Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 10:48 PM BST

PDB ID	:	4QZV
Title	:	Bat-derived coronavirus HKU4 uses MERS-CoV receptor human CD26 for cell entry
Authors	:	Gao, F.G.; Wang, Q.H.; Qi, J.X.; Lu, G.W.
Deposited on	:	2014-07-29
Resolution	:	2.59 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 ①) were used in the production of this report:

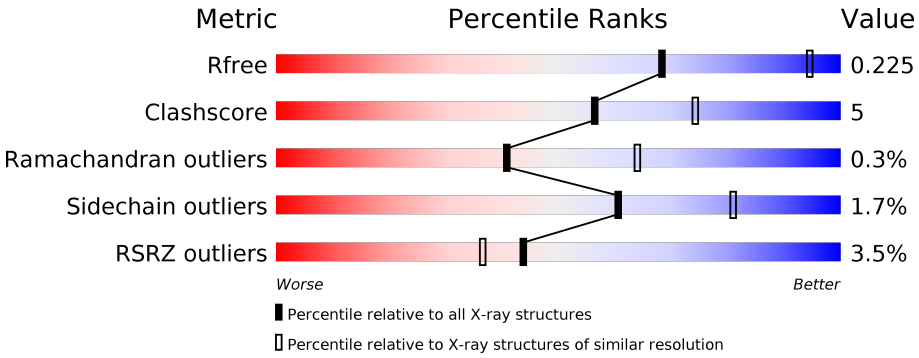
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	734	2% 90% 9%
1	C	734	3% 89% 10%
2	B	246	5% 66% 17% 15%
2	D	246	7% 65% 16% 15%
3	E	2	100%
3	G	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	H	2	50% 50%
3	I	2	50% 50%
3	K	2	100%
3	L	2	50% 50%
4	F	3	33% 67%
4	J	3	33% 67%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15900 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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5957	3824	981	1126	26			
1	C	727	Total	C	N	O	S	0	0	0
			5957	3824	981	1126	26			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	767	HIS	-	expression tag	UNP P27487
A	768	HIS	-	expression tag	UNP P27487
A	769	HIS	-	expression tag	UNP P27487
A	770	HIS	-	expression tag	UNP P27487
A	771	HIS	-	expression tag	UNP P27487
A	772	HIS	-	expression tag	UNP P27487
C	767	HIS	-	expression tag	UNP P27487
C	768	HIS	-	expression tag	UNP P27487
C	769	HIS	-	expression tag	UNP P27487
C	770	HIS	-	expression tag	UNP P27487
C	771	HIS	-	expression tag	UNP P27487
C	772	HIS	-	expression tag	UNP P27487

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	208	Total	C	N	O	S	0	0	0
			1597	1017	260	306	14			
2	D	208	Total	C	N	O	S	0	0	0
			1597	1017	260	306	14			

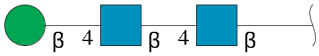
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	241	HIS	-	expression tag	UNP A3EX94
B	242	HIS	-	expression tag	UNP A3EX94
B	243	HIS	-	expression tag	UNP A3EX94
B	244	HIS	-	expression tag	UNP A3EX94
B	245	HIS	-	expression tag	UNP A3EX94
B	246	HIS	-	expression tag	UNP A3EX94
D	241	HIS	-	expression tag	UNP A3EX94
D	242	HIS	-	expression tag	UNP A3EX94
D	243	HIS	-	expression tag	UNP A3EX94
D	244	HIS	-	expression tag	UNP A3EX94
D	245	HIS	-	expression tag	UNP A3EX94
D	246	HIS	-	expression tag	UNP A3EX94

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

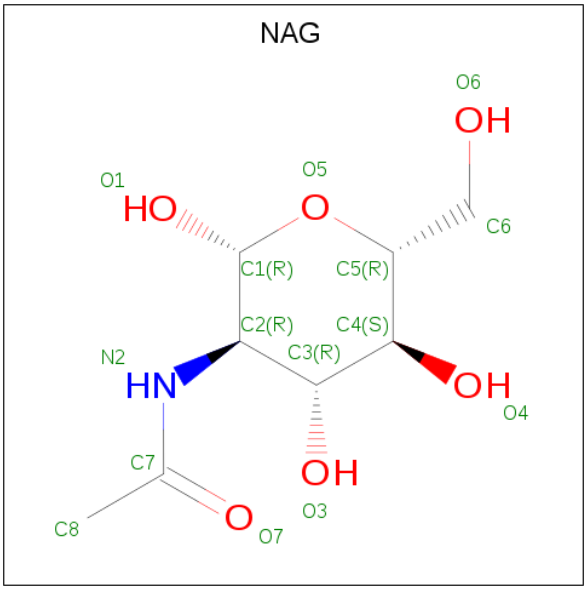
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	E	2	Total C N O 28 16 2 10	0	0	0
3	G	2	Total C N O 28 16 2 10	0	0	0
3	H	2	Total C N O 28 16 2 10	0	0	0
3	I	2	Total C N O 28 16 2 10	0	0	0
3	K	2	Total C N O 28 16 2 10	0	0	0
3	L	2	Total C N O 28 16 2 10	0	0	0

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



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	195	Total O 195 195	0	0
6	B	26	Total O 26 26	0	0

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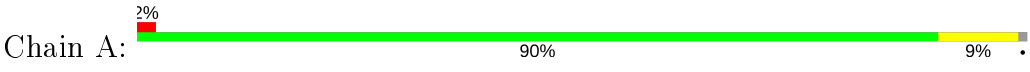
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	239	Total O 239 239	0	0
6	D	16	Total O 16 16	0	0

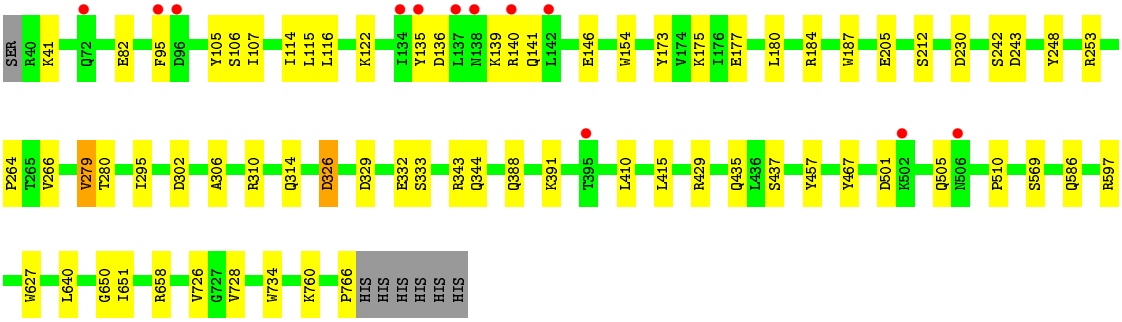
3 Residue-property plots (i)

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: Dipeptidyl peptidase 4

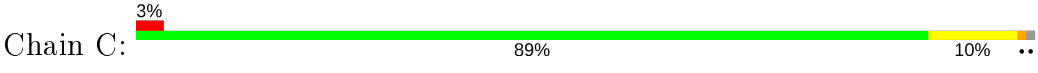
Chain A:

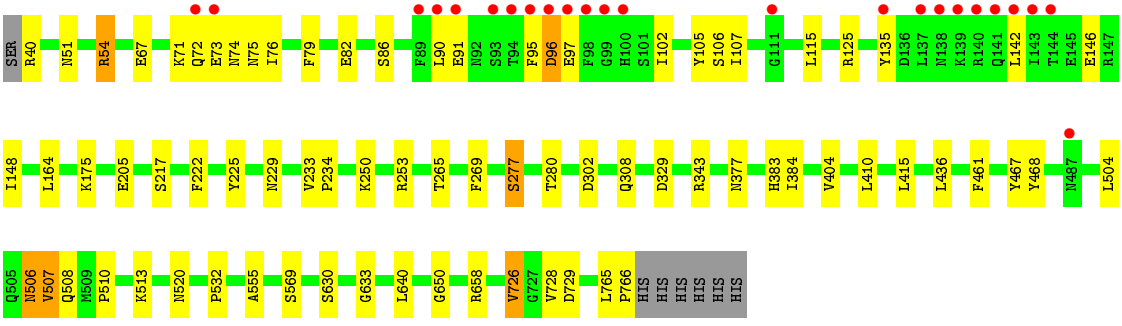




- Molecule 1: Dipeptidyl peptidase 4

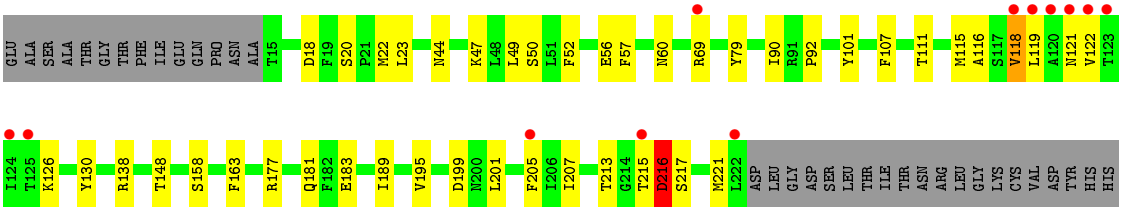
Chain C:





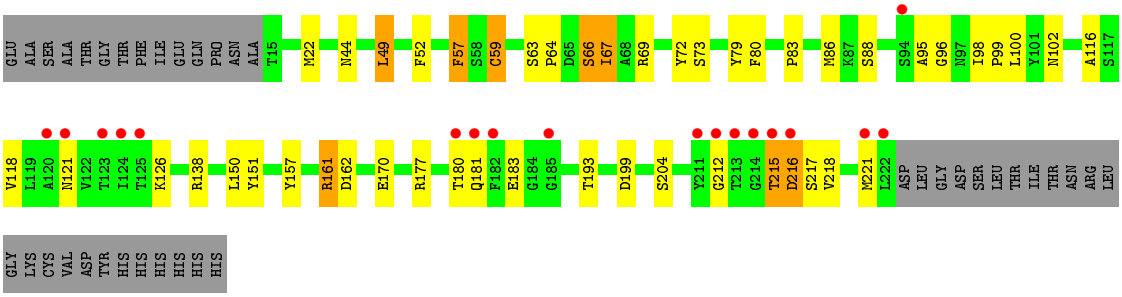
- Molecule 2: Spike protein S1

Chain B:



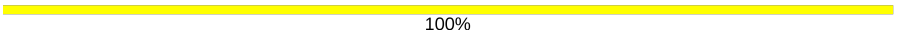
• Molecule 2: Spike protein S1

Chain D:



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

Chain E:



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

Chain G:

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

Chain H:

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

Chain I:

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

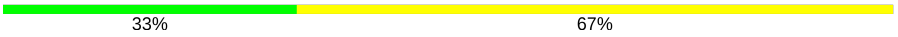
Chain K:

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

Chain L:

