Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 02:27 AM EDT

PDB ID	:	4QC0
Title	:	Crystal structure of human TLR8 in complex with XG-1-236
Authors	:	Tanji, H.; Ohto, U.; Shimizu, T.
Deposited on	:	2014-05-09
Resolution	:	2.10 Å(reported)

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

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

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

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

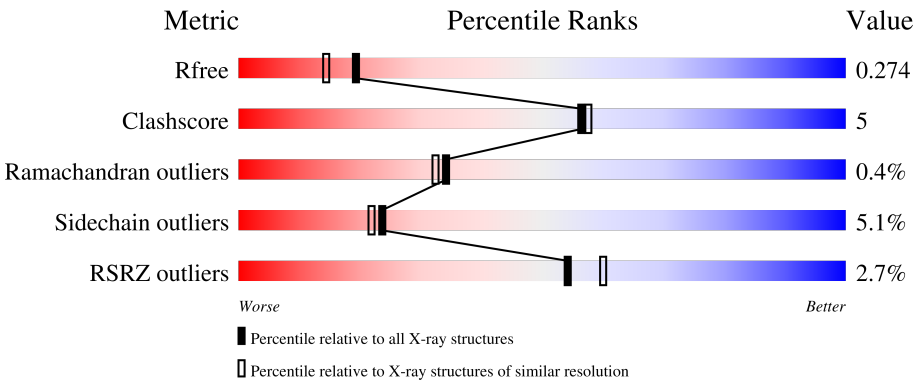
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	811	2%, 78%, 13%, • 8%
1	B	811	3%, 77%, 13%, • 8%
2	C	3	67%, 33%
2	D	3	100%
2	F	3	100%

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Mol	Chain	Length	Quality of chain
3	E	4	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12433 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.

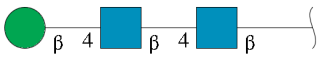
- Molecule 1 is a protein called Toll-like receptor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	746	5988	3831	1018	1120	19	0	0	0
1	B	745	5996	3835	1020	1122	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 beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

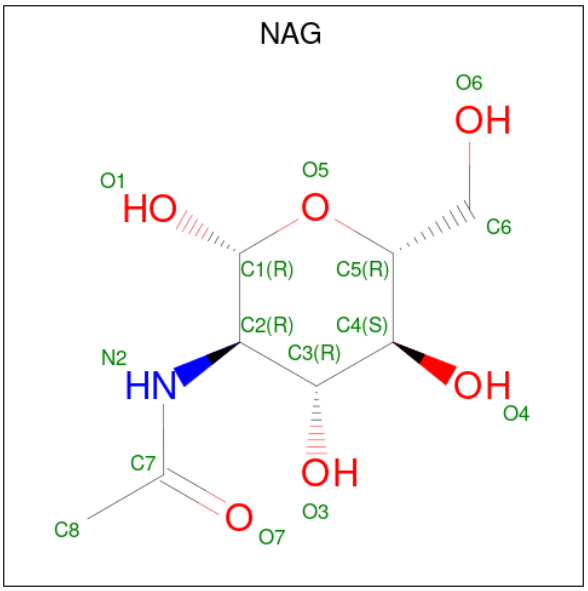


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	3	39	22	2	15	0	0	0
2	D	3	39	22	2	15	0	0	0
2	F	3	39	22	2	15	0	0	0

- Molecule 3 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.

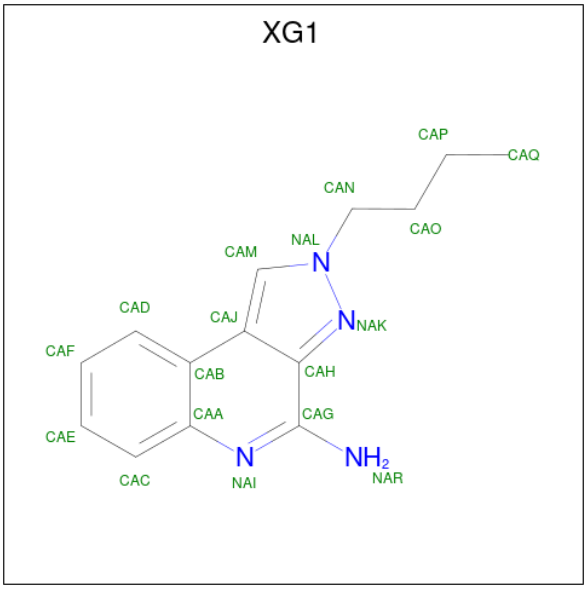
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	4	50	28	2	20	0	0	0

- Molecule 4 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		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	B	1	14	8	1	5	0	0
			Total	C	N	O		
4	B	1	14	8	1	5	0	0

- Molecule 5 is 2-butyl-2H-pyrazolo[3,4-c]quinolin-4-amine (three-letter code: XG1) (formula: $C_{14}H_{16}N_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
5	A	1	18	14	4	0	0
			Total	C	N		
5	B	1	18	14	4	0	0

- Molecule 6 is water.

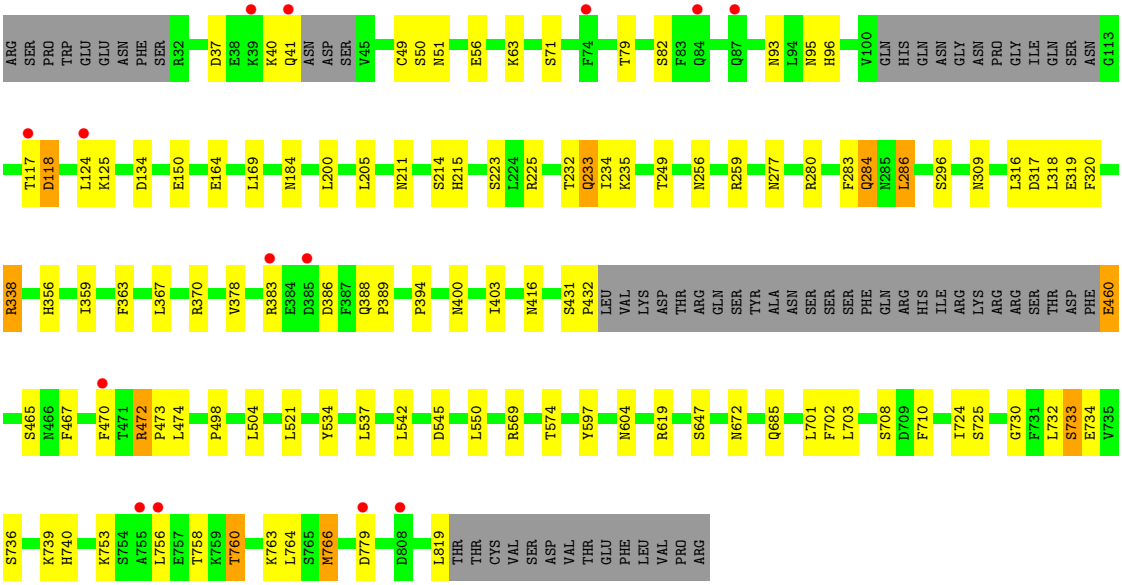
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	87	87	87	0	0
			Total	O		
6	B	89	89	89	0	0

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.

