1026	1132	19			
1	B	739	Total	C	N	O	S	0	0	0
			5957	3810	1012	1116	19			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	-	expression tag	UNP Q9NR97
A	24	SER	-	expression tag	UNP Q9NR97
A	25	PRO	-	expression tag	UNP Q9NR97
A	26	TRP	-	expression tag	UNP Q9NR97
A	828	GLU	-	expression tag	UNP Q9NR97
A	829	PHE	-	expression tag	UNP Q9NR97
A	830	LEU	-	expression tag	UNP Q9NR97
A	831	VAL	-	expression tag	UNP Q9NR97
A	832	PRO	-	expression tag	UNP Q9NR97
A	833	ARG	-	expression tag	UNP Q9NR97
B	23	ARG	-	expression tag	UNP Q9NR97
B	24	SER	-	expression tag	UNP Q9NR97
B	25	PRO	-	expression tag	UNP Q9NR97
B	26	TRP	-	expression tag	UNP Q9NR97
B	828	GLU	-	expression tag	UNP Q9NR97
B	829	PHE	-	expression tag	UNP Q9NR97
B	830	LEU	-	expression tag	UNP Q9NR97
B	831	VAL	-	expression tag	UNP Q9NR97
B	832	PRO	-	expression tag	UNP Q9NR97
B	833	ARG	-	expression tag	UNP Q9NR97

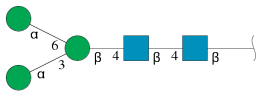
- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	0	0	0
			50	28	2	20			

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

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

- Molecule 4 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.

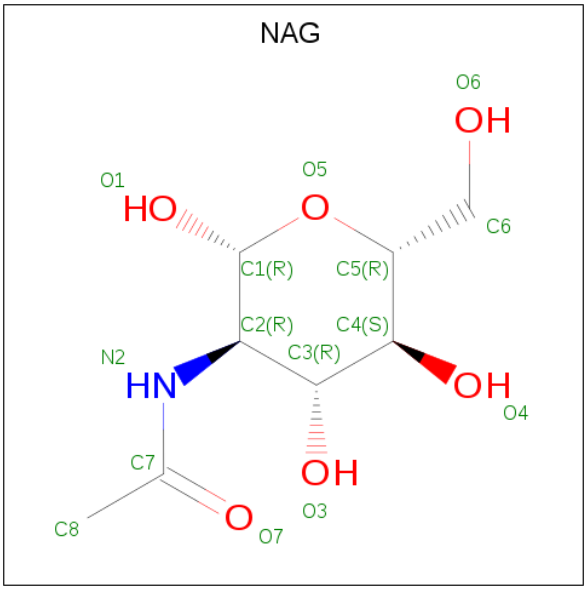


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is an oligosaccharide called 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.

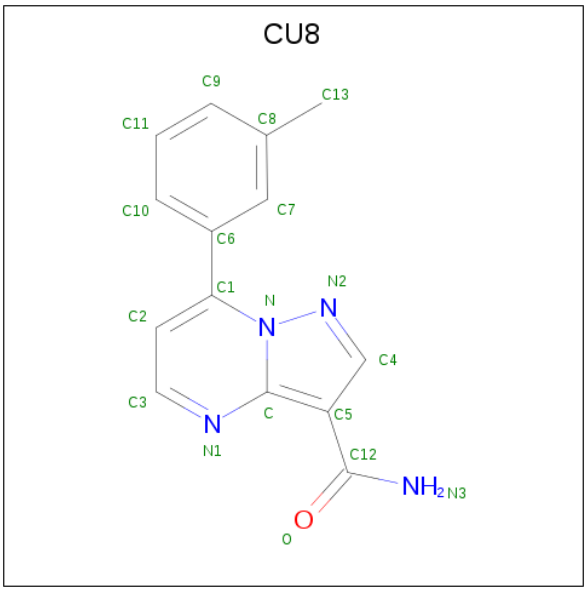
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	F	4	Total C N O 50 28 2 20	0	0	0
5	H	4	Total C N O 50 28 2 20	0	0	0

- 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 7-(3-methylphenyl)pyrazolo[1,5-a]pyrimidine-3-carboxamide (three-letter code: CU8) (formula: $C_{14}H_{12}N_4O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			19	14	4	1		
7	B	1	Total	C	N	O	0	0
			19	14	4	1		

- Molecule 8 is water.

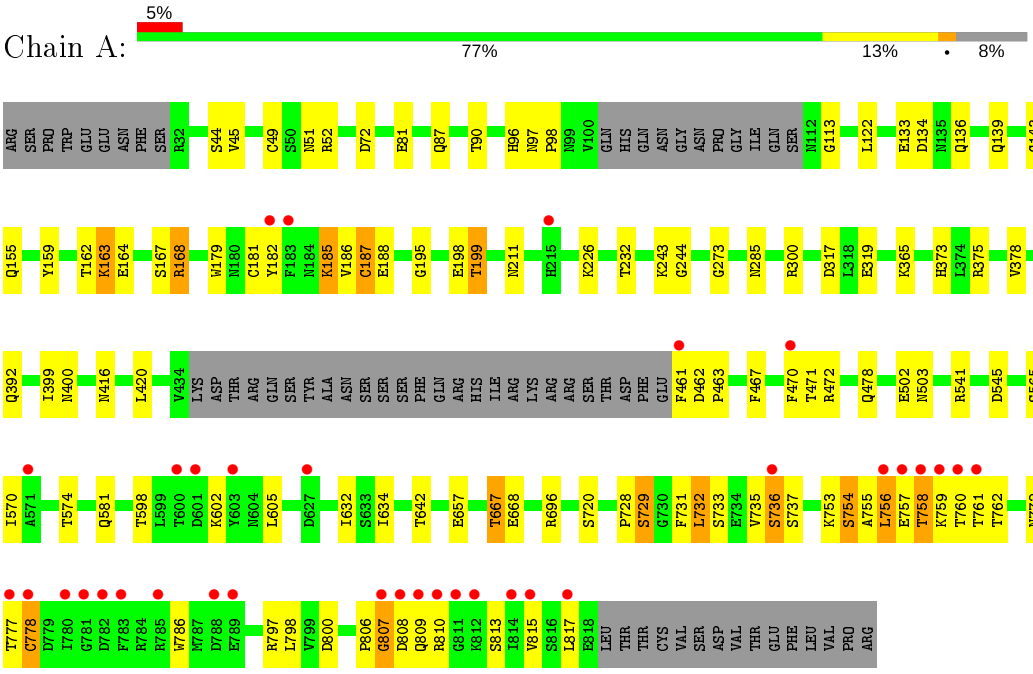
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	133	Total	O	0	0
			133	133		
8	B	104	Total	O	0	0
			104	104		

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.

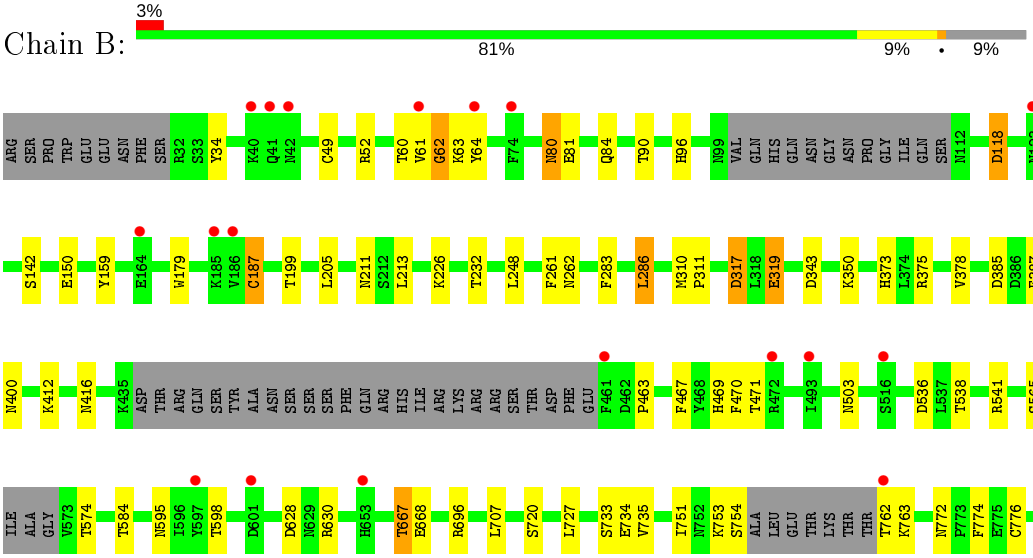
- Molecule 1: Toll-like receptor 8

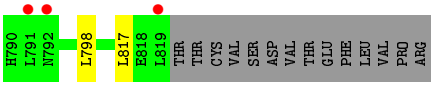
Chain A:



- Molecule 1: Toll-like receptor 8

Chain B:





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

Chain C:

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

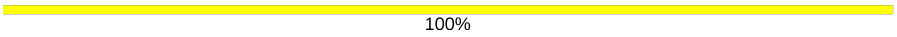
Chain D:

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

Chain G:

• Molecule 4: 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 E:

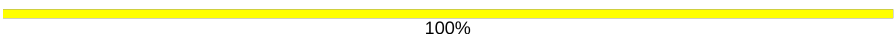


• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

• Molecule 5: 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:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	144.14Å 99.15Å 140.25Å 90.00° 108.07° 90.00°	Depositor
Resolution (Å)	40.16 – 2.40 40.16 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.16-2.40) 99.6 (40.16-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.81 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.201 , 0.256 0.206 , 0.258	Depositor DCC
R_{free} test set	3589 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	50.8	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 40.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12621	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: CU8, BMA, NAG, 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	0.68	0/6162	0.81	2/8358 (0.0%)
1	B	0.68	0/6078	0.78	2/8240 (0.0%)
All	All	0.68	0/12240	0.80	4/16598 (0.0%)

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

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	62	GLY	N-CA-C	-6.09	97.88	113.10
1	B	317	ASP	CB-CG-OD1	-5.65	113.21	118.30
1	A	778	CYS	CA-CB-SG	5.34	123.61	114.00
1	A	163	LYS	N-CA-C	-5.02	97.44	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	185	LYS	Peptide
1	A	187	CYS	Peptide
1	A	807	GLY	Peptide

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	6038	0	6032	116	0
1	B	5957	0	5950	59	0
2	C	50	0	43	2	0
3	D	28	0	25	0	0
3	G	28	0	25	0	0
4	E	61	0	52	0	0
5	F	50	0	43	4	0
5	H	50	0	43	0	0
6	A	56	0	52	0	0
6	B	28	0	26	0	0
7	A	19	0	0	0	0
7	B	19	0	0	0	0
8	A	133	0	0	8	0
8	B	104	0	0	3	0
All	All	12621	0	12291	174	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 7.