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

Chain F:



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

Chain J:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.80Å 203.17Å 207.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.30 – 2.59 46.30 – 2.59	Depositor EDS
% Data completeness (in resolution range)	98.0 (46.30-2.59) 93.2 (46.30-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.190 , 0.224 0.193 , 0.225	Depositor DCC
R_{free} test set	5113 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	36.7	Xtriage
Anisotropy	0.732	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 37.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.007 for -h,l,k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	15900	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 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	0.29	0/6129	0.46	0/8336
1	C	0.32	0/6129	0.49	1/8336 (0.0%)
2	B	0.39	0/1635	0.49	0/2222
2	D	0.40	0/1635	0.51	0/2222
All	All	0.32	0/15528	0.48	1/21116 (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	C	0	1
2	B	0	1
2	D	0	2
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	96	ASP	CB-CG-OD2	5.28	123.05	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	121	ASN	Peptide
1	C	96	ASP	Peptide

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Mol	Chain	Res	Type	Group
2	D	121	ASN	Peptide
2	D	215	THR	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	5957	0	5673	45	0
1	C	5957	0	5674	54	0
2	B	1597	0	1553	26	0
2	D	1597	0	1553	28	0
3	E	28	0	25	1	0
3	G	28	0	25	1	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
4	F	39	0	34	0	0
4	J	39	0	34	2	0
5	A	42	0	39	0	0
5	C	28	0	26	0	0
6	A	195	0	0	12	0
6	B	26	0	0	1	0
6	C	239	0	0	12	0
6	D	16	0	0	2	0
All	All	15900	0	14736	152	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 (152) 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:658:ARG:NH1	6:A:1029:HOH:O	1.88	1.06
1:A:253:ARG:HH21	1:C:253:ARG:HH21	1.16	0.91
2:D:180:THR:HG22	2:D:183:GLU:HG2	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:63:SER:OG	2:D:66:SER:OG	1.96	0.84
2:D:138:ARG:NH2	2:D:183:GLU:O	2.11	0.83
2:D:216:ASP:OD1	2:D:217:SER:N	2.11	0.82
2:B:148:THR:OG1	6:B:317:HOH:O	1.98	0.80
2:D:157:TYR:O	6:D:307:HOH:O	2.04	0.76
1:C:40:ARG:NH2	1:C:506:ASN:O	2.19	0.76
1:C:146:GLU:O	1:C:175:LYS:NZ	2.20	0.74
6:A:935:HOH:O	3:G:2:NAG:O4	2.07	0.73
1:A:766:PRO:O	6:A:1040:HOH:O	2.07	0.72
2:D:150:LEU:O	6:D:310:HOH:O	2.07	0.72
1:C:233:VAL:O	6:C:1015:HOH:O	2.08	0.71
1:A:122:LYS:O	6:A:993:HOH:O	2.08	0.71
1:A:597:ARG:NH2	6:A:945:HOH:O	2.23	0.71
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.73	0.69
1:C:302:ASP:OD1	6:C:931:HOH:O	2.10	0.69
1:C:513:LYS:NZ	6:C:930:HOH:O	2.26	0.68
2:B:69:ARG:HH11	2:B:69:ARG:HG2	1.61	0.66
1:A:253:ARG:HH21	1:C:253:ARG:NH2	1.91	0.66
2:D:177:ARG:NH1	2:D:183:GLU:OE2	2.29	0.65
1:A:139:LYS:HG3	1:A:141:GLN:HB2	1.79	0.65
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.78	0.65
1:A:734:TRP:O	6:A:914:HOH:O	2.14	0.65
2:D:126:LYS:NZ	2:D:199:ASP:O	2.30	0.64
1:C:76:ILE:HD12	1:C:90:LEU:HD23	1.80	0.64
2:D:73:SER:HB2	2:D:212:GLY:H	1.63	0.64
2:B:118:VAL:HG12	2:B:122:VAL:HG11	1.80	0.64
1:A:205:GLU:HG2	6:A:1041:HOH:O	1.97	0.64
1:A:329:ASP:OD1	1:A:343:ARG:NH1	2.31	0.63
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.80	0.62
2:D:161:ARG:NH1	2:D:162:ASP:OD1	2.32	0.62
1:A:177:GLU:HB2	1:A:180:LEU:HG	1.82	0.62
1:C:95:PHE:O	1:C:95:PHE:CD2	2.53	0.61
1:C:308:GLN:NE2	6:C:1090:HOH:O	2.30	0.61
1:C:82:GLU:OE1	1:C:467:TYR:OH	2.11	0.61
1:C:135:TYR:CE1	1:C:142:LEU:HB2	2.36	0.60
1:C:95:PHE:HE1	1:C:135:TYR:CZ	2.20	0.60
1:C:555:ALA:O	6:C:983:HOH:O	2.16	0.60
1:A:388:GLN:HB2	1:A:391:LYS:HB2	1.85	0.58
1:C:95:PHE:HE1	1:C:135:TYR:HH	1.50	0.58
1:A:146:GLU:O	1:A:175:LYS:NZ	2.35	0.58
2:D:64:PRO:O	2:D:67:ILE:HG22	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:67:ILE:HG13	2:D:67:ILE:O	2.05	0.57
1:C:658:ARG:NH2	6:C:1091:HOH:O	2.37	0.57
1:A:136:ASP:HB3	1:A:139:LYS:HG2	1.87	0.57
2:B:126:LYS:NZ	2:B:199:ASP:O	2.37	0.57
1:C:729:ASP:OD2	6:C:977:HOH:O	2.16	0.57
2:D:72:TYR:O	2:D:218:VAL:N	2.33	0.56
1:C:67:GLU:OE1	6:C:964:HOH:O	2.18	0.55
1:C:766:PRO:O	6:C:1064:HOH:O	2.18	0.55
1:C:726:VAL:HG12	1:C:728:VAL:HG23	1.89	0.55
1:A:154:TRP:CE2	1:A:212:SER:HB2	2.41	0.54
2:B:118:VAL:CG1	2:B:122:VAL:HG11	2.37	0.54
1:C:95:PHE:HE1	1:C:135:TYR:OH	1.91	0.54
1:A:326:ASP:OD1	1:A:344:GLN:HG2	2.08	0.54
1:C:125:ARG:NE	1:C:205:GLU:OE1	2.32	0.53
1:C:91:GLU:OE1	1:C:91:GLU:N	2.30	0.53
2:B:47:LYS:O	2:B:50:SER:OG	2.22	0.53
1:A:640:LEU:O	6:A:1048:HOH:O	2.19	0.52
2:B:138:ARG:NH2	2:B:183:GLU:O	2.42	0.52
1:C:106:SER:HB3	1:C:115:LEU:HB3	1.90	0.52
1:C:532:PRO:O	6:C:1114:HOH:O	2.19	0.51
1:C:40:ARG:HB3	1:C:508:GLN:NE2	2.26	0.51
1:A:295:ILE:HG22	2:B:189:ILE:HD11	1.92	0.50
1:C:329:ASP:OD1	1:C:343:ARG:NH1	2.44	0.50
1:C:384:ILE:HG13	1:C:404:VAL:HG21	1.93	0.50
2:D:44:ASN:HB2	2:D:221:MET:HE2	1.92	0.50
2:B:90:ILE:HG21	2:B:115:MET:HE1	1.93	0.49
2:D:80:PHE:CE2	2:D:204:SER:HB3	2.48	0.49
1:A:140:ARG:HD3	1:A:140:ARG:N	2.27	0.49
1:A:435:GLN:HE21	1:A:437:SER:HG	1.52	0.48
1:C:75:ASN:HB3	1:C:91:GLU:HA	1.95	0.48
1:A:586:GLN:OE1	6:A:939:HOH:O	2.20	0.48
2:B:22:MET:HA	2:B:79:TYR:CE1	2.48	0.48
1:A:230:ASP:OD1	1:A:264:PRO:HB3	2.14	0.48
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.96	0.48
1:A:279:VAL:HG12	1:A:280:THR:HG23	1.95	0.48
1:C:410:LEU:HD13	1:C:415:LEU:HD23	1.95	0.48
2:B:181:GLN:OE1	2:B:181:GLN:HA	2.14	0.48
1:A:435:GLN:NE2	1:A:437:SER:OG	2.27	0.47
2:B:92:PRO:HG3	2:B:107:PHE:CZ	2.50	0.47
2:B:215:THR:O	2:B:216:ASP:HB2	2.14	0.47
1:C:277:SER:HG	1:C:280:THR:H	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:510:PRO:HD3	1:C:569:SER:HB2	1.97	0.47
1:A:82:GLU:HB2	1:A:467:TYR:OH	2.15	0.46
1:C:415:LEU:HB2	1:C:436:LEU:HD21	1.98	0.46
2:B:18:ASP:OD1	2:B:20:SER:OG	2.25	0.46
2:B:205:PHE:HE1	2:B:207:ILE:HD11	1.79	0.46
6:A:1031:HOH:O	3:E:2:NAG:O4	2.20	0.46
1:C:461:PHE:CD2	1:C:468:TYR:HB3	2.51	0.46
1:C:148:ILE:HD11	1:C:164:LEU:HD13	1.97	0.45
1:C:217:SER:HB3	1:C:222:PHE:HB2	1.97	0.45
1:C:280:THR:O	6:C:1050:HOH:O	2.21	0.45
2:D:95:ALA:HA	2:D:96:GLY:HA3	1.63	0.45
2:D:57:PHE:HE2	2:D:59:CYS:SG	2.40	0.45
2:D:98:ILE:HA	2:D:102:ASN:HD22	1.81	0.45
1:C:79:PHE:CE1	1:C:86:SER:HB3	2.51	0.44
1:A:627:TRP:HB2	1:A:651:ILE:HB	1.99	0.44
1:C:51:ASN:OD1	1:C:54:ARG:CZ	2.65	0.44
2:D:22:MET:HA	2:D:79:TYR:CE1	2.51	0.44
1:C:71:LYS:HE3	1:C:105:TYR:CE2	2.52	0.44
1:A:242:SER:OG	1:A:243:ASP:N	2.51	0.44
2:D:49:LEU:HD21	2:D:57:PHE:HE1	1.83	0.44
2:D:170:GLU:HB2	4:J:2:NAG:H61	1.98	0.44
2:D:95:ALA:HB1	2:D:99:PRO:HG2	2.00	0.44
1:A:410:LEU:HD13	1:A:415:LEU:HD23	2.00	0.44
1:C:504:LEU:HA	1:C:507:VAL:HG12	2.00	0.43
4:J:2:NAG:O3	4:J:3:BMA:H2	2.18	0.43
2:B:130:TYR:HB2	2:B:195:VAL:HB	2.00	0.43
2:D:73:SER:HB2	2:D:212:GLY:N	2.30	0.43
2:D:215:THR:O	2:D:216:ASP:HB2	2.18	0.43
1:A:306:ALA:HB3	1:A:310:ARG:HG2	2.00	0.43
1:A:106:SER:HB3	1:A:115:LEU:HB3	2.01	0.42
1:C:377:ASN:ND2	1:C:383:HIS:HD2	2.18	0.42
1:C:630:SER:O	1:C:633:GLY:N	2.52	0.42
2:B:44:ASN:HB2	2:B:221:MET:HE2	2.01	0.42
1:A:105:TYR:HB2	1:A:114:ILE:HD11	2.00	0.42
1:C:95:PHE:CE2	1:C:102:ILE:HD11	2.55	0.42
1:A:429:ARG:HB2	1:A:457:TYR:H	1.84	0.42
1:C:506:ASN:N	1:C:506:ASN:HD22	2.16	0.42
2:B:118:VAL:HG23	2:B:201:LEU:O	2.20	0.42
1:C:72:GLN:HB3	1:C:75:ASN:OD1	2.20	0.42
2:B:23:LEU:HD12	2:B:23:LEU:HA	1.77	0.41
1:C:225:TYR:CZ	1:C:269:PHE:HB2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:504:LEU:O	6:C:1005:HOH:O	2.21	0.41
1:A:332:GLU:HG3	1:A:333:SER:N	2.35	0.41
1:A:760:LYS:NZ	6:A:1054:HOH:O	2.45	0.41
2:B:52:PHE:HB3	2:B:116:ALA:HB1	2.03	0.41
1:C:229:ASN:HB3	1:C:265:THR:OG1	2.20	0.41
2:D:52:PHE:HB3	2:D:116:ALA:HB1	2.03	0.41
2:D:83:PRO:HG2	2:D:86:MET:HG3	2.01	0.41
2:B:56:GLU:HB3	2:B:115:MET:HB2	2.02	0.41
2:B:49:LEU:HD21	2:B:57:PHE:HE2	1.86	0.41
2:B:119:LEU:O	2:B:122:VAL:HG12	2.21	0.41
1:A:501:ASP:O	1:A:505:GLN:HG3	2.21	0.41
1:A:726:VAL:HG13	1:A:728:VAL:HG23	2.02	0.41
1:A:184:ARG:HD3	1:A:187:TRP:CE2	2.56	0.41
1:C:765:LEU:HA	1:C:766:PRO:HD3	1.95	0.41
2:D:100:LEU:HD22	2:D:151:TYR:CD1	2.56	0.41
2:D:161:ARG:O	2:D:161:ARG:HG2	2.19	0.41
1:A:248:TYR:CZ	1:C:234:PRO:HB2	2.56	0.41
1:A:266:VAL:O	6:A:1008:HOH:O	2.22	0.41
1:C:71:LYS:HE3	1:C:105:TYR:CD2	2.56	0.40
1:C:51:ASN:OD1	1:C:54:ARG:NH2	2.54	0.40
2:B:101:TYR:O	2:B:158:SER:HB2	2.21	0.40
1:A:173:TYR:CE2	1:A:184:ARG:HG3	2.56	0.40
1:A:95:PHE:CZ	1:A:116:LEU:HD11	2.56	0.40
1:C:640:LEU:HD11	1:C:650:GLY:HA3	2.02	0.40
2:B:163:PHE:CE1	2:B:177:ARG:HB2	2.57	0.40
2:B:215:THR:O	2:B:215:THR:OG1	2.32	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	725/734 (99%)	694 (96%)	31 (4%)	0	100	100
1	C	725/734 (99%)	688 (95%)	34 (5%)	3 (0%)	34	57
2	B	206/246 (84%)	189 (92%)	16 (8%)	1 (0%)	29	52
2	D	206/246 (84%)	195 (95%)	10 (5%)	1 (0%)	29	52
All	All	1862/1960 (95%)	1766 (95%)	91 (5%)	5 (0%)	41	64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	216	ASP
1	C	97	GLU
1	C	520	ASN
1	C	73	GLU
2	D	216	ASP