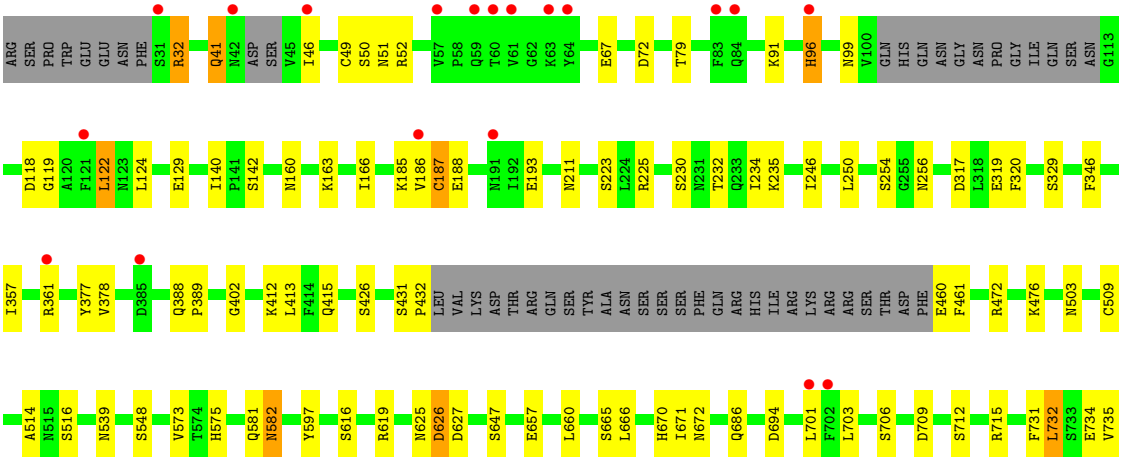
- Molecule 1: Toll-like receptor 8

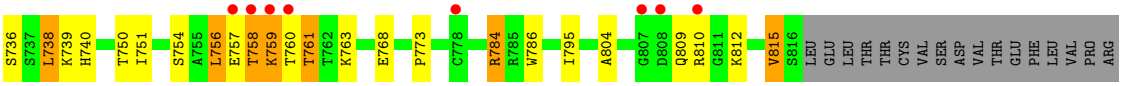
Chain A:



- Molecule 1: Toll-like receptor 8

Chain B:



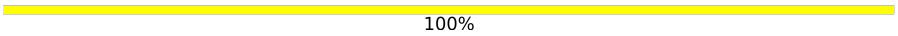


• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

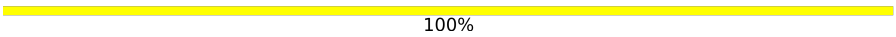
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



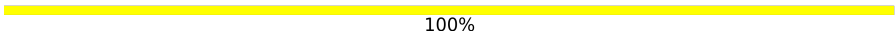
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



• Molecule 3: 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 E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.51Å 149.22Å 85.83Å 90.00° 103.50° 90.00°	Depositor
Resolution (Å)	83.46 – 2.10 38.78 – 2.10	Depositor EDS
% Data completeness (in resolution range)	88.5 (83.46-2.10) 88.5 (38.78-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.213 , 0.271 0.218 , 0.274	Depositor DCC
R_{free} test set	4509 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	29.5	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 39.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12433	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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: NAG, MAN, XG1, BMA

