Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2023 – 02:30 AM EDT

PDB ID	:	4GZS
Title	:	N2 neuraminidase D151G mutant of a/Tanzania/205/2010 H3N2 in complex with hepes
Authors	:	Zhu, X.; Wilson, I.A.
Deposited on	:	2012-09-06
Resolution	:	2.35 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

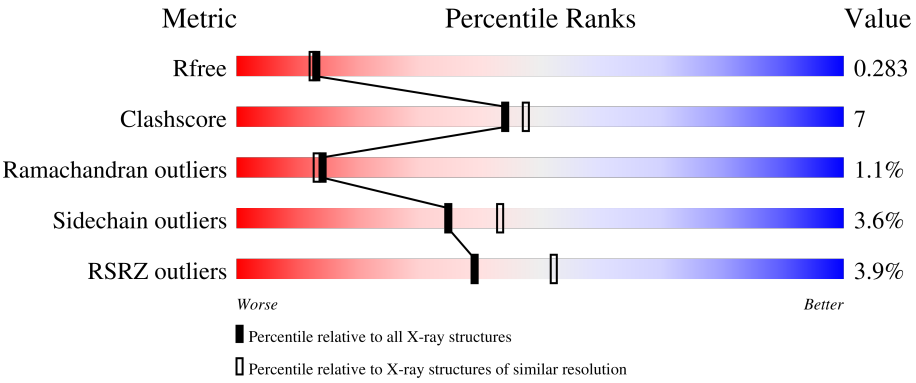
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	393	3% 83% 15%
1	B	393	5% 82% 16%
1	C	393	5% 80% 16%
1	D	393	2% 80% 18%
2	E	5	100%

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Mol	Chain	Length	Quality of chain
2	G	5	20% 60% 20%
2	I	5	100%
2	K	5	60% 40%
3	F	2	50% 50%
3	H	2	100%
3	J	2	100%
4	L	2	100%

2 Entry composition (i)

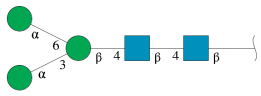
There are 8 unique types of molecules in this entry. The entry contains 12862 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	0	0
			2998	1858	531	587	22			
1	B	388	Total	C	N	O	S	0	0	0
			2998	1858	531	587	22			
1	C	388	Total	C	N	O	S	0	0	0
			2998	1858	531	587	22			
1	D	388	Total	C	N	O	S	0	0	0
			2998	1858	531	587	22			

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



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

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	F	2	Total C N O 24 14 1 9	0	0	0
3	H	2	Total C N O 24 14 1 9	0	0	0
3	J	2	Total C N O 24 14 1 9	0	0	0

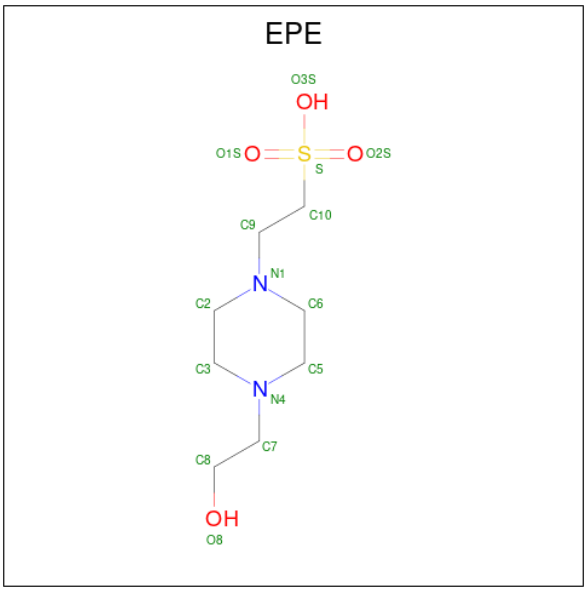
- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	L	2	Total C N O 28 16 2 10	0	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

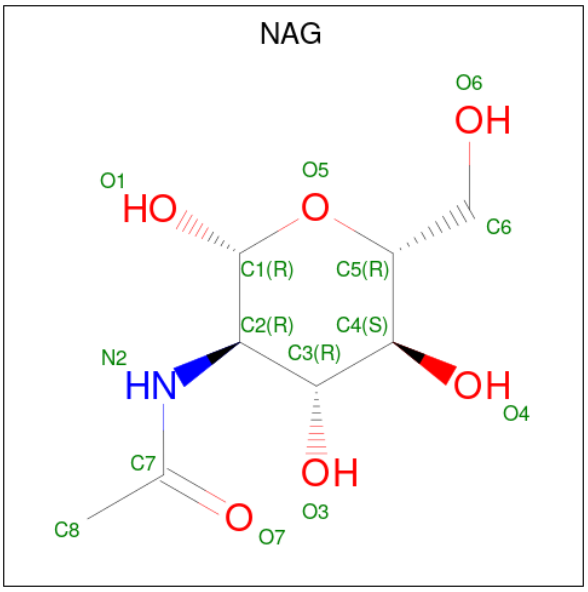
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	B	1	Total Ca 1 1	0	0
5	C	2	Total Ca 2 2	0	0
5	D	1	Total Ca 1 1	0	0

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O S 15 8 2 4 1	0	0
6	B	1	Total C N O S 15 8 2 4 1	0	0
6	C	1	Total C N O S 15 8 2 4 1	0	0
6	D	1	Total C N O S 15 8 2 4 1	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
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is water.

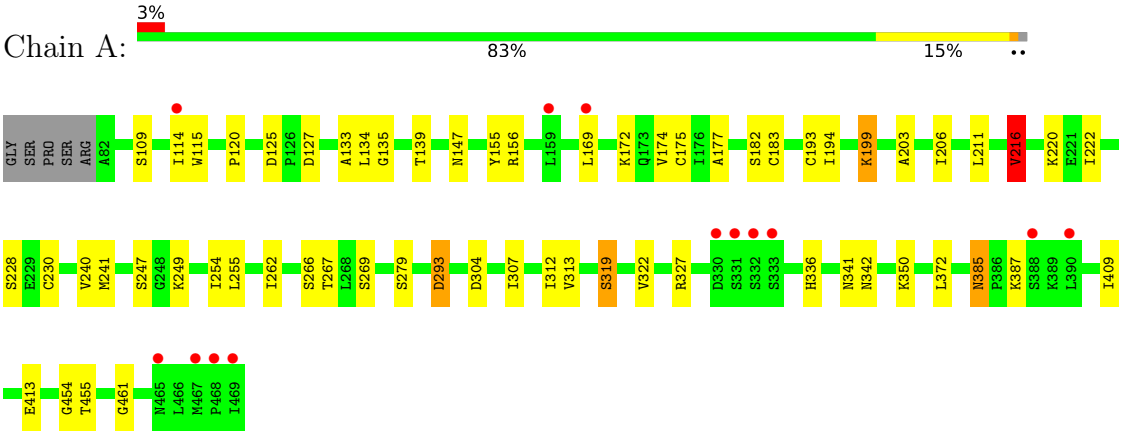
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	91	Total	O	0	0
			91	91		
8	B	89	Total	O	0	0
			89	89		
8	C	93	Total	O	0	0
			93	93		
8	D	90	Total	O	0	0
			90	90		

3 Residue-property plots

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.

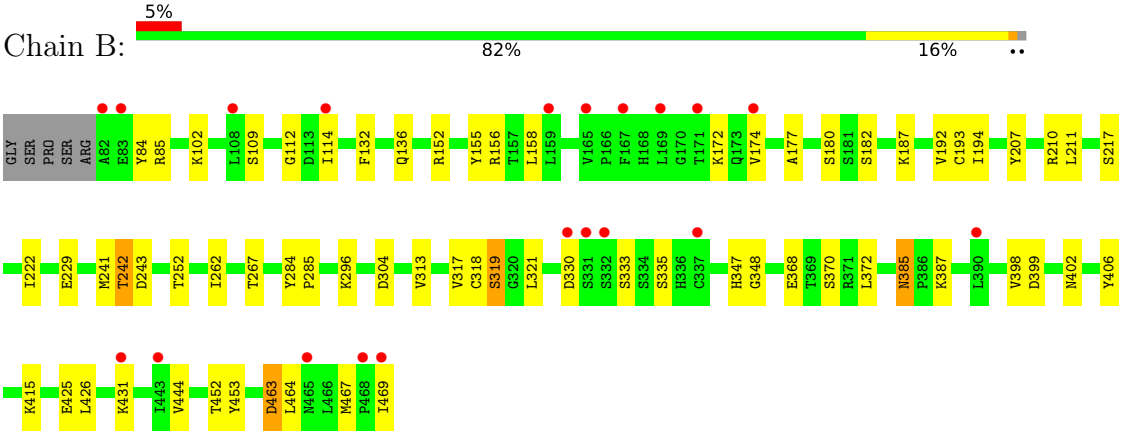
• Molecule 1: Neuraminidase

Chain A:



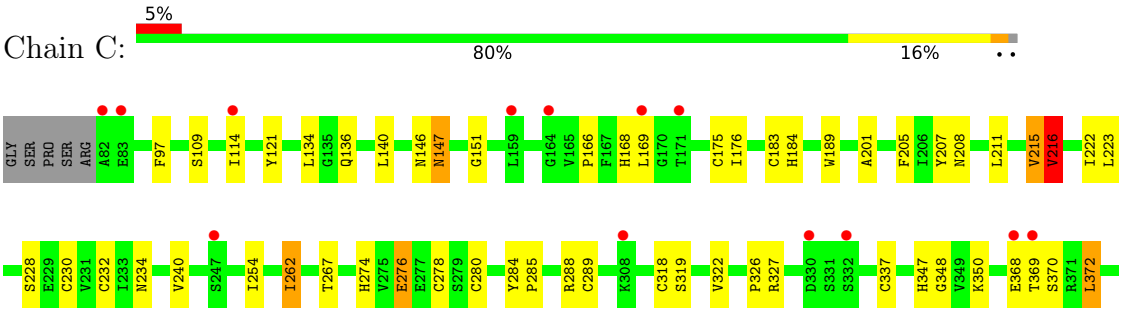
• Molecule 1: Neuraminidase

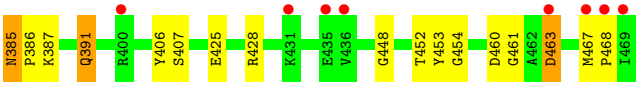
Chain B:



• Molecule 1: Neuraminidase

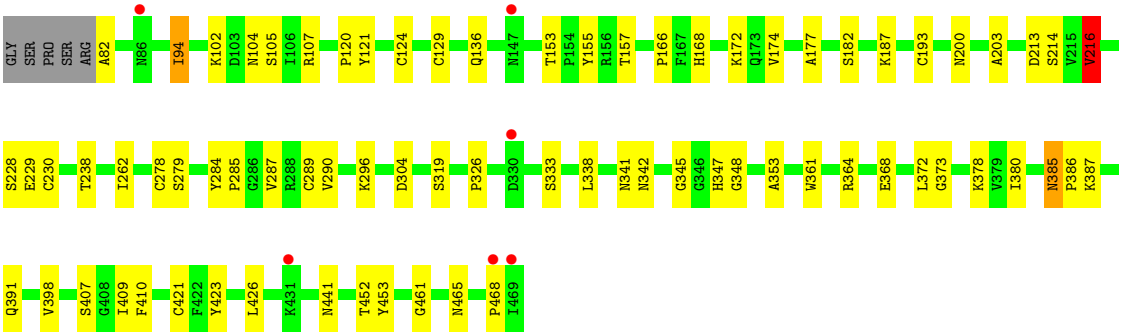
Chain C:





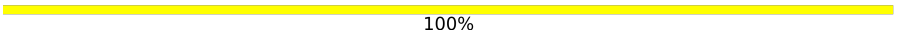
• Molecule 1: Neuraminidase

Chain D:



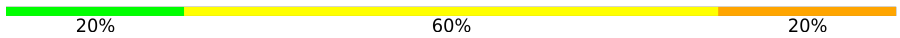
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



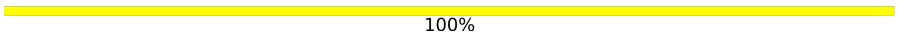
• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

Chain I:



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

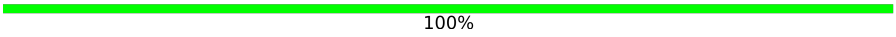
Chain K:

• Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

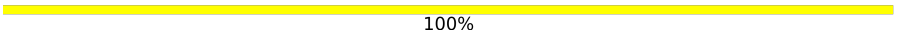
• Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



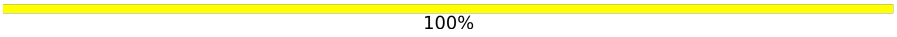
• Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