All (174) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:GLY:O	1:A:300:ARG:NH2	1.74	1.18
1:A:753:LYS:HA	1:A:756:LEU:HB3	1.45	0.99
1:A:167:SER:HB2	1:A:199:THR:HG21	1.44	0.98
1:A:777:THR:HB	1:A:778:CYS:HA	1.46	0.98
1:B:34:TYR:O	1:B:60:THR:HG21	1.67	0.95
1:B:469:HIS:CD2	1:B:470:PHE:CD2	2.56	0.94
1:A:735:VAL:HA	1:A:736:SER:CB	2.01	0.91
1:A:732:LEU:HD22	1:A:755:ALA:O	1.73	0.87
1:A:735:VAL:HA	1:A:736:SER:HB3	1.57	0.86
1:A:319:GLU:HG2	8:A:1055:HOH:O	1.74	0.85
1:A:167:SER:O	1:A:168:ARG:HB2	1.77	0.84
1:A:167:SER:CB	1:A:199:THR:HG21	2.07	0.83
1:B:62:GLY:HA3	1:B:63:LYS:HG3	1.60	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:HIS:CD2	1:B:470:PHE:HD2	1.99	0.81
1:A:732:LEU:CD2	1:A:755:ALA:O	2.32	0.77
1:B:776:CYS:HB3	1:B:817:LEU:HD21	1.68	0.76
1:A:754:SER:N	1:A:756:LEU:O	2.19	0.75
1:A:187:CYS:SG	1:A:188:GLU:O	2.44	0.75
1:A:186:VAL:HA	1:A:187:CYS:C	2.06	0.74
1:A:732:LEU:O	1:A:762:THR:HG21	1.88	0.73
1:B:469:HIS:NE2	1:B:470:PHE:CD2	2.57	0.72
1:B:319:GLU:OE1	1:B:469:HIS:HB2	1.88	0.72
1:A:807:GLY:HA2	1:A:810:ARG:H	1.54	0.72
1:A:777:THR:CB	1:A:778:CYS:HA	2.19	0.69
1:A:753:LYS:CA	1:A:756:LEU:HB3	2.20	0.68
1:B:226:LYS:NZ	5:F:2:NAG:H81	2.07	0.68
1:A:187:CYS:CB	1:A:188:GLU:O	2.42	0.68
1:A:733:SER:OG	1:A:757:GLU:HG2	1.94	0.67
1:A:545:ASP:OD2	8:A:1001:HOH:O	2.11	0.67
1:A:187:CYS:HB2	1:A:188:GLU:O	1.94	0.67
1:A:122:LEU:HD13	1:A:143:GLY:O	1.95	0.67
1:B:62:GLY:CA	1:B:63:LYS:HG3	2.24	0.67
1:B:63:LYS:O	1:B:64:TYR:HB2	1.95	0.66
1:A:807:GLY:HA3	1:A:810:ARG:HB3	1.75	0.65
1:A:154:ILE:HD13	1:A:463:PRO:HG2	1.79	0.65
1:A:809:GLN:NE2	1:A:817:LEU:HD11	2.11	0.65
1:A:777:THR:HB	1:A:778:CYS:CA	2.27	0.64
1:A:807:GLY:HA2	1:A:809:GLN:N	2.13	0.63
1:A:467:PHE:HB3	2:C:1:NAG:H81	1.81	0.63
1:B:735:VAL:HG23	8:B:1014:HOH:O	1.99	0.63
1:B:375:ARG:HD2	1:B:400:ASN:HD21	1.63	0.62
1:A:632:ILE:HD12	1:A:657:GLU:HG2	1.82	0.61
1:A:735:VAL:HG13	1:A:736:SER:OG	2.01	0.60
1:A:195:GLY:O	1:A:198:GLU:HG2	2.02	0.60
1:A:732:LEU:O	1:A:762:THR:CG2	2.48	0.60
1:A:760:THR:H	1:A:761:THR:HA	1.65	0.60
1:B:584:THR:HG22	8:B:1092:HOH:O	2.02	0.59
1:A:179:TRP:CD1	1:A:463:PRO:HB3	2.38	0.58
1:A:807:GLY:CA	1:A:810:ARG:H	2.15	0.58
1:A:754:SER:H	1:A:756:LEU:C	2.06	0.57
1:A:541:ARG:HA	1:A:565:SER:O	2.03	0.57
1:A:159:TYR:CD1	1:A:187:CYS:HB3	2.40	0.57
1:A:163:LYS:O	1:A:164:GLU:CB	2.52	0.56
1:B:469:HIS:NE2	1:B:470:PHE:CE2	2.73	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ASN:O	1:A:232:THR:HA	2.05	0.56
1:B:80:ASN:N	1:B:80:ASN:OD1	2.39	0.56
1:A:776:CYS:O	1:A:806:PRO:CD	2.55	0.55
1:A:243:LYS:HD2	1:A:285:ASN:HD22	1.72	0.55
1:A:728:PRO:O	1:A:731:PHE:HB3	2.06	0.55
1:A:776:CYS:O	1:A:806:PRO:HD3	2.06	0.55
1:B:226:LYS:HZ2	5:F:2:NAG:H81	1.70	0.55
1:A:243:LYS:HD2	1:A:285:ASN:ND2	2.23	0.54
1:B:211:ASN:O	1:B:232:THR:HA	2.07	0.54
1:B:129:GLU:HG2	1:B:150:GLU:HB3	1.89	0.54
1:A:375:ARG:HD2	1:A:400:ASN:HD21	1.73	0.54
1:A:758:THR:OG1	1:A:759:LYS:HA	2.07	0.54
1:B:317:ASP:HB2	1:B:343:ASP:HB3	1.91	0.53
1:A:756:LEU:HG	1:A:786:TRP:CD1	2.44	0.53
1:B:261:PHE:CE2	1:B:350:LYS:HD3	2.43	0.53
1:B:541:ARG:HA	1:B:565:SER:O	2.08	0.53
1:A:732:LEU:HD23	1:A:732:LEU:C	2.29	0.53
1:A:735:VAL:HA	1:A:736:SER:OG	2.07	0.53
1:A:392:GLN:HB2	8:A:1002:HOH:O	2.08	0.52
1:B:470:PHE:O	1:B:471:THR:HB	2.09	0.52
1:B:469:HIS:NE2	1:B:470:PHE:HD2	1.99	0.52
1:B:734:GLU:HA	1:B:735:VAL:C	2.28	0.52
1:A:226:LYS:NZ	2:C:2:NAG:H81	2.24	0.52
1:A:728:PRO:HB2	1:A:731:PHE:HB2	1.92	0.52
1:B:96:HIS:HD2	1:B:134:ASP:OD2	1.93	0.52
1:A:642:THR:CG2	8:A:1117:HOH:O	2.60	0.50
1:A:181:CYS:SG	1:A:187:CYS:N	2.84	0.50
1:A:605:LEU:HD13	1:A:634:ILE:HG12	1.92	0.50
1:A:777:THR:CB	1:A:778:CYS:CA	2.86	0.50
1:A:566:HIS:HE1	1:B:262:ASN:O	1.95	0.50
1:B:34:TYR:O	1:B:60:THR:CG2	2.49	0.50
1:A:566:HIS:HD2	1:A:568:PHE:H	1.59	0.49
1:A:470:PHE:CZ	1:A:472:ARG:HG2	2.48	0.49
1:A:185:LYS:N	1:A:186:VAL:O	2.45	0.49
1:B:776:CYS:HB3	1:B:817:LEU:CD2	2.41	0.49
1:A:113:GLY:HA3	1:A:136:GLN:HB2	1.95	0.49
1:A:162:THR:C	1:A:163:LYS:O	2.47	0.49
1:A:44:SER:HB3	8:A:1122:HOH:O	2.12	0.49
1:A:797:ARG:NH1	1:A:800:ASP:OD2	2.46	0.49
1:A:96:HIS:HD2	1:A:134:ASP:OD2	1.96	0.49
1:B:373:HIS:HA	1:B:400:ASN:HB3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:VAL:HG12	1:B:62:GLY:N	2.28	0.48
1:A:416:ASN:ND2	8:A:1008:HOH:O	2.46	0.48
1:A:753:LYS:O	1:A:754:SER:OG	2.29	0.48
1:B:261:PHE:CE2	1:B:350:LYS:CD	2.96	0.48
1:A:155:GLN:HE21	1:A:463:PRO:HG3	1.78	0.48
1:A:502:GLU:O	1:A:503:ASN:HB2	2.13	0.47
1:A:185:LYS:CG	1:A:186:VAL:H	2.28	0.47
1:A:729:SER:HA	1:A:754:SER:C	2.34	0.47
1:A:813:SER:OG	1:A:815:VAL:HG22	2.14	0.47
1:B:226:LYS:HZ3	5:F:2:NAG:H81	1.79	0.47
1:B:179:TRP:CD1	1:B:463:PRO:HB3	2.49	0.47
1:A:731:PHE:O	1:A:732:LEU:HD22	2.14	0.47
1:A:146:GLU:CD	1:A:146:GLU:H	2.17	0.47
1:A:754:SER:H	1:A:756:LEU:CA	2.28	0.47
1:B:387:PHE:O	1:B:391:MET:HG3	2.15	0.47
1:B:707:LEU:HD23	1:B:735:VAL:HG11	1.96	0.46
1:B:283:PHE:HA	1:B:286:LEU:HD22	1.96	0.46
1:B:772:ASN:HB2	1:B:774:PHE:CE2	2.50	0.46
1:A:733:SER:HB2	1:A:757:GLU:HB3	1.97	0.46
1:A:807:GLY:HA2	1:A:808:ASP:C	2.36	0.46
1:B:467:PHE:HB3	5:F:1:NAG:H81	1.98	0.46
1:A:461:PHE:CG	1:A:462:ASP:N	2.83	0.45
1:A:817:LEU:HA	8:A:1077:HOH:O	2.16	0.45
1:A:373:HIS:HA	1:A:400:ASN:HB3	1.98	0.45
1:A:243:LYS:CB	1:A:244:GLY:HA2	2.46	0.45
1:A:735:VAL:HG12	1:A:737:SER:N	2.31	0.45
1:B:667:THR:HG22	1:B:668:GLU:HG3	1.97	0.45
1:A:182:TYR:HD1	1:A:182:TYR:H	1.63	0.45
1:A:696:ARG:HG2	1:A:720:SER:OG	2.16	0.45
1:A:753:LYS:CB	1:A:756:LEU:HD13	2.46	0.45
1:B:470:PHE:O	1:B:471:THR:CB	2.64	0.45
1:B:412:LYS:HB3	1:B:503:ASN:HB3	1.99	0.44
1:B:310:MET:N	1:B:311:PRO:HD3	2.32	0.44
1:A:807:GLY:HA2	1:A:810:ARG:N	2.28	0.44
1:B:205:LEU:HD23	1:B:205:LEU:C	2.37	0.44
1:B:159:TYR:CG	1:B:187:CYS:HB2	2.53	0.44
1:B:696:ARG:HG2	1:B:720:SER:OG	2.18	0.44
1:A:735:VAL:CA	1:A:736:SER:CB	2.84	0.44
1:A:574:THR:HG22	1:A:598:THR:HG23	2.00	0.44
1:A:181:CYS:HB2	1:A:187:CYS:HB3	1.93	0.44
1:A:733:SER:CB	1:A:757:GLU:HB3	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:584:THR:CG2	8:B:1092:HOH:O	2.63	0.43
1:B:118:ASP:N	1:B:118:ASP:OD2	2.51	0.43
1:A:754:SER:N	1:A:756:LEU:N	2.66	0.43
1:A:756:LEU:HD23	1:A:756:LEU:C	2.39	0.43
1:A:185:LYS:O	1:A:187:CYS:O	2.35	0.43
1:A:667:THR:HG22	1:A:668:GLU:HG3	2.01	0.43
1:B:733:SER:O	1:B:734:GLU:C	2.57	0.43
1:A:97:ASN:HA	1:A:98:PRO:HA	1.81	0.43
1:B:471:THR:HG22	1:B:471:THR:O	2.19	0.43
1:A:122:LEU:HD12	1:A:122:LEU:HA	1.81	0.43
1:A:133:GLU:CG	1:A:154:ILE:HG13	2.49	0.43
1:B:536:ASP:OD1	1:B:538:THR:HG23	2.18	0.43
1:A:568:PHE:C	1:A:570:ILE:H	2.21	0.42
1:A:733:SER:OG	1:A:757:GLU:CG	2.64	0.42
1:A:735:VAL:HG12	1:A:737:SER:H	1.84	0.42
1:A:754:SER:HA	1:A:755:ALA:C	2.40	0.42
1:B:310:MET:N	1:B:311:PRO:CD	2.83	0.42
1:A:51:ASN:HA	1:A:72:ASP:O	2.19	0.42
1:A:133:GLU:HG2	1:A:154:ILE:HG13	2.00	0.42
1:B:574:THR:HG22	1:B:598:THR:HG23	2.01	0.41
1:A:757:GLU:HG3	1:A:758:THR:N	2.34	0.41
1:B:628:ASP:HB2	1:B:630:ARG:HD3	2.02	0.41
1:B:707:LEU:HD23	1:B:735:VAL:CG1	2.50	0.41
1:A:155:GLN:HE21	1:A:463:PRO:CG	2.34	0.41
1:A:735:VAL:CA	1:A:736:SER:HB3	2.39	0.41
1:B:753:LYS:O	1:B:754:SER:C	2.59	0.41
1:B:727:LEU:HD23	1:B:751:ILE:HG23	2.03	0.41
1:A:776:CYS:C	1:A:777:THR:HG23	2.41	0.41
1:A:365:LYS:NZ	8:A:1015:HOH:O	2.53	0.41
1:A:776:CYS:HB3	1:A:777:THR:CG2	2.50	0.41
1:A:772:ASN:HB2	1:A:774:PHE:CE2	2.56	0.41
1:A:399:ILE:HG13	1:A:420:LEU:HD21	2.02	0.40
1:B:375:ARG:HD2	1:B:400:ASN:ND2	2.32	0.40
1:A:375:ARG:HD2	1:A:400:ASN:ND2	2.35	0.40
1:B:763:LYS:HA	1:B:763:LYS:HD3	1.90	0.40
1:A:753:LYS:HB3	1:A:756:LEU:HD13	2.03	0.40
1:A:798:LEU:HD23	1:A:798:LEU:HA	1.96	0.40
1:B:319:GLU:HG3	1:B:319:GLU:H	1.64	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	744/811 (92%)	692 (93%)	48 (6%)	4 (0%)	29	41
1	B	729/811 (90%)	686 (94%)	42 (6%)	1 (0%)	51	68
All	All	1473/1622 (91%)	1378 (94%)	90 (6%)	5 (0%)	41	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	168	ARG
1	A	736	SER
1	A	378	VAL
1	B	378	VAL
1	A	754	SER