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	0.58	0/6111	0.81	2/8287 (0.0%)
1	B	0.55	0/6119	0.79	0/8297
All	All	0.56	0/12230	0.80	2/16584 (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	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	259	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	338	ARG	NE-CZ-NH2	5.08	122.84	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	186	VAL	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	5988	0	5961	61	0
1	B	5996	0	5985	63	0
2	C	39	0	34	1	0
2	D	39	0	34	0	0
2	F	39	0	34	0	0
3	E	50	0	43	0	0
4	A	42	0	39	2	0
4	B	28	0	26	1	0
5	A	18	0	16	0	0
5	B	18	0	16	0	0
6	A	87	0	0	5	0
6	B	89	0	0	5	0
All	All	12433	0	12188	123	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 (123) 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:472:ARG:NH1	1:A:473:PRO:O	2.07	0.86
1:B:329:SER:O	1:B:329:SER:OG	1.97	0.79
1:B:735:VAL:HB	1:B:738:LEU:CB	2.14	0.78
1:B:768:GLU:HA	6:B:1043:HOH:O	1.85	0.75
1:B:735:VAL:HB	1:B:738:LEU:HB3	1.68	0.72
1:B:163:LYS:HD2	6:B:1084:HOH:O	1.95	0.66
1:A:215:HIS:ND1	6:A:1079:HOH:O	2.29	0.65
1:A:79:THR:HG22	1:A:117:THR:HG21	1.80	0.64
1:B:706:SER:HB3	1:B:709:ASP:OD2	1.97	0.63
1:A:498:PRO:HA	6:A:1077:HOH:O	1.98	0.63
1:B:211:ASN:O	1:B:232:THR:HA	1.98	0.63
1:B:732:LEU:O	1:B:758:THR:HG22	2.00	0.62
1:B:760:THR:HG22	1:B:761:THR:H	1.64	0.62
1:A:460:GLU:HG2	1:B:625:ASN:HD22	1.65	0.62
1:B:625:ASN:OD1	1:B:626:ASP:N	2.33	0.62
1:B:317:ASP:OD1	1:B:319:GLU:OE1	2.18	0.61
1:A:283:PHE:HA	1:A:286:LEU:HD22	1.81	0.61
1:B:581:GLN:HG2	1:B:582:ASN:OD1	2.00	0.61
1:B:431:SER:HB2	1:B:432:PRO:HD2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:733:SER:CB	6:A:1024:HOH:O	2.49	0.60
1:A:317:ASP:OD1	1:A:319:GLU:OE1	2.21	0.58
1:A:734:GLU:HB2	1:A:760:THR:HG21	1.85	0.57
1:B:185:LYS:O	1:B:187:CYS:HB2	2.04	0.57
1:A:732:LEU:HB3	1:A:758:THR:HG23	1.85	0.57
1:B:735:VAL:HB	1:B:738:LEU:HB2	1.86	0.56
1:B:193:GLU:HG2	6:B:1084:HOH:O	2.05	0.56
1:A:431:SER:HB2	1:A:432:PRO:CD	2.36	0.55
1:A:545:ASP:OD1	1:A:574:THR:OG1	2.23	0.55
1:B:234:ILE:O	1:B:256:ASN:HB3	2.07	0.54
1:B:582:ASN:OD1	1:B:582:ASN:N	2.39	0.54
1:A:732:LEU:HD12	1:A:756:LEU:HA	1.89	0.54
1:A:467:PHE:HB3	2:C:1:NAG:H81	1.90	0.54
1:A:537:LEU:HD22	1:A:542:LEU:HD11	1.89	0.54
1:A:739:LYS:HG2	1:A:763:LYS:HB3	1.89	0.54
1:A:96:HIS:ND1	1:A:134:ASP:OD2	2.40	0.53
1:A:521:LEU:HD13	1:A:550:LEU:HD21	1.89	0.53
1:B:51:ASN:HA	1:B:72:ASP:O	2.07	0.53
1:A:234:ILE:O	1:A:256:ASN:HB3	2.08	0.53
1:A:223:SER:O	1:A:225:ARG:NH1	2.42	0.52
1:A:214:SER:HA	1:A:233:GLN:O	2.10	0.52
1:A:431:SER:HB2	1:A:432:PRO:HD2	1.90	0.52
1:B:320:PHE:HA	1:B:346:PHE:O	2.10	0.52
1:B:357:ILE:HG13	1:B:377:TYR:CZ	2.45	0.52
1:A:703:LEU:HD21	1:A:724:ILE:CD1	2.39	0.52
1:B:784:ARG:NH1	1:B:815:VAL:O	2.43	0.51
1:B:573:VAL:O	1:B:575:HIS:CE1	2.64	0.51
1:A:118:ASP:HB3	6:A:1086:HOH:O	2.11	0.51
1:A:732:LEU:HD13	1:A:756:LEU:O	2.11	0.50
1:A:708:SER:HB2	1:A:734:GLU:HG3	1.94	0.49
1:A:597:TYR:HB3	1:A:619:ARG:HB2	1.92	0.49
1:B:230:SER:HA	1:B:254:SER:O	2.13	0.49
1:B:96:HIS:CE1	1:B:99:ASN:OD1	2.65	0.48
1:A:79:THR:HG22	1:A:117:THR:CG2	2.43	0.48
1:B:809:GLN:OE1	1:B:812:LYS:HD2	2.12	0.48
1:B:67:GLU:OE2	1:B:91:LYS:HE3	2.14	0.48
1:B:250:LEU:C	1:B:250:LEU:HD23	2.33	0.48
1:A:118:ASP:OD1	1:A:118:ASP:N	2.45	0.47
1:B:625:ASN:OD1	1:B:625:ASN:C	2.51	0.47
1:B:41:GLN:HG2	1:B:46:ILE:CD1	2.44	0.47
1:A:753:LYS:HA	1:A:756:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:SER:O	1:B:225:ARG:NH1	2.48	0.47
1:B:119:GLY:HA2	1:B:122:LEU:HG	1.97	0.47
1:A:730:GLY:O	1:A:733:SER:HB2	2.15	0.47
1:A:739:LYS:HA	1:A:764:LEU:HA	1.97	0.47
1:A:184:ASN:HB2	1:B:627:ASP:O	2.15	0.46
1:A:647:SER:HA	1:A:672:ASN:O	2.16	0.46
1:B:597:TYR:HB3	1:B:619:ARG:HB2	1.98	0.46
1:B:706:SER:O	1:B:709:ASP:HB2	2.15	0.46
1:B:731:PHE:O	1:B:734:GLU:HB3	2.15	0.46
4:B:910:NAG:H4	6:B:1080:HOH:O	2.16	0.46
1:A:359:ILE:HG23	1:A:363:PHE:CD1	2.51	0.46
1:A:400:ASN:OD1	1:A:400:ASN:C	2.53	0.45
1:A:685:GLN:HG3	1:A:710:PHE:HA	1.98	0.45
1:A:703:LEU:HD21	1:A:724:ILE:HD13	1.97	0.45
1:B:647:SER:HB2	1:B:672:ASN:O	2.17	0.45
1:A:403:ILE:HG22	1:A:403:ILE:O	2.17	0.45
1:A:316:LEU:HD21	1:A:318:LEU:HD11	1.99	0.45
1:B:50:SER:O	1:B:52:ARG:HG2	2.17	0.45
1:A:388:GLN:HB2	1:A:389:PRO:HD3	1.98	0.44
1:B:140:ILE:HD13	1:B:166:ILE:HD11	2.00	0.44
1:B:757:GLU:O	1:B:758:THR:OG1	2.35	0.44
1:B:402:GLY:HA2	1:B:426:SER:O	2.18	0.44
1:B:665:SER:O	1:B:666:LEU:C	2.55	0.44
1:A:736:SER:O	1:A:763:LYS:HD3	2.18	0.43
1:B:32:ARG:NH1	1:B:795:ILE:HG12	2.33	0.43
1:B:431:SER:HB2	1:B:432:PRO:CD	2.46	0.43
1:A:604:ASN:HB3	6:A:1045:HOH:O	2.18	0.43
1:B:754:SER:O	1:B:757:GLU:HB3	2.18	0.43
1:B:357:ILE:HG13	1:B:377:TYR:CE2	2.53	0.43
1:B:773:PRO:HA	1:B:804:ALA:HB2	2.00	0.42
1:B:388:GLN:HB2	1:B:389:PRO:HD3	2.00	0.42
1:A:394:PRO:HG2	4:A:904:NAG:H82	2.01	0.42
1:A:277:ASN:OD1	1:A:277:ASN:C	2.58	0.42
1:B:514:ALA:HA	1:B:539:ASN:O	2.20	0.42
1:A:93:ASN:OD1	1:A:93:ASN:C	2.57	0.42
1:A:383:ARG:HD3	1:A:386:ASP:OD2	2.19	0.42
1:B:91:LYS:HG2	1:B:129:GLU:HB3	2.02	0.42
1:B:671:ILE:HG22	1:B:671:ILE:O	2.19	0.42
1:B:750:THR:OG1	1:B:751:ILE:N	2.52	0.42
1:A:474:LEU:HD23	1:A:474:LEU:HA	1.90	0.42
1:B:415:GLN:HG3	1:B:503:ASN:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:670:HIS:HA	1:B:694:ASP:HB3	2.02	0.42
1:A:211:ASN:O	1:A:232:THR:HA	2.19	0.42
1:A:356:HIS:NE2	1:A:383:ARG:HD2	2.35	0.42
1:B:124:LEU:HD23	1:B:124:LEU:N	2.34	0.42
1:B:732:LEU:HA	1:B:735:VAL:HG13	2.01	0.42
1:B:756:LEU:HD22	1:B:786:TRP:CG	2.55	0.42
1:B:660:LEU:HD22	1:B:686:GLN:HG3	2.02	0.41
1:A:284:GLN:HA	1:A:309:ASN:HD22	1.84	0.41
1:B:460:GLU:OE1	1:B:461:PHE:CE2	2.73	0.41
1:B:759:LYS:O	1:B:759:LYS:HD3	2.20	0.41
1:B:763:LYS:N	6:B:1047:HOH:O	2.53	0.41
1:A:40:LYS:O	1:A:41:GLN:C	2.58	0.41
1:A:169:LEU:O	1:A:200:LEU:HD22	2.19	0.41
1:A:205:LEU:C	1:A:205:LEU:HD23	2.41	0.41
1:A:370:ARG:HH22	4:A:904:NAG:H61	1.85	0.41
1:A:296:SER:HA	1:A:320:PHE:O	2.21	0.40
1:A:367:LEU:HD23	1:A:367:LEU:HA	1.95	0.40
1:A:356:HIS:CD2	1:A:383:ARG:HD2	2.57	0.40
1:B:738:LEU:HD21	1:B:740:HIS:O	2.22	0.40
1:A:504:LEU:HD23	1:A:504:LEU:HA	1.94	0.40
1:A:740:HIS:CD2	1:A:766:MET:HG2	2.56	0.40
1:A:71:SER:HA	1:A:95:ASN:O	2.22	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	738/811 (91%)	679 (92%)	56 (8%)	3 (0%)	34	32
1	B	737/811 (91%)	669 (91%)	65 (9%)	3 (0%)	34	32
All	All	1475/1622 (91%)	1348 (91%)	121 (8%)	6 (0%)	34	32