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	652/659 (99%)	648 (99%)	4 (1%)	86	95
1	C	652/659 (99%)	644 (99%)	8 (1%)	71	87
2	B	180/212 (85%)	174 (97%)	6 (3%)	38	64
2	D	180/212 (85%)	169 (94%)	11 (6%)	18	38
All	All	1664/1742 (96%)	1635 (98%)	29 (2%)	60	81

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	107	ILE
1	A	279	VAL
1	A	326	ASP
2	B	60	ASN
2	B	111	THR

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Mol	Chain	Res	Type
2	B	118	VAL
2	B	213	THR
2	B	216	ASP
2	B	217	SER
1	C	54	ARG
1	C	74	ASN
1	C	107	ILE
1	C	250	LYS
1	C	277	SER
1	C	506	ASN
1	C	507	VAL
1	C	726	VAL
2	D	49	LEU
2	D	57	PHE
2	D	59	CYS
2	D	66	SER
2	D	67	ILE
2	D	69	ARG
2	D	88	SER
2	D	118	VAL
2	D	161	ARG
2	D	181	GLN
2	D	193	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	731	GLN
2	B	121	ASN
1	C	506	ASN
2	D	153	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)

18 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	$\#\|Z\| > 2$
3	NAG	E	1	1,3	14,14,15	0.55	0	17,19,21	0.86	1 (5%)
3	NAG	E	2	3	14,14,15	0.51	0	17,19,21	0.49	0
4	NAG	F	1	1,4	14,14,15	0.86	1 (7%)	17,19,21	0.58	0
4	NAG	F	2	4	14,14,15	0.36	0	17,19,21	0.70	0
4	BMA	F	3	4	11,11,12	1.87	3 (27%)	15,15,17	1.72	3 (20%)
3	NAG	G	1	1,3	14,14,15	0.33	0	17,19,21	0.53	0
3	NAG	G	2	3	14,14,15	0.19	0	17,19,21	0.63	0
3	NAG	H	1	1,3	14,14,15	0.63	1 (7%)	17,19,21	0.49	0
3	NAG	H	2	3	14,14,15	0.30	0	17,19,21	0.45	0
3	NAG	I	1	1,3	14,14,15	0.56	0	17,19,21	0.83	1 (5%)
3	NAG	I	2	3	14,14,15	0.38	0	17,19,21	0.35	0
4	NAG	J	1	1,4	14,14,15	0.82	1 (7%)	17,19,21	0.57	0
4	NAG	J	2	4	14,14,15	0.67	1 (7%)	17,19,21	0.42	0
4	BMA	J	3	4	11,11,12	1.86	3 (27%)	15,15,17	1.89	5 (33%)
3	NAG	K	1	1,3	14,14,15	0.27	0	17,19,21	0.52	0
3	NAG	K	2	3	14,14,15	0.25	0	17,19,21	0.62	0
3	NAG	L	1	1,3	14,14,15	0.60	1 (7%)	17,19,21	0.47	0
3	NAG	L	2	3	14,14,15	0.15	0	17,19,21	0.72	0

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

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

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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	3	BMA	O5-C5	3.40	1.50	1.43
4	F	3	BMA	C4-C3	-3.27	1.44	1.52
4	J	3	BMA	C4-C3	-3.17	1.44	1.52
4	F	3	BMA	O5-C5	3.09	1.49	1.43
4	F	3	BMA	C2-C3	-2.99	1.48	1.52
4	F	1	NAG	O5-C1	-2.96	1.39	1.43
4	J	3	BMA	C2-C3	-2.84	1.48	1.52
4	J	1	NAG	O5-C1	-2.56	1.39	1.43
4	J	2	NAG	O5-C1	-2.39	1.39	1.43
3	H	1	NAG	O5-C1	-2.25	1.40	1.43
3	L	1	NAG	O5-C1	-2.14	1.40	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	3	BMA	C3-C4-C5	4.68	118.59	110.24
4	F	3	BMA	C3-C4-C5	4.38	118.05	110.24
4	J	3	BMA	C2-C3-C4	2.89	115.90	110.89
3	I	1	NAG	C1-O5-C5	2.78	115.96	112.19
3	E	1	NAG	C1-O5-C5	2.75	115.91	112.19
4	F	3	BMA	C2-C3-C4	2.62	115.43	110.89
4	J	3	BMA	O6-C6-C5	2.26	119.05	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	3	BMA	O5-C5-C4	2.13	116.01	110.83
4	J	3	BMA	O5-C5-C6	2.09	110.49	107.20
4	J	3	BMA	O5-C5-C4	2.08	115.89	110.83

There are no chirality outliers.

All (28) torsion outliers are listed below:

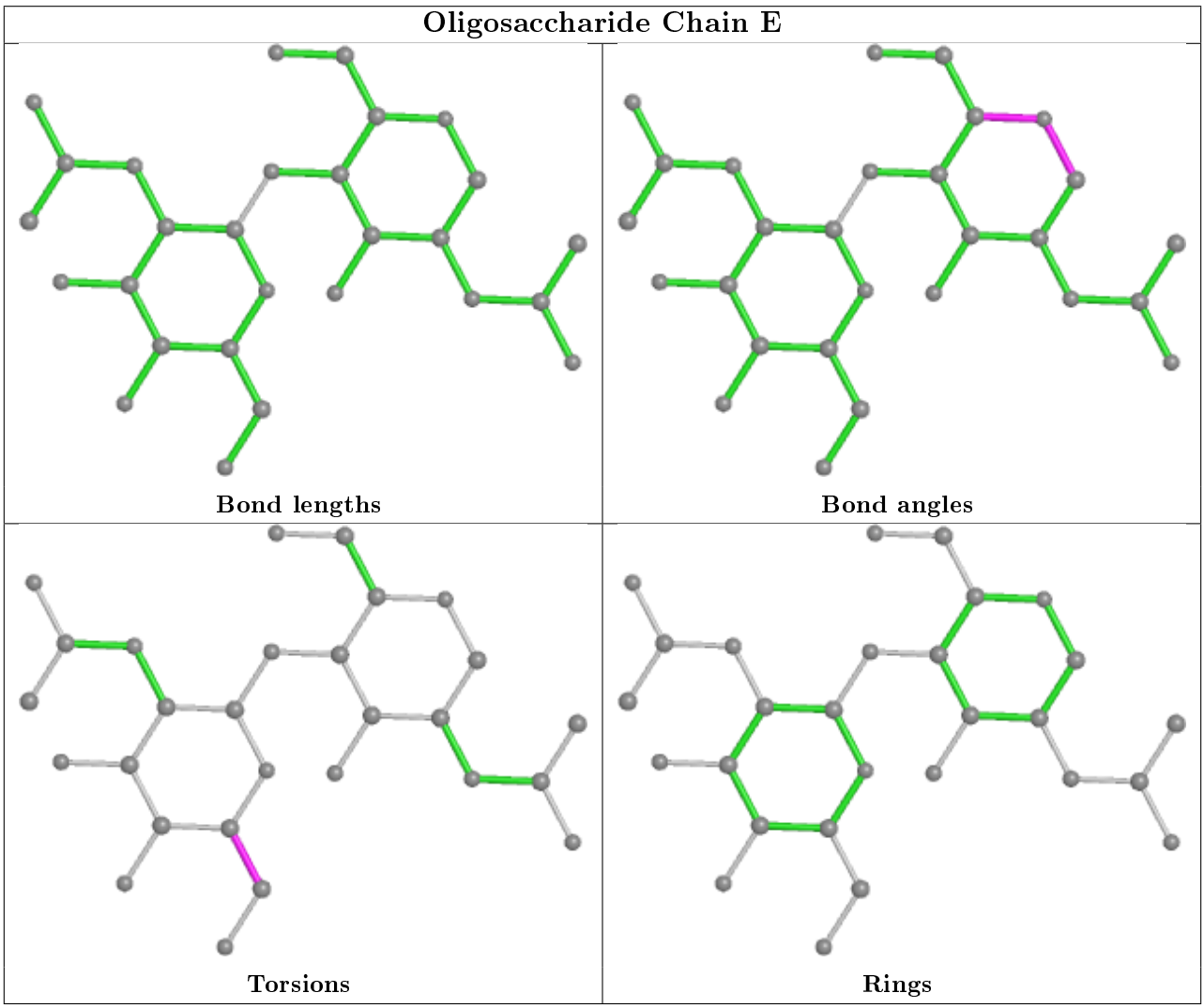
Mol	Chain	Res	Type	Atoms
4	F	2	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	J	3	BMA	C4-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
3	H	2	NAG	C4-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6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

There are no ring outliers.