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	697/755 (92%)	676 (97%)	21 (3%)	41	61
1	B	689/755 (91%)	668 (97%)	21 (3%)	41	61
All	All	1386/1510 (92%)	1344 (97%)	42 (3%)	41	61

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	49	CYS
1	A	52	ARG
1	A	81	GLU
1	A	87	GLN
1	A	90	THR
1	A	139	GLN
1	A	146	GLU
1	A	199	THR
1	A	317	ASP
1	A	384	GLU
1	A	388	GLN
1	A	471	THR
1	A	478	GLN
1	A	581	GLN
1	A	602	LYS
1	A	667	THR
1	A	729	SER
1	A	732	LEU
1	A	756	LEU
1	A	758	THR
1	B	49	CYS
1	B	52	ARG
1	B	80	ASN
1	B	81	GLU
1	B	84	GLN
1	B	90	THR
1	B	118	ASP
1	B	142	SER
1	B	187	CYS
1	B	199	THR
1	B	213	LEU
1	B	248	LEU
1	B	286	LEU
1	B	319	GLU
1	B	385	ASP
1	B	416	ASN
1	B	595	ASN
1	B	667	THR
1	B	762	THR
1	B	780	ILE
1	B	798	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	96	HIS
1	A	155	GLN
1	A	285	ASN
1	A	469	HIS
1	A	499	ASN
1	A	566	HIS
1	A	581	GLN
1	A	604	ASN
1	B	77	HIS
1	B	87	GLN
1	B	96	HIS
1	B	99	ASN
1	B	160	ASN
1	B	585	ASN
1	B	686	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

21 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	0.90	1 (7%)	17,19,21	1.75	3 (17%)
2	NAG	C	2	2	14,14,15	0.60	0	17,19,21	1.53	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BMA	C	3	2	11,11,12	0.90	0	15,15,17	1.75	5 (33%)
2	MAN	C	4	2	11,11,12	0.79	0	15,15,17	1.51	3 (20%)
3	NAG	D	1	1,3	14,14,15	1.12	1 (7%)	17,19,21	1.73	4 (23%)
3	NAG	D	2	3	14,14,15	1.10	1 (7%)	17,19,21	1.73	6 (35%)
4	NAG	E	1	1,4	14,14,15	0.60	0	17,19,21	1.45	3 (17%)
4	NAG	E	2	4	14,14,15	1.04	1 (7%)	17,19,21	1.64	5 (29%)
4	BMA	E	3	4	11,11,12	0.65	0	15,15,17	1.64	4 (26%)
4	MAN	E	4	4	11,11,12	0.62	0	15,15,17	1.16	2 (13%)
4	MAN	E	5	4	11,11,12	0.66	0	15,15,17	1.90	5 (33%)
5	NAG	F	1	1,5	14,14,15	0.74	0	17,19,21	1.51	3 (17%)
5	NAG	F	2	5	14,14,15	1.08	1 (7%)	17,19,21	2.03	7 (41%)
5	BMA	F	3	5	11,11,12	0.92	0	15,15,17	1.40	2 (13%)
5	MAN	F	4	5	11,11,12	1.09	1 (9%)	15,15,17	2.54	5 (33%)
3	NAG	G	1	1,3	14,14,15	1.17	2 (14%)	17,19,21	1.64	4 (23%)
3	NAG	G	2	3	14,14,15	0.72	0	17,19,21	1.14	1 (5%)
5	NAG	H	1	1,5	14,14,15	0.84	0	17,19,21	1.36	2 (11%)
5	NAG	H	2	5	14,14,15	0.92	1 (7%)	17,19,21	1.59	5 (29%)
5	BMA	H	3	5	11,11,12	0.88	0	15,15,17	1.84	5 (33%)
5	MAN	H	4	5	11,11,12	0.68	0	15,15,17	1.74	2 (13%)

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	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	1/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	2/2/19/22	0/1/1/1
4	MAN	E	5	4	-	1/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	4	MAN	C2-C3	3.33	1.57	1.52
5	F	2	NAG	O5-C1	-2.67	1.39	1.43
4	E	2	NAG	O5-C1	-2.55	1.39	1.43
5	H	2	NAG	O5-C1	-2.21	1.40	1.43
3	D	1	NAG	O5-C1	-2.11	1.40	1.43
3	G	1	NAG	C2-N2	-2.10	1.42	1.46
2	C	1	NAG	C1-C2	-2.07	1.49	1.52
3	D	2	NAG	O5-C1	-2.07	1.40	1.43
3	G	1	NAG	O5-C1	-2.02	1.40	1.43

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	4	MAN	C1-C2-C3	6.18	117.27	109.67
5	H	4	MAN	O5-C5-C6	5.73	116.18	107.20
4	E	5	MAN	O5-C5-C6	4.75	114.66	107.20
2	C	1	NAG	O5-C1-C2	-4.47	104.22	111.29
3	D	2	NAG	O5-C5-C6	4.45	114.19	107.20
5	F	4	MAN	O5-C5-C6	4.40	114.11	107.20
5	F	2	NAG	O5-C1-C2	-4.21	104.64	111.29
5	H	3	BMA	C1-C2-C3	3.86	114.41	109.67
2	C	3	BMA	O5-C5-C6	3.84	113.22	107.20
4	E	2	NAG	C4-C3-C2	-3.50	105.89	111.02
5	F	1	NAG	O5-C1-C2	-3.47	105.81	111.29
5	H	3	BMA	C2-C3-C4	-3.44	104.93	110.89
5	F	4	MAN	C2-C3-C4	3.37	116.72	110.89
5	F	3	BMA	O5-C1-C2	-3.24	105.77	110.77
3	G	1	NAG	O3-C3-C4	3.16	117.66	110.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	2	NAG	C4-C3-C2	-3.14	106.42	111.02
5	F	2	NAG	O7-C7-C8	-3.10	116.30	122.06
3	D	1	NAG	C1-C2-N2	-3.09	105.22	110.49
5	H	1	NAG	C1-O5-C5	3.07	116.35	112.19
4	E	3	BMA	O3-C3-C2	3.06	115.86	109.99
4	E	1	NAG	O5-C1-C2	-2.98	106.58	111.29
2	C	3	BMA	C3-C4-C5	2.94	115.49	110.24
4	E	5	MAN	O5-C1-C2	-2.93	106.25	110.77
3	D	1	NAG	C6-C5-C4	-2.90	106.22	113.00
2	C	1	NAG	O7-C7-C8	-2.87	116.72	122.06
3	G	1	NAG	C1-C2-N2	-2.86	105.61	110.49
2	C	2	NAG	O5-C1-C2	-2.85	106.78	111.29
5	H	2	NAG	O6-C6-C5	-2.84	101.55	111.29
3	D	1	NAG	C1-O5-C5	-2.82	108.38	112.19
5	F	2	NAG	O5-C5-C6	2.81	111.62	107.20
5	F	2	NAG	C3-C4-C5	-2.80	105.25	110.24
5	H	3	BMA	O3-C3-C4	2.74	116.68	110.35
5	F	3	BMA	O5-C5-C6	2.72	111.47	107.20
2	C	4	MAN	C3-C4-C5	2.65	114.97	110.24
5	F	2	NAG	C1-C2-N2	2.62	114.97	110.49
5	F	1	NAG	O3-C3-C2	2.62	114.89	109.47
4	E	3	BMA	O5-C1-C2	-2.60	106.75	110.77
3	G	1	NAG	C4-C3-C2	-2.58	107.24	111.02
5	H	2	NAG	C1-O5-C5	2.57	115.67	112.19
4	E	1	NAG	C8-C7-N2	2.57	120.44	116.10
5	F	4	MAN	O5-C1-C2	-2.56	106.81	110.77
4	E	3	BMA	C1-O5-C5	-2.55	108.74	112.19
4	E	2	NAG	C6-C5-C4	-2.52	107.11	113.00
5	H	3	BMA	O4-C4-C5	-2.50	103.08	109.30
3	D	2	NAG	C1-O5-C5	2.48	115.56	112.19
2	C	2	NAG	O5-C5-C6	2.45	111.05	107.20
4	E	4	MAN	O2-C2-C1	-2.45	104.14	109.15
3	D	2	NAG	O5-C1-C2	-2.42	107.46	111.29
3	G	1	NAG	O3-C3-C2	-2.41	104.48	109.47
2	C	2	NAG	C1-O5-C5	-2.39	108.95	112.19
4	E	3	BMA	O4-C4-C3	-2.38	104.84	110.35
2	C	3	BMA	O4-C4-C3	-2.35	104.92	110.35
3	G	2	NAG	O5-C1-C2	-2.33	107.61	111.29
2	C	1	NAG	C4-C3-C2	2.33	114.43	111.02
2	C	3	BMA	C1-O5-C5	2.32	115.34	112.19
5	F	2	NAG	C1-O5-C5	-2.31	109.06	112.19
3	D	1	NAG	O5-C5-C6	2.29	110.79	107.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	5	MAN	C1-O5-C5	-2.27	109.12	112.19
5	H	4	MAN	O5-C1-C2	-2.26	107.28	110.77
2	C	3	BMA	O6-C6-C5	2.24	118.97	111.29
4	E	2	NAG	O5-C5-C6	2.23	110.71	107.20
5	F	4	MAN	O2-C2-C3	2.22	114.58	110.14
5	H	2	NAG	C6-C5-C4	-2.21	107.83	113.00
2	C	4	MAN	C2-C3-C4	2.19	114.68	110.89
5	H	2	NAG	O4-C4-C5	-2.18	103.88	109.30
5	F	1	NAG	O7-C7-N2	2.18	125.96	121.95
2	C	4	MAN	O3-C3-C4	-2.17	105.32	110.35
5	F	2	NAG	C8-C7-N2	2.17	119.78	116.10
2	C	2	NAG	O7-C7-C8	-2.15	118.06	122.06
4	E	1	NAG	O4-C4-C3	-2.15	105.38	110.35
3	D	2	NAG	C3-C4-C5	-2.14	106.42	110.24
4	E	2	NAG	O4-C4-C5	-2.13	104.00	109.30
3	D	2	NAG	C1-C2-N2	2.11	114.09	110.49
4	E	5	MAN	O2-C2-C1	-2.07	104.92	109.15
5	H	3	BMA	O5-C5-C6	2.06	110.44	107.20
4	E	5	MAN	C2-C3-C4	2.05	114.45	110.89
5	H	1	NAG	C1-C2-N2	2.04	113.97	110.49
4	E	2	NAG	O5-C5-C4	-2.03	105.88	110.83
4	E	4	MAN	O3-C3-C2	2.01	113.85	109.99
3	D	2	NAG	C4-C3-C2	-2.01	108.07	111.02