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	758	THR
1	A	82	SER
1	A	124	LEU
1	B	736	SER
1	B	378	VAL
1	A	378	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	686/755 (91%)	654 (95%)	32 (5%)	26	25
1	B	690/755 (91%)	652 (94%)	38 (6%)	21	19
All	All	1376/1510 (91%)	1306 (95%)	70 (5%)	24	22

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ASP
1	A	49	CYS
1	A	50	SER
1	A	51	ASN
1	A	56	GLU
1	A	63	LYS
1	A	118	ASP
1	A	125	LYS
1	A	150	GLU
1	A	164	GLU
1	A	233	GLN
1	A	235	LYS
1	A	249	THR
1	A	280	ARG
1	A	284	GLN
1	A	286	LEU
1	A	338	ARG

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Mol	Chain	Res	Type
1	A	416	ASN
1	A	460	GLU
1	A	465	SER
1	A	470	PHE
1	A	472	ARG
1	A	534	TYR
1	A	569	ARG
1	A	701	LEU
1	A	702	PHE
1	A	725	SER
1	A	733	SER
1	A	760	THR
1	A	766	MET
1	A	779	ASP
1	A	819	LEU
1	B	32	ARG
1	B	41	GLN
1	B	49	CYS
1	B	79	THR
1	B	96	HIS
1	B	118	ASP
1	B	122	LEU
1	B	142	SER
1	B	160	ASN
1	B	187	CYS
1	B	188	GLU
1	B	235	LYS
1	B	246	ILE
1	B	361	ARG
1	B	412	LYS
1	B	413	LEU
1	B	472	ARG
1	B	476	LYS
1	B	509	CYS
1	B	516	SER
1	B	548	SER
1	B	582	ASN
1	B	616	SER
1	B	626	ASP
1	B	657	GLU
1	B	701	LEU
1	B	703	LEU

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Mol	Chain	Res	Type
1	B	712	SER
1	B	715	ARG
1	B	732	LEU
1	B	738	LEU
1	B	739	LYS
1	B	756	LEU
1	B	759	LYS
1	B	761	THR
1	B	784	ARG
1	B	810	ARG
1	B	815	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	99	ASN
1	A	123	ASN
1	A	309	ASN
1	A	388	GLN
1	A	408	GLN
1	A	625	ASN
1	A	809	GLN
1	B	41	GLN
1	B	77	HIS
1	B	135	ASN
1	B	247	ASN
1	B	285	ASN
1	B	416	ASN
1	B	752	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)

13 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	C	1	2,1	14,14,15	0.83	1 (7%)	17,19,21	1.20	2 (11%)
2	NAG	C	2	2	14,14,15	0.81	0	17,19,21	1.46	3 (17%)
2	BMA	C	3	2	11,11,12	0.84	0	15,15,17	3.37	8 (53%)
2	NAG	D	1	2,1	14,14,15	0.66	0	17,19,21	1.55	3 (17%)
2	NAG	D	2	2	14,14,15	1.06	1 (7%)	17,19,21	2.02	7 (41%)
2	BMA	D	3	2	11,11,12	0.49	0	15,15,17	1.99	2 (13%)
3	NAG	E	1	3,1	14,14,15	0.72	0	17,19,21	1.72	5 (29%)
3	NAG	E	2	3	14,14,15	0.87	1 (7%)	17,19,21	1.83	4 (23%)
3	BMA	E	3	3	11,11,12	0.37	0	15,15,17	1.81	4 (26%)
3	MAN	E	4	3	11,11,12	0.94	1 (9%)	15,15,17	1.75	4 (26%)
2	NAG	F	1	2,1	14,14,15	0.63	0	17,19,21	1.40	3 (17%)
2	NAG	F	2	2	14,14,15	0.69	0	17,19,21	1.27	2 (11%)
2	BMA	F	3	2	11,11,12	0.58	0	15,15,17	2.17	5 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	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	-	2/2/19/22	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
3	NAG	E	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	NAG	O5-C1	-2.30	1.40	1.43
2	C	1	NAG	O5-C1	-2.27	1.40	1.43
3	E	4	MAN	O5-C1	-2.23	1.40	1.43
2	D	2	NAG	O5-C1	-2.06	1.40	1.43

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3	BMA	C1-O5-C5	8.61	123.85	112.19
2	F	3	BMA	C1-O5-C5	5.73	119.95	112.19
2	C	3	BMA	C1-C2-C3	5.02	115.83	109.67
2	D	3	BMA	O5-C5-C6	4.59	114.40	107.20
2	D	3	BMA	O4-C4-C3	-4.00	101.10	110.35
3	E	3	BMA	C1-O5-C5	3.97	117.58	112.19
3	E	4	MAN	C2-C3-C4	3.90	117.64	110.89
2	C	3	BMA	O3-C3-C2	-3.73	102.86	109.99
3	E	3	BMA	O5-C5-C6	3.72	113.03	107.20
2	C	3	BMA	C3-C4-C5	3.69	116.83	110.24
3	E	2	NAG	C6-C5-C4	-3.62	104.52	113.00
3	E	2	NAG	C1-O5-C5	3.60	117.08	112.19
2	D	1	NAG	O7-C7-C8	-3.60	115.37	122.06
3	E	4	MAN	C3-C4-C5	3.56	116.59	110.24
2	D	2	NAG	C1-C2-N2	3.52	116.50	110.49
2	C	2	NAG	O5-C1-C2	-3.51	105.74	111.29
2	C	3	BMA	O2-C2-C3	-3.51	103.11	110.14
3	E	1	NAG	C6-C5-C4	-3.47	104.89	113.00
2	F	3	BMA	C3-C4-C5	3.36	116.23	110.24
2	D	2	NAG	O7-C7-N2	3.31	128.04	121.95
2	C	3	BMA	O5-C1-C2	3.27	115.82	110.77
2	F	1	NAG	O7-C7-C8	-3.24	116.04	122.06
2	D	2	NAG	C4-C3-C2	-3.09	106.49	111.02
2	F	2	NAG	O3-C3-C2	-2.77	103.72	109.47
2	F	3	BMA	O4-C4-C5	-2.75	102.46	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2	NAG	O3-C3-C4	-2.74	104.01	110.35
3	E	1	NAG	C3-C4-C5	2.67	115.01	110.24
3	E	1	NAG	O5-C5-C4	2.59	117.14	110.83
2	F	2	NAG	C4-C3-C2	-2.53	107.31	111.02
3	E	2	NAG	O5-C1-C2	-2.50	107.33	111.29
2	F	3	BMA	C1-C2-C3	2.43	112.65	109.67
3	E	3	BMA	O3-C3-C4	-2.43	104.74	110.35
3	E	2	NAG	O6-C6-C5	-2.41	103.04	111.29
2	C	3	BMA	O5-C5-C4	2.38	116.63	110.83
2	D	2	NAG	C8-C7-N2	-2.37	112.08	116.10
2	D	2	NAG	O6-C6-C5	-2.30	103.40	111.29
2	F	1	NAG	C2-N2-C7	2.29	126.17	122.90
2	D	1	NAG	O5-C5-C6	2.26	110.75	107.20
2	F	3	BMA	C6-C5-C4	-2.25	107.73	113.00
2	C	3	BMA	O5-C5-C6	2.25	110.73	107.20
2	F	1	NAG	C1-C2-N2	2.24	114.31	110.49
3	E	1	NAG	O7-C7-N2	2.23	126.06	121.95
2	D	2	NAG	O4-C4-C3	-2.23	105.19	110.35
2	C	1	NAG	C8-C7-N2	2.23	119.87	116.10
2	C	1	NAG	O3-C3-C4	2.22	115.49	110.35
2	D	1	NAG	O4-C4-C3	-2.17	105.32	110.35
2	C	2	NAG	O3-C3-C4	-2.17	105.33	110.35
3	E	3	BMA	C1-C2-C3	-2.15	107.02	109.67
3	E	1	NAG	O6-C6-C5	-2.14	103.96	111.29
3	E	4	MAN	O2-C2-C3	2.13	114.40	110.14
3	E	4	MAN	C1-O5-C5	-2.07	109.39	112.19
2	C	2	NAG	C1-C2-N2	2.02	113.94	110.49