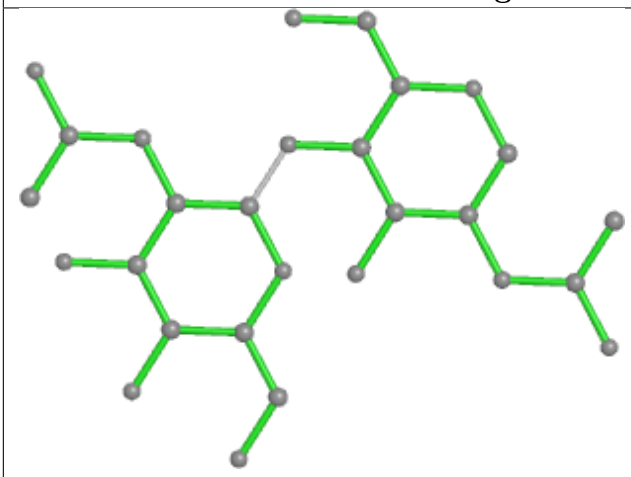
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	2	NAG	2	0
3	G	2	NAG	1	0
3	E	2	NAG	1	0
4	J	3	BMA	1	0

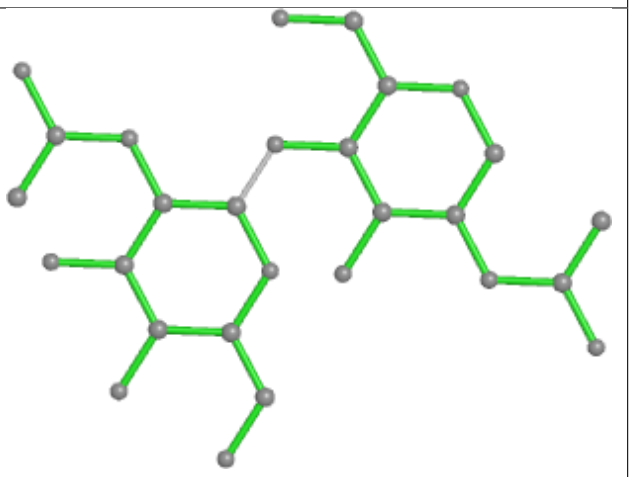
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



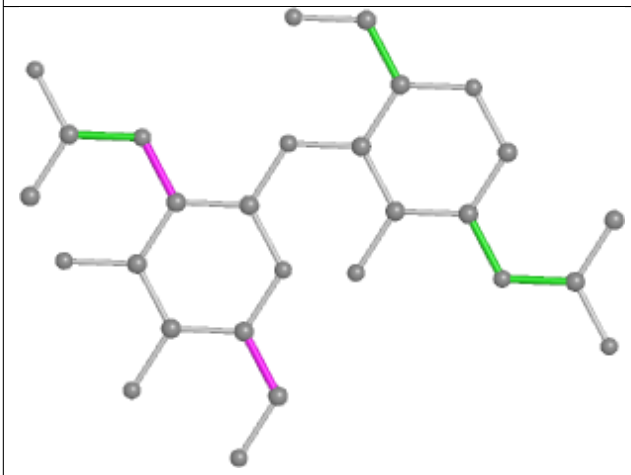
Oligosaccharide Chain G



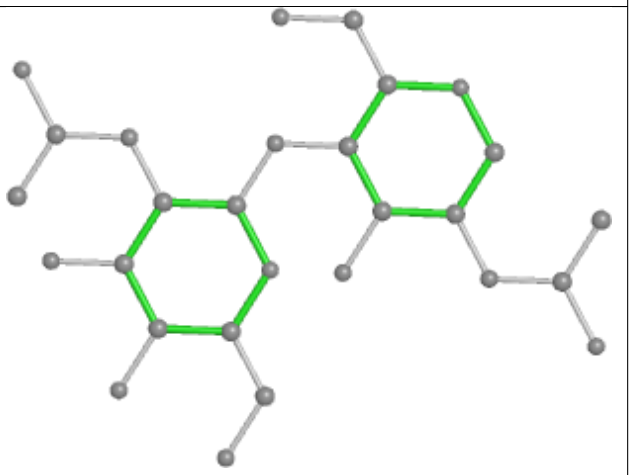
Bond lengths



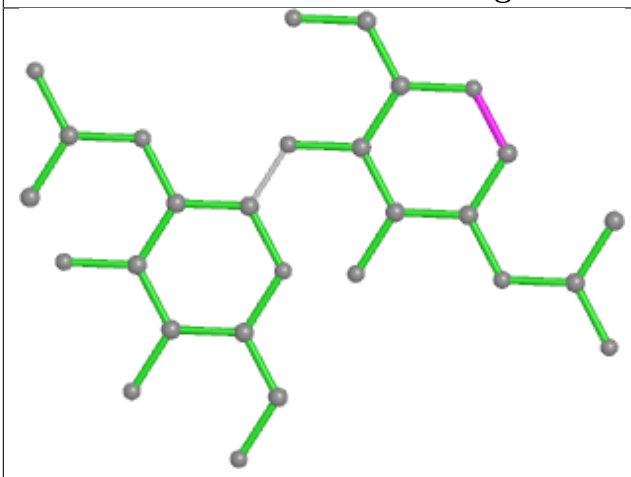
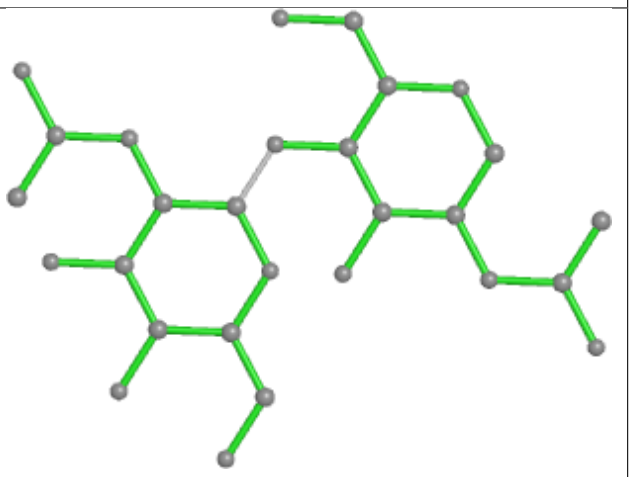
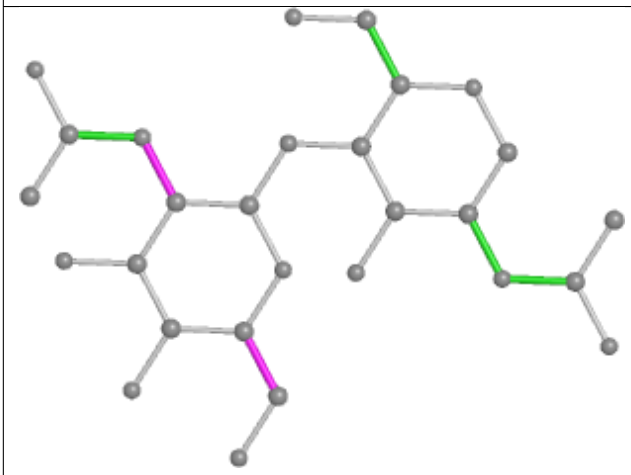
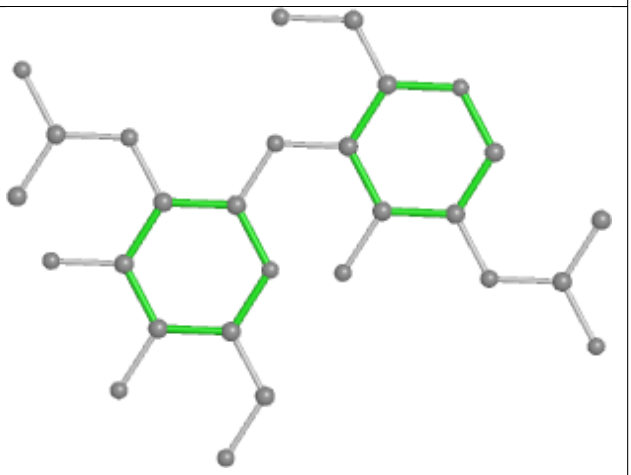
Bond angles