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	4	MAN	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
5	F	2	NAG	C8-C7-N2-C2
5	F	2	NAG	O7-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
4	E	4	MAN	C4-C5-C6-O6
5	F	4	MAN	O5-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6
5	H	4	MAN	O5-C5-C6-O6
4	E	4	MAN	O5-C5-C6-O6
4	E	5	MAN	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	F	2	NAG	O5-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6

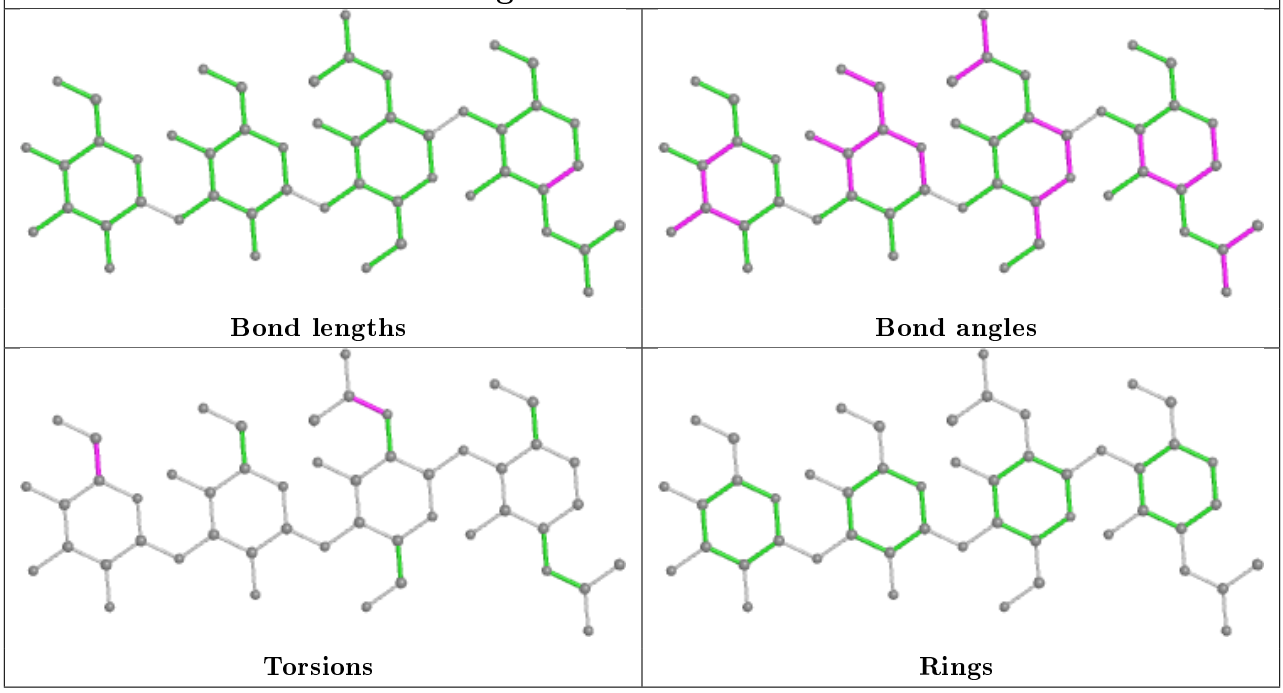
There are no ring outliers.

4 monomers are involved in 6 short contacts:

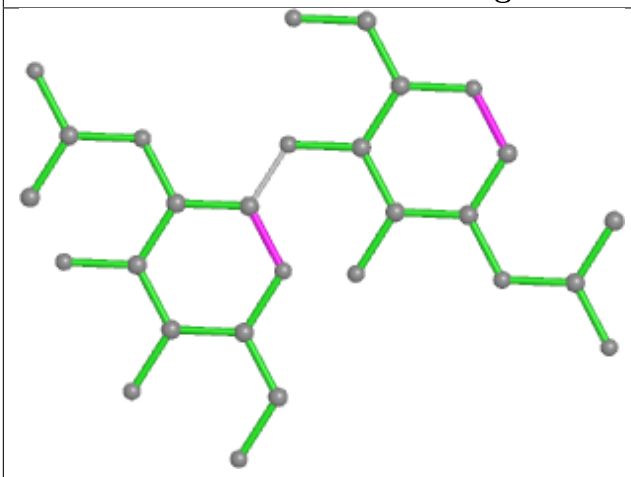
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0
5	F	2	NAG	3	0
5	F	1	NAG	1	0
2	C	2	NAG	1	0

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

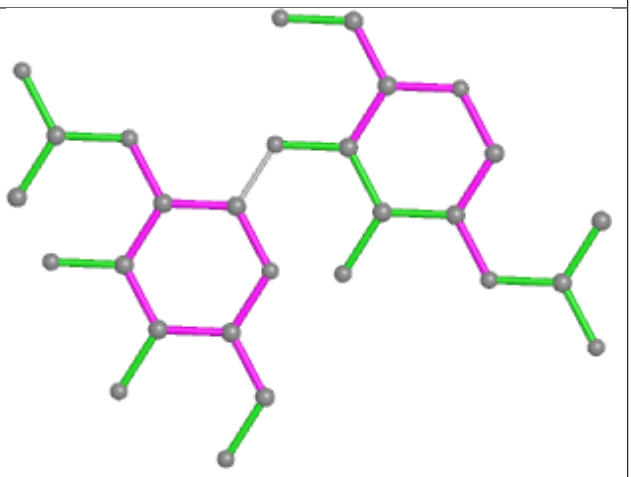
Oligosaccharide Chain C



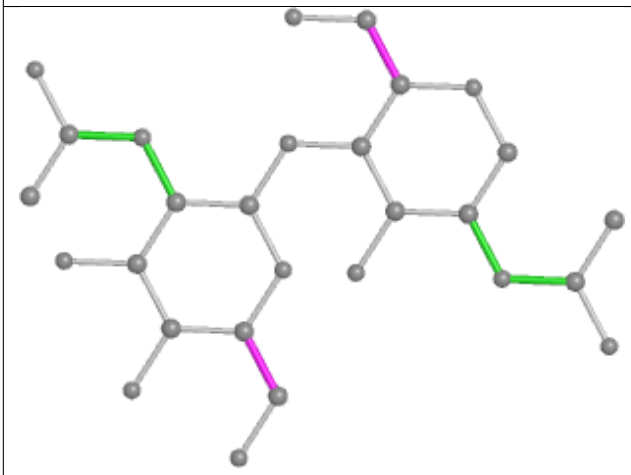
Oligosaccharide Chain D



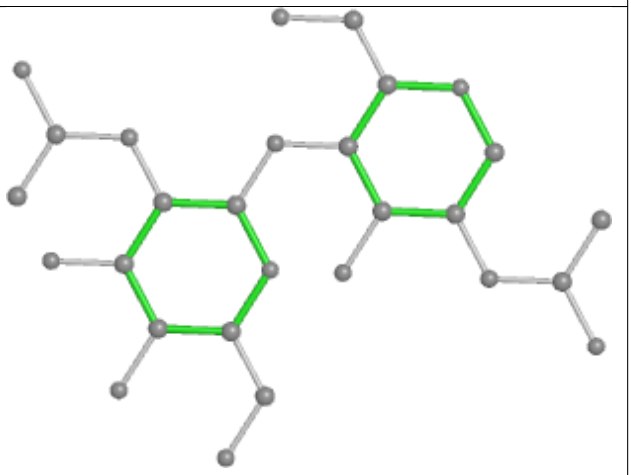
Bond lengths



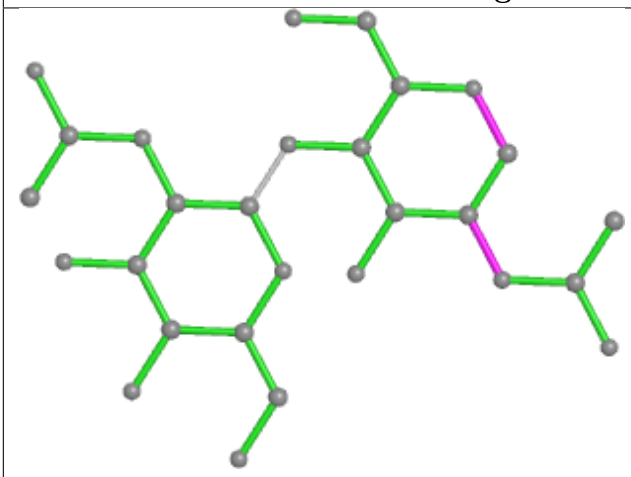
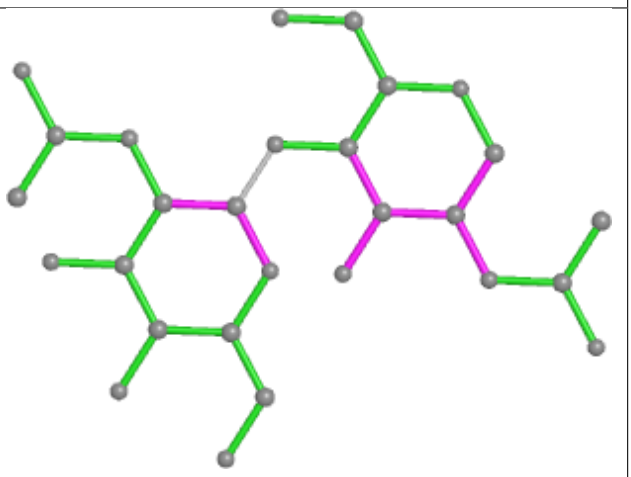
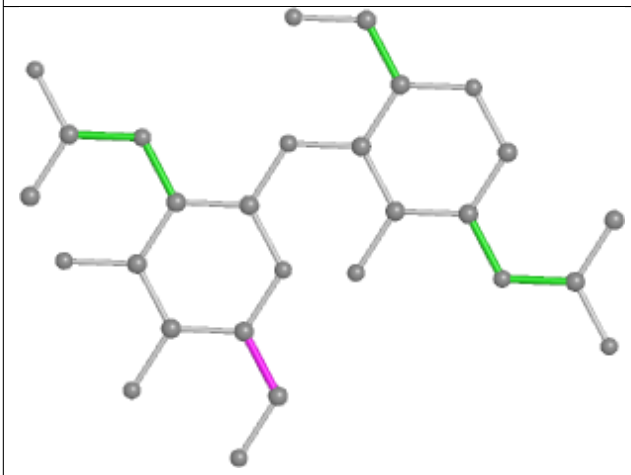
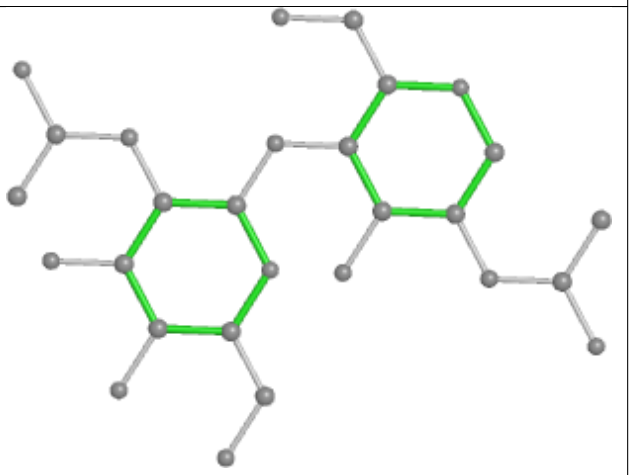
Bond angles