There are no chirality outliers.

All (12) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6

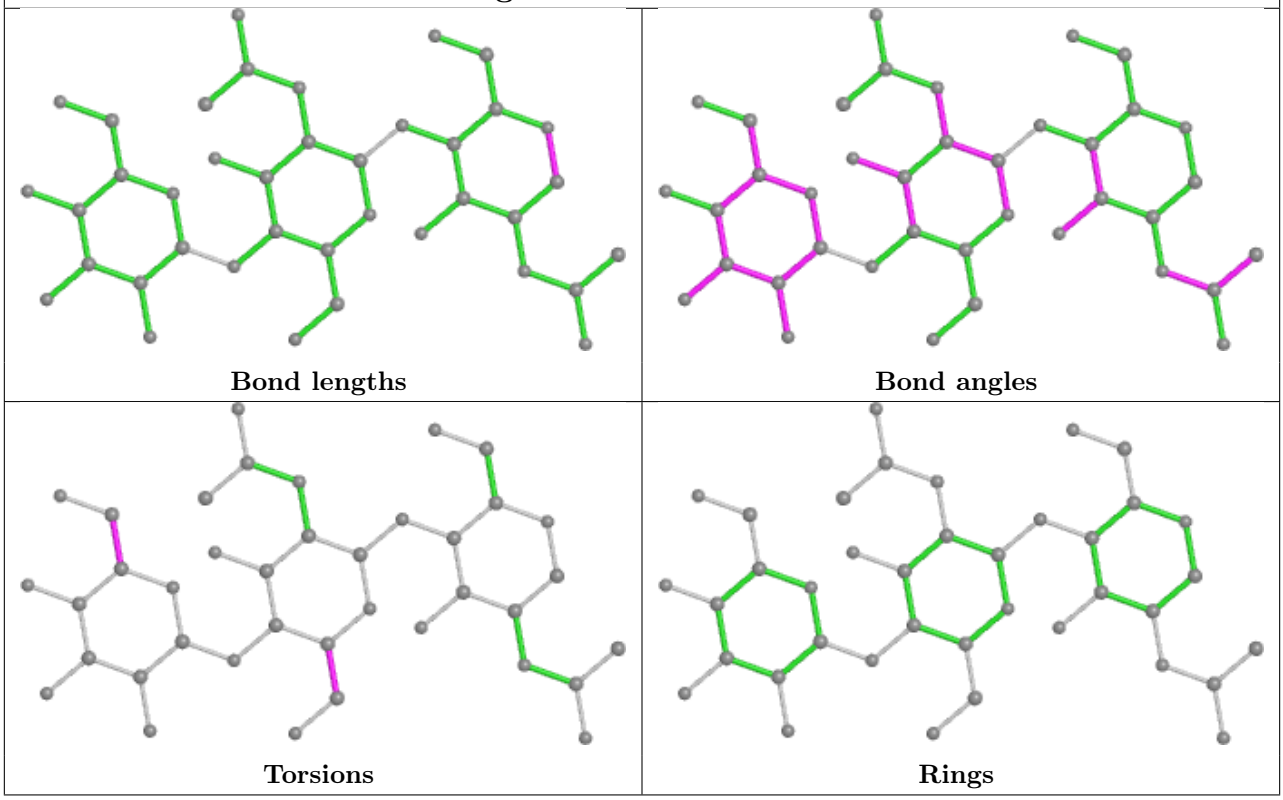
There are no ring outliers.

1 monomer is involved in 1 short contact:

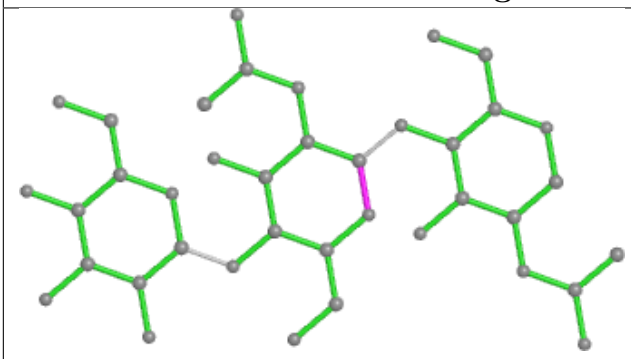
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0