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

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	80.81Å 110.20Å 110.59Å 90.00° 97.46° 90.00°	Depositor
Resolution (Å)	50.00 – 2.35 44.21 – 2.34	Depositor EDS
% Data completeness (in resolution range)	92.4 (50.00-2.35) 91.8 (44.21-2.34)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.225 , 0.287 0.225 , 0.283	Depositor DCC
R_{free} test set	3724 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	26.4	Xtriage
Anisotropy	1.073	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 33.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12862	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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: EPE, FUC, NAG, BMA, CA, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.56	0/3065	0.70	1/4156 (0.0%)
1	B	0.57	0/3065	0.68	0/4156
1	C	0.59	0/3065	0.71	1/4156 (0.0%)
1	D	0.58	0/3065	0.70	1/4156 (0.0%)
All	All	0.58	0/12260	0.70	3/16624 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	216	VAL	CB-CA-C	-7.38	97.37	111.40
1	C	216	VAL	CB-CA-C	-5.48	100.98	111.40
1	D	216	VAL	CB-CA-C	-5.43	101.09	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2998	0	2856	37	0
1	B	2998	0	2855	43	0
1	C	2998	0	2855	50	0
1	D	2998	0	2855	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	61	0	52	0	0
2	G	61	0	52	1	0
2	I	61	0	52	0	0
2	K	61	0	52	2	0
3	F	24	0	22	1	0
3	H	24	0	22	0	0
3	J	24	0	22	0	0
4	L	28	0	25	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
6	A	15	0	17	2	0
6	B	15	0	17	2	0
6	C	15	0	17	1	0
6	D	15	0	17	2	0
7	A	14	0	13	0	0
7	B	28	0	26	0	0
7	C	28	0	26	0	0
7	D	28	0	26	0	0
8	A	91	0	0	1	0
8	B	89	0	0	2	0
8	C	93	0	0	0	0
8	D	90	0	0	3	0
All	All	12862	0	11879	160	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (160) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:THR:HB	1:C:216:VAL:CG2	2.02	0.88
1:A:177:ALA:HB2	1:A:193:CYS:HB3	1.60	0.84
1:C:452:THR:HB	1:D:216:VAL:HG22	1.68	0.73
1:B:452:THR:HB	1:C:216:VAL:HG22	1.69	0.73
1:A:216:VAL:HG13	1:D:453:TYR:C	2.13	0.69
1:B:385:ASN:ND2	1:B:387:LYS:H	1.94	0.66
1:B:452:THR:HB	1:C:216:VAL:HG23	1.78	0.66
1:C:453:TYR:C	1:D:216:VAL:HG13	2.17	0.65
1:B:152:ARG:HH11	6:B:502:EPE:H81	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:ALA:HB2	1:D:193:CYS:HB3	1.80	0.64
1:B:242:THR:HG23	1:B:252:THR:OG1	1.99	0.63
1:B:385:ASN:HD22	1:B:387:LYS:H	1.44	0.63
1:B:136:GLN:OE1	1:B:156:ARG:CZ	2.47	0.62
1:C:347:HIS:CG	1:C:348:GLY:H	2.18	0.61
6:D:502:EPE:H32	6:D:502:EPE:H102	1.81	0.61
1:D:385:ASN:ND2	1:D:387:LYS:H	1.97	0.61
1:A:455:THR:HG22	8:A:665:HOH:O	2.00	0.61
1:C:146:ASN:O	1:C:147:ASN:HB2	2.00	0.61
1:C:278:CYS:HB3	1:C:289:CYS:HB3	1.84	0.60
1:C:337:CYS:SG	1:C:386:PRO:HG3	2.42	0.60
1:B:304:ASP:HB2	1:B:313:VAL:HG22	1.85	0.58
1:B:102:LYS:HG3	1:B:444:VAL:HG23	1.86	0.57
1:C:151:GLY:HA3	6:C:503:EPE:H51	1.86	0.57
1:D:136:GLN:HE21	1:D:136:GLN:HA	1.70	0.56
1:A:155:TYR:CE1	1:D:461:GLY:HA3	2.40	0.56
1:A:385:ASN:ND2	1:A:387:LYS:H	2.04	0.56
1:C:453:TYR:O	1:D:216:VAL:HG13	2.04	0.56
1:B:180:SER:HA	1:B:192:VAL:O	2.06	0.55
1:B:177:ALA:HB2	1:B:193:CYS:HB3	1.87	0.55
1:B:102:LYS:HB2	1:C:176:ILE:HG12	1.89	0.55
1:A:279:SER:HB3	1:A:409:ILE:HG22	1.89	0.55
1:C:109:SER:HB3	1:C:114:ILE:HB	1.89	0.55
1:A:194:ILE:HD11	1:A:241:MET:HE3	1.88	0.54
1:A:216:VAL:HG22	1:D:452:THR:HB	1.90	0.54
1:B:463:ASP:O	1:B:467:MET:HG2	2.08	0.54
1:D:278:CYS:HB3	1:D:289:CYS:HB3	1.90	0.53
1:C:391:GLN:OE1	2:K:3:BMA:O2	2.23	0.53
1:B:385:ASN:HD22	1:B:385:ASN:C	2.11	0.53
1:D:465:ASN:HD22	1:D:465:ASN:H	1.57	0.52
1:A:147:ASN:HD21	3:F:1:NAG:H62	1.74	0.52
1:A:228:SER:HB3	1:A:350:LYS:HE2	1.92	0.52
1:B:109:SER:HB3	1:B:114:ILE:HB	1.91	0.51
1:A:109:SER:HB3	1:A:114:ILE:HB	1.92	0.51
1:A:194:ILE:HD11	1:A:241:MET:CE	2.40	0.51
1:C:385:ASN:C	1:C:385:ASN:HD22	2.13	0.51
1:A:461:GLY:HA3	1:B:155:TYR:CE1	2.46	0.51
1:C:97:PHE:CD1	1:C:448:GLY:HA2	2.46	0.51
1:B:194:ILE:HD11	1:B:241:MET:CE	2.41	0.51
1:D:102:LYS:NZ	1:D:104:ASN:OD1	2.44	0.50
1:B:347:HIS:CG	1:B:348:GLY:H	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:TYR:CG	1:C:228:SER:HA	2.46	0.50
1:B:172:LYS:HD3	1:B:174:VAL:HG12	1.93	0.50
1:D:385:ASN:C	1:D:385:ASN:HD22	2.15	0.50
1:A:135:GLY:O	1:A:156:ARG:HA	2.11	0.50
1:A:254:ILE:HD13	1:A:312:ILE:HG13	1.94	0.50
1:B:398:VAL:HG21	1:B:426:LEU:HD21	1.92	0.50
1:D:279:SER:HB3	1:D:409:ILE:HG22	1.95	0.49
1:A:134:LEU:O	1:A:156:ARG:NH2	2.45	0.49
1:A:385:ASN:HD22	1:A:385:ASN:C	2.16	0.49
1:C:428:ARG:NH1	1:C:460:ASP:OD2	2.45	0.49
1:B:85:ARG:HD3	8:B:609:HOH:O	2.11	0.48
1:D:385:ASN:HD22	1:D:386:PRO:N	2.11	0.48
1:C:228:SER:HB3	1:C:350:LYS:HE2	1.95	0.48
8:D:614:HOH:O	2:K:1:NAG:H82	2.14	0.48
1:B:467:MET:O	1:B:469:ILE:HG13	2.14	0.48
1:C:385:ASN:ND2	1:C:387:LYS:H	2.12	0.48
1:A:304:ASP:HB2	1:A:313:VAL:HG22	1.96	0.48
1:D:407:SER:HA	1:D:423:TYR:O	2.14	0.48
1:C:454:GLY:HA3	1:D:200:ASN:O	2.13	0.48
1:B:112:GLY:HA3	1:C:169:LEU:HD11	1.96	0.47
1:D:238:THR:HG21	1:D:287:VAL:HG21	1.96	0.47
1:C:201:ALA:HB3	1:C:223:LEU:HB3	1.96	0.47
1:D:82:ALA:O	1:D:187:LYS:HE2	2.14	0.47
1:B:284:TYR:CD1	1:B:285:PRO:HA	2.50	0.47
1:B:370:SER:OG	1:B:372:LEU:HD13	2.15	0.47
1:D:378:LYS:O	1:D:391:GLN:HA	2.15	0.47
6:A:502:EPE:H102	6:A:502:EPE:H61	1.65	0.47
1:C:347:HIS:CG	1:C:348:GLY:N	2.83	0.47
1:A:115:TRP:HA	1:A:139:THR:HA	1.96	0.47
1:D:182:SER:O	1:D:229:GLU:HA	2.16	0.46
1:B:318:CYS:O	1:B:319:SER:C	2.54	0.46
1:B:321:LEU:HD22	1:B:330:ASP:OD1	2.14	0.46
1:C:134:LEU:HD23	1:C:134:LEU:HA	1.78	0.46
1:A:255:LEU:N	1:A:255:LEU:HD12	2.31	0.46
1:A:240:VAL:HG22	1:A:254:ILE:HG13	1.97	0.46
1:A:454:GLY:HA2	2:G:1:NAG:O5	2.16	0.46
1:B:132:PHE:HB3	1:B:158:LEU:HD11	1.98	0.46
1:A:413:GLU:O	1:B:210:ARG:NH1	2.49	0.45
1:D:107:ARG:HG3	8:D:609:HOH:O	2.16	0.45
1:A:216:VAL:HG13	1:D:453:TYR:O	2.17	0.45
1:D:398:VAL:HG21	1:D:426:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:LEU:HA	1:B:467:MET:HG2	1.99	0.45
1:D:121:TYR:CG	1:D:228:SER:HA	2.51	0.45
1:B:284:TYR:CG	1:B:285:PRO:HA	2.52	0.45
6:B:502:EPE:H61	6:B:502:EPE:H101	1.55	0.45
1:C:215:VAL:HG22	1:C:262:ILE:CD1	2.46	0.45
1:C:322:VAL:HG23	1:C:327:ARG:HD2	1.99	0.45
1:C:280:CYS:HA	1:C:288:ARG:O	2.18	0.44
1:D:136:GLN:HA	1:D:136:GLN:NE2	2.32	0.44
1:D:172:LYS:HD3	1:D:174:VAL:HG12	1.99	0.44
1:B:217:SER:OG	1:B:243:ASP:OD2	2.26	0.44
1:B:399:ASP:OD2	1:B:402:ASN:ND2	2.50	0.44
1:A:199:LYS:O	1:A:220:LYS:HB3	2.18	0.44
1:B:453:TYR:C	1:C:216:VAL:HG13	2.37	0.44
1:D:120:PRO:HG3	1:D:441:ASN:ND2	2.33	0.44
1:C:318:CYS:O	1:C:386:PRO:HA	2.18	0.43
1:A:293:ASP:OD1	1:A:293:ASP:C	2.56	0.43
8:B:602:HOH:O	1:C:175:CYS:HB2	2.18	0.43
1:D:290:VAL:HG21	1:D:353:ALA:HB3	1.99	0.43
1:A:322:VAL:HG23	1:A:327:ARG:HD2	2.00	0.43
1:C:463:ASP:O	1:C:467:MET:HG2	2.18	0.43
1:D:364:ARG:HA	8:D:668:HOH:O	2.18	0.43
1:A:172:LYS:HD3	1:A:174:VAL:HG12	2.00	0.43
6:A:502:EPE:H31	6:A:502:EPE:H81	1.48	0.43
1:D:385:ASN:ND2	1:D:385:ASN:C	2.71	0.43
1:C:184:HIS:HD2	1:C:189:TRP:NE1	2.17	0.43
1:C:385:ASN:C	1:C:385:ASN:ND2	2.72	0.43
1:A:120:PRO:HA	1:A:133:ALA:HA	1.99	0.43
1:A:175:CYS:HB3	1:A:206:ILE:HD12	1.99	0.43
1:A:228:SER:HB3	1:A:350:LYS:CE	2.49	0.43
1:C:326:PRO:HA	1:C:368:GLU:O	2.18	0.43
1:D:94:ILE:HG22	1:D:361:TRP:CE2	2.53	0.43
6:D:502:EPE:H102	6:D:502:EPE:C3	2.48	0.42
1:D:296:LYS:C	1:D:345:GLY:HA3	2.39	0.42
1:A:194:ILE:HG12	1:A:203:ALA:HB2	2.00	0.42
1:B:194:ILE:HD11	1:B:241:MET:HE3	2.01	0.42
1:B:296:LYS:HE3	1:B:296:LYS:HB2	1.75	0.42
1:C:274:HIS:CE1	1:C:276:GLU:OE1	2.72	0.42
1:C:370:SER:HB3	1:C:372:LEU:HD22	2.01	0.42
1:B:406:TYR:HB2	1:B:425:GLU:OE1	2.19	0.42
1:A:385:ASN:ND2	1:A:385:ASN:C	2.72	0.42
1:B:182:SER:O	1:B:229:GLU:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:ASN:O	1:D:342:ASN:HB2	2.19	0.42
1:B:84:TYR:CE1	1:B:187:LYS:HD2	2.54	0.42
1:C:205:PHE:HE1	1:C:215:VAL:HG23	1.85	0.42
1:C:240:VAL:HG22	1:C:254:ILE:HG13	2.02	0.42
1:C:207:TYR:O	1:C:208:ASN:C	2.59	0.42
1:C:109:SER:OG	1:C:140:LEU:HD13	2.19	0.41
1:C:385:ASN:HD22	1:C:386:PRO:N	2.18	0.41
1:B:207:TYR:O	1:B:210:ARG:HG2	2.20	0.41
1:D:347:HIS:CG	1:D:348:GLY:H	2.38	0.41
1:D:124:CYS:HA	1:D:129:CYS:HA	2.02	0.41
1:D:203:ALA:O	1:D:214:SER:HA	2.20	0.41
1:A:125:ASP:OD1	1:A:127:ASP:N	2.49	0.41
1:C:284:TYR:CD1	1:C:285:PRO:HA	2.55	0.41
1:C:183:CYS:SG	1:C:232:CYS:SG	3.19	0.41
1:D:166:PRO:O	1:D:168:HIS:HD2	2.03	0.41
1:A:341:ASN:O	1:A:342:ASN:HB2	2.21	0.41
1:C:183:CYS:N	1:C:230:CYS:SG	2.94	0.41
1:C:97:PHE:HD1	1:C:448:GLY:HA2	1.85	0.40
1:C:461:GLY:HA3	1:D:155:TYR:CZ	2.56	0.40
1:C:166:PRO:O	1:C:168:HIS:HD2	2.04	0.40
1:A:169:LEU:HD23	1:A:169:LEU:HA	1.86	0.40
1:C:406:TYR:HB2	1:C:425:GLU:OE1	2.20	0.40
1:D:284:TYR:HA	1:D:285:PRO:HA	1.91	0.40
1:D:326:PRO:HA	1:D:368:GLU:O	2.22	0.40
1:D:410:PHE:CZ	1:D:421:CYS:HB2	2.56	0.40
1:B:453:TYR:N	1:C:216:VAL:HG22	2.37	0.40
1:A:182:SER:C	1:A:230:CYS:SG	3.00	0.40
1:B:318:CYS:O	1:B:335:SER:HB3	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	386/393 (98%)	361 (94%)	21 (5%)	4 (1%)	15	15
1	B	386/393 (98%)	358 (93%)	24 (6%)	4 (1%)	15	15
1	C	386/393 (98%)	354 (92%)	27 (7%)	5 (1%)	12	10
1	D	386/393 (98%)	357 (92%)	25 (6%)	4 (1%)	15	15
All	All	1544/1572 (98%)	1430 (93%)	97 (6%)	17 (1%)	14	13

