Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 04:16 AM EDT

PDB ID	:	5WYZ
Title	:	Crystal structure of human TLR8 in complex with CU-CPT9b
Authors	:	Tanji, H.; Ohto, U.; Shimizu, T.
Deposited on	:	2017-01-16
Resolution	:	2.30 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

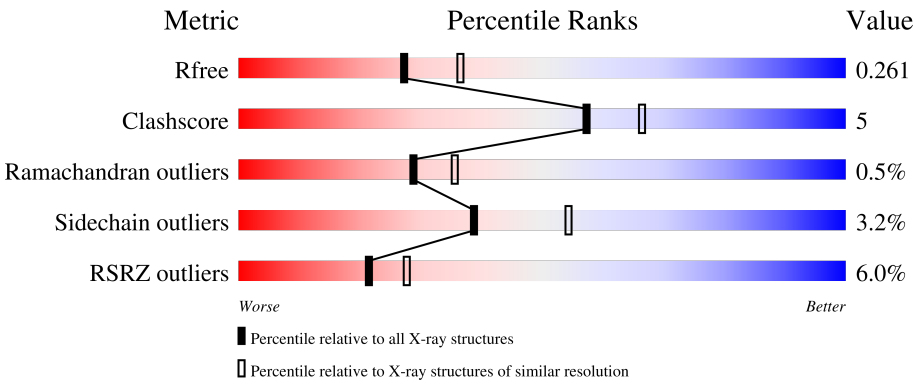
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	811	5% 81% 10% • 8%
1	B	811	6% 79% 12% • 8%
2	C	4	100%
3	D	2	100%
3	G	2	100%

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Mol	Chain	Length	Quality of chain
4	E	5	100%
5	F	4	75% 25%
5	H	4	75% 25%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 12600 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
			Total	C	N	O	S			
1	A	750	6038	3861	1026	1132	19	0	0	0
1	B	745	6004	3840	1021	1124	19	0	0	0

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

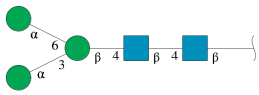
- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

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

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

- 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.

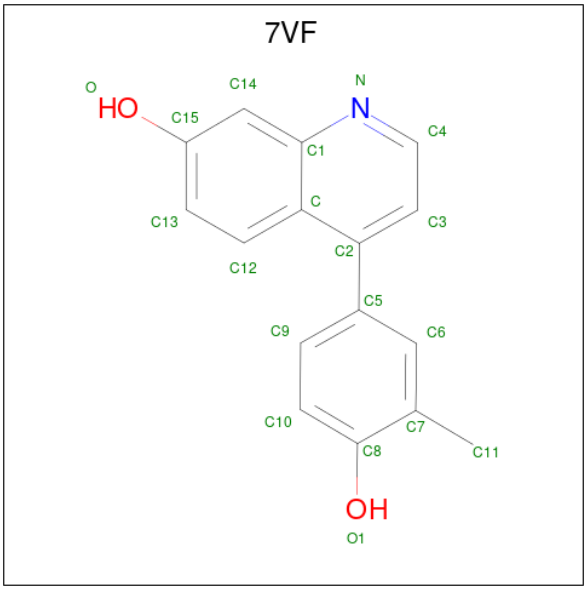


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	E	5	61	34	2	25	0	0	0

- 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.

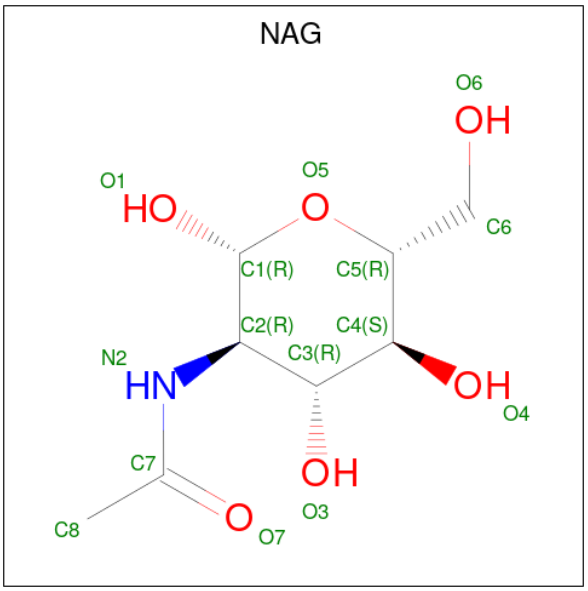
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	F	4	50	28	2	20	0	0	0
			Total	C	N	O			
5	H	4	50	28	2	20	0	0	0

- Molecule 6 is 4-(3-methyl-4-oxidanyl-phenyl)quinolin-7-ol (three-letter code: 7VF) (formula: $C_{16}H_{13}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	19	16	1	2	0	0
			Total	C	N	O		
6	B	1	19	16	1	2	0	0

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



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

- Molecule 8 is water.

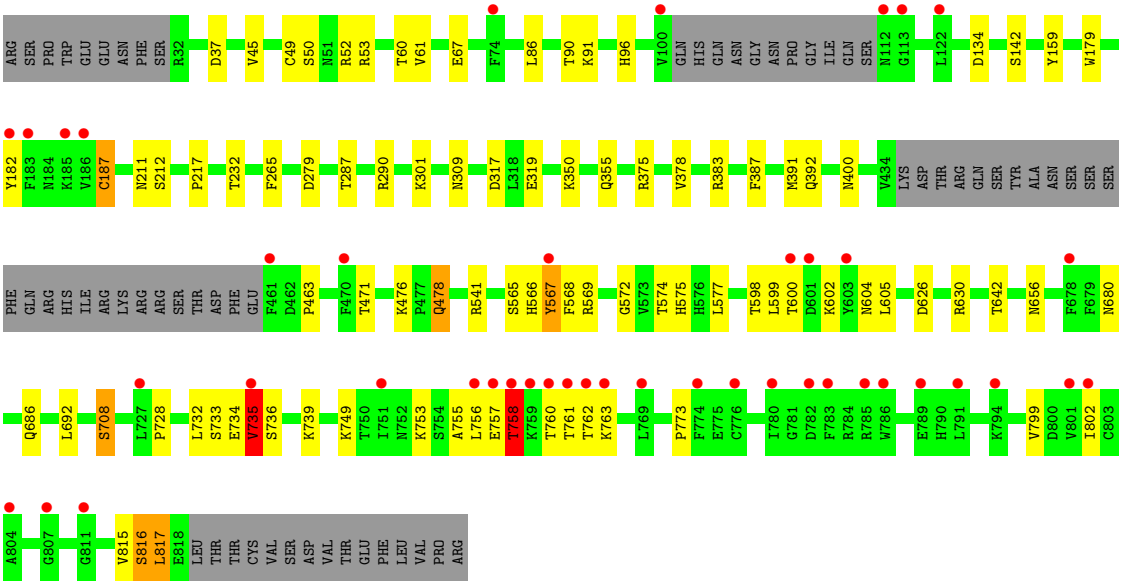
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	116	116	116	0	0
			Total	O		
8	B	81	81	81	0	0

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.

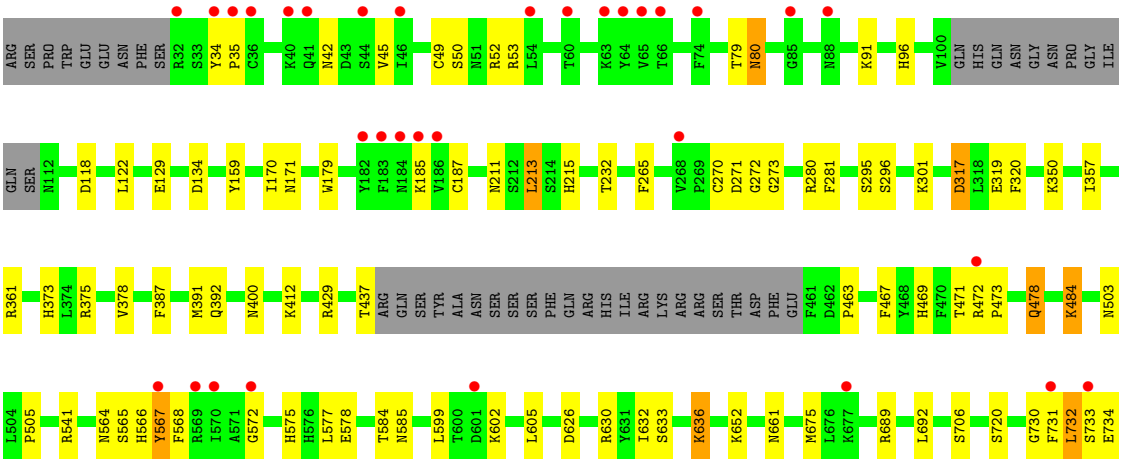
- Molecule 1: Toll-like receptor 8

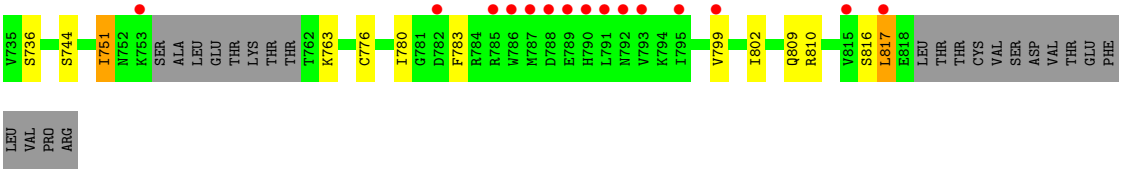
Chain A:



- 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: 100%

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

Chain D: 100%

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

Chain G: 100%

• 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: 100%

• 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: 75% 25%

• 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: 75% 25%

NAG1
NAG2
BMA3
MAN4

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	143.62Å 98.95Å 139.52Å 90.00° 108.39° 90.00°	Depositor
Resolution (Å)	132.39 – 2.30 44.13 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (132.39-2.30) 100.0 (44.13-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.208 , 0.260 0.213 , 0.261	Depositor DCC
R_{free} test set	4197 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	50.0	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12600	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 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 7VF, MAN, NAG

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	0.69	0/6162	0.79	3/8358 (0.0%)
1	B	0.68	0/6127	0.81	6/8308 (0.1%)
All	All	0.68	0/12289	0.80	9/16666 (0.1%)

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	1
1	B	0	4
All	All	0	5

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	689	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	B	689	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	B	213	LEU	N-CA-C	-6.48	93.51	111.00
1	B	80	ASN	N-CA-C	-6.09	94.56	111.00
1	A	279	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	A	290	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	B	429	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	B	272	GLY	N-CA-C	-5.39	99.61	113.10
1	A	290	ARG	NE-CZ-NH2	-5.14	117.73	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	758	THR	Peptide
1	B	271	ASP	Peptide
1	B	731	PHE	Peptide
1	B	79	THR	Peptide
1	B	80	ASN	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	6033	61	0
1	B	6004	0	5997	62	0
2	C	50	0	43	0	0
3	D	28	0	24	0	0
3	G	28	0	25	0	0
4	E	61	0	52	0	0
5	F	50	0	43	2	0
5	H	50	0	43	1	0
6	A	19	0	0	0	0
6	B	19	0	0	0	0
7	A	42	0	38	0	0
7	B	14	0	13	0	0
8	A	116	0	0	5	0
8	B	81	0	0	2	0
All	All	12600	0	12311	122	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 5.