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

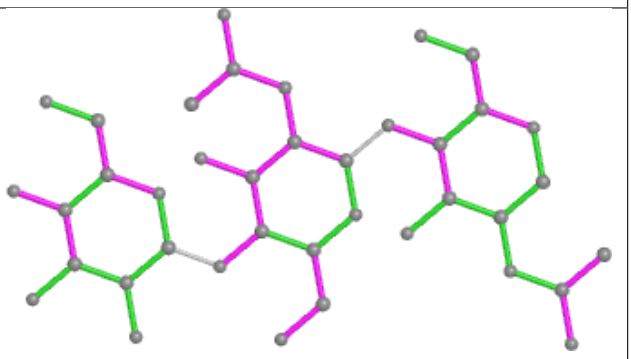
Oligosaccharide Chain C



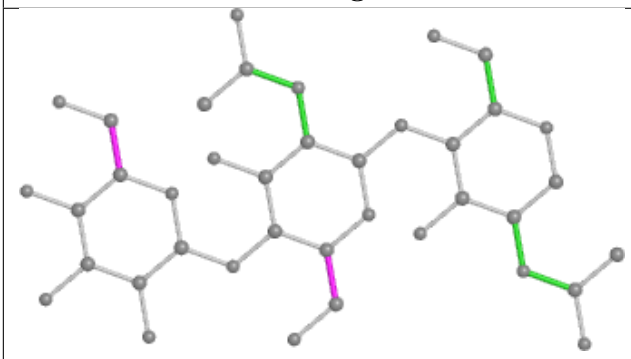
Oligosaccharide Chain D



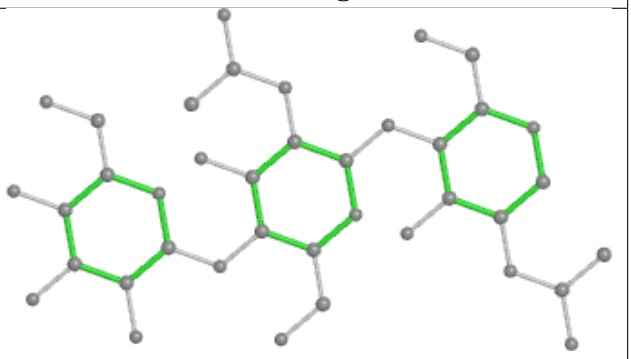
Bond lengths



Bond angles

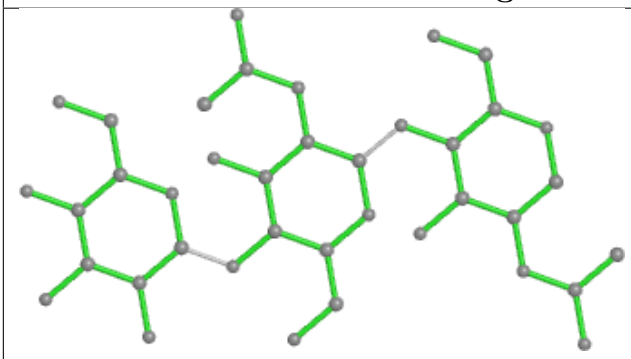


Torsions

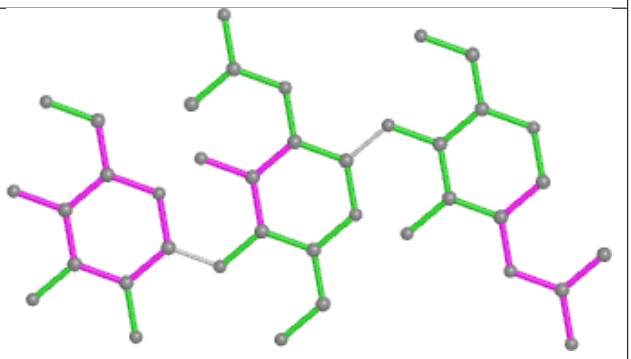


Rings

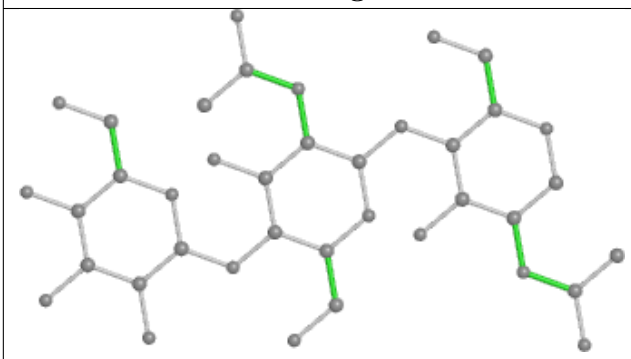
Oligosaccharide Chain F



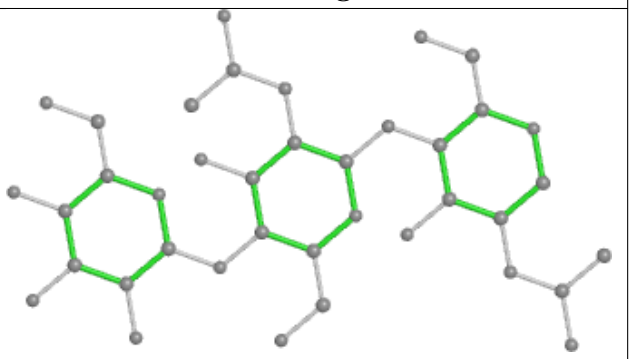
Bond lengths



Bond angles

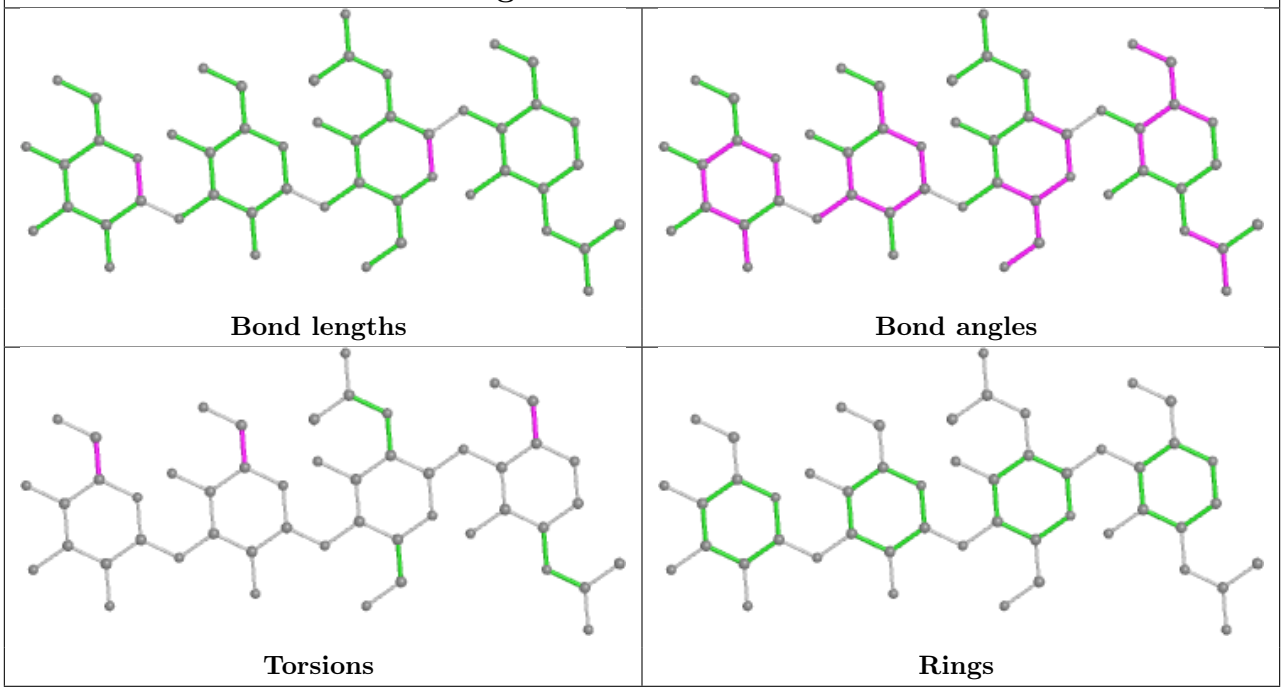


Torsions



Rings

Oligosaccharide Chain E



5.6 Ligand geometry (i)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	904	1	14,14,15	0.55	0	17,19,21	1.47	3 (17%)
4	NAG	B	906	1	14,14,15	0.61	0	17,19,21	1.54	5 (29%)
5	XG1	B	901	-	18,20,20	1.07	1 (5%)	19,28,28	1.72	3 (15%)
5	XG1	A	910	-	18,20,20	1.25	2 (11%)	19,28,28	1.31	4 (21%)
4	NAG	A	905	1	14,14,15	0.53	0	17,19,21	1.28	2 (11%)
4	NAG	A	909	1	14,14,15	0.70	0	17,19,21	1.37	3 (17%)
4	NAG	B	910	1	14,14,15	0.74	0	17,19,21	1.07	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	904	1	-	2/6/23/26	0/1/1/1
4	NAG	B	906	1	-	0/6/23/26	0/1/1/1
5	XG1	B	901	-	-	3/4/4/4	0/3/3/3
5	XG1	A	910	-	-	1/4/4/4	0/3/3/3
4	NAG	A	905	1	-	2/6/23/26	0/1/1/1
4	NAG	A	909	1	-	2/6/23/26	0/1/1/1
4	NAG	B	910	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	910	XG1	CAJ-CAH	2.51	1.47	1.42
5	A	910	XG1	CAC-CAA	-2.10	1.38	1.41
5	B	901	XG1	CAJ-CAH	2.08	1.46	1.42

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	901	XG1	CAH-CAG-NAI	-5.39	117.47	121.01
4	A	904	NAG	O3-C3-C2	-3.27	102.70	109.47
4	B	906	NAG	C4-C3-C2	-2.77	106.95	111.02
4	A	904	NAG	C3-C4-C5	2.74	115.12	110.24
4	B	906	NAG	C1-C2-N2	-2.73	105.83	110.49
5	B	901	XG1	NAR-CAG-NAI	2.71	124.32	117.09
4	A	905	NAG	C1-C2-N2	-2.69	105.89	110.49
4	A	909	NAG	O6-C6-C5	-2.63	102.26	111.29
4	A	904	NAG	O5-C5-C4	-2.62	104.46	110.83
4	B	906	NAG	C2-N2-C7	2.59	126.59	122.90
4	A	909	NAG	C4-C3-C2	-2.50	107.36	111.02
5	A	910	XG1	NAR-CAG-NAI	2.39	123.45	117.09
4	A	909	NAG	C1-C2-N2	-2.37	106.44	110.49
5	A	910	XG1	CAM-NAL-NAK	2.34	113.28	111.45
4	B	906	NAG	C3-C4-C5	-2.28	106.16	110.24
4	B	910	NAG	C4-C3-C2	-2.28	107.68	111.02
5	A	910	XG1	CAH-CAG-NAI	-2.28	119.51	121.01
4	A	905	NAG	O7-C7-C8	-2.26	117.86	122.06