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	468	PRO
1	B	333	SER
1	C	234	ASN
1	D	468	PRO
1	A	319	SER
1	C	147	ASN
1	B	319	SER
1	D	319	SER
1	A	262	ILE
1	A	336	HIS
1	D	262	ILE
1	C	262	ILE
1	A	222	ILE
1	D	373	GLY
1	B	262	ILE
1	B	222	ILE
1	C	222	ILE

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	337/341 (99%)	323 (96%)	14 (4%)	30	36
1	B	337/341 (99%)	328 (97%)	9 (3%)	44	55
1	C	337/341 (99%)	324 (96%)	13 (4%)	32	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	337/341 (99%)	324 (96%)	13 (4%)	32 40
All	All	1348/1364 (99%)	1299 (96%)	49 (4%)	35 43

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	CYS
1	A	199	LYS
1	A	211	LEU
1	A	216	VAL
1	A	247	SER
1	A	249	LYS
1	A	266	SER
1	A	267	THR
1	A	269	SER
1	A	293	ASP
1	A	307	ILE
1	A	319	SER
1	A	372	LEU
1	A	385	ASN
1	B	211	LEU
1	B	242	THR
1	B	267	THR
1	B	317	VAL
1	B	368	GLU
1	B	385	ASN
1	B	415	LYS
1	B	431	LYS
1	B	463	ASP
1	C	136	GLN
1	C	211	LEU
1	C	215	VAL
1	C	216	VAL
1	C	267	THR
1	C	276	GLU
1	C	319	SER
1	C	369	THR
1	C	372	LEU
1	C	385	ASN
1	C	391	GLN
1	C	407	SER
1	C	463	ASP

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Mol	Chain	Res	Type
1	D	94	ILE
1	D	105	SER
1	D	153	THR
1	D	157	THR
1	D	213	ASP
1	D	216	VAL
1	D	230	CYS
1	D	304	ASP
1	D	333	SER
1	D	338	LEU
1	D	372	LEU
1	D	380	ILE
1	D	385	ASN

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	86	ASN
1	A	147	ASN
1	A	234	ASN
1	A	385	ASN
1	B	168	HIS
1	B	385	ASN
1	B	393	ASN
1	C	136	GLN
1	C	168	HIS
1	C	385	ASN
1	C	393	ASN
1	D	136	GLN
1	D	168	HIS
1	D	385	ASN
1	D	393	ASN
1	D	465	ASN

5.3.3 RNA

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)

28 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	E	1	2,1	14,14,15	0.65	0	17,19,21	1.15	2 (11%)
2	NAG	E	2	2	14,14,15	0.40	0	17,19,21	1.39	2 (11%)
2	BMA	E	3	2	11,11,12	0.72	0	15,15,17	0.89	1 (6%)
2	MAN	E	4	2	11,11,12	0.67	0	15,15,17	1.63	3 (20%)
2	MAN	E	5	2	11,11,12	0.73	0	15,15,17	2.43	5 (33%)
3	NAG	F	1	3,1	14,14,15	0.63	0	17,19,21	1.55	3 (17%)
3	FUC	F	2	3	10,10,11	0.58	0	14,14,16	0.73	0
2	NAG	G	1	2,1	14,14,15	0.44	0	17,19,21	1.32	1 (5%)
2	NAG	G	2	2	14,14,15	0.54	0	17,19,21	0.82	0
2	BMA	G	3	2	11,11,12	0.97	0	15,15,17	1.58	3 (20%)
2	MAN	G	4	2	11,11,12	0.68	0	15,15,17	1.55	3 (20%)
2	MAN	G	5	2	11,11,12	0.59	0	15,15,17	2.22	4 (26%)
3	NAG	H	1	3,1	14,14,15	0.61	0	17,19,21	0.86	0
3	FUC	H	2	3	10,10,11	0.68	0	14,14,16	0.73	0
2	NAG	I	1	2,1	14,14,15	0.79	1 (7%)	17,19,21	1.16	2 (11%)
2	NAG	I	2	2	14,14,15	0.60	0	17,19,21	1.19	1 (5%)
2	BMA	I	3	2	11,11,12	0.53	0	15,15,17	1.25	2 (13%)
2	MAN	I	4	2	11,11,12	0.58	0	15,15,17	1.92	3 (20%)
2	MAN	I	5	2	11,11,12	0.66	0	15,15,17	2.14	3 (20%)
3	NAG	J	1	3,1	14,14,15	0.52	0	17,19,21	1.27	1 (5%)
3	FUC	J	2	3	10,10,11	0.85	0	14,14,16	2.11	3 (21%)
2	NAG	K	1	2,1	14,14,15	0.70	0	17,19,21	1.28	2 (11%)
2	NAG	K	2	2	14,14,15	0.53	0	17,19,21	1.06	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BMA	K	3	2	11,11,12	0.75	0	15,15,17	1.08	1 (6%)
2	MAN	K	4	2	11,11,12	0.60	0	15,15,17	1.36	1 (6%)
2	MAN	K	5	2	11,11,12	0.61	0	15,15,17	1.92	5 (33%)
4	NAG	L	1	4,1	14,14,15	0.47	0	17,19,21	1.54	2 (11%)
4	NAG	L	2	4	14,14,15	0.56	0	17,19,21	1.22	2 (11%)

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	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
2	MAN	E	4	2	-	2/2/19/22	0/1/1/1
2	MAN	E	5	2	-	2/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	FUC	F	2	3	-	-	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	BMA	G	3	2	-	2/2/19/22	0/1/1/1
2	MAN	G	4	2	-	0/2/19/22	0/1/1/1
2	MAN	G	5	2	-	1/2/19/22	0/1/1/1
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1
3	FUC	H	2	3	-	-	0/1/1/1
2	NAG	I	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	BMA	I	3	2	-	2/2/19/22	0/1/1/1
2	MAN	I	4	2	-	0/2/19/22	0/1/1/1
2	MAN	I	5	2	-	0/2/19/22	0/1/1/1
3	NAG	J	1	3,1	-	2/6/23/26	0/1/1/1
3	FUC	J	2	3	-	-	0/1/1/1
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	BMA	K	3	2	-	2/2/19/22	0/1/1/1
2	MAN	K	4	2	-	0/2/19/22	0/1/1/1
2	MAN	K	5	2	-	2/2/19/22	0/1/1/1
4	NAG	L	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	L	2	4	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1	NAG	O5-C1	-2.10	1.40	1.43