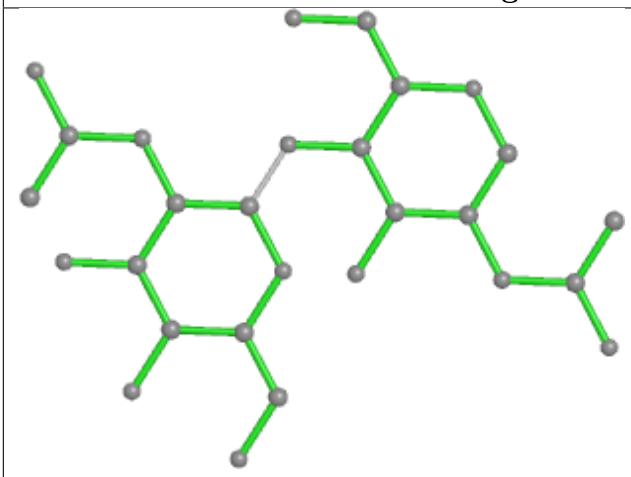
Torsions



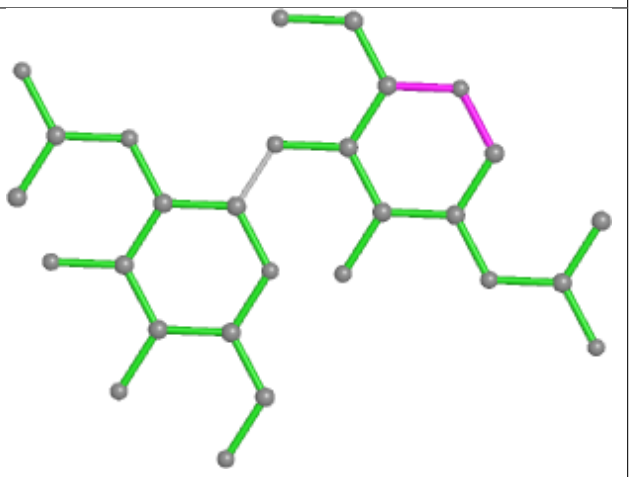
Rings

Oligosaccharide Chain H	
 Bond lengths	 Bond angles
 Torsions	 Rings

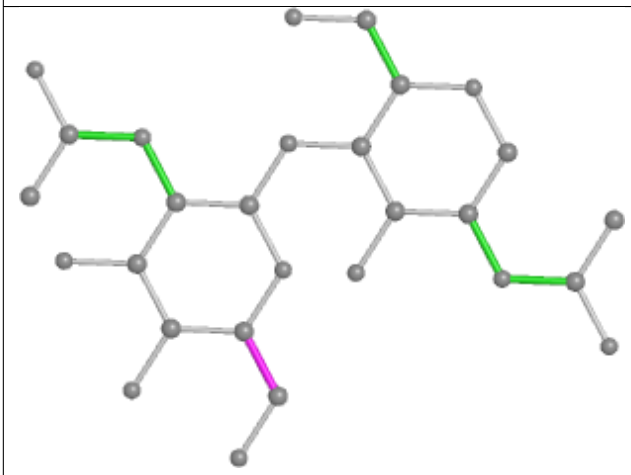
Oligosaccharide Chain I



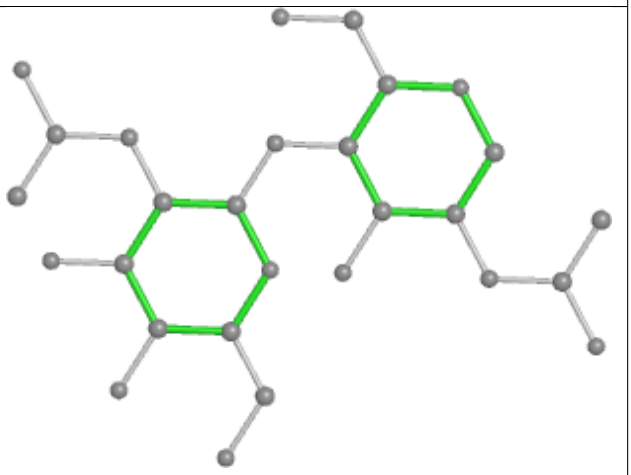
Bond lengths



Bond angles

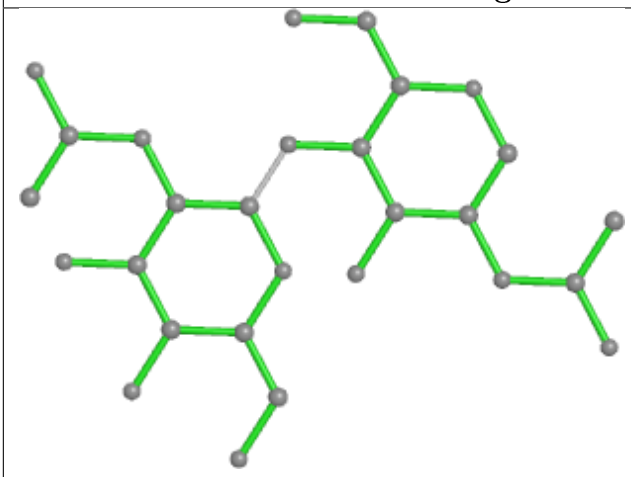


Torsions

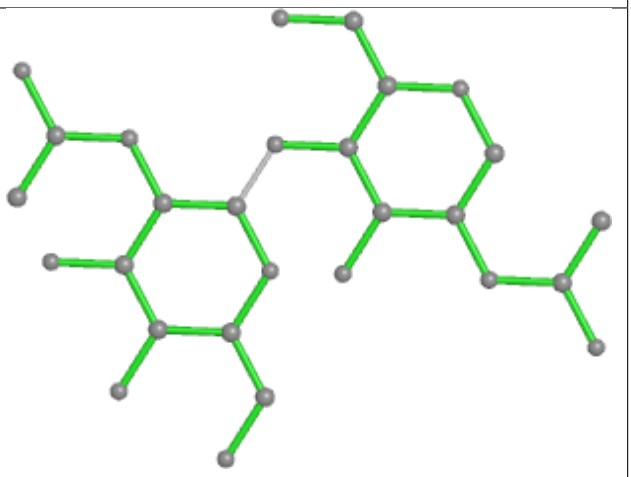


Rings

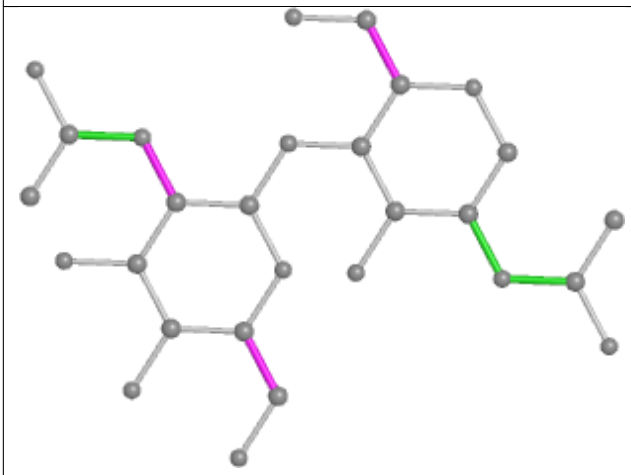
Oligosaccharide Chain K



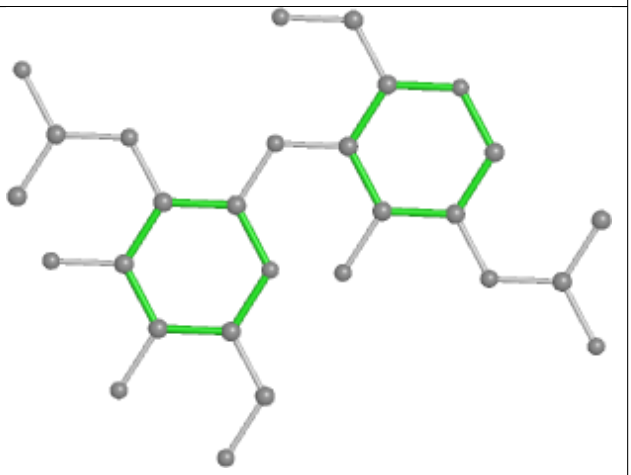
Bond lengths



Bond angles

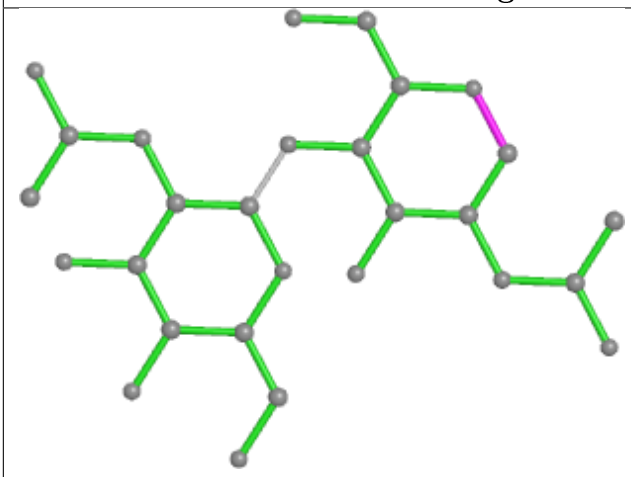


Torsions

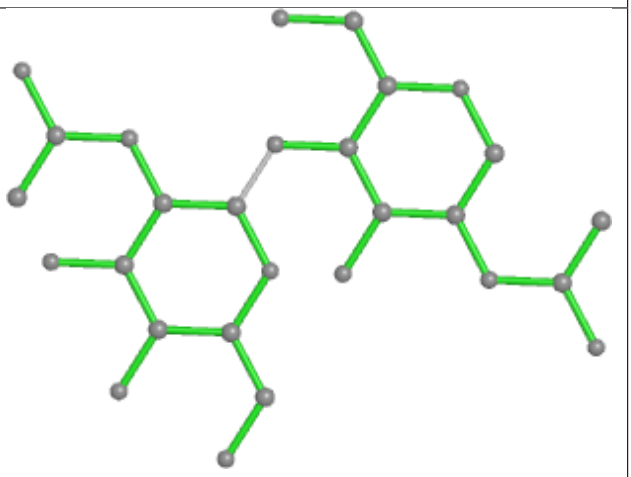


Rings

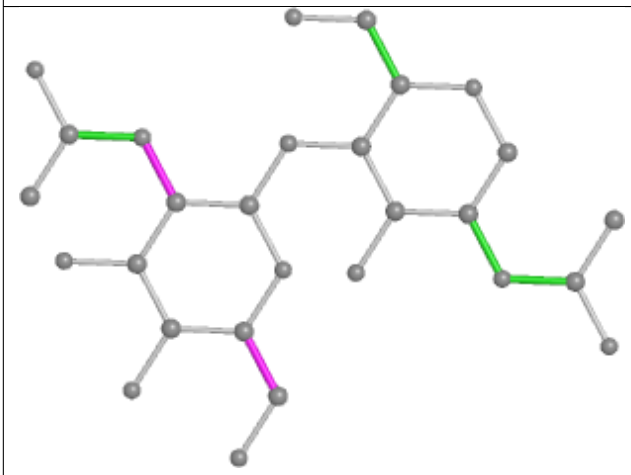
Oligosaccharide Chain L



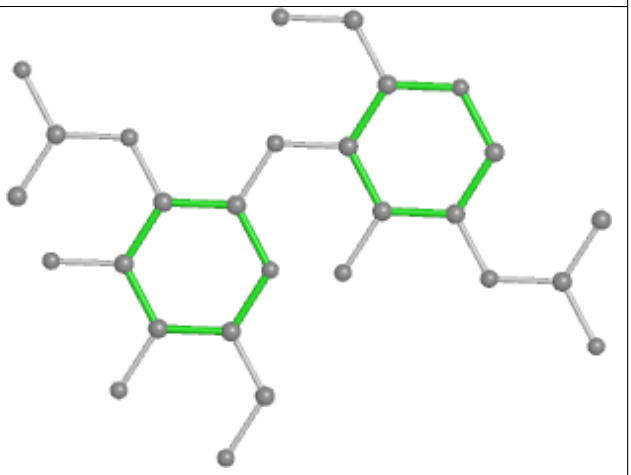
Bond lengths



Bond angles

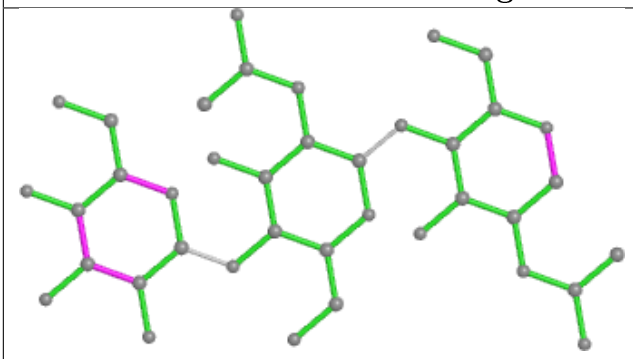


Torsions

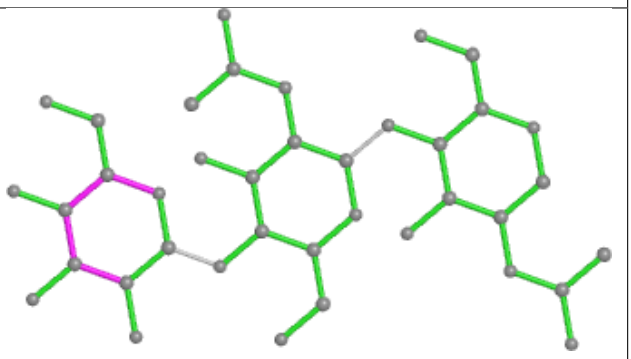


Rings

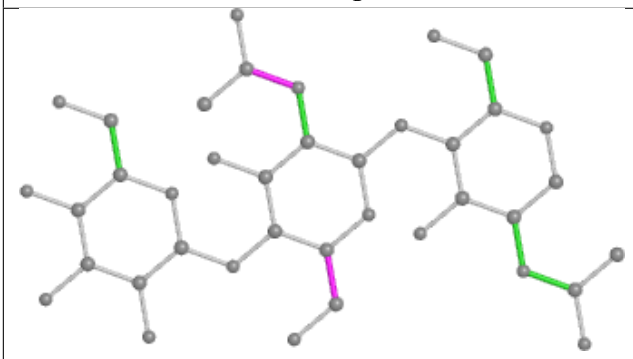
Oligosaccharide Chain F



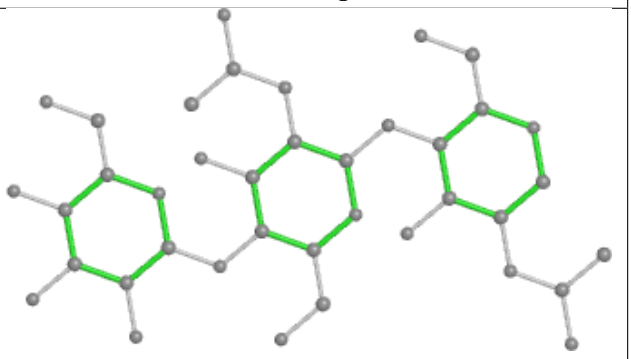
Bond lengths



Bond angles

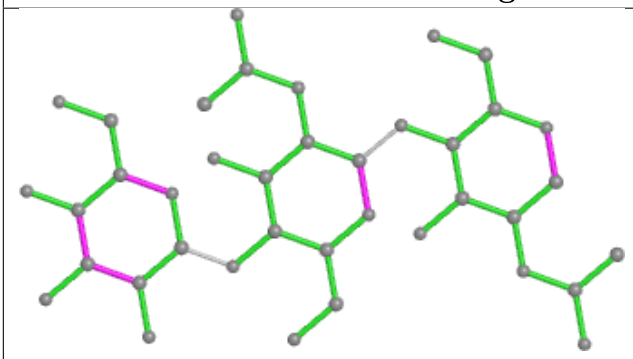


Torsions

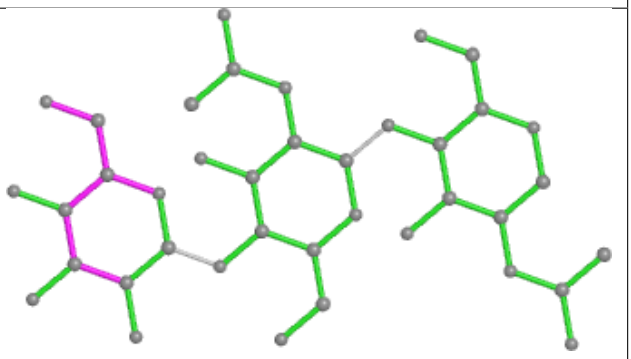


Rings

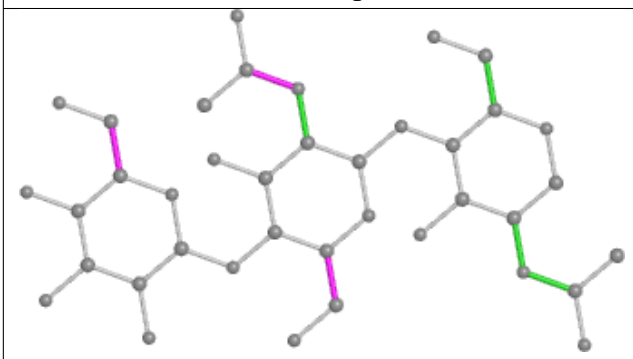
Oligosaccharide Chain J



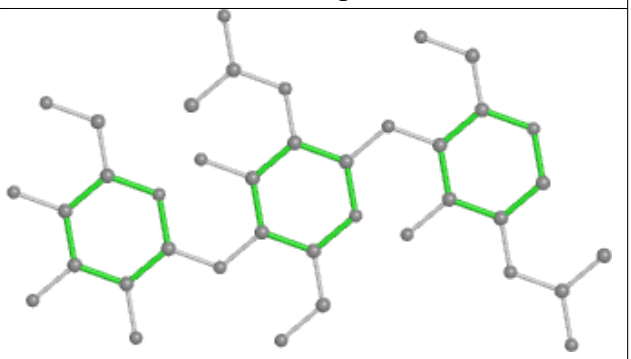
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	C	803	1	14,14,15	0.44	0	17,19,21	0.52	0
5	NAG	A	803	1	14,14,15	0.35	0	17,19,21	0.47	0
5	NAG	A	804	1	14,14,15	0.30	0	17,19,21	0.33	0
5	NAG	A	812	1	14,14,15	0.34	0	17,19,21	0.54	0
5	NAG	C	804	1	14,14,15	0.32	0	17,19,21	0.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	803	1	-	0/6/23/26	0/1/1/1
5	NAG	A	803	1	-	0/6/23/26	0/1/1/1
5	NAG	A	804	1	-	0/6/23/26	0/1/1/1
5	NAG	A	812	1	-	1/6/23/26	0/1/1/1