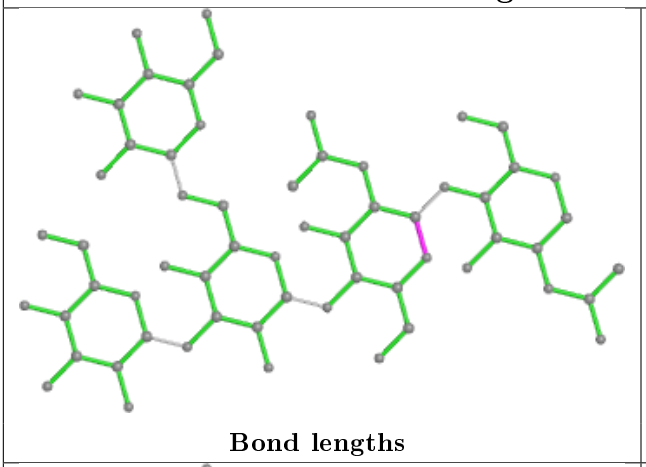
Torsions



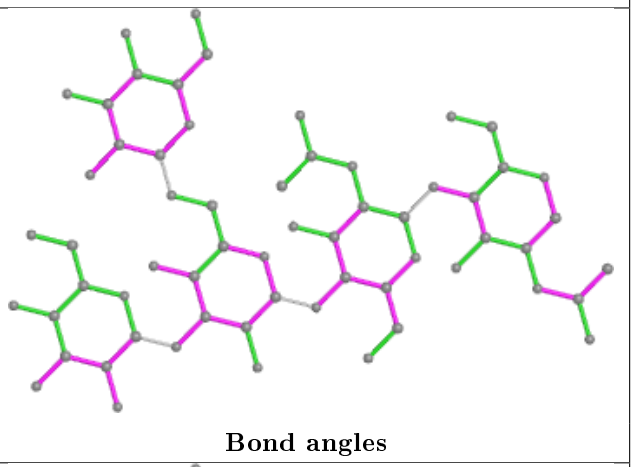
Rings

Oligosaccharide Chain G	
 Bond lengths	 Bond angles
 Torsions	 Rings

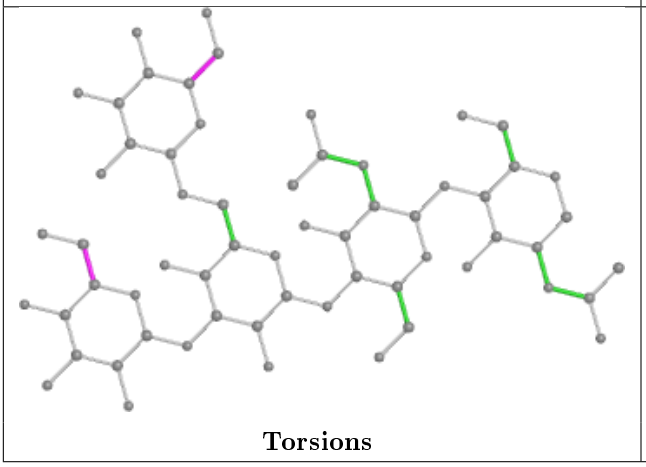
Oligosaccharide Chain E



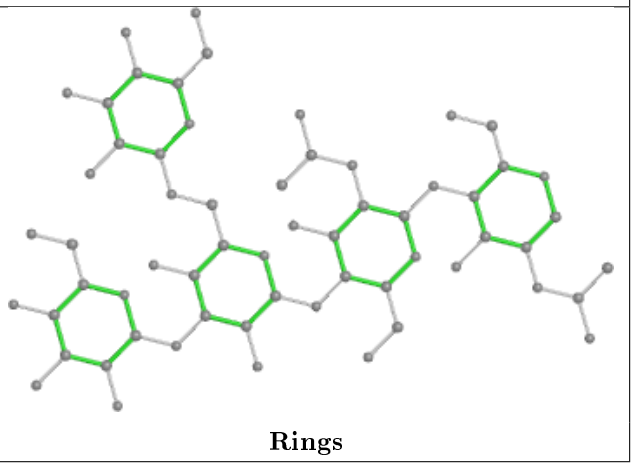
Bond lengths



Bond angles

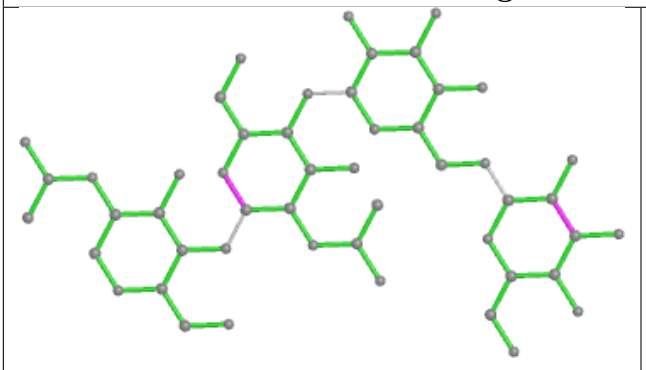


Torsions

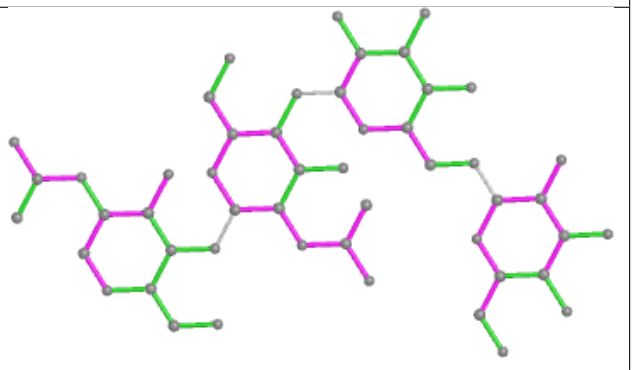


Rings

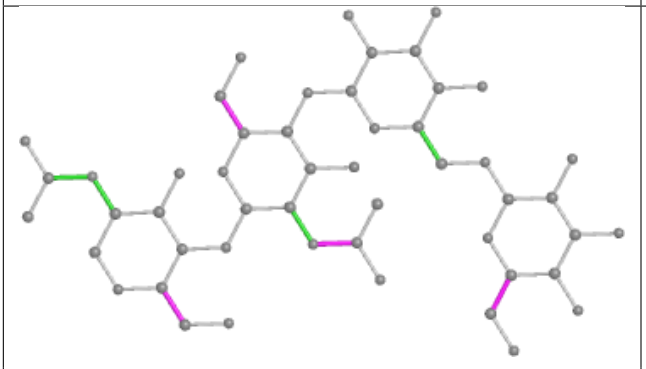
Oligosaccharide Chain F



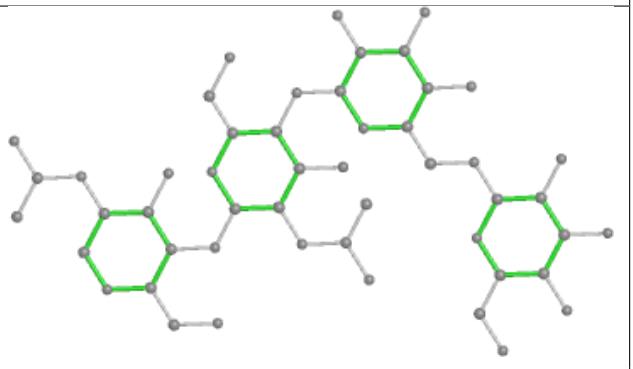
Bond lengths



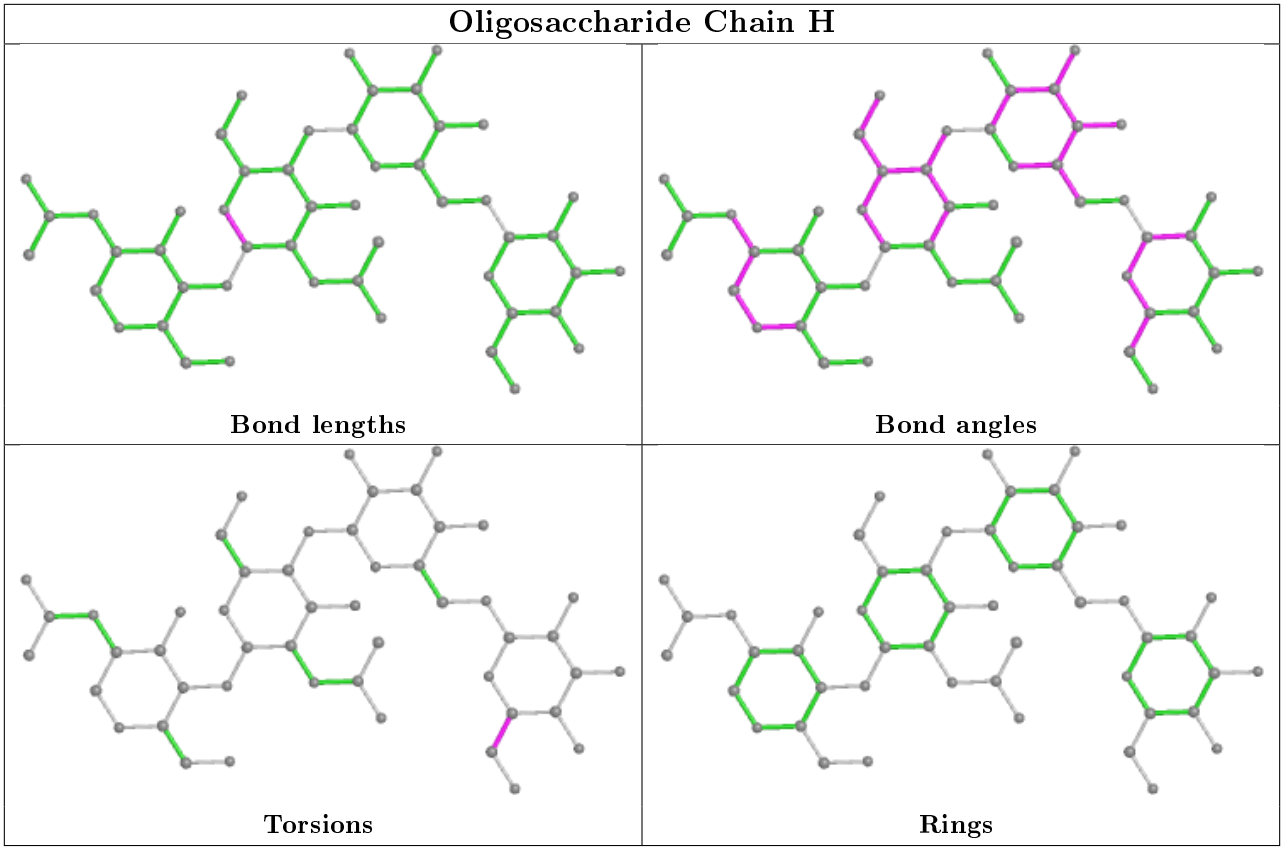
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	A	915	1	14,14,15	0.67	0	17,19,21	1.55	3 (17%)
6	NAG	A	914	1	14,14,15	0.85	0	17,19,21	1.70	3 (17%)
6	NAG	B	913	1	14,14,15	0.88	1 (7%)	17,19,21	1.30	3 (17%)
7	CU8	A	916	-	17,21,21	1.79	3 (17%)	20,30,30	2.03	6 (30%)
6	NAG	A	901	1	14,14,15	0.49	0	17,19,21	2.53	5 (29%)
6	NAG	A	906	1	14,14,15	0.78	0	17,19,21	1.85	4 (23%)
7	CU8	B	901	-	17,21,21	1.75	3 (17%)	20,30,30	1.98	5 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	B	902	1	14,14,15	0.65	0	17,19,21	1.69	6 (35%)