All (122) 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:758:THR:HA	1:A:760:THR:OG1	1.45	1.17
1:B:478:GLN:HE21	1:B:478:GLN:H	1.04	0.97
1:A:478:GLN:HE21	1:A:478:GLN:H	1.12	0.97
1:A:760:THR:HB	1:A:761:THR:HA	1.49	0.94
1:A:61:VAL:CG2	1:A:86:LEU:HD11	1.98	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:733:SER:N	1:B:734:GLU:HA	1.87	0.89
1:A:61:VAL:HG21	1:A:86:LEU:HD11	1.55	0.89
1:A:760:THR:CB	1:A:761:THR:HA	2.05	0.86
1:B:732:LEU:C	1:B:734:GLU:HA	2.02	0.79
1:A:758:THR:CA	1:A:760:THR:OG1	2.29	0.78
1:A:757:GLU:O	1:A:758:THR:HG22	1.83	0.78
1:B:584:THR:HG22	1:B:585:ASN:ND2	2.02	0.74
1:A:37:ASP:OD2	1:A:52:ARG:NH1	2.21	0.73
1:A:760:THR:HB	1:A:761:THR:CA	2.18	0.72
1:B:295:SER:OG	1:B:319:GLU:OE1	2.07	0.71
1:B:319:GLU:OE2	1:B:469:HIS:HB2	1.91	0.69
1:B:478:GLN:H	1:B:478:GLN:NE2	1.85	0.68
1:B:375:ARG:HD2	1:B:400:ASN:HD21	1.58	0.66
1:A:733:SER:HB3	1:A:757:GLU:HB3	1.75	0.66
1:A:478:GLN:H	1:A:478:GLN:NE2	1.91	0.66
1:A:211:ASN:O	1:A:232:THR:HA	1.96	0.66
1:A:753:LYS:O	1:A:756:LEU:O	2.14	0.65
1:B:35:PRO:O	1:B:52:ARG:NH1	2.32	0.63
1:A:383:ARG:NH1	8:A:1002:HOH:O	2.23	0.62
1:A:61:VAL:HG22	1:A:86:LEU:HD11	1.79	0.62
1:B:478:GLN:HE21	1:B:478:GLN:N	1.87	0.61
1:B:50:SER:O	1:B:52:ARG:HG2	2.02	0.60
1:A:375:ARG:HD2	1:A:400:ASN:HD21	1.67	0.58
1:B:317:ASP:OD1	1:B:319:GLU:OE2	2.21	0.58
1:A:642:THR:HG23	8:A:1095:HOH:O	2.02	0.58
1:A:182:TYR:O	1:A:182:TYR:CD2	2.57	0.58
1:A:656:ASN:OD1	1:A:680:ASN:ND2	2.37	0.57
1:A:574:THR:HG22	1:A:598:THR:HG23	1.86	0.57
1:A:761:THR:HG22	1:A:762:THR:N	2.20	0.57
1:A:642:THR:CG2	8:A:1095:HOH:O	2.53	0.57
1:A:541:ARG:HA	1:A:565:SER:O	2.05	0.57
1:B:484:LYS:HE2	1:B:505:PRO:HB2	1.86	0.57
1:B:626:ASP:OD1	1:B:630:ARG:NH1	2.37	0.57
1:B:730:GLY:O	1:B:733:SER:HA	2.05	0.56
1:A:749:LYS:HG3	1:A:773:PRO:O	2.06	0.56
1:B:541:ARG:HA	1:B:565:SER:O	2.06	0.55
1:A:187:CYS:SG	1:A:187:CYS:O	2.65	0.55
1:A:686:GLN:O	1:A:686:GLN:HG3	2.07	0.55
1:B:733:SER:N	1:B:734:GLU:CA	2.67	0.54
1:A:319:GLU:HG2	8:A:1067:HOH:O	2.07	0.54
1:A:476:LYS:HD3	8:A:1102:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:PHE:HB2	5:F:1:NAG:H81	1.90	0.54
1:B:736:SER:HB2	1:B:763:LYS:HE2	1.90	0.53
1:B:211:ASN:O	1:B:232:THR:HA	2.08	0.53
1:B:185:LYS:N	1:B:185:LYS:HE2	2.23	0.53
1:A:577:LEU:HD12	1:A:605:LEU:HD11	1.90	0.53
1:A:574:THR:HG22	1:A:598:THR:CG2	2.39	0.53
1:B:577:LEU:HD12	1:B:605:LEU:HD11	1.91	0.52
1:B:159:TYR:CE1	1:B:187:CYS:HB2	2.46	0.51
1:A:50:SER:O	1:A:52:ARG:HG3	2.09	0.51
1:A:572:GLY:HA3	1:B:265:PHE:HE2	1.75	0.51
1:A:159:TYR:CE1	1:A:187:CYS:HB2	2.44	0.51
1:B:270:CYS:O	1:B:273:GLY:N	2.43	0.51
1:A:61:VAL:HG21	1:A:86:LEU:CD1	2.32	0.50
1:A:478:GLN:HE21	1:A:478:GLN:N	1.94	0.50
1:A:708:SER:OG	1:A:735:VAL:N	2.45	0.50
1:B:472:ARG:NH1	1:B:473:PRO:O	2.45	0.49
1:A:566:HIS:C	1:A:568:PHE:H	2.15	0.49
1:B:626:ASP:OD2	1:B:630:ARG:HD3	2.13	0.49
1:A:692:LEU:C	1:A:692:LEU:HD23	2.33	0.49
1:B:159:TYR:CD1	1:B:187:CYS:HB2	2.48	0.49
1:B:692:LEU:C	1:B:692:LEU:HD23	2.32	0.49
1:B:575:HIS:O	1:B:599:LEU:HA	2.14	0.48
1:B:213:LEU:O	1:B:232:THR:O	2.32	0.48
1:B:357:ILE:HG22	8:B:1017:HOH:O	2.14	0.48
1:B:467:PHE:CB	5:F:1:NAG:H81	2.43	0.48
1:B:179:TRP:CD1	1:B:463:PRO:HB3	2.49	0.47
1:B:816:SER:O	1:B:817:LEU:HD22	2.13	0.47
1:A:602:LYS:HD2	1:A:604:ASN:H	1.78	0.47
1:B:809:GLN:O	1:B:810:ARG:C	2.53	0.47
5:H:4:MAN:O6	5:H:4:MAN:O4	2.28	0.47
1:B:578:GLU:HG3	1:B:602:LYS:HE2	1.97	0.47
1:A:734:GLU:O	1:A:736:SER:N	2.43	0.47
1:B:52:ARG:NH1	1:B:52:ARG:HG3	2.30	0.47
1:A:799:VAL:O	1:A:802:ILE:HD11	2.15	0.47
1:A:575:HIS:O	1:A:599:LEU:HA	2.13	0.47
1:A:728:PRO:O	1:A:755:ALA:HA	2.14	0.47
1:A:733:SER:CB	1:A:757:GLU:HB3	2.44	0.47
1:A:265:PHE:HE2	1:B:572:GLY:HA3	1.79	0.46
1:B:53:ARG:NH2	1:B:799:VAL:HG12	2.30	0.46
1:A:816:SER:O	1:A:817:LEU:HD22	2.15	0.46
1:A:757:GLU:O	1:A:758:THR:CG2	2.60	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:751:ILE:HG12	1:B:783:PHE:CD1	2.51	0.45
1:B:720:SER:HA	1:B:744:SER:O	2.17	0.44
1:A:179:TRP:CD1	1:A:463:PRO:HB3	2.51	0.44
1:B:52:ARG:HG3	1:B:52:ARG:HH11	1.82	0.44
1:B:566:HIS:C	1:B:568:PHE:H	2.20	0.44
1:A:67:GLU:HG2	1:A:91:LYS:HB3	2.00	0.44
1:B:632:ILE:HG22	1:B:661:ASN:ND2	2.34	0.43
1:A:96:HIS:HD2	1:A:134:ASP:OD2	2.02	0.43
1:B:96:HIS:HD2	1:B:134:ASP:OD2	2.01	0.43
1:A:739:LYS:HD2	1:A:763:LYS:O	2.18	0.43
1:B:373:HIS:HA	1:B:400:ASN:HB3	2.00	0.42
1:B:564:ASN:HB2	8:B:1002:HOH:O	2.18	0.42
1:A:732:LEU:HD11	1:A:756:LEU:HA	2.01	0.42
1:B:732:LEU:CD1	1:B:732:LEU:N	2.83	0.42
1:B:34:TYR:CG	1:B:35:PRO:HA	2.55	0.42
1:B:412:LYS:HB3	1:B:503:ASN:HB3	2.01	0.42
1:B:633:SER:O	1:B:636:LYS:HB2	2.20	0.42
1:A:53:ARG:NH2	1:A:799:VAL:HG12	2.35	0.42
1:B:632:ILE:HG22	1:B:661:ASN:HD22	1.85	0.42
1:A:761:THR:CG2	1:A:762:THR:N	2.83	0.41
1:B:91:LYS:HA	1:B:129:GLU:O	2.21	0.41
1:B:652:LYS:HA	1:B:675:MET:O	2.21	0.41
1:A:387:PHE:O	1:A:391:MET:HG3	2.21	0.41
1:A:758:THR:CB	1:A:760:THR:OG1	2.69	0.41
1:A:287:THR:HA	1:A:309:ASN:O	2.21	0.41
1:A:733:SER:HA	1:A:734:GLU:HA	1.77	0.41
1:B:751:ILE:CG1	1:B:783:PHE:CD1	3.04	0.40
1:B:799:VAL:O	1:B:802:ILE:HD11	2.21	0.40
1:A:179:TRP:HE3	1:A:182:TYR:CE1	2.39	0.40
1:A:626:ASP:OD1	1:A:630:ARG:NH2	2.51	0.40
1:B:776:CYS:HA	1:B:780:ILE:HG12	2.03	0.40
1:B:280:ARG:NH1	1:B:281:PHE:CE2	2.89	0.40
1:B:296:SER:HA	1:B:320:PHE:O	2.21	0.40
1:B:170:ILE:HD12	1:B:171:ASN:N	2.36	0.40
1:B:387:PHE:O	1:B:391:MET:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	744/811 (92%)	698 (94%)	41 (6%)	5 (1%)	22	26
1	B	737/811 (91%)	698 (95%)	37 (5%)	2 (0%)	41	50
All	All	1481/1622 (91%)	1396 (94%)	78 (5%)	7 (0%)	29	35