4	B	906	NAG	O4-C4-C5	2.19	114.74	109.30
5	A	910	XG1	CAH-CAG-NAR	-2.19	117.02	120.35
5	B	901	XG1	CAG-NAI-CAA	2.17	124.46	118.39

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	904	NAG	O5-C5-C6-O6
4	A	904	NAG	C4-C5-C6-O6
5	A	910	XG1	NAL-CAN-CAO-CAP
5	B	901	XG1	NAL-CAN-CAO-CAP
4	A	905	NAG	C4-C5-C6-O6
4	A	909	NAG	C4-C5-C6-O6
4	A	905	NAG	O5-C5-C6-O6
5	B	901	XG1	CAO-CAN-NAL-NAK
4	A	909	NAG	O5-C5-C6-O6
5	B	901	XG1	CAN-CAO-CAP-CAQ

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	904	NAG	2	0
4	B	910	NAG	1	0

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	746/811 (91%)	-0.07	14 (1%)	66	71	18, 33, 62, 92	0
1	B	745/811 (91%)	0.09	27 (3%)	42	49	18, 36, 67, 85	0
All	All	1491/1622 (91%)	0.01	41 (2%)	54	60	18, 34, 66, 92	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	756	LEU	6.4
1	B	758	THR	4.8
1	B	760	THR	4.3
1	B	46	ILE	4.2
1	B	808	ASP	4.1
1	B	757	GLU	3.9
1	B	807	GLY	3.7
1	B	759	LYS	3.7
1	A	779	ASP	3.4
1	B	42	ASN	3.3
1	A	39	LYS	3.2
1	B	84	GLN	3.0
1	B	59	GLN	2.8
1	B	385	ASP	2.8
1	B	701	LEU	2.8
1	B	31	SER	2.7
1	A	470	PHE	2.7
1	B	778	CYS	2.6
1	B	83	PHE	2.5
1	B	702	PHE	2.5
1	B	810	ARG	2.4
1	B	191	ASN	2.4
1	A	124	LEU	2.4
1	B	57	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	808	ASP	2.4
1	A	84	GLN	2.3
1	B	60	THR	2.3
1	A	74	PHE	2.3
1	A	87	GLN	2.3
1	A	117	THR	2.3
1	B	361	ARG	2.3
1	B	64	TYR	2.3
1	B	121	PHE	2.3
1	A	383	ARG	2.3
1	B	63	LYS	2.2
1	A	41	GLN	2.2
1	B	61	VAL	2.2
1	B	186	VAL	2.2
1	B	96	HIS	2.1
1	A	385	ASP	2.1
1	A	755	ALA	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BMA	E	3	11/12	0.78	0.12	46,49,51,51	0
2	BMA	C	3	11/12	0.88	0.16	34,39,42,43	0
3	MAN	E	4	11/12	0.89	0.11	42,45,48,48	0
2	BMA	F	3	11/12	0.92	0.22	35,37,40,42	0
2	BMA	D	3	11/12	0.93	0.20	35,38,41,42	0
3	NAG	E	2	14/15	0.94	0.13	27,34,43,45	0
3	NAG	E	1	14/15	0.95	0.15	23,27,30,36	0
2	NAG	F	2	14/15	0.96	0.11	25,27,32,37	0
2	NAG	D	2	14/15	0.96	0.09	22,22,29,36	0
2	NAG	D	1	14/15	0.96	0.08	17,20,22,24	0
2	NAG	C	1	14/15	0.97	0.11	22,24,29,29	0

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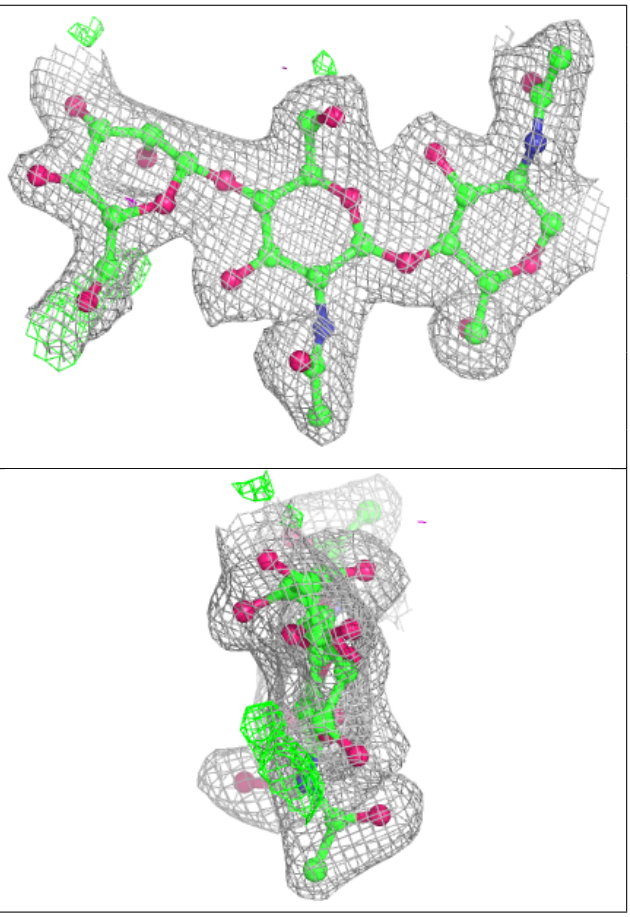
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	C	2	14/15	0.97	0.07	24,30,35,37	0
2	NAG	F	1	14/15	0.98	0.08	19,22,24,26	0

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.