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	5	MAN	C1-C2-C3	7.12	118.42	109.67
2	I	5	MAN	C1-O5-C5	5.32	119.40	112.19
2	I	4	MAN	C1-O5-C5	5.19	119.22	112.19
2	G	5	MAN	C1-O5-C5	4.93	118.87	112.19
4	L	1	NAG	C1-O5-C5	4.73	118.59	112.19
2	G	5	MAN	C1-C2-C3	4.52	115.22	109.67
3	J	2	FUC	C3-C4-C5	4.47	116.73	109.77
2	G	1	NAG	C1-O5-C5	4.35	118.09	112.19
3	J	1	NAG	O5-C5-C6	4.15	113.71	107.20
3	J	2	FUC	O5-C1-C2	-4.05	104.53	110.77
2	I	5	MAN	O5-C1-C2	4.04	117.01	110.77
3	J	2	FUC	O5-C5-C4	3.96	116.62	109.52
2	K	4	MAN	C1-O5-C5	3.85	117.41	112.19
2	I	5	MAN	C1-C2-C3	3.83	114.37	109.67
2	E	4	MAN	C1-O5-C5	3.78	117.32	112.19
2	G	5	MAN	O5-C1-C2	3.77	116.59	110.77
2	G	3	BMA	C1-C2-C3	3.74	114.27	109.67
2	K	5	MAN	C2-C3-C4	3.63	117.19	110.89
2	E	2	NAG	O5-C5-C6	3.57	112.80	107.20
2	G	4	MAN	C1-O5-C5	3.56	117.01	112.19
2	E	5	MAN	C1-O5-C5	3.41	116.81	112.19
2	K	5	MAN	C1-C2-C3	3.36	113.79	109.67
3	F	1	NAG	O3-C3-C4	3.35	118.10	110.35
2	I	4	MAN	C3-C4-C5	-3.30	104.36	110.24
4	L	2	NAG	C1-O5-C5	3.17	116.49	112.19
2	E	5	MAN	O5-C1-C2	3.02	115.43	110.77
2	E	1	NAG	C1-O5-C5	2.98	116.23	112.19
2	E	5	MAN	C2-C3-C4	2.96	116.02	110.89
2	K	5	MAN	C1-O5-C5	2.93	116.17	112.19
2	E	4	MAN	O5-C5-C6	2.89	111.74	107.20
2	K	5	MAN	O5-C5-C6	2.88	111.72	107.20
2	K	1	NAG	C1-O5-C5	2.88	116.09	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	5	MAN	C2-C3-C4	2.83	115.79	110.89
2	K	5	MAN	C3-C4-C5	2.76	115.16	110.24
4	L	1	NAG	O3-C3-C2	-2.72	103.83	109.47
2	K	1	NAG	C4-C3-C2	2.70	114.98	111.02
2	I	1	NAG	C2-N2-C7	-2.60	119.20	122.90
3	F	1	NAG	O5-C5-C6	2.58	111.25	107.20
2	K	3	BMA	C1-C2-C3	2.58	112.83	109.67
2	I	3	BMA	O5-C5-C6	2.56	111.22	107.20
2	G	4	MAN	C3-C4-C5	-2.55	105.70	110.24
2	K	2	NAG	C3-C4-C5	-2.49	105.79	110.24
3	F	1	NAG	O4-C4-C3	2.38	115.85	110.35
2	G	4	MAN	O2-C2-C1	2.33	113.92	109.15
2	I	1	NAG	C1-C2-N2	-2.23	106.67	110.49
2	G	3	BMA	O5-C5-C4	-2.22	105.41	110.83
2	I	4	MAN	O5-C1-C2	2.15	114.08	110.77
2	E	5	MAN	O5-C5-C6	2.14	110.56	107.20
2	I	2	NAG	C1-C2-N2	2.14	114.14	110.49
2	E	4	MAN	C1-C2-C3	2.13	112.28	109.67
2	I	3	BMA	O6-C6-C5	-2.12	104.01	111.29
2	G	3	BMA	C6-C5-C4	2.06	117.82	113.00
2	E	1	NAG	O4-C4-C3	-2.04	105.63	110.35
4	L	2	NAG	C4-C3-C2	2.03	114.00	111.02
2	E	2	NAG	C3-C4-C5	-2.02	106.64	110.24
2	E	3	BMA	C6-C5-C4	2.00	117.69	113.00

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	5	MAN	O5-C5-C6-O6
2	E	4	MAN	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
2	K	3	BMA	O5-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6
2	E	5	MAN	O5-C5-C6-O6
2	E	4	MAN	C4-C5-C6-O6
2	K	5	MAN	C4-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
2	E	5	MAN	C4-C5-C6-O6
2	K	3	BMA	C4-C5-C6-O6
2	I	3	BMA	C4-C5-C6-O6
2	G	3	BMA	O5-C5-C6-O6

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

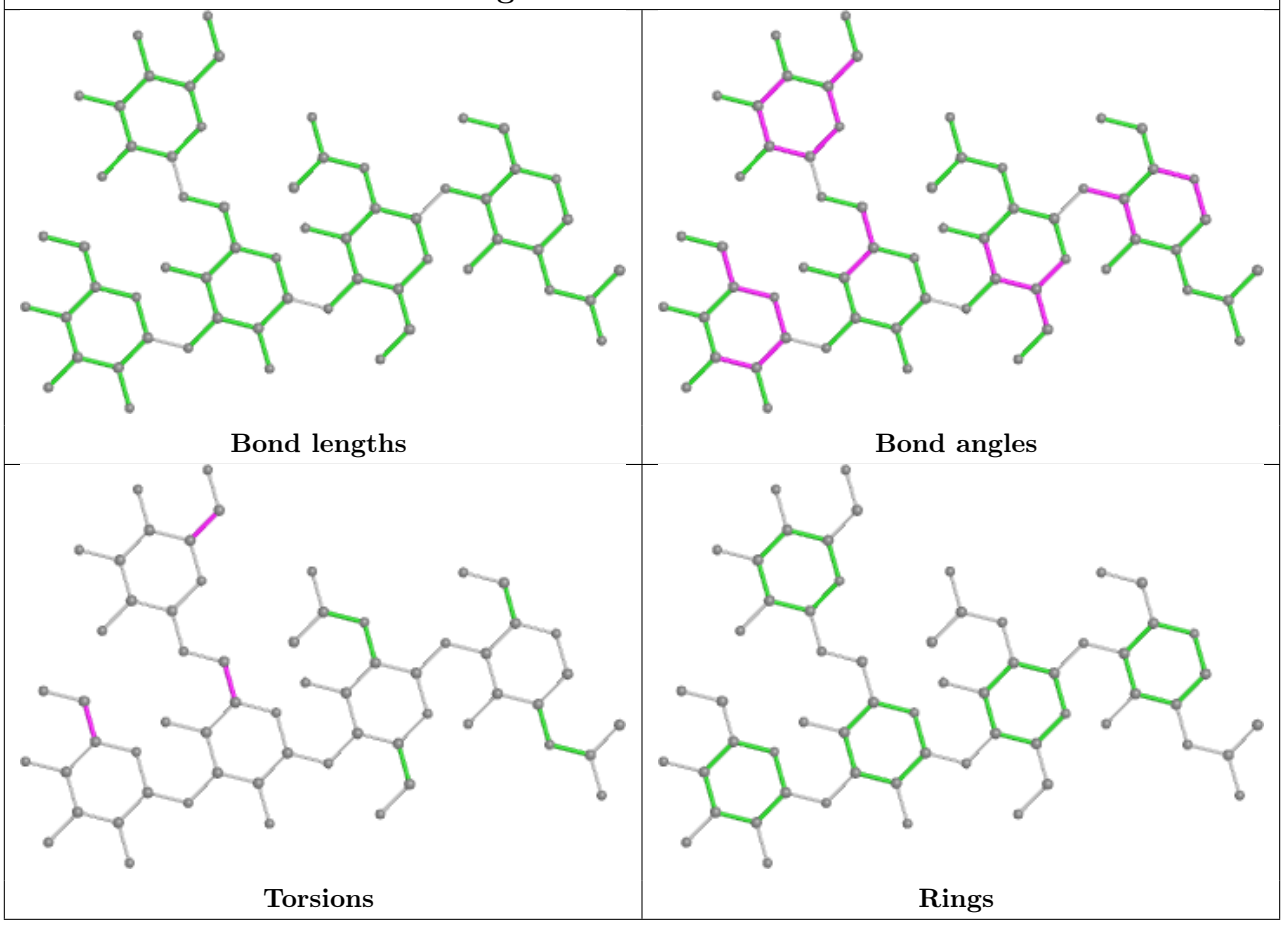
There are no ring outliers.

4 monomers are involved in 4 short contacts:

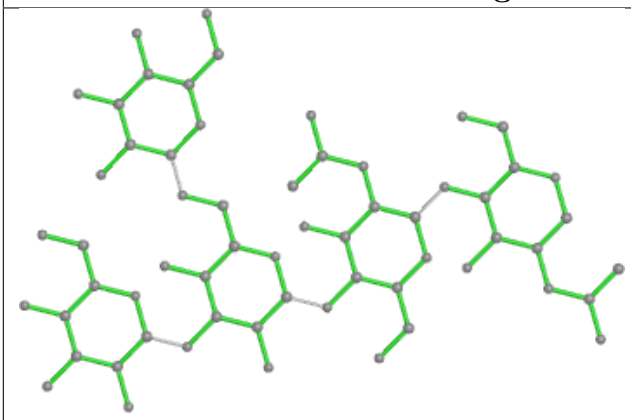
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	1	NAG	1	0
2	G	1	NAG	1	0
3	F	1	NAG	1	0
2	K	3	BMA	1	0