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	567	TYR
1	A	600	THR
1	B	567	TYR
1	A	378	VAL
1	A	758	THR
1	B	378	VAL
1	A	735	VAL

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%)	674 (97%)	23 (3%)	38	53
1	B	693/755 (92%)	672 (97%)	21 (3%)	41	57
All	All	1390/1510 (92%)	1346 (97%)	44 (3%)	39	54

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	VAL
1	A	49	CYS
1	A	60	THR
1	A	90	THR
1	A	142	SER
1	A	187	CYS
1	A	212	SER
1	A	217	PRO
1	A	301	LYS
1	A	317	ASP
1	A	350	LYS
1	A	355	GLN
1	A	392	GLN
1	A	471	THR
1	A	478	GLN
1	A	567	TYR
1	A	569	ARG
1	A	708	SER
1	A	735	VAL
1	A	758	THR
1	A	815	VAL
1	A	816	SER
1	A	817	LEU
1	B	42	ASN
1	B	45	VAL
1	B	49	CYS
1	B	118	ASP
1	B	122	LEU
1	B	215	HIS
1	B	301	LYS
1	B	317	ASP
1	B	350	LYS
1	B	361	ARG
1	B	392	GLN
1	B	437	THR
1	B	471	THR
1	B	478	GLN
1	B	484	LYS
1	B	567	TYR
1	B	636	LYS
1	B	706	SER
1	B	732	LEU
1	B	751	ILE

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Mol	Chain	Res	Type
1	B	817	LEU

Sometimes 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	233	GLN
1	A	478	GLN
1	A	566	HIS
1	A	581	GLN
1	A	604	ASN
1	A	752	ASN
1	B	96	HIS
1	B	123	ASN
1	B	155	GLN
1	B	478	GLN
1	B	585	ASN
1	B	604	ASN
1	B	792	ASN

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)

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	0.68	0	17,19,21	1.78	3 (17%)
2	NAG	C	2	2	14,14,15	0.93	0	17,19,21	1.30	3 (17%)
2	BMA	C	3	2	11,11,12	0.86	0	15,15,17	2.17	7 (46%)
2	MAN	C	4	2	11,11,12	0.85	0	15,15,17	1.37	3 (20%)
3	NAG	D	1	3,1	14,14,15	1.18	1 (7%)	17,19,21	1.37	4 (23%)
3	NAG	D	2	3	14,14,15	1.35	2 (14%)	17,19,21	1.35	3 (17%)
4	NAG	E	1	4,1	14,14,15	0.76	0	17,19,21	1.85	5 (29%)
4	NAG	E	2	4	14,14,15	0.94	0	17,19,21	2.01	4 (23%)
4	BMA	E	3	4	11,11,12	0.66	0	15,15,17	1.65	3 (20%)
4	MAN	E	4	4	11,11,12	0.74	0	15,15,17	1.53	2 (13%)
4	MAN	E	5	4	11,11,12	0.54	0	15,15,17	1.88	5 (33%)
5	NAG	F	1	1,5	14,14,15	0.73	0	17,19,21	1.62	3 (17%)
5	NAG	F	2	5	14,14,15	0.72	0	17,19,21	2.02	4 (23%)
5	BMA	F	3	5	11,11,12	0.80	0	15,15,17	2.73	4 (26%)
5	MAN	F	4	5	11,11,12	1.07	1 (9%)	15,15,17	3.25	7 (46%)
3	NAG	G	1	3,1	14,14,15	0.96	1 (7%)	17,19,21	1.74	5 (29%)
3	NAG	G	2	3	14,14,15	0.91	1 (7%)	17,19,21	1.63	3 (17%)
5	NAG	H	1	1,5	14,14,15	1.45	3 (21%)	17,19,21	1.31	3 (17%)
5	NAG	H	2	5	14,14,15	0.93	1 (7%)	17,19,21	1.27	2 (11%)
5	BMA	H	3	5	11,11,12	1.02	1 (9%)	15,15,17	1.31	3 (20%)
5	MAN	H	4	5	11,11,12	0.76	0	15,15,17	2.34	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	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	2	4	-	2/6/23/26	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
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	1/6/23/26	0/1/1/1
5	BMA	F	3	5	-	2/2/19/22	0/1/1/1
5	MAN	F	4	5	-	2/2/19/22	0/1/1/1
3	NAG	G	1	3,1	-	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 (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2	NAG	O5-C1	-3.70	1.37	1.43
5	H	1	NAG	C1-C2	3.21	1.57	1.52
5	H	1	NAG	C8-C7	2.81	1.56	1.50
3	D	1	NAG	O3-C3	-2.72	1.36	1.43
5	H	3	BMA	O5-C1	-2.50	1.39	1.43
5	F	4	MAN	C2-C3	2.41	1.56	1.52
3	G	2	NAG	O5-C1	-2.36	1.39	1.43
5	H	2	NAG	O5-C1	-2.31	1.40	1.43
3	D	2	NAG	C1-C2	2.26	1.55	1.52
5	H	1	NAG	O5-C1	-2.09	1.40	1.43
3	G	1	NAG	O5-C1	-2.04	1.40	1.43

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	3	BMA	C1-O5-C5	7.92	122.93	112.19
5	F	4	MAN	C1-C2-C3	7.51	118.90	109.67
5	H	4	MAN	O5-C5-C6	7.49	118.95	107.20
5	F	4	MAN	C1-O5-C5	7.20	121.94	112.19
4	E	2	NAG	C1-O5-C5	-5.20	105.14	112.19
5	F	2	NAG	O5-C1-C2	-4.73	103.82	111.29
2	C	3	BMA	O5-C5-C6	4.70	114.57	107.20
5	F	3	BMA	C3-C4-C5	4.63	118.50	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	NAG	O7-C7-C8	-4.60	113.52	122.06
4	E	1	NAG	O5-C1-C2	-4.22	104.62	111.29
4	E	5	MAN	O5-C5-C6	4.21	113.80	107.20
4	E	3	BMA	O3-C3-C2	4.08	117.80	109.99
5	F	2	NAG	C1-C2-N2	4.02	117.35	110.49
5	F	2	NAG	O5-C5-C6	3.96	113.41	107.20
3	G	2	NAG	O5-C1-C2	-3.89	105.15	111.29
3	G	1	NAG	C1-C2-N2	-3.68	104.20	110.49
3	G	2	NAG	C2-N2-C7	-3.56	117.83	122.90
2	C	3	BMA	C3-C4-C5	3.52	116.51	110.24
5	F	4	MAN	O5-C5-C6	3.42	112.56	107.20
3	D	2	NAG	C1-O5-C5	3.34	116.71	112.19
4	E	2	NAG	C4-C3-C2	-3.25	106.25	111.02
5	F	4	MAN	O3-C3-C2	3.22	116.16	109.99
4	E	1	NAG	O7-C7-C8	-3.14	116.22	122.06
5	F	1	NAG	O6-C6-C5	-3.13	100.56	111.29
4	E	4	MAN	C1-O5-C5	3.06	116.34	112.19
5	H	1	NAG	C1-O5-C5	3.05	116.33	112.19
5	H	4	MAN	C1-O5-C5	-3.05	108.06	112.19
5	F	1	NAG	O5-C1-C2	-3.04	106.48	111.29
4	E	2	NAG	O4-C4-C3	-3.03	103.34	110.35
4	E	3	BMA	O2-C2-C3	3.03	116.20	110.14
4	E	1	NAG	C8-C7-N2	3.02	121.21	116.10
2	C	1	NAG	O7-C7-N2	3.00	127.47	121.95
5	F	1	NAG	C3-C4-C5	-2.99	104.91	110.24
4	E	5	MAN	C3-C4-C5	2.84	115.31	110.24
3	D	1	NAG	O4-C4-C5	-2.84	102.25	109.30
2	C	3	BMA	C1-O5-C5	2.80	115.98	112.19
4	E	5	MAN	O5-C1-C2	-2.74	106.54	110.77
3	G	1	NAG	O7-C7-C8	-2.66	117.12	122.06
2	C	3	BMA	O6-C6-C5	2.58	120.14	111.29
4	E	3	BMA	O5-C1-C2	-2.55	106.83	110.77
2	C	2	NAG	O5-C1-C2	-2.52	107.30	111.29
3	G	1	NAG	O3-C3-C4	2.52	116.18	110.35
2	C	4	MAN	C3-C4-C5	2.50	114.70	110.24
2	C	4	MAN	O2-C2-C3	2.50	115.15	110.14
4	E	1	NAG	C1-O5-C5	2.48	115.56	112.19
5	F	4	MAN	C6-C5-C4	-2.45	107.25	113.00
2	C	3	BMA	C2-C3-C4	2.44	115.12	110.89
3	D	2	NAG	O4-C4-C5	2.41	115.28	109.30
2	C	3	BMA	O4-C4-C3	-2.40	104.81	110.35
2	C	3	BMA	O5-C1-C2	-2.37	107.11	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	3	BMA	O3-C3-C2	2.37	114.54	109.99
4	E	5	MAN	C1-C2-C3	-2.33	106.81	109.67
5	F	4	MAN	O3-C3-C4	-2.32	104.98	110.35
2	C	2	NAG	C1-C2-N2	2.32	114.45	110.49
5	F	4	MAN	O5-C1-C2	2.30	114.31	110.77
5	F	3	BMA	O5-C5-C6	2.29	110.79	107.20
3	G	2	NAG	O4-C4-C5	2.27	114.95	109.30
4	E	4	MAN	C3-C4-C5	2.27	114.29	110.24
5	H	2	NAG	C4-C3-C2	-2.24	107.73	111.02
2	C	4	MAN	C2-C3-C4	2.21	114.72	110.89
4	E	2	NAG	C1-C2-N2	2.20	114.25	110.49
5	H	2	NAG	O6-C6-C5	-2.20	103.76	111.29
5	F	2	NAG	O7-C7-C8	-2.18	118.00	122.06
2	C	1	NAG	O4-C4-C3	-2.18	105.31	110.35
4	E	1	NAG	O5-C5-C4	-2.18	105.53	110.83
5	H	3	BMA	C2-C3-C4	-2.16	107.16	110.89
3	G	1	NAG	C8-C7-N2	2.16	119.76	116.10
3	D	1	NAG	C6-C5-C4	-2.10	108.08	113.00
3	D	2	NAG	O5-C1-C2	-2.09	107.99	111.29
3	D	1	NAG	C1-C2-N2	-2.07	106.95	110.49
5	H	3	BMA	O5-C5-C6	2.05	110.42	107.20
2	C	2	NAG	C1-O5-C5	-2.04	109.42	112.19
3	D	1	NAG	O5-C5-C6	2.04	110.40	107.20
5	H	1	NAG	O4-C4-C5	2.02	114.32	109.30
5	F	3	BMA	O4-C4-C5	-2.02	104.29	109.30
3	G	1	NAG	O3-C3-C2	-2.02	105.30	109.47
5	H	1	NAG	O5-C1-C2	-2.01	108.11	111.29
4	E	5	MAN	C1-O5-C5	-2.00	109.48	112.19

There are no chirality outliers.