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	915	1	-	2/6/23/26	0/1/1/1
6	NAG	A	914	1	-	0/6/23/26	0/1/1/1
6	NAG	B	913	1	-	0/6/23/26	0/1/1/1
7	CU8	A	916	-	-	0/5/8/8	0/3/3/3
6	NAG	A	901	1	-	2/6/23/26	0/1/1/1
6	NAG	A	906	1	-	2/6/23/26	0/1/1/1
7	CU8	B	901	-	-	0/5/8/8	0/3/3/3
6	NAG	B	902	1	-	2/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	901	CU8	C1-N	-4.93	1.32	1.41
7	A	916	CU8	C1-N	-4.86	1.32	1.41
7	A	916	CU8	O-C12	-3.42	1.17	1.24
7	B	901	CU8	O-C12	-3.09	1.18	1.24
6	B	913	NAG	C1-C2	2.62	1.56	1.52
7	A	916	CU8	C5-C12	-2.35	1.46	1.50
7	B	901	CU8	C12-N3	-2.12	1.28	1.33

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	901	NAG	C1-O5-C5	7.90	122.90	112.19
7	B	901	CU8	C2-C3-N1	-5.07	116.73	124.58
7	A	916	CU8	C2-C3-N1	-4.94	116.93	124.58
6	A	906	NAG	C1-O5-C5	4.41	118.16	112.19
6	A	915	NAG	C1-O5-C5	4.28	117.99	112.19
7	A	916	CU8	C3-C2-C1	4.14	121.06	117.29
6	A	914	NAG	C1-O5-C5	3.99	117.60	112.19
7	B	901	CU8	C3-C2-C1	3.79	120.74	117.29
6	A	901	NAG	C8-C7-N2	3.52	122.07	116.10
6	A	906	NAG	C4-C3-C2	-3.37	106.09	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	906	NAG	C2-N2-C7	-3.36	118.12	122.90
6	B	913	NAG	O5-C5-C6	3.36	112.47	107.20
6	A	914	NAG	O5-C5-C6	-3.28	102.06	107.20
6	A	915	NAG	O5-C1-C2	-2.88	106.74	111.29
6	B	902	NAG	O5-C5-C6	2.79	111.58	107.20
6	A	901	NAG	C4-C3-C2	-2.78	106.95	111.02
6	B	902	NAG	C4-C3-C2	2.78	115.09	111.02
6	B	902	NAG	C1-C2-N2	-2.78	105.75	110.49
6	B	902	NAG	O5-C1-C2	2.61	115.40	111.29
6	B	902	NAG	C3-C4-C5	2.54	114.77	110.24
7	B	901	CU8	C6-C7-C8	-2.48	119.47	121.28
6	A	906	NAG	O3-C3-C2	-2.47	104.35	109.47
7	A	916	CU8	C6-C7-C8	-2.43	119.50	121.28
7	B	901	CU8	C3-N1-C	2.41	119.76	116.77
6	A	915	NAG	C1-C2-N2	-2.38	106.42	110.49
7	B	901	CU8	C10-C6-C1	-2.31	117.17	121.00
6	B	913	NAG	O5-C1-C2	-2.12	107.94	111.29
7	A	916	CU8	C4-N2-N	2.12	107.28	103.94
6	B	913	NAG	O7-C7-C8	-2.09	118.17	122.06
6	A	901	NAG	C2-N2-C7	2.09	125.88	122.90
6	A	901	NAG	O5-C1-C2	2.06	114.53	111.29
6	A	914	NAG	O6-C6-C5	-2.05	104.27	111.29
7	A	916	CU8	C6-C1-N	2.05	120.83	117.82
7	A	916	CU8	C9-C8-C7	2.00	120.96	117.95
6	B	902	NAG	C6-C5-C4	-2.00	108.31	113.00

There are no chirality outliers.

All (8) torsion outliers are listed below:

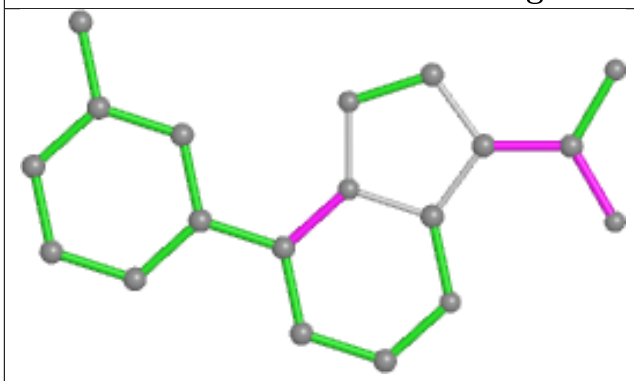
Mol	Chain	Res	Type	Atoms
6	B	902	NAG	O5-C5-C6-O6
6	A	915	NAG	O5-C5-C6-O6
6	A	915	NAG	C4-C5-C6-O6
6	B	902	NAG	C4-C5-C6-O6
6	A	901	NAG	C8-C7-N2-C2
6	A	901	NAG	O7-C7-N2-C2
6	A	906	NAG	O5-C5-C6-O6
6	A	906	NAG	C4-C5-C6-O6

There are no ring outliers.

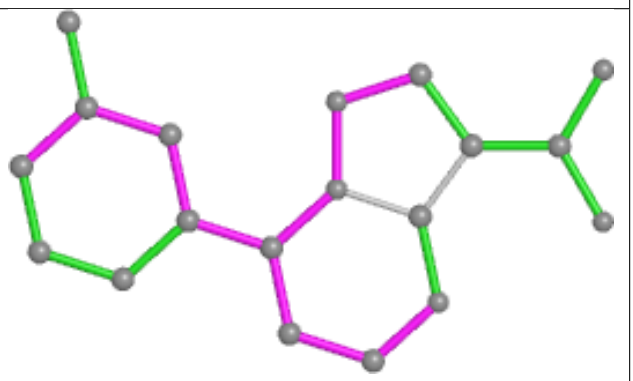
No monomer is involved in short contacts.

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.