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

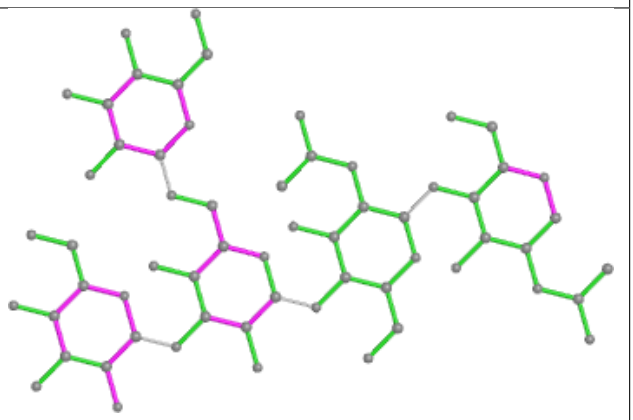
Oligosaccharide Chain E



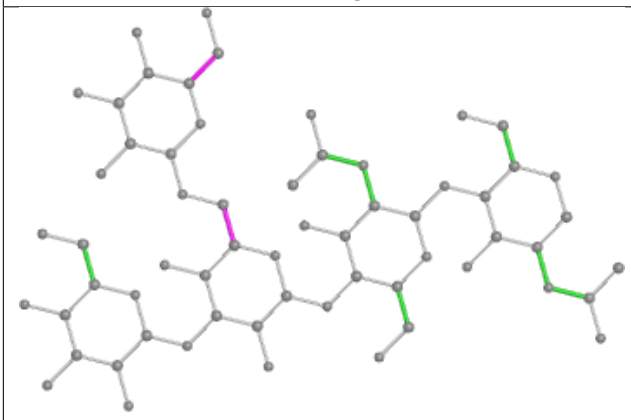
Oligosaccharide Chain G



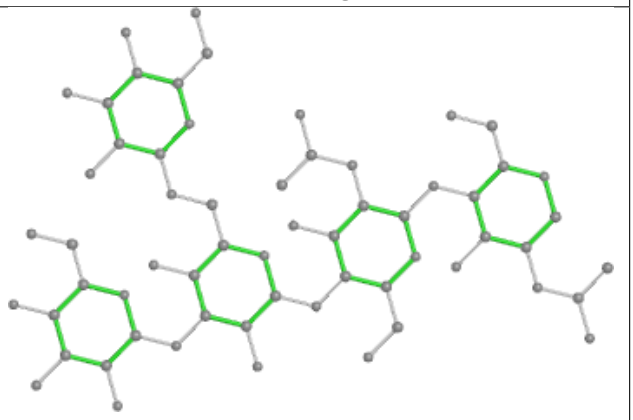
Bond lengths



Bond angles

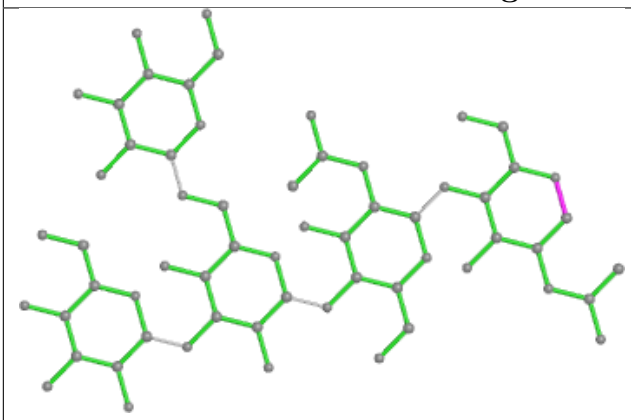


Torsions

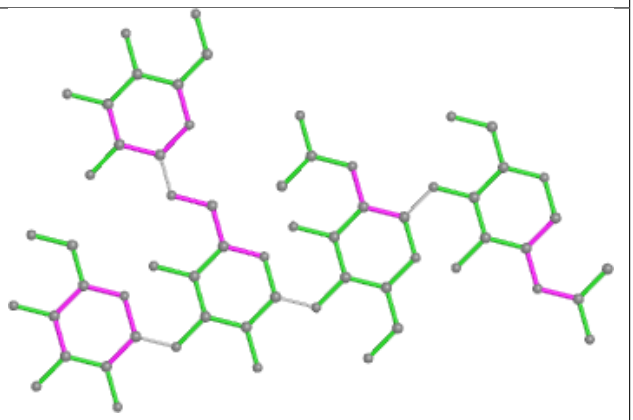


Rings

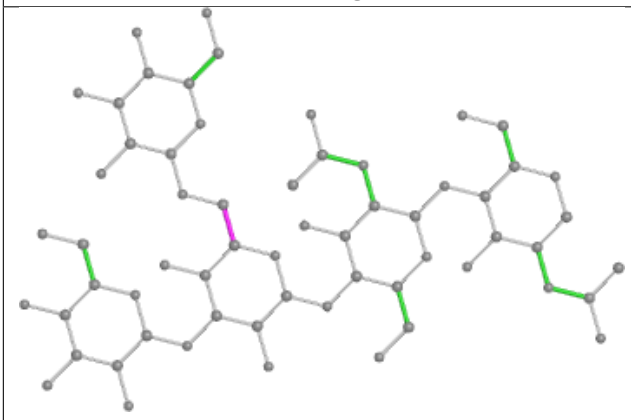
Oligosaccharide Chain I



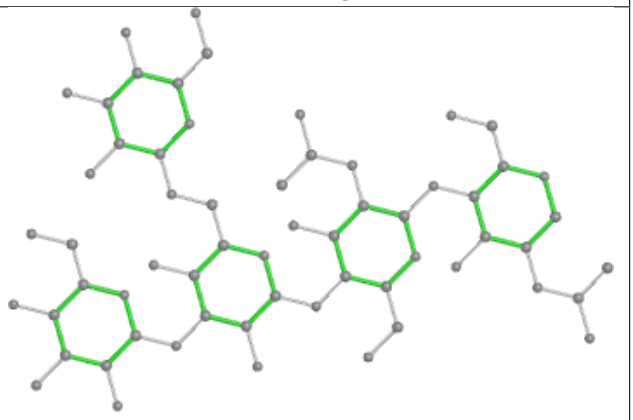
Bond lengths



Bond angles

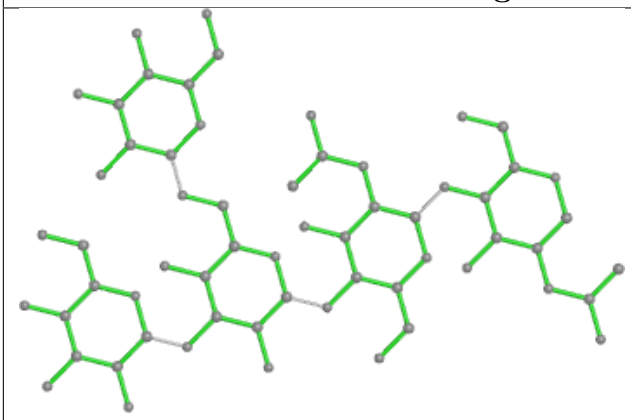


Torsions

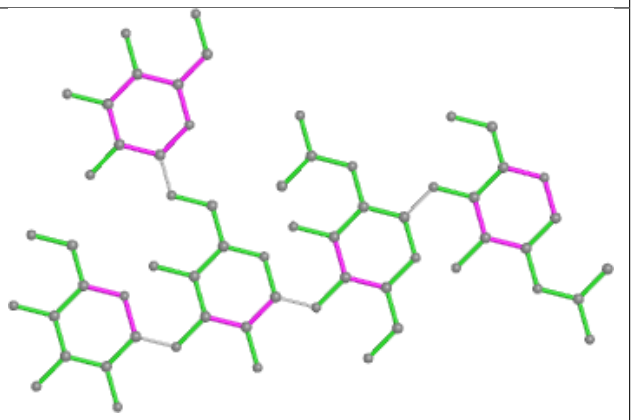


Rings

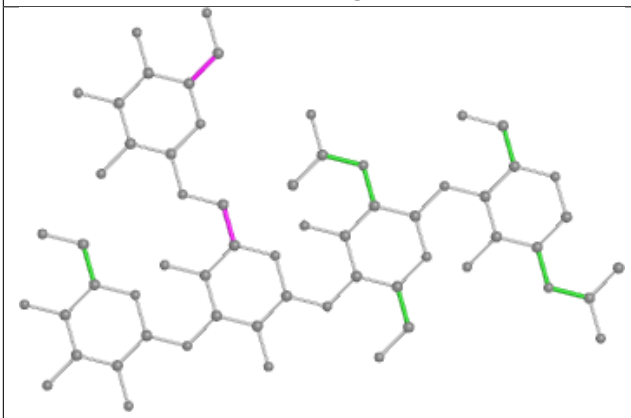
Oligosaccharide Chain K



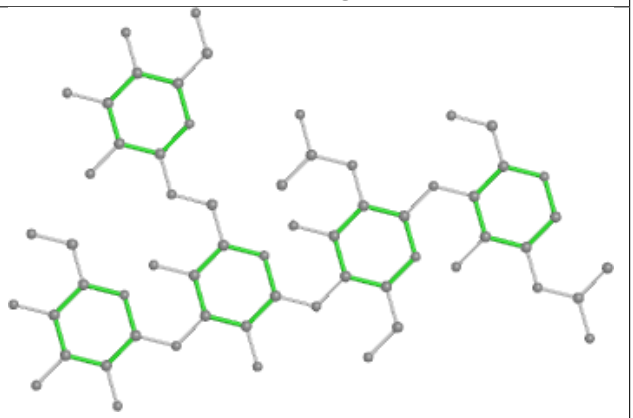
Bond lengths



Bond angles

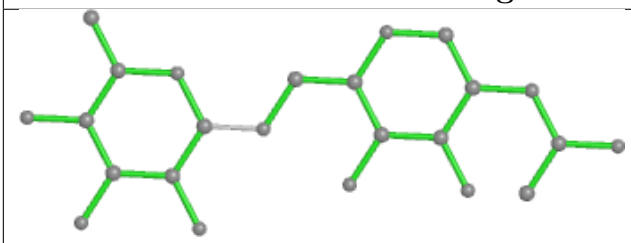


Torsions

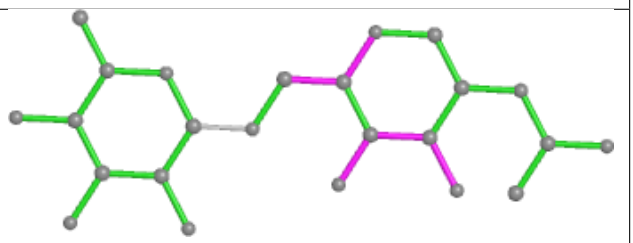


Rings

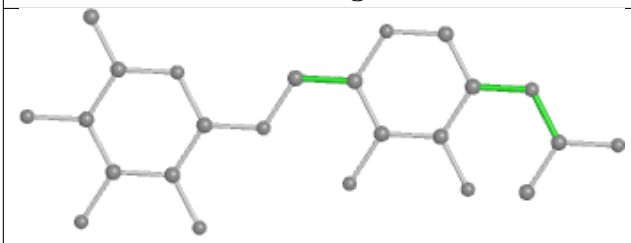
Oligosaccharide Chain F



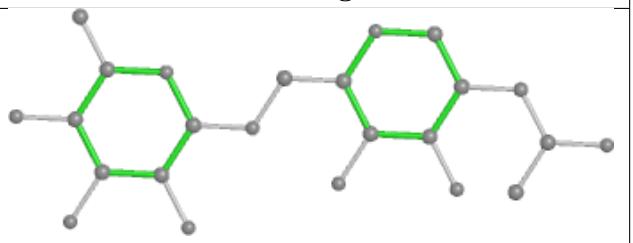
Bond lengths



Bond angles

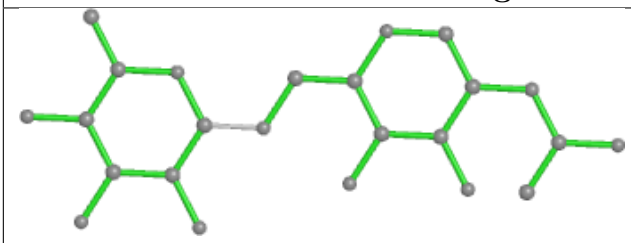


Torsions

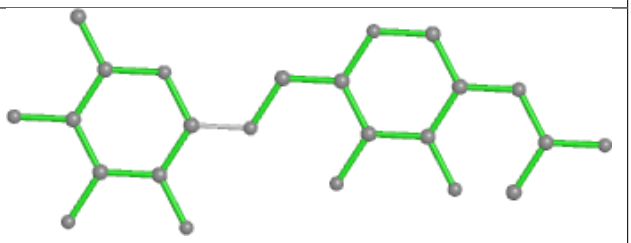


Rings

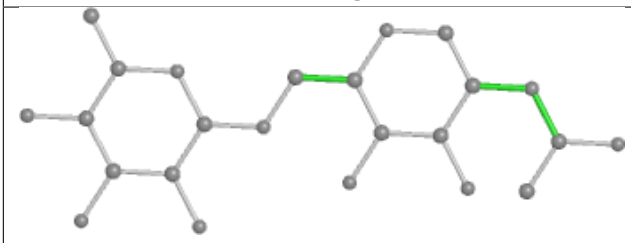