All (15) torsion outliers are listed below:

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

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

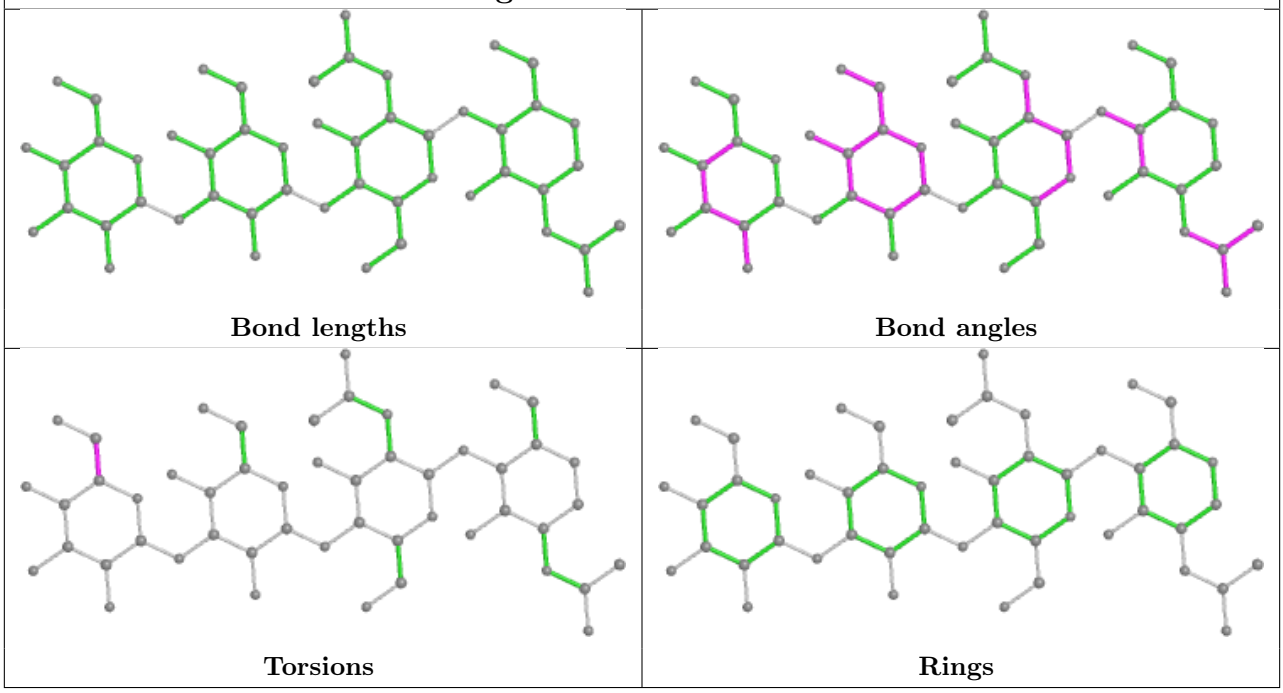
There are no ring outliers.

2 monomers are involved in 3 short contacts:

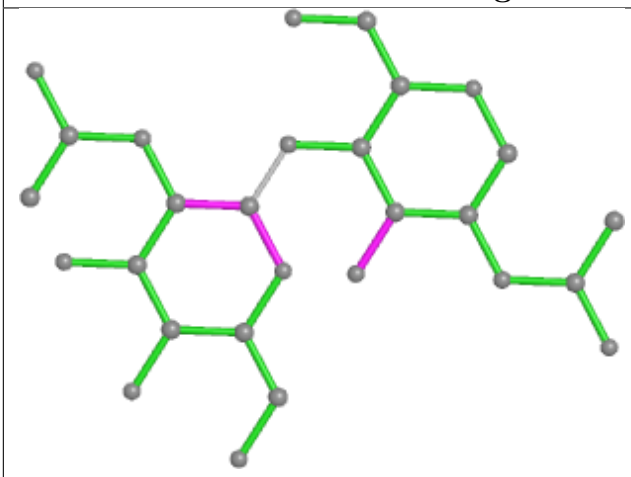
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	4	MAN	1	0
5	F	1	NAG	2	0