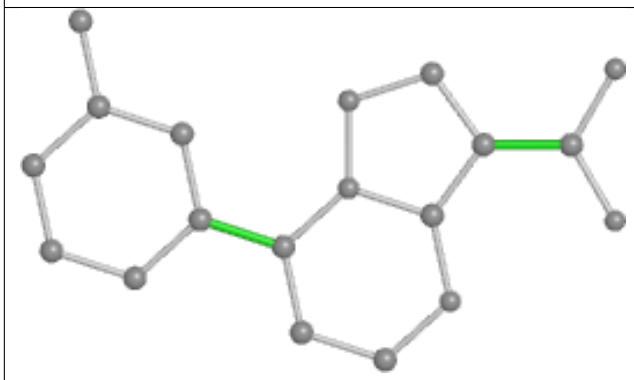
Ligand CU8 A 916



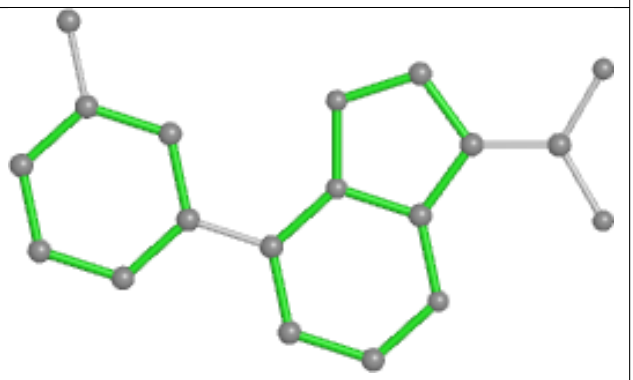
Bond lengths



Bond angles

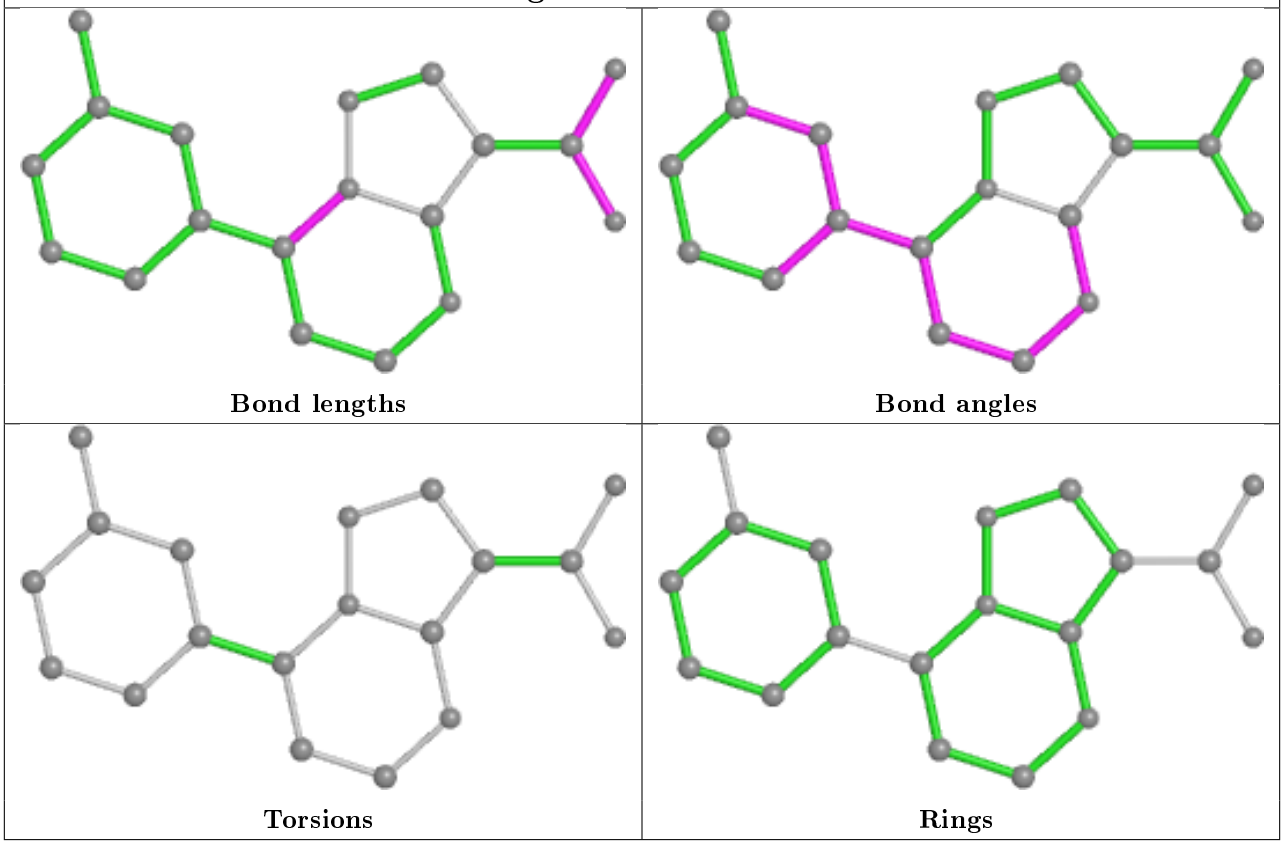


Torsions



Rings

Ligand CU8 B 901



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	750/811 (92%)	0.16	38 (5%)	28	26	29, 57, 103, 151	0
1	B	739/811 (91%)	0.10	25 (3%)	45	44	30, 55, 98, 134	0
All	All	1489/1622 (91%)	0.13	63 (4%)	36	35	29, 56, 99, 151	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	756	LEU	7.9
1	A	182	TYR	4.9
1	B	185	LYS	4.6
1	A	183	PHE	4.6
1	A	780	ILE	4.6
1	B	461	PHE	4.5
1	A	461	PHE	4.3
1	A	758	THR	4.1
1	A	759	LYS	4.0
1	A	776	CYS	3.8
1	A	760	THR	3.5
1	A	812	LYS	3.5
1	A	809	GLN	3.3
1	A	777	THR	3.3
1	A	571	ALA	3.2
1	A	783	PHE	3.1
1	B	819	LEU	3.1
1	B	493	ILE	3.1
1	A	808	ASP	3.0
1	B	601	ASP	2.9
1	A	782	ASP	2.9
1	B	392	GLN	2.8
1	A	789	GLU	2.8
1	A	778	CYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	792	ASN	2.7
1	A	807	GLY	2.7
1	A	736	SER	2.6
1	B	567	TYR	2.6
1	A	774	PHE	2.6
1	B	61	VAL	2.6
1	B	791	LEU	2.6
1	B	40	LYS	2.6
1	A	817	LEU	2.5
1	B	597	TYR	2.5
1	A	569	ARG	2.5
1	A	788	ASP	2.5
1	B	123	ASN	2.5
1	A	810	ARG	2.4
1	B	64	TYR	2.4
1	A	215	HIS	2.4
1	B	762	THR	2.4
1	A	811	GLY	2.4
1	B	186	VAL	2.4
1	B	41	GLN	2.3
1	A	785	ARG	2.3
1	A	603	TYR	2.3
1	A	627	ASP	2.3
1	B	789	GLU	2.3
1	A	601	ASP	2.2
1	B	42	ASN	2.2
1	A	757	GLU	2.2
1	A	815	VAL	2.2
1	B	164	GLU	2.2
1	B	653	HIS	2.1
1	A	600	THR	2.1
1	A	761	THR	2.1
1	A	814	ILE	2.1
1	A	470	PHE	2.1
1	B	472	ARG	2.1
1	B	788	ASP	2.1
1	B	516	SER	2.0
1	B	74	PHE	2.0
1	A	781	GLY	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)

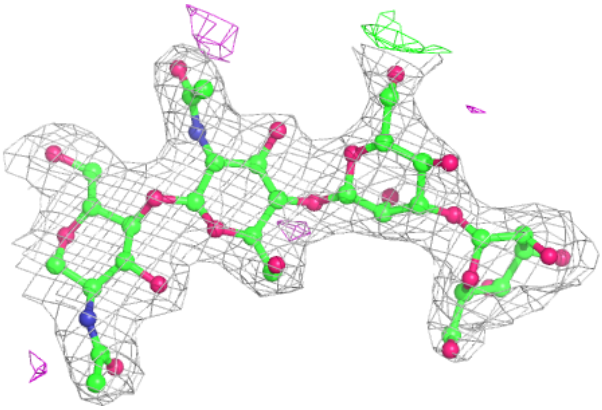
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

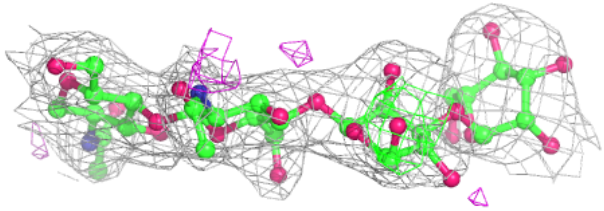
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MAN	H	4	11/12	0.70	0.22	73,96,113,114	0
5	MAN	F	4	11/12	0.72	0.20	79,91,97,98	0
5	BMA	H	3	11/12	0.83	0.14	53,59,80,103	0
4	MAN	E	5	11/12	0.83	0.19	79,84,89,96	0
2	BMA	C	3	11/12	0.84	0.19	55,67,79,82	0
2	MAN	C	4	11/12	0.86	0.23	74,84,88,91	0
5	BMA	F	3	11/12	0.87	0.13	63,68,84,85	0
3	NAG	G	2	14/15	0.88	0.17	55,71,82,95	0
3	NAG	D	2	14/15	0.89	0.16	49,62,79,81	0
4	MAN	E	4	11/12	0.91	0.18	87,95,108,110	0
4	BMA	E	3	11/12	0.95	0.10	49,59,69,73	0
2	NAG	C	1	14/15	0.97	0.13	35,40,47,47	0
3	NAG	G	1	14/15	0.97	0.12	34,38,46,51	0
5	NAG	H	1	14/15	0.97	0.13	33,36,37,38	0
5	NAG	F	2	14/15	0.97	0.13	33,45,58,64	0
2	NAG	C	2	14/15	0.97	0.12	38,46,52,61	0
4	NAG	E	2	14/15	0.98	0.12	31,37,46,53	0
5	NAG	H	2	14/15	0.98	0.12	36,41,45,50	0
4	NAG	E	1	14/15	0.98	0.12	27,35,38,38	0
3	NAG	D	1	14/15	0.98	0.11	31,36,41,41	0
5	NAG	F	1	14/15	0.98	0.13	33,37,46,55	0

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

Electron density around Chain C:

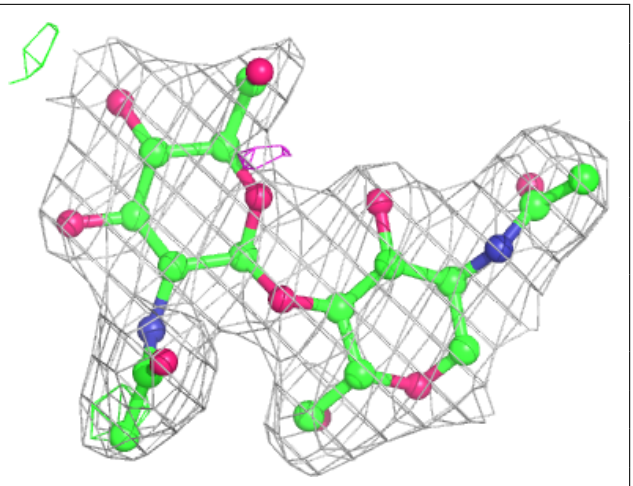
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

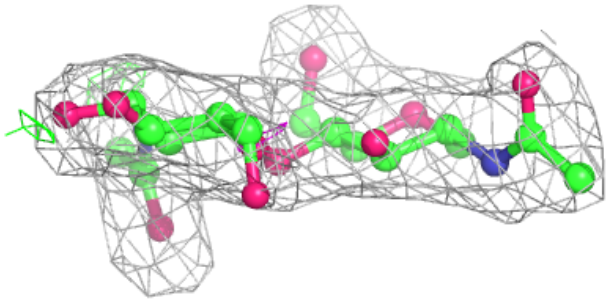


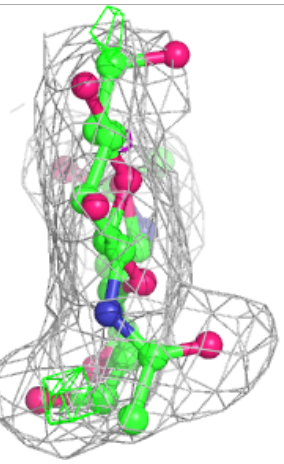


Electron density around Chain D:

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

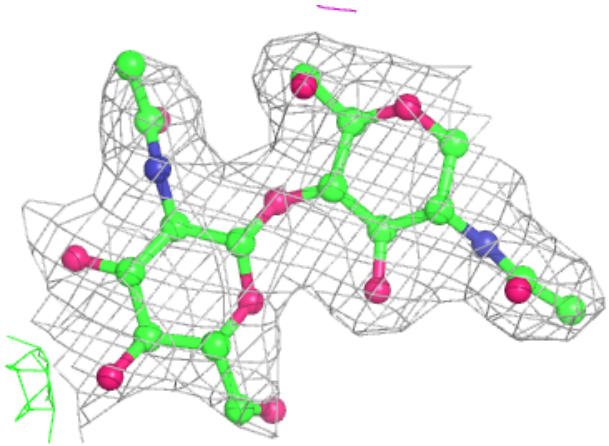


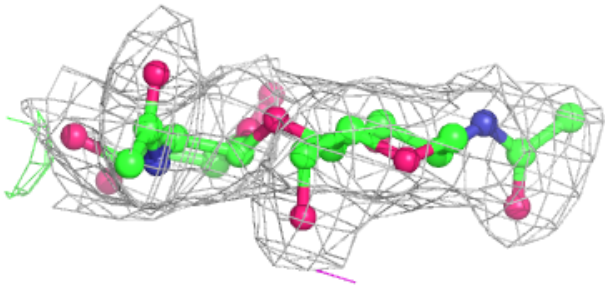


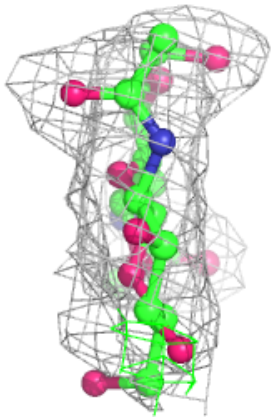


Electron density around Chain G:

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

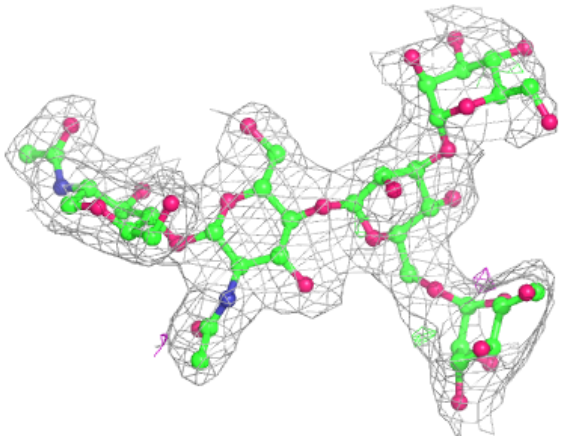


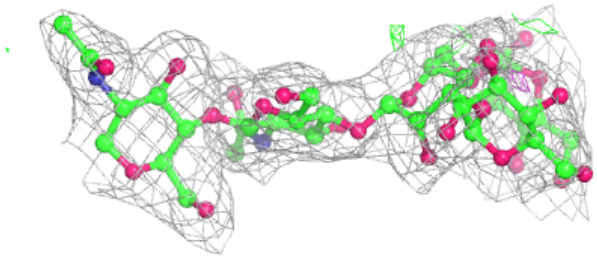


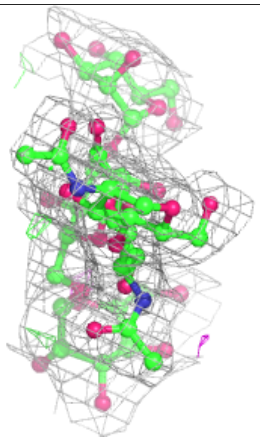


Electron density around Chain E:

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

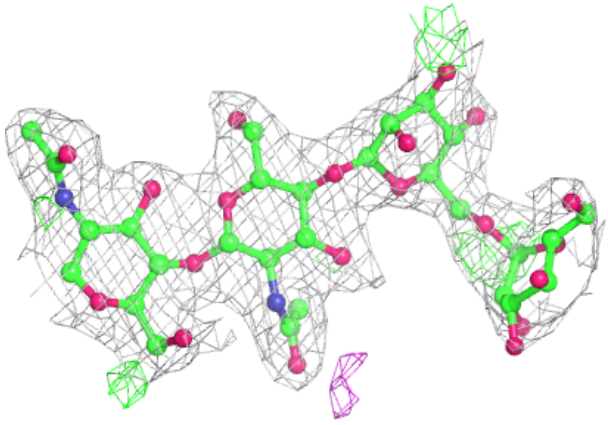


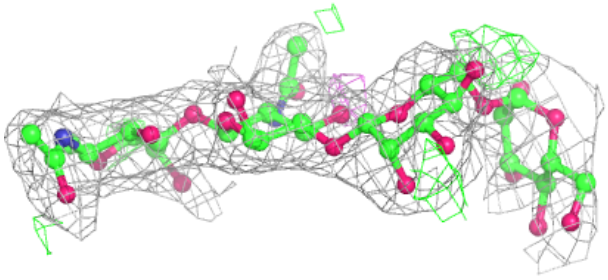




Electron density around Chain F:

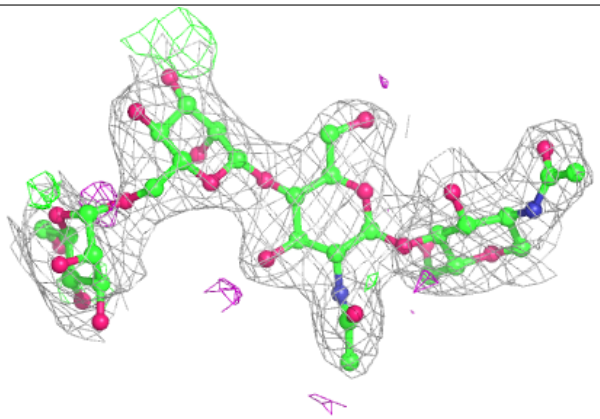
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

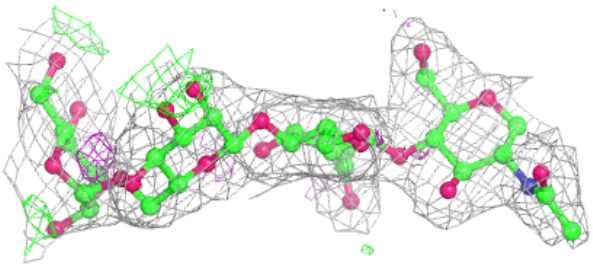




Electron density around Chain H:

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





6.4 Ligands

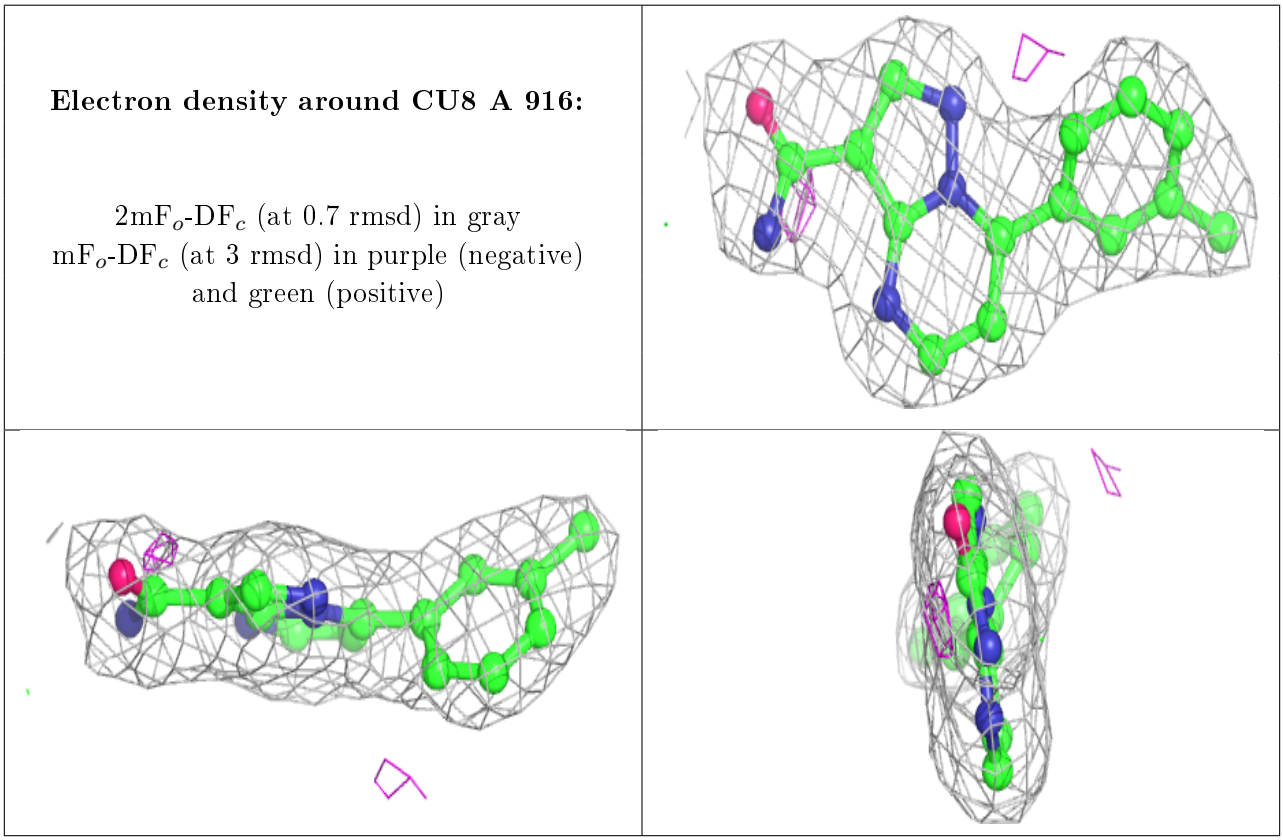
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	A	915	14/15	0.78	0.22	76,90,106,106	0
6	NAG	B	902	14/15	0.83	0.24	79,87,98,100	0
6	NAG	A	901	14/15	0.87	0.18	76,85,90,92	0
6	NAG	B	913	14/15	0.93	0.15	53,61,71,72	0
6	NAG	A	906	14/15	0.96	0.10	52,62,69,72	0
7	CU8	A	916	19/19	0.96	0.14	33,39,51,53	0
7	CU8	B	901	19/19	0.97	0.21	36,42,49,53	0
6	NAG	A	914	14/15	0.97	0.13	40,44,57,61	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.

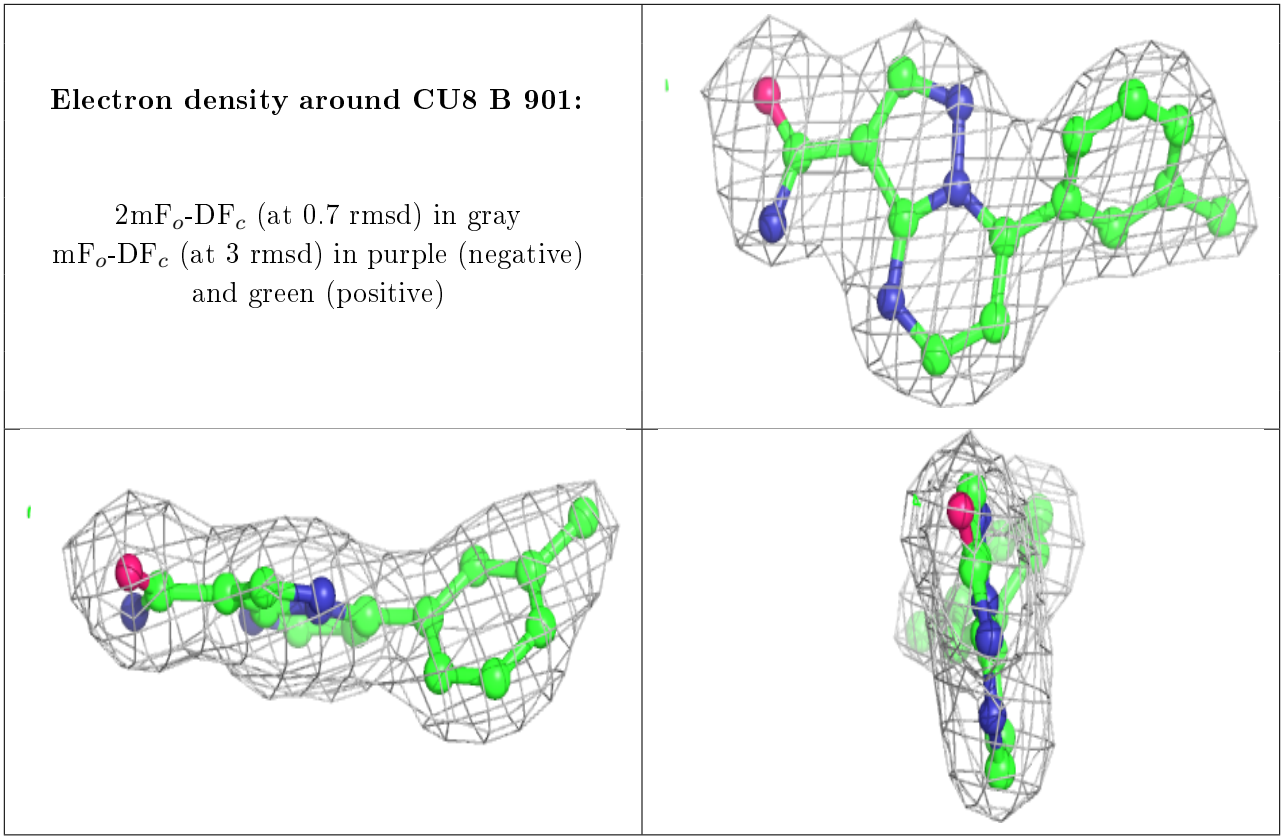
Electron density around CU8 A 916:

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



Electron density around CU8 B 901:

$2mF_o$-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.