Oligosaccharide Chain H



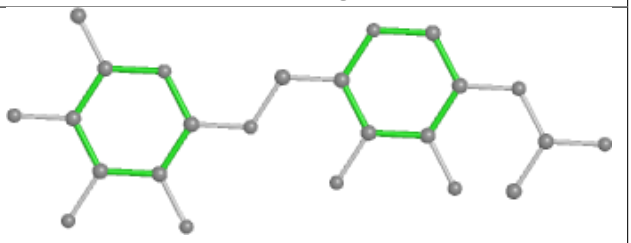
Bond lengths



Bond angles

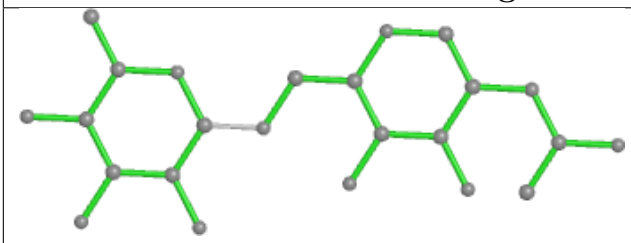


Torsions

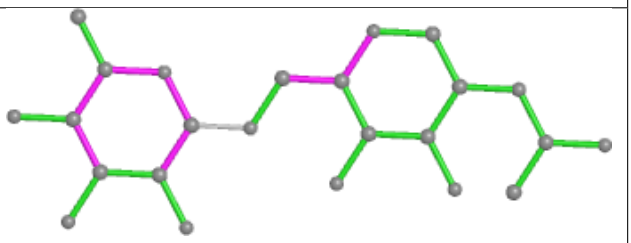


Rings

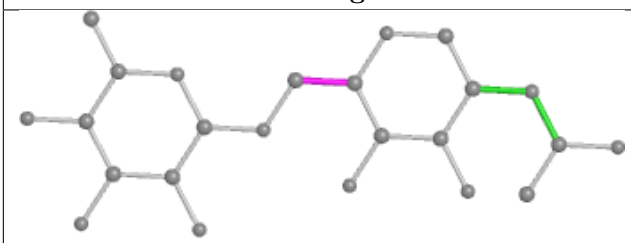
Oligosaccharide Chain J



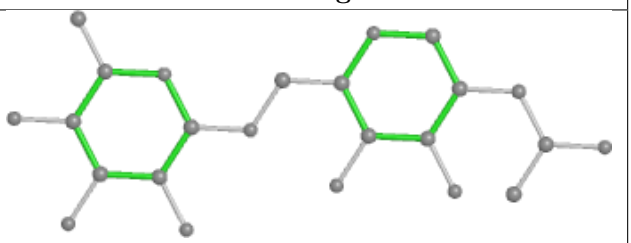
Bond lengths



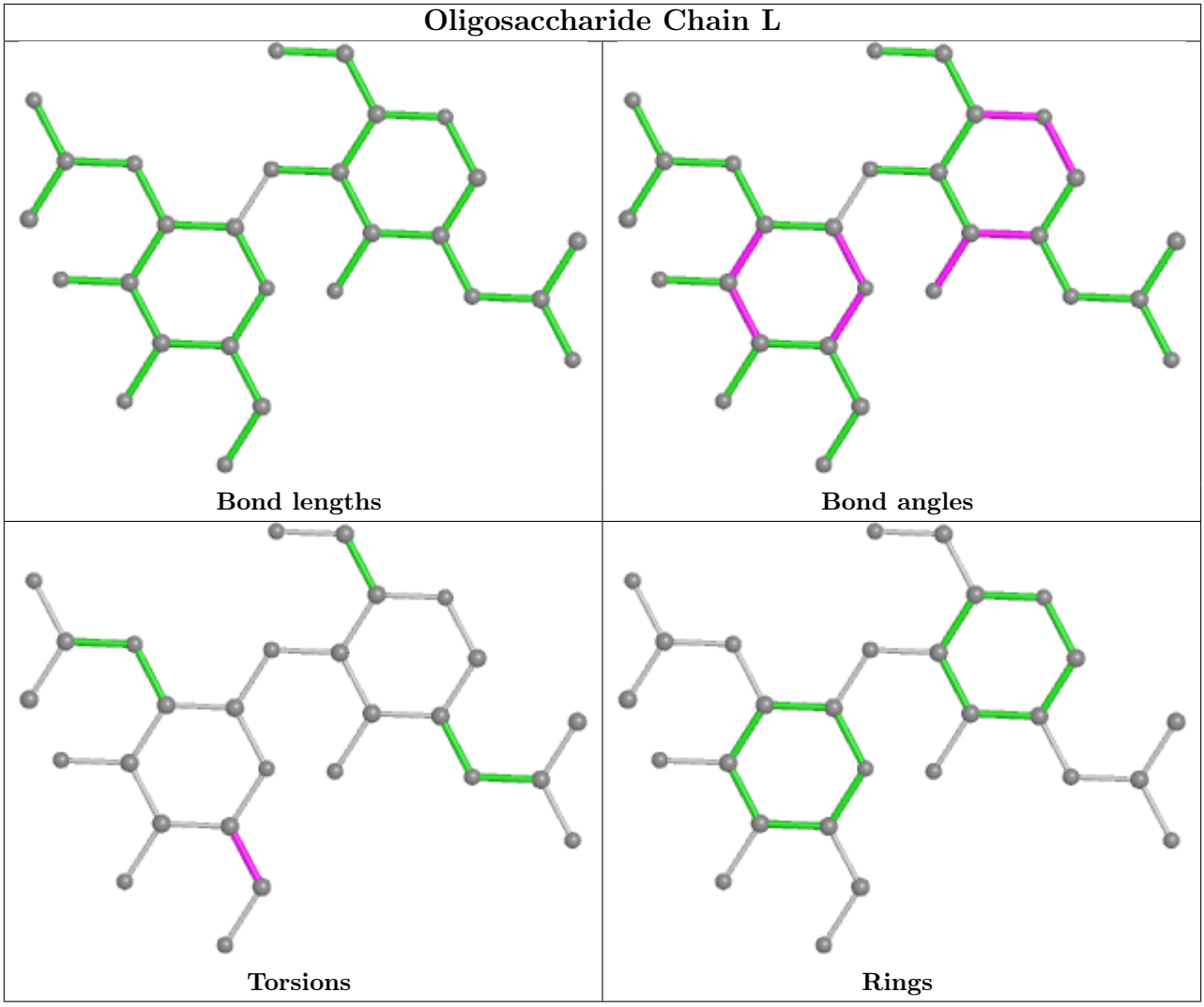
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 5 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	B	511	1	14,14,15	0.58	0	17,19,21	2.18	2 (11%)
7	NAG	D	508	1	14,14,15	0.50	0	17,19,21	0.90	1 (5%)
7	NAG	D	511	1	14,14,15	0.46	0	17,19,21	1.85	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	EPE	D	502	-	15,15,15	1.18	1 (6%)	18,20,20	2.54	6 (33%)
7	NAG	C	512	1	14,14,15	0.67	1 (7%)	17,19,21	1.62	1 (5%)
6	EPE	A	502	-	15,15,15	1.00	1 (6%)	18,20,20	2.52	5 (27%)
7	NAG	C	509	1	14,14,15	0.57	0	17,19,21	1.75	4 (23%)
7	NAG	B	508	1	14,14,15	0.45	0	17,19,21	1.74	1 (5%)
6	EPE	B	502	-	15,15,15	1.04	1 (6%)	18,20,20	2.34	8 (44%)
6	EPE	C	503	-	15,15,15	0.91	1 (6%)	18,20,20	2.23	6 (33%)
7	NAG	A	510	1	14,14,15	0.67	0	17,19,21	1.19	2 (11%)