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

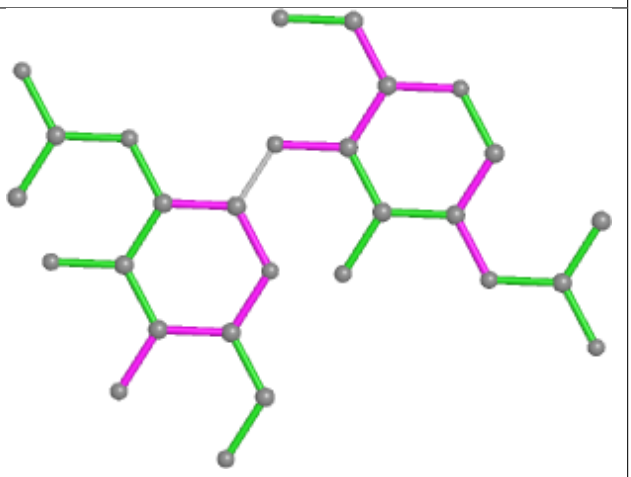
Oligosaccharide Chain C



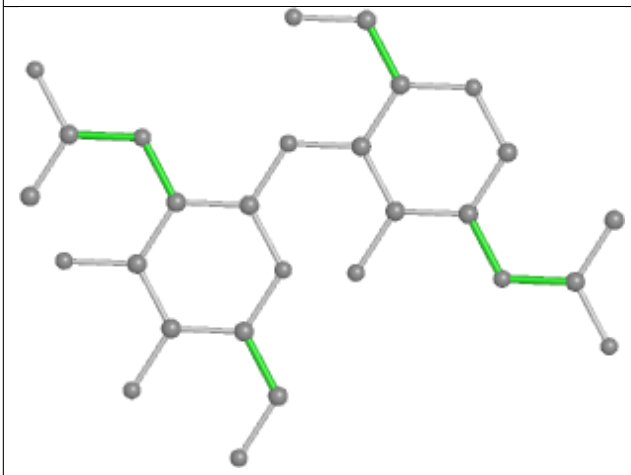
Oligosaccharide Chain D



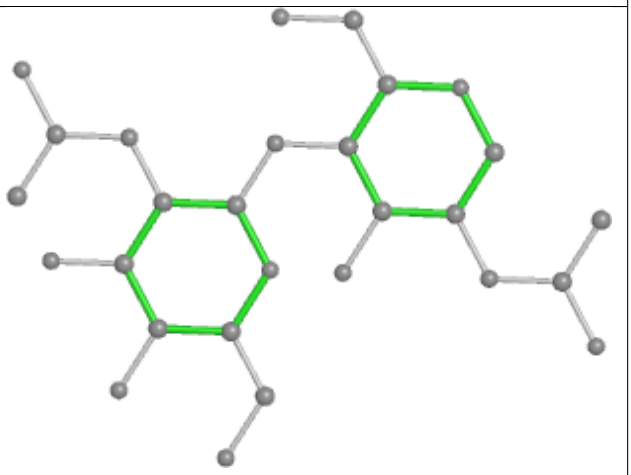
Bond lengths



Bond angles

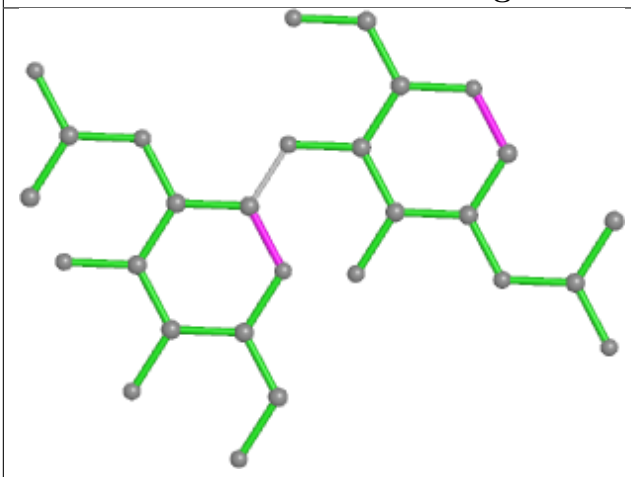


Torsions

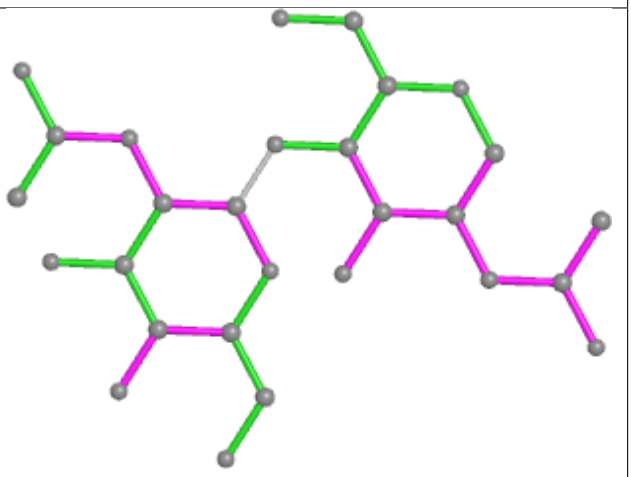


Rings

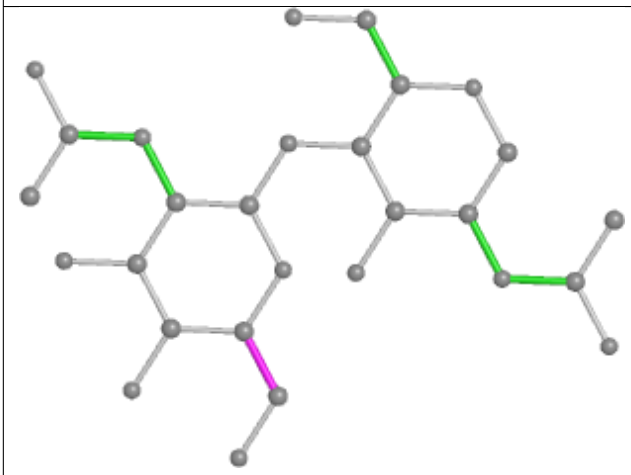
Oligosaccharide Chain G



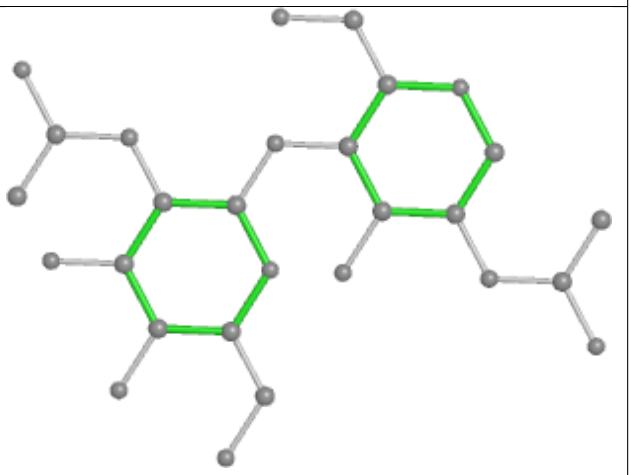
Bond lengths



Bond angles

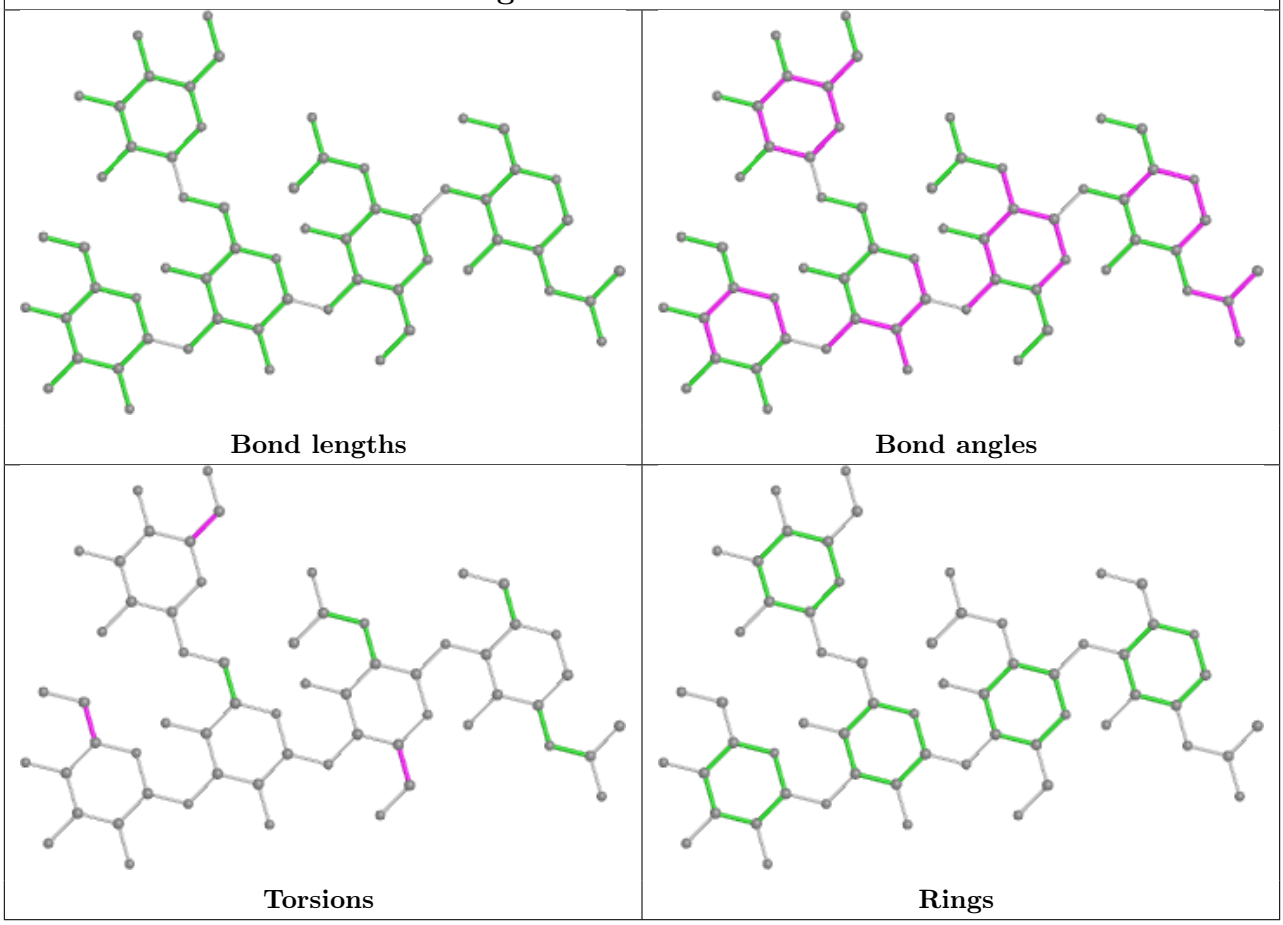


Torsions

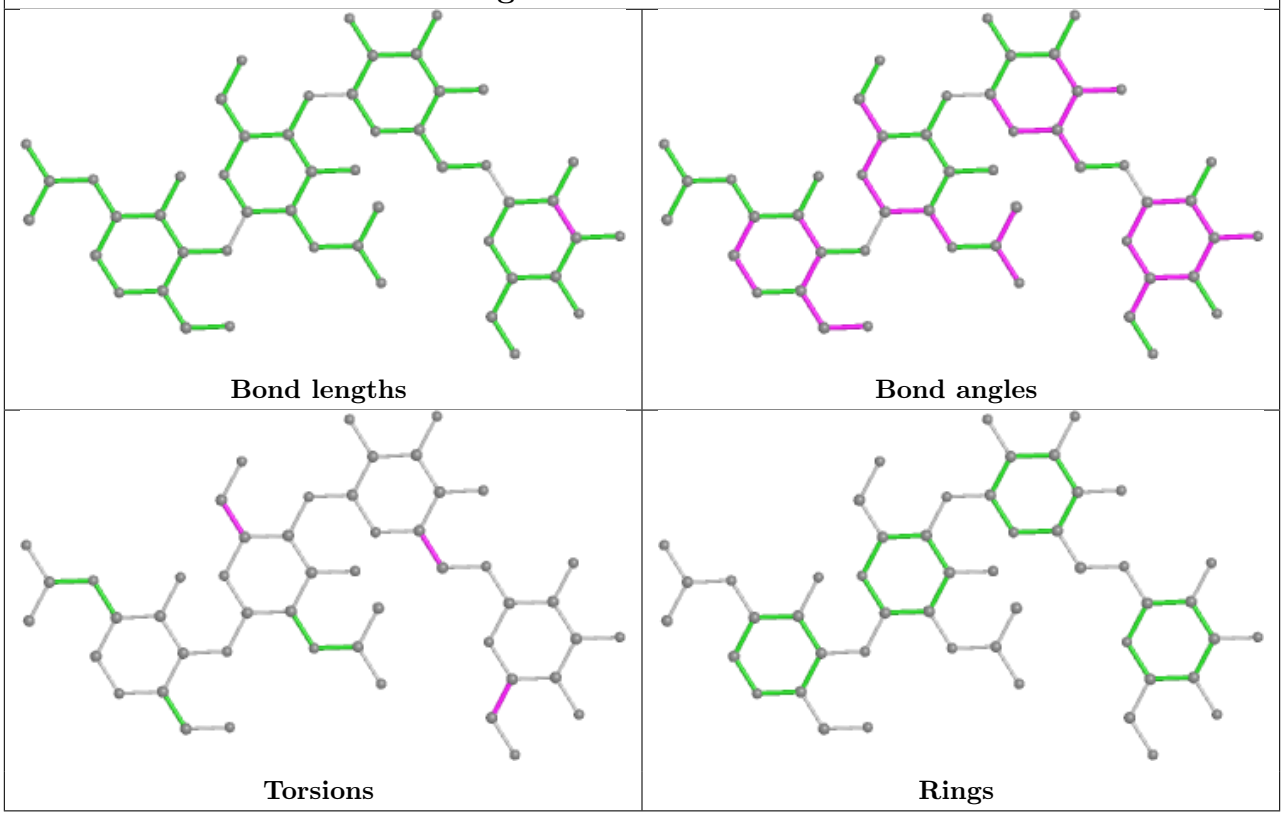


Rings

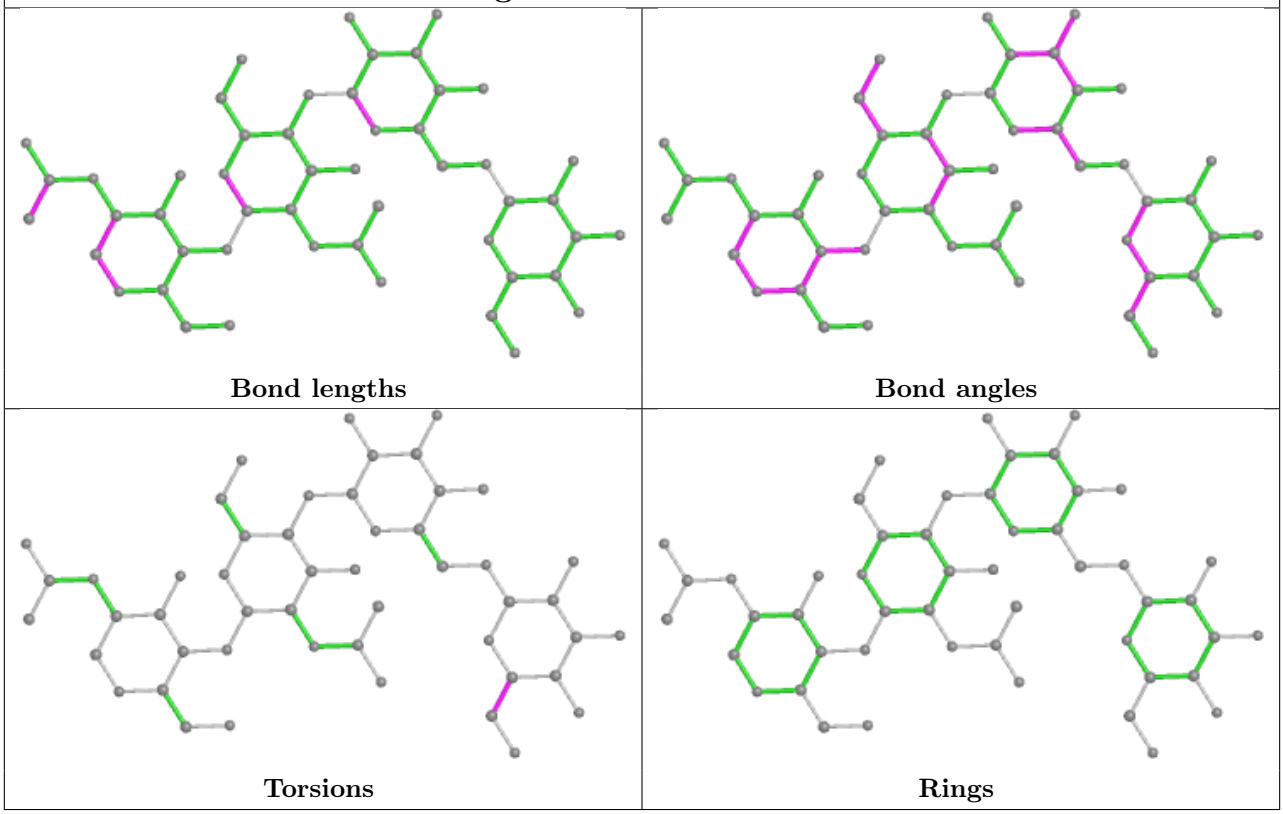
Oligosaccharide Chain E



Oligosaccharide Chain F



Oligosaccharide Chain H



5.6 Ligand geometry (i)

6 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	7VF	A	901	-	21,21,21	1.65	3 (14%)	30,30,30	1.63	6 (20%)
7	NAG	B	912	1	14,14,15	1.14	1 (7%)	17,19,21	1.62	3 (17%)
7	NAG	A	915	1	14,14,15	0.53	0	17,19,21	2.35	3 (17%)
6	7VF	B	901	-	21,21,21	1.79	4 (19%)	30,30,30	1.41	4 (13%)
7	NAG	A	906	1	14,14,15	0.72	0	17,19,21	1.66	3 (17%)
7	NAG	A	914	1	14,14,15	1.28	2 (14%)	17,19,21	2.33	4 (23%)

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	7VF	A	901	-	-	0/4/4/4	0/3/3/3
7	NAG	B	912	1	-	0/6/23/26	0/1/1/1
7	NAG	A	915	1	-	0/6/23/26	0/1/1/1
6	7VF	B	901	-	-	0/4/4/4	0/3/3/3
7	NAG	A	906	1	-	0/6/23/26	0/1/1/1
7	NAG	A	914	1	-	2/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	901	7VF	C8-C7	6.23	1.48	1.40
6	A	901	7VF	C8-C7	4.53	1.46	1.40
6	A	901	7VF	C-C1	3.49	1.48	1.42
7	B	912	NAG	C1-C2	3.28	1.57	1.52