5	NAG	C	804	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	812	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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

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	727/734 (99%)	0.02	12 (1%)	70	66	22, 41, 69, 142	0
1	C	727/734 (99%)	0.04	24 (3%)	46	39	21, 39, 68, 199	0
2	B	208/246 (84%)	0.34	12 (5%)	23	17	34, 55, 96, 119	0
2	D	208/246 (84%)	0.59	18 (8%)	10	7	33, 58, 124, 171	0
All	All	1870/1960 (95%)	0.13	66 (3%)	44	36	21, 43, 84, 199	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	95	PHE	10.3
2	D	213	THR	8.8
2	D	215	THR	8.2
2	D	214	GLY	7.8
1	C	135	TYR	7.2
1	C	94	THR	7.2
1	C	96	ASP	6.9
2	D	222	LEU	6.3
2	D	124	ILE	6.1
2	B	123	THR	5.8
2	D	120	ALA	5.8
2	D	121	ASN	5.5
1	C	97	GLU	4.6
2	B	119	LEU	4.4
2	D	212	GLY	4.3
1	C	142	LEU	4.2
1	A	95	PHE	4.1
2	D	182	PHE	4.0
1	A	135	TYR	3.9
1	C	98	PHE	3.8
1	A	142	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
2	D	94	SER	3.6
1	C	139	LYS	3.5
2	B	124	ILE	3.4
1	C	140	ARG	3.4
1	C	141	GLN	3.3
1	C	143	ILE	3.2
1	C	93	SER	3.2
2	B	118	VAL	3.2
1	C	137	LEU	3.2
2	B	205	PHE	3.0
2	B	222	LEU	3.0
1	A	72	GLN	3.0
1	A	506	ASN	2.9
1	A	96	ASP	2.8
1	C	73	GLU	2.8
1	C	99	GLY	2.8
2	D	181	GLN	2.7
2	B	121	ASN	2.7
2	B	69	ARG	2.7
2	B	120	ALA	2.7
1	A	137	LEU	2.7
2	D	185	GLY	2.6
2	D	221	MET	2.6
1	A	138	ASN	2.5
1	C	111	GLY	2.5
2	D	123	THR	2.5
1	A	140	ARG	2.5
2	D	216	ASP	2.4
1	C	89	PHE	2.4
2	B	125	THR	2.4
1	C	138	ASN	2.3
1	C	72	GLN	2.3
2	D	211	TYR	2.3
1	A	395	THR	2.3
2	B	215	THR	2.2
1	C	100	HIS	2.2
2	D	125	THR	2.1
1	C	91	GLU	2.1
1	A	134	ILE	2.1
1	C	144	THR	2.1
2	B	122	VAL	2.1
1	A	502	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	487	ASN	2.1
2	D	180	THR	2.0
1	C	90	LEU	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)

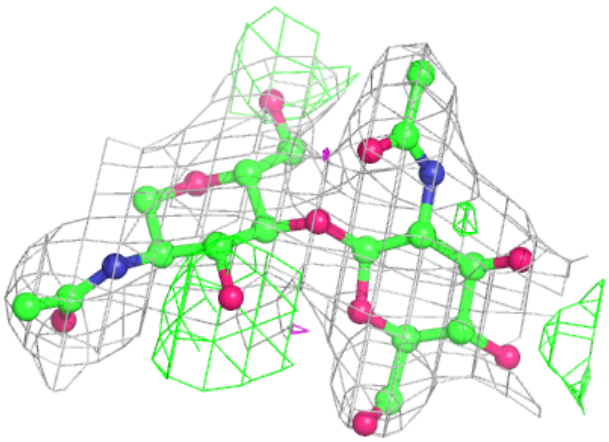
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