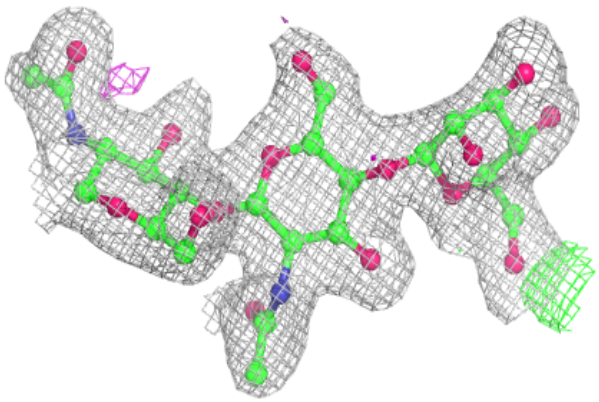
Electron density around Chain C:

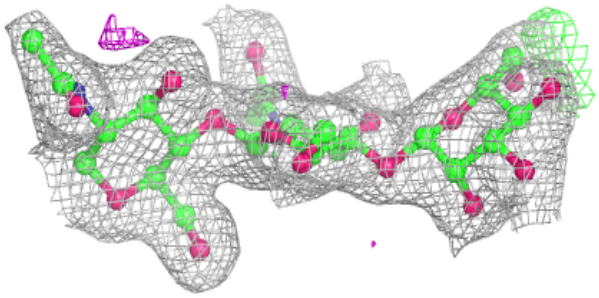
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

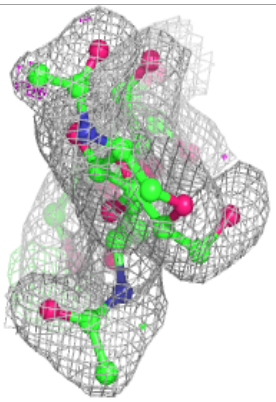


Electron density around Chain D:

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

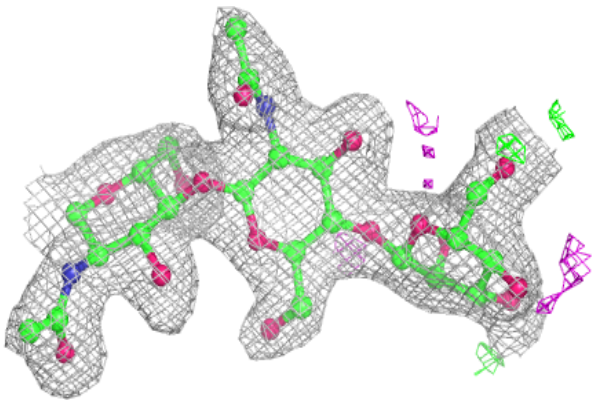


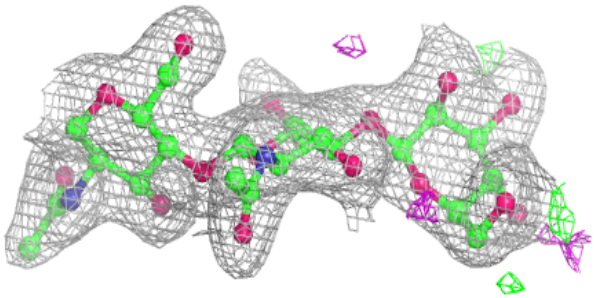


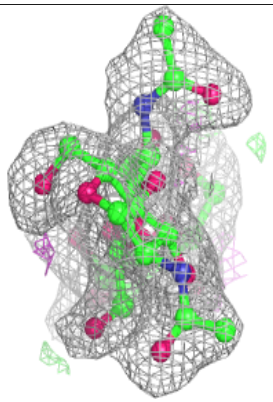


Electron density around Chain F:

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

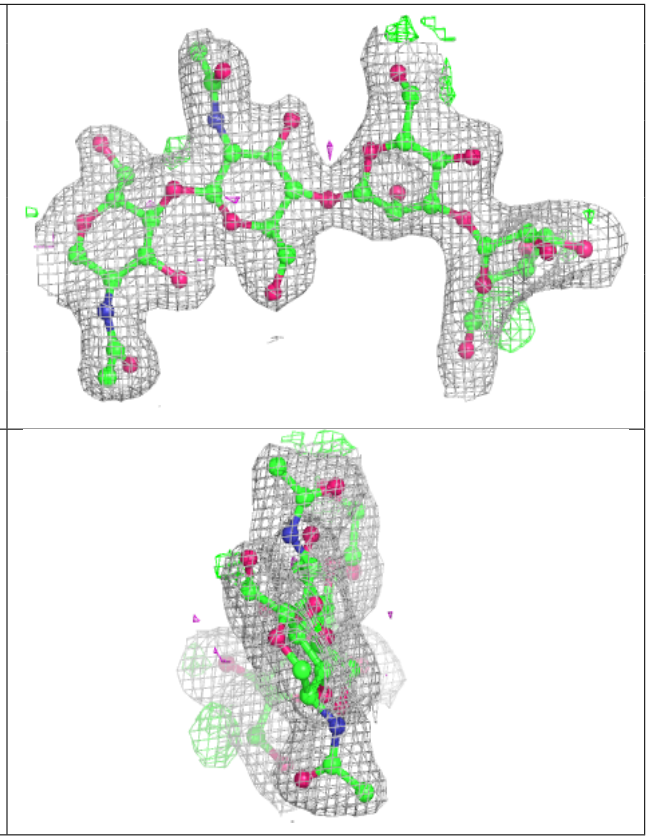






Electron density around Chain E:

$2mF_o$-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
4	NAG	A	904	14/15	0.93	0.13	38,41,45,45	0
4	NAG	B	910	14/15	0.94	0.10	39,49,57,61	0
4	NAG	B	906	14/15	0.95	0.10	22,26,30,30	0
4	NAG	A	909	14/15	0.96	0.11	24,36,44,45	0
5	XG1	A	910	18/18	0.96	0.10	17,19,22,24	0
4	NAG	A	905	14/15	0.97	0.10	21,23,26,29	0
5	XG1	B	901	18/18	0.97	0.10	21,22,25,26	0

6.5 Other polymers (i)

There are no such residues in this entry.