7	A	914	NAG	O5-C1	-2.87	1.39	1.43
7	A	914	NAG	O5-C5	-2.87	1.37	1.43
6	B	901	7VF	C2-C	2.72	1.49	1.42
6	B	901	7VF	C-C1	2.50	1.46	1.42
6	A	901	7VF	C2-C	2.42	1.48	1.42
6	B	901	7VF	C14-C1	-2.06	1.38	1.41

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	915	NAG	C1-O5-C5	7.82	122.79	112.19
7	A	914	NAG	O5-C5-C6	-6.23	97.43	107.20
7	A	914	NAG	O6-C6-C5	-4.74	95.04	111.29
7	A	906	NAG	C1-O5-C5	4.46	118.23	112.19
7	B	912	NAG	O5-C1-C2	-4.31	104.49	111.29
6	B	901	7VF	C11-C7-C8	4.11	124.48	120.73
7	A	914	NAG	O5-C1-C2	-4.06	104.88	111.29
6	A	901	7VF	C2-C-C1	4.04	119.62	117.44
6	A	901	7VF	C14-C1-N	3.59	122.06	117.97
7	A	906	NAG	O3-C3-C2	-3.33	102.58	109.47
6	A	901	7VF	C-C1-N	-3.27	119.35	122.83
7	A	915	NAG	C4-C3-C2	-3.10	106.48	111.02
7	B	912	NAG	O3-C3-C2	3.00	115.68	109.47
7	A	915	NAG	O3-C3-C2	2.75	115.15	109.47
6	B	901	7VF	C4-N-C1	2.56	120.89	116.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	912	NAG	C1-C2-N2	-2.54	106.15	110.49
6	B	901	7VF	C14-C1-N	2.39	120.70	117.97
6	A	901	7VF	C11-C7-C8	-2.35	118.58	120.73
6	B	901	7VF	C-C1-N	-2.22	120.47	122.83
6	A	901	7VF	O-C15-C13	-2.17	113.83	120.02
7	A	906	NAG	O5-C5-C6	2.15	110.58	107.20
7	A	914	NAG	O5-C5-C4	2.14	116.04	110.83
6	A	901	7VF	C4-N-C1	2.12	120.22	116.93

There are no chirality outliers.

All (2) torsion outliers are listed below:

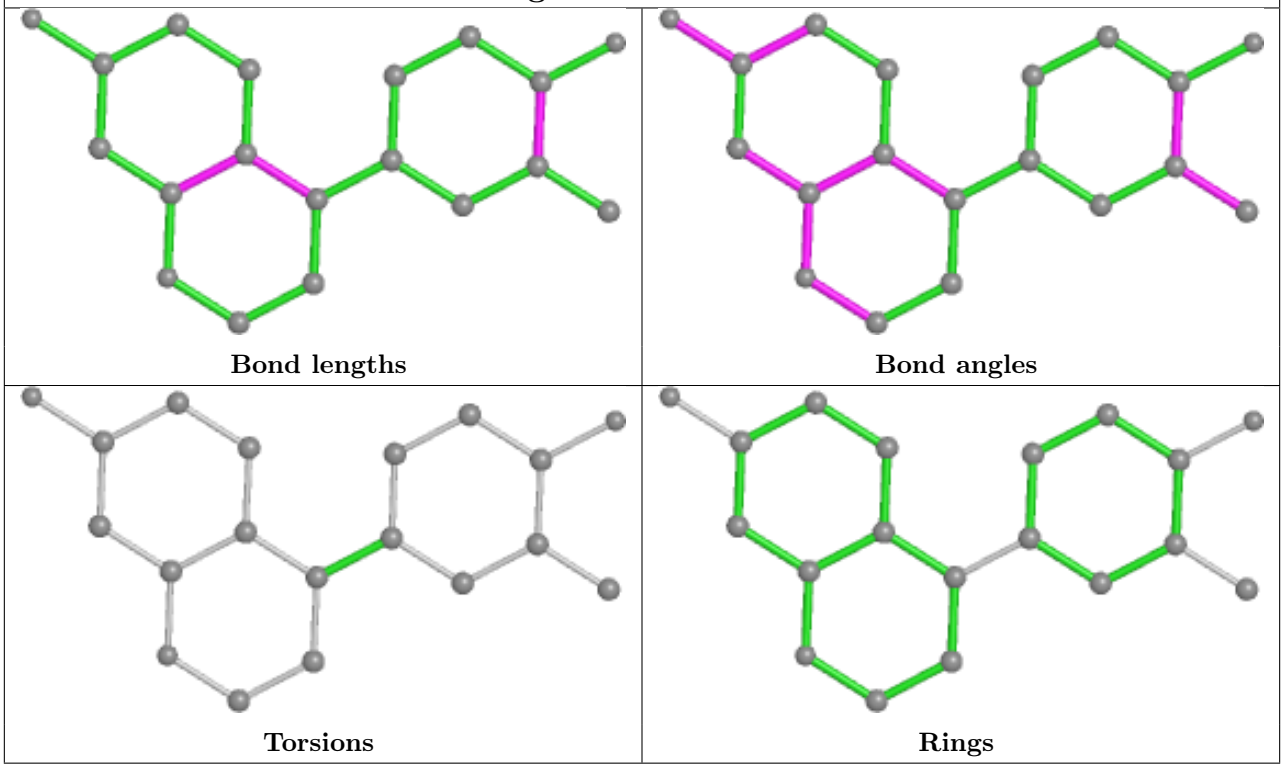
Mol	Chain	Res	Type	Atoms
7	A	914	NAG	C4-C5-C6-O6
7	A	914	NAG	O5-C5-C6-O6

There are no ring outliers.

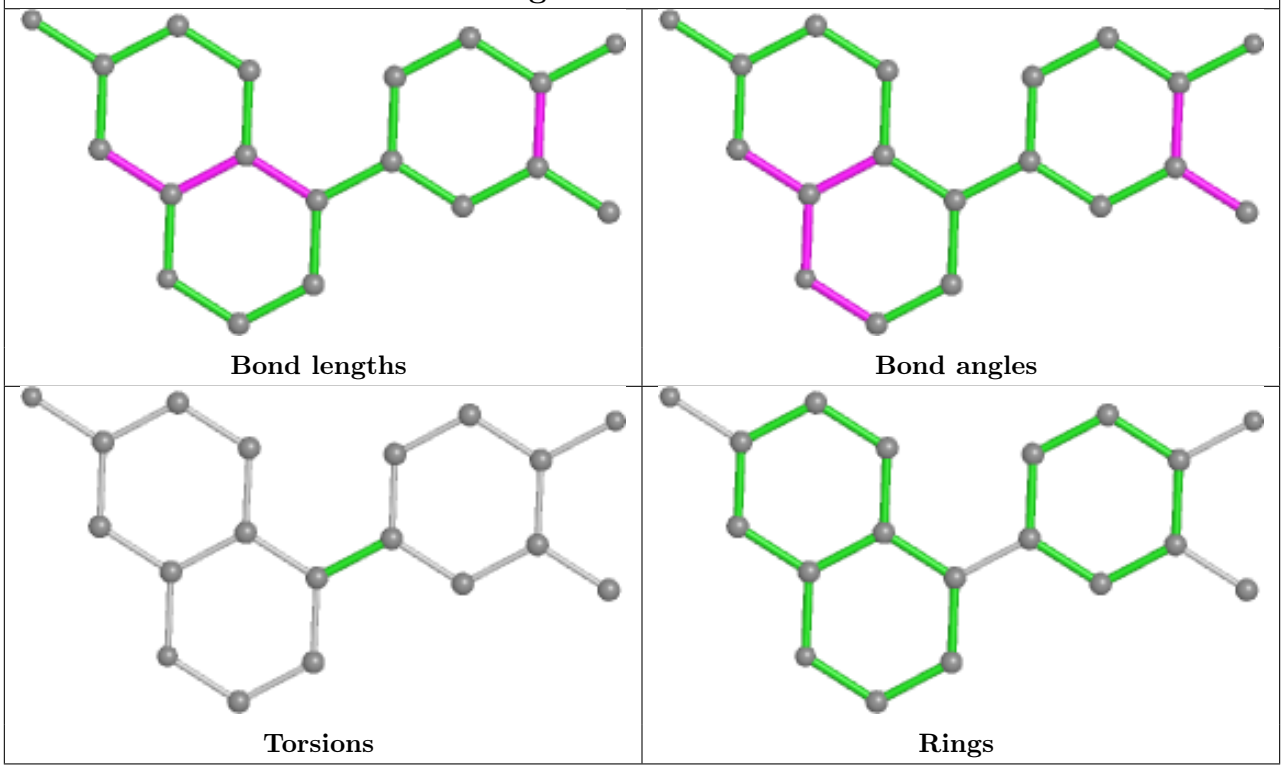
No monomer is involved in short contacts.