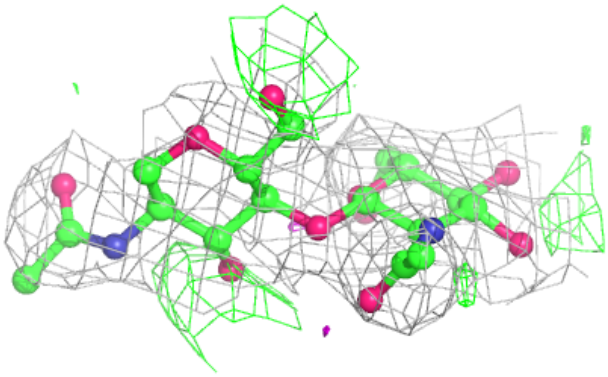
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BMA	J	3	11/12	0.63	0.29	98,109,123,126	0
3	NAG	L	2	14/15	0.77	0.32	76,91,94,95	0
3	NAG	E	1	14/15	0.79	0.16	60,63,69,73	0
3	NAG	I	1	14/15	0.83	0.17	65,81,92,102	0
4	BMA	F	3	11/12	0.83	0.31	110,122,127,129	0
3	NAG	K	2	14/15	0.83	0.23	51,70,77,92	0
3	NAG	K	1	14/15	0.84	0.16	51,59,62,62	0
4	NAG	J	2	14/15	0.85	0.26	60,71,79,80	0
3	NAG	I	2	14/15	0.86	0.26	105,114,123,127	0
4	NAG	F	2	14/15	0.86	0.17	51,65,79,84	0
3	NAG	G	2	14/15	0.87	0.26	62,73,79,85	0
3	NAG	H	2	14/15	0.88	0.26	80,86,91,94	0
3	NAG	G	1	14/15	0.89	0.19	46,51,59,61	0
3	NAG	L	1	14/15	0.89	0.26	49,58,66,78	0
3	NAG	E	2	14/15	0.92	0.19	50,60,68,70	0
3	NAG	H	1	14/15	0.94	0.20	57,67,76,82	0
4	NAG	F	1	14/15	0.96	0.16	33,39,54,59	0
4	NAG	J	1	14/15	0.96	0.11	23,40,52,59	0

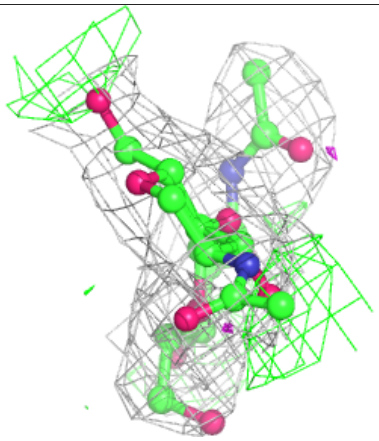
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

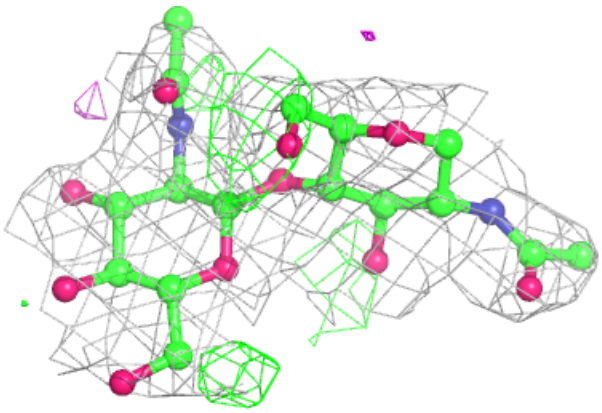


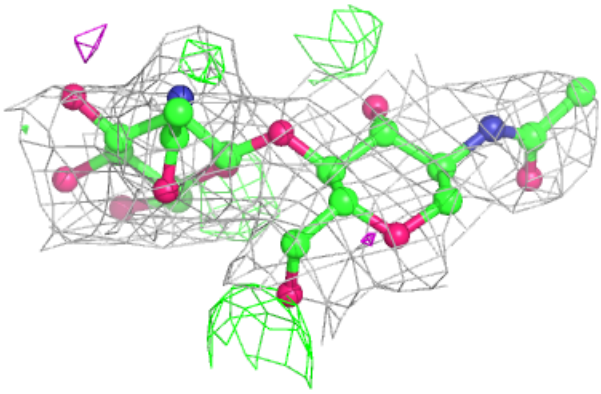


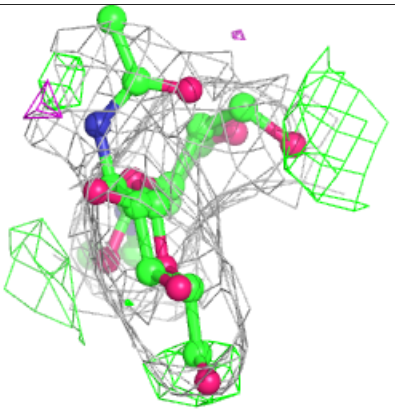


Electron density around Chain G:

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

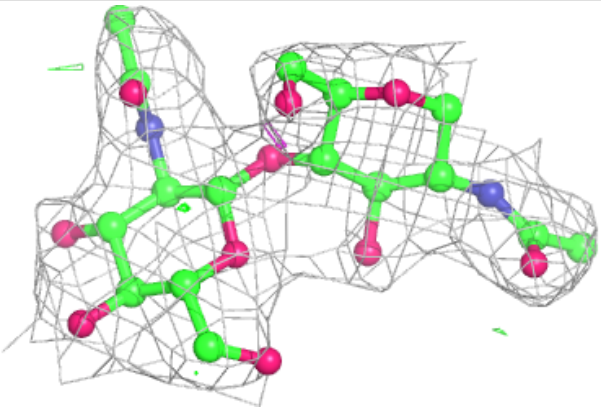


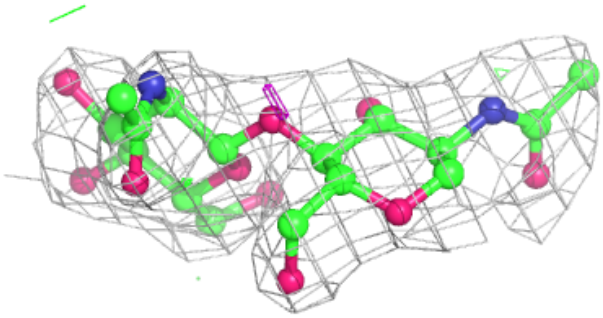


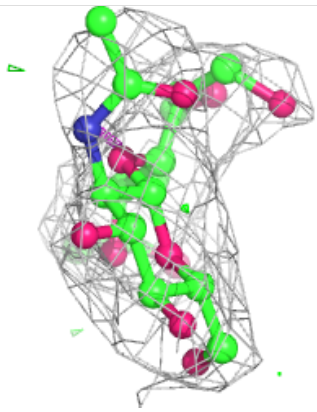


Electron density around Chain H:

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

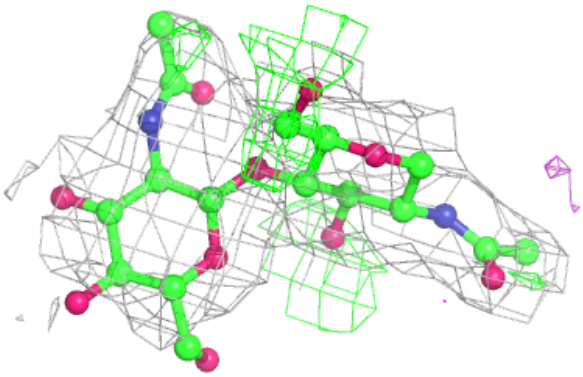


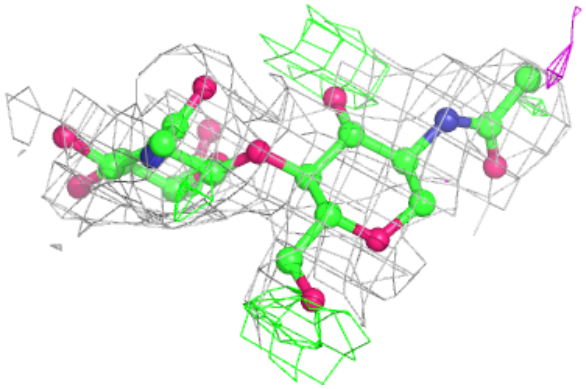


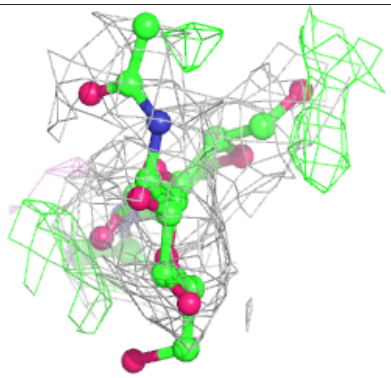


Electron density around Chain I:

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

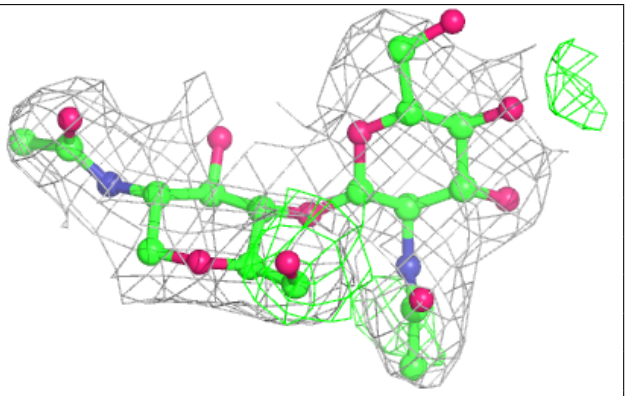


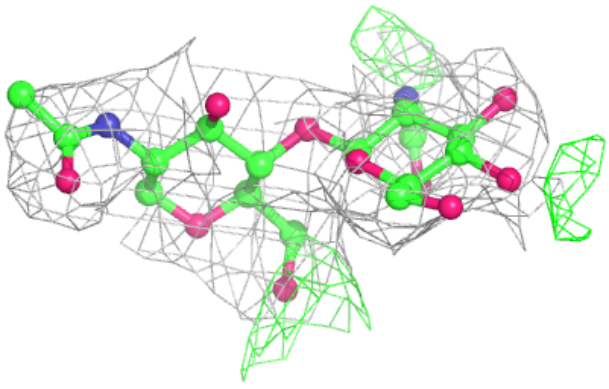


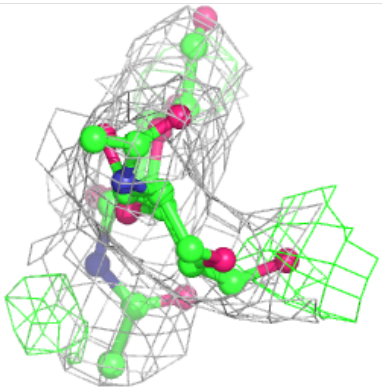


Electron density around Chain K:

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

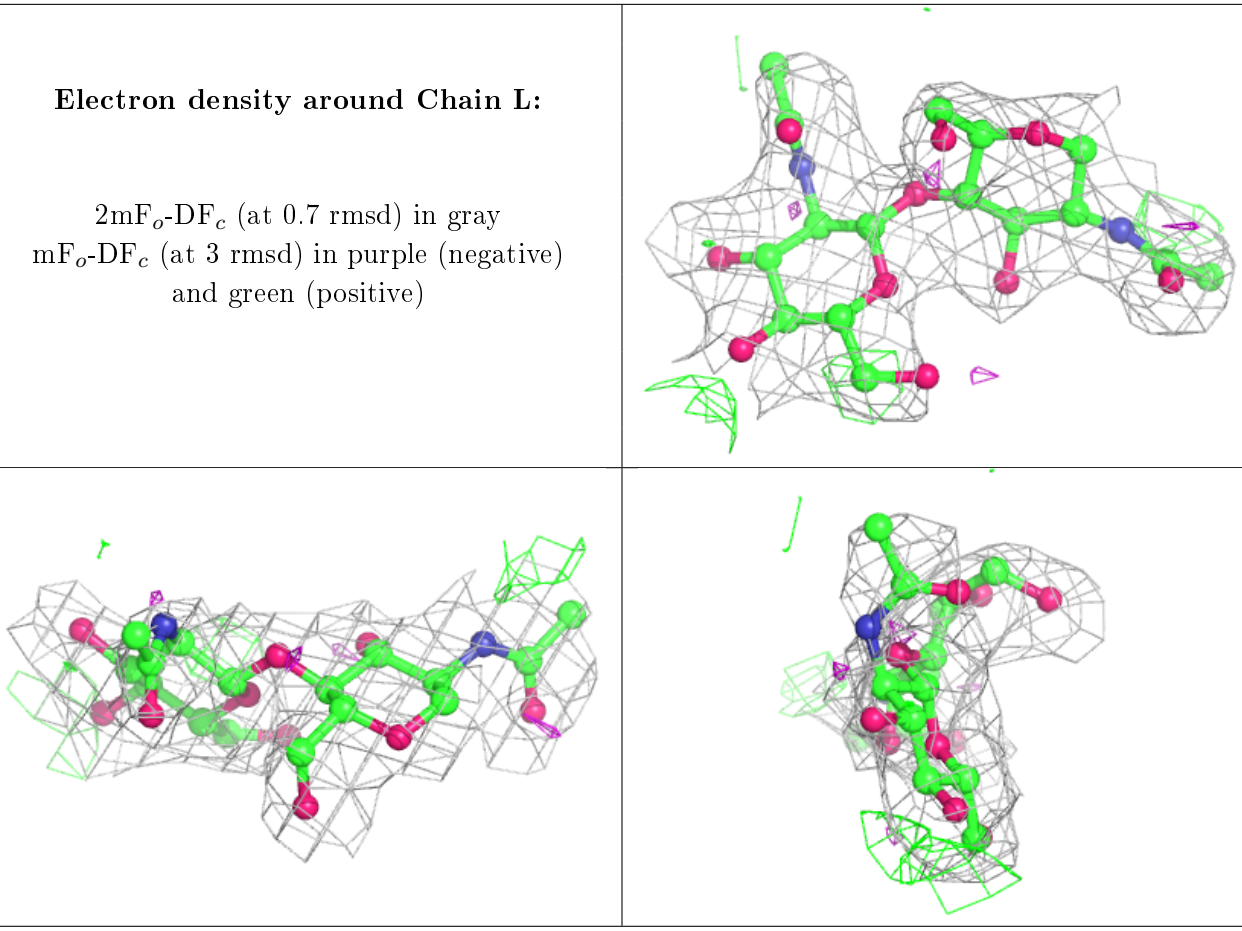






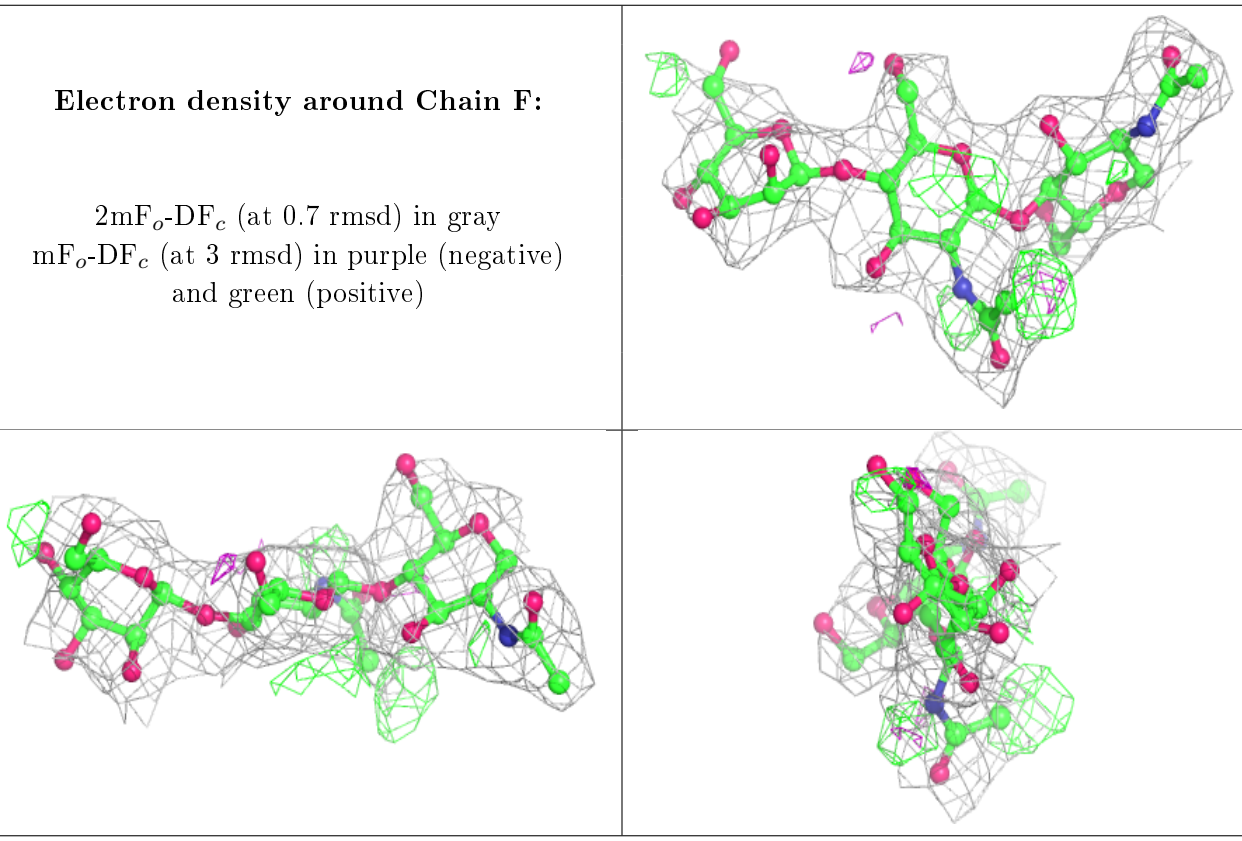
Electron density around Chain L:

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



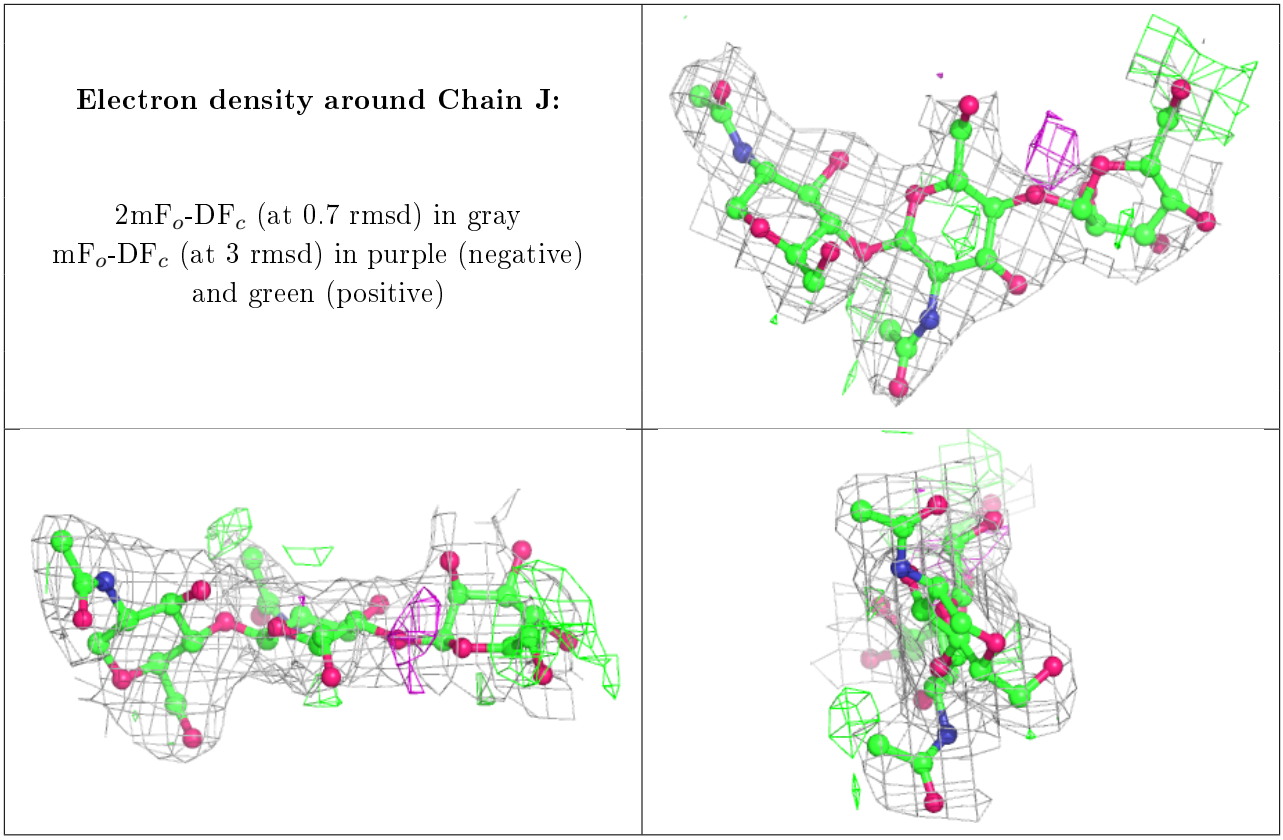
Electron density around Chain F:

$2mF_o$-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 J:

$2mF_o$-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
5	NAG	A	812	14/15	0.77	0.28	98,105,114,114	0
5	NAG	A	803	14/15	0.81	0.24	59,82,88,89	0
5	NAG	C	804	14/15	0.83	0.22	71,81,90,92	0
5	NAG	A	804	14/15	0.87	0.15	61,70,78,80	0
5	NAG	C	803	14/15	0.90	0.27	61,80,84,86	0

6.5 Other polymers

There are no such residues in this entry.