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 7VF A 901



Ligand 7VF B 901



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	750/811 (92%)	0.33	43 (5%)	23	30	30, 55, 100, 158	0
1	B	745/811 (91%)	0.38	47 (6%)	20	25	34, 56, 100, 124	0
All	All	1495/1622 (92%)	0.36	90 (6%)	21	28	30, 56, 100, 158	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	186	VAL	6.6
1	A	756	LEU	5.8
1	A	185	LYS	5.6
1	B	64	TYR	5.5
1	A	759	LYS	5.4
1	A	791	LEU	5.4
1	A	780	ILE	5.2
1	A	774	PHE	4.7
1	B	793	VAL	4.3
1	B	792	ASN	4.2
1	B	41	GLN	4.2
1	B	785	ARG	4.2
1	B	46	ILE	4.2
1	B	182	TYR	4.1
1	A	727	LEU	4.1
1	B	472	ARG	4.1
1	A	461	PHE	4.1
1	B	786	TRP	4.0
1	A	735	VAL	4.0
1	A	760	THR	4.0
1	B	791	LEU	4.0
1	B	183	PHE	4.0
1	B	186	VAL	3.9
1	B	185	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	600	THR	3.8
1	B	817	LEU	3.7
1	A	182	TYR	3.7
1	A	786	TRP	3.5
1	A	183	PHE	3.5
1	A	783	PHE	3.5
1	B	789	GLU	3.5
1	A	751	ILE	3.4
1	B	569	ARG	3.3
1	A	801	VAL	3.3
1	A	758	THR	3.2
1	A	601	ASP	3.1
1	B	34	TYR	3.1
1	B	787	MET	3.0
1	B	32	ARG	3.0
1	A	470	PHE	3.0
1	B	40	LYS	3.0
1	B	572	GLY	3.0
1	B	788	ASP	3.0
1	A	113	GLY	2.9
1	A	100	VAL	2.9
1	A	802	ILE	2.8
1	B	795	ILE	2.8
1	B	184	ASN	2.7
1	B	66	THR	2.7
1	A	761	THR	2.7
1	B	782	ASP	2.7
1	A	804	ALA	2.6
1	A	769	LEU	2.6
1	B	567	TYR	2.6
1	A	763	LYS	2.6
1	A	678	PHE	2.6
1	B	36	CYS	2.6
1	B	731	PHE	2.6
1	A	757	GLU	2.6
1	A	762	THR	2.5
1	A	811	GLY	2.5
1	B	268	VAL	2.5
1	B	63	LYS	2.5
1	B	677	LYS	2.5
1	B	35	PRO	2.5
1	B	74	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	753	LYS	2.4
1	B	85	GLY	2.4
1	B	60	THR	2.4
1	B	54	LEU	2.4
1	A	603	TYR	2.4
1	A	785	ARG	2.4
1	A	567	TYR	2.3
1	B	799	VAL	2.3
1	A	122	LEU	2.2
1	B	601	ASP	2.2
1	A	789	GLU	2.2
1	B	65	VAL	2.2
1	A	807	GLY	2.2
1	B	815	VAL	2.2
1	B	570	ILE	2.2
1	B	88	ASN	2.1
1	A	74	PHE	2.1
1	A	112	ASN	2.1
1	B	790	HIS	2.1
1	A	794	LYS	2.1
1	B	44	SER	2.1
1	B	733	SER	2.0
1	A	782	ASP	2.0
1	A	776	CYS	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MAN	F	4	11/12	0.68	0.19	75,88,96,97	0
5	MAN	H	4	11/12	0.78	0.17	72,94,98,111	0
2	MAN	C	4	11/12	0.80	0.24	71,87,92,92	0
4	MAN	E	5	11/12	0.84	0.13	81,87,91,98	0

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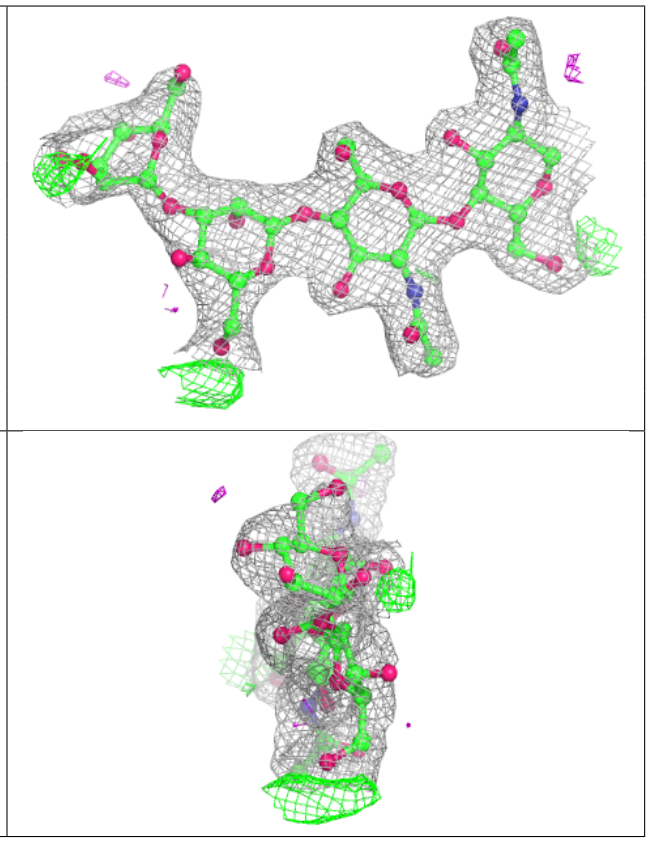
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MAN	E	4	11/12	0.86	0.12	85,96,102,105	0
2	BMA	C	3	11/12	0.87	0.14	56,68,75,88	0
3	NAG	G	2	14/15	0.88	0.15	51,64,81,88	0
5	BMA	F	3	11/12	0.89	0.16	68,82,86,88	0
4	BMA	E	3	11/12	0.93	0.10	49,64,73,74	0
5	BMA	H	3	11/12	0.93	0.12	51,60,79,94	0
3	NAG	D	2	14/15	0.93	0.11	45,57,68,69	0
5	NAG	F	2	14/15	0.96	0.17	38,45,59,67	0
5	NAG	F	1	14/15	0.97	0.17	35,41,45,54	0
2	NAG	C	2	14/15	0.97	0.11	34,42,50,55	0
3	NAG	G	1	14/15	0.97	0.14	32,39,48,52	0
3	NAG	D	1	14/15	0.98	0.12	32,35,40,41	0
5	NAG	H	1	14/15	0.98	0.13	33,36,39,43	0
5	NAG	H	2	14/15	0.98	0.12	36,41,44,51	0
2	NAG	C	1	14/15	0.98	0.13	30,37,42,50	0
4	NAG	E	1	14/15	0.98	0.15	32,36,38,41	0
4	NAG	E	2	14/15	0.99	0.13	28,37,46,48	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.

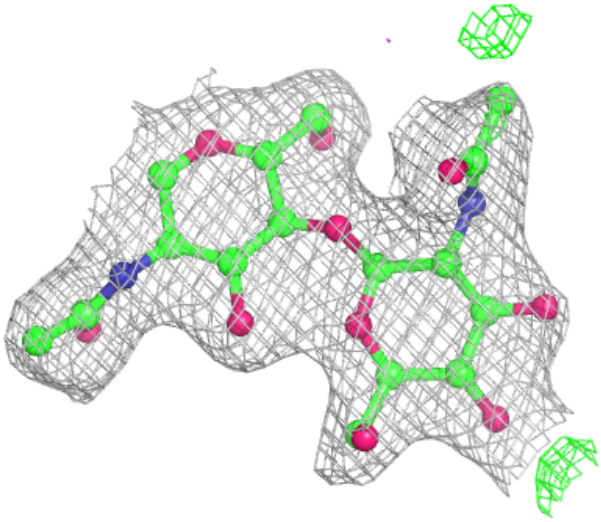
Electron density around Chain C:

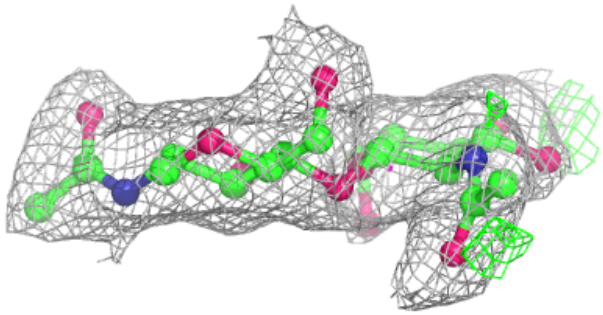
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

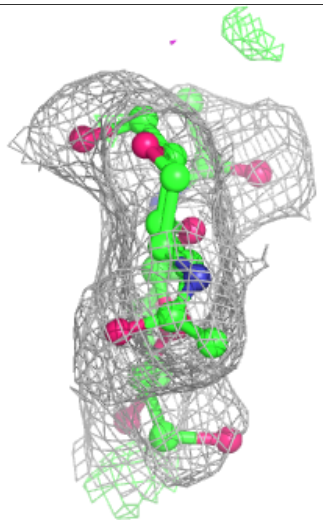


Electron density around Chain D:

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

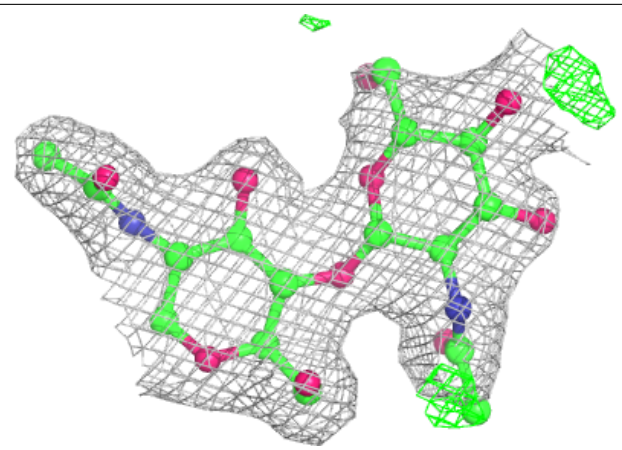


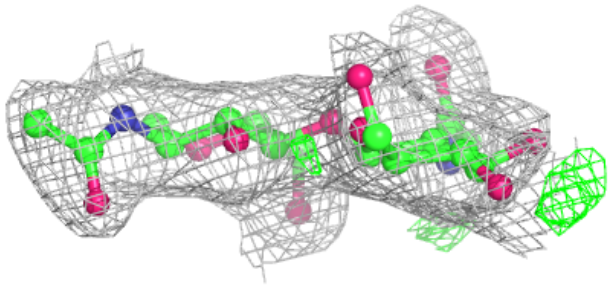


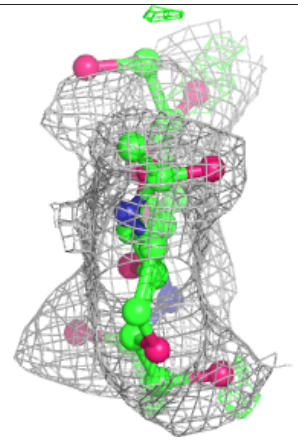


Electron density around Chain G:

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

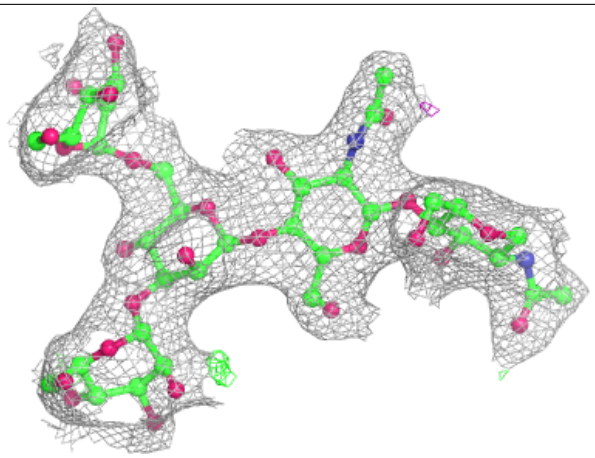


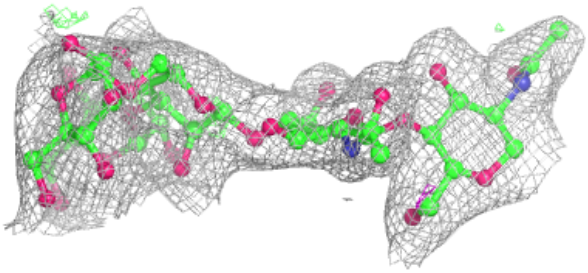


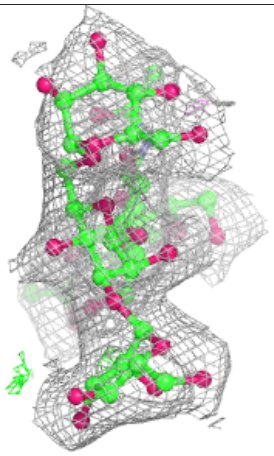


Electron density around Chain E:

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

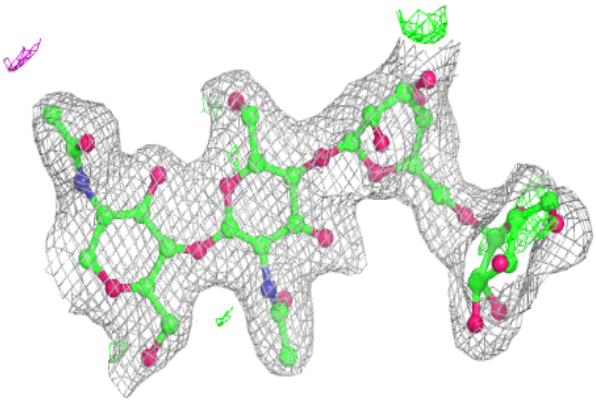


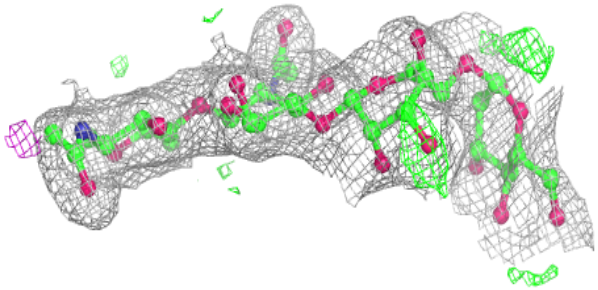


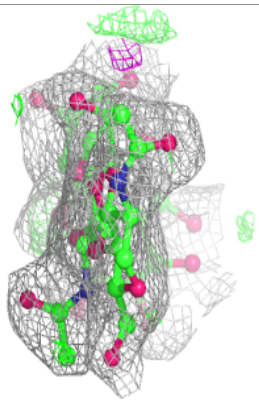


Electron density around Chain F:

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

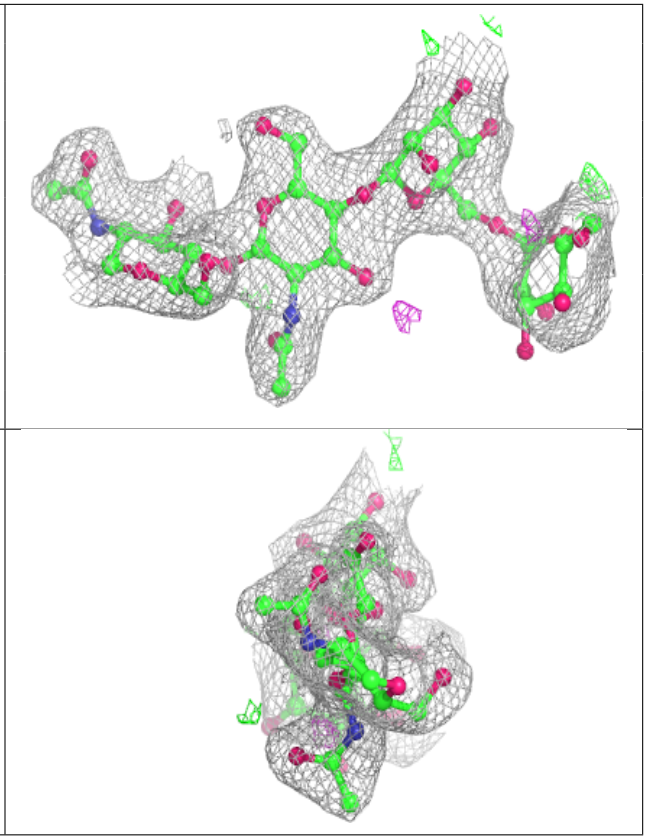






Electron density around Chain H:

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



6.4 Ligands (i)

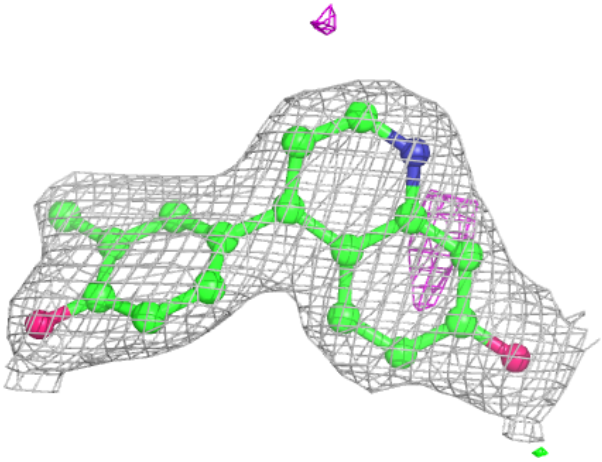
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

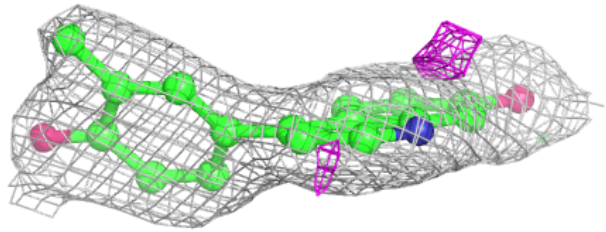
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	A	915	14/15	0.82	0.20	73,83,98,99	0
7	NAG	B	912	14/15	0.95	0.14	54,65,76,76	0
7	NAG	A	914	14/15	0.96	0.11	36,45,50,56	0
6	7VF	B	901	19/19	0.96	0.13	34,38,43,46	0
7	NAG	A	906	14/15	0.96	0.10	47,58,64,64	0
6	7VF	A	901	19/19	0.97	0.14	34,38,43,43	0

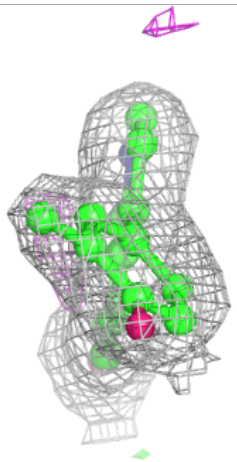
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 7VF 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)

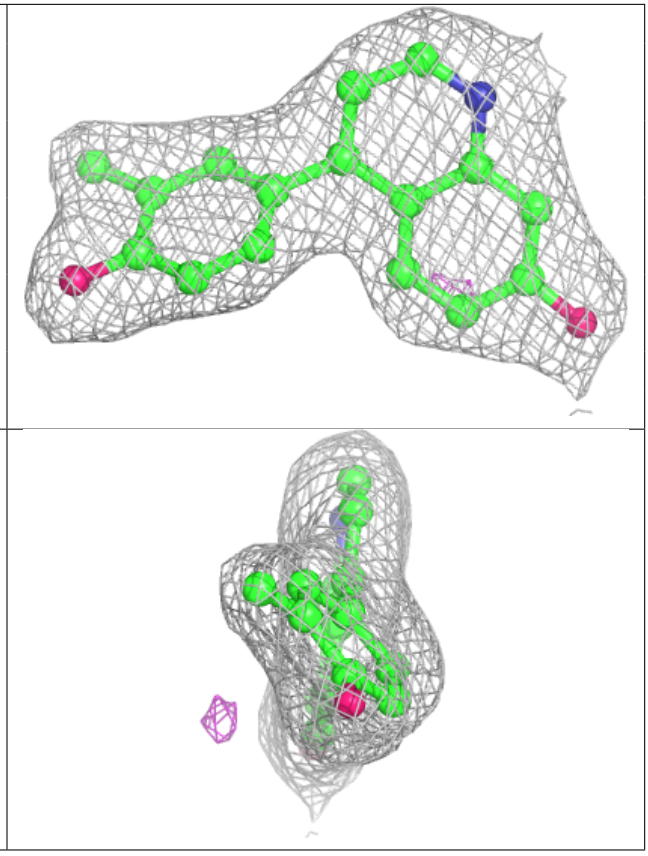






Electron density around 7VF A 901:

$2mF_o$-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 (i)

There are no such residues in this entry.