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
7	NAG	B	511	1	-	1/6/23/26	0/1/1/1
7	NAG	D	508	1	-	2/6/23/26	0/1/1/1
7	NAG	D	511	1	-	0/6/23/26	0/1/1/1
6	EPE	D	502	-	-	1/9/19/19	0/1/1/1
7	NAG	C	512	1	-	2/6/23/26	0/1/1/1
6	EPE	A	502	-	-	8/9/19/19	0/1/1/1
7	NAG	C	509	1	-	2/6/23/26	0/1/1/1
7	NAG	B	508	1	-	2/6/23/26	0/1/1/1
6	EPE	B	502	-	-	5/9/19/19	0/1/1/1
6	EPE	C	503	-	-	5/9/19/19	0/1/1/1
7	NAG	A	510	1	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	502	EPE	C10-S	3.52	1.82	1.77
6	B	502	EPE	C10-S	3.50	1.82	1.77
6	A	502	EPE	C10-S	2.87	1.81	1.77
6	C	503	EPE	C10-S	2.70	1.81	1.77
7	C	512	NAG	C1-C2	2.05	1.55	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	511	NAG	C1-O5-C5	7.89	122.88	112.19
6	A	502	EPE	O2S-S-C10	7.14	115.51	106.92
6	D	502	EPE	O2S-S-C10	6.85	115.17	106.92
7	B	508	NAG	C1-O5-C5	6.18	120.56	112.19
7	C	512	NAG	C1-O5-C5	5.46	119.59	112.19
6	D	502	EPE	C5-N4-C3	4.96	119.99	108.83
6	C	503	EPE	C6-N1-C2	4.95	119.97	108.83
6	A	502	EPE	C5-N4-C3	4.76	119.54	108.83
6	B	502	EPE	O2S-S-C10	4.68	112.55	106.92
7	D	511	NAG	C4-C3-C2	-4.25	104.78	111.02
6	B	502	EPE	C5-N4-C3	4.17	118.22	108.83
7	C	509	NAG	C3-C4-C5	4.17	117.68	110.24
6	C	503	EPE	C7-N4-C3	4.09	121.69	111.23
6	C	503	EPE	C5-N4-C3	3.63	117.00	108.83
6	B	502	EPE	C6-N1-C2	3.62	116.97	108.83
6	A	502	EPE	C7-N4-C3	3.58	120.39	111.23
7	A	510	NAG	C1-O5-C5	3.46	116.88	112.19
6	C	503	EPE	O3S-S-C10	3.35	111.19	105.77
7	D	511	NAG	C1-C2-N2	3.30	116.13	110.49
6	D	502	EPE	C7-N4-C3	3.25	119.54	111.23
6	B	502	EPE	C7-N4-C3	3.22	119.48	111.23
7	C	509	NAG	O5-C1-C2	-3.19	106.25	111.29
6	C	503	EPE	C7-N4-C5	3.14	119.26	111.23
7	C	509	NAG	C1-O5-C5	3.07	116.36	112.19
6	D	502	EPE	C7-N4-C5	3.05	119.03	111.23
6	A	502	EPE	C7-N4-C5	2.93	118.72	111.23
6	A	502	EPE	C6-N1-C2	2.89	115.33	108.83
6	B	502	EPE	C5-C6-N1	2.89	116.57	110.64
6	C	503	EPE	C3-C2-N1	2.80	116.39	110.64
6	D	502	EPE	C6-N1-C2	2.80	115.12	108.83
7	B	511	NAG	C1-C2-N2	2.52	114.79	110.49
7	D	511	NAG	O5-C1-C2	-2.50	107.35	111.29
6	B	502	EPE	C7-N4-C5	2.48	117.57	111.23
6	B	502	EPE	O1S-S-C10	2.41	109.82	106.92
7	D	511	NAG	C2-N2-C7	-2.36	119.54	122.90
7	C	509	NAG	C4-C3-C2	2.35	114.47	111.02
7	D	508	NAG	C1-O5-C5	2.35	115.37	112.19
7	D	511	NAG	O5-C5-C6	2.24	110.71	107.20
6	D	502	EPE	C5-C6-N1	2.23	115.21	110.64
7	A	510	NAG	O5-C5-C6	2.10	110.49	107.20
6	B	502	EPE	C9-N1-C6	2.05	116.48	111.23

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	502	EPE	C10-C9-N1-C6
6	A	502	EPE	C8-C7-N4-C3
6	A	502	EPE	S-C10-C9-N1
6	B	502	EPE	C10-C9-N1-C6
6	B	502	EPE	S-C10-C9-N1
6	C	503	EPE	C9-C10-S-O2S
6	C	503	EPE	C9-C10-S-O3S
7	B	508	NAG	O5-C5-C6-O6
7	C	509	NAG	O5-C5-C6-O6
7	B	508	NAG	C4-C5-C6-O6
7	C	512	NAG	C4-C5-C6-O6
7	A	510	NAG	C4-C5-C6-O6
7	C	509	NAG	C4-C5-C6-O6
7	A	510	NAG	O5-C5-C6-O6
7	C	512	NAG	O5-C5-C6-O6
6	A	502	EPE	C9-C10-S-O3S
6	B	502	EPE	N4-C7-C8-O8
7	D	508	NAG	C4-C5-C6-O6
7	B	511	NAG	O5-C5-C6-O6
6	A	502	EPE	N4-C7-C8-O8
6	C	503	EPE	C8-C7-N4-C5
7	D	508	NAG	O5-C5-C6-O6
6	C	503	EPE	C8-C7-N4-C3
6	A	502	EPE	C9-C10-S-O1S
6	A	502	EPE	C9-C10-S-O2S
6	C	503	EPE	C9-C10-S-O1S
6	B	502	EPE	C8-C7-N4-C5
6	D	502	EPE	C8-C7-N4-C5
6	A	502	EPE	C10-C9-N1-C2
6	B	502	EPE	C9-C10-S-O1S

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	502	EPE	2	0
6	A	502	EPE	2	0
6	B	502	EPE	2	0
6	C	503	EPE	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

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	388/393 (98%)	0.48	13 (3%)	45	57	14, 28, 42, 61	0
1	B	388/393 (98%)	0.56	20 (5%)	27	39	16, 28, 43, 57	0
1	C	388/393 (98%)	0.54	21 (5%)	25	37	11, 28, 42, 59	0
1	D	388/393 (98%)	0.38	6 (1%)	73	81	12, 27, 42, 61	0
All	All	1552/1572 (98%)	0.49	60 (3%)	39	52	11, 28, 42, 61	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	469	ILE	10.4
1	A	469	ILE	8.8
1	D	468	PRO	7.3
1	D	469	ILE	6.6
1	B	469	ILE	5.5
1	A	468	PRO	3.7
1	C	468	PRO	3.6
1	B	114	ILE	3.4
1	A	333	SER	3.3
1	B	169	LEU	3.3
1	A	465	ASN	3.1
1	C	169	LEU	3.0
1	C	431	LYS	2.9
1	D	431	LYS	2.9
1	B	465	ASN	2.7
1	A	330	ASP	2.7
1	C	308	LYS	2.6
1	D	147	ASN	2.6
1	B	332	SER	2.6
1	B	174	VAL	2.6
1	B	390	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	82	ALA	2.5
1	C	330	ASP	2.5
1	D	86	ASN	2.5
1	B	167	PHE	2.5
1	C	436	VAL	2.5
1	B	330	ASP	2.5
1	B	468	PRO	2.5
1	B	337	CYS	2.4
1	C	159	LEU	2.4
1	C	114	ILE	2.4
1	C	247	SER	2.4
1	D	330	ASP	2.3
1	A	390	LEU	2.3
1	C	82	ALA	2.3
1	A	467	MET	2.3
1	A	331	SER	2.3
1	B	331	SER	2.3
1	B	83	GLU	2.3
1	B	159	LEU	2.3
1	B	171	THR	2.3
1	A	388	SER	2.3
1	B	165	VAL	2.3
1	A	114	ILE	2.3
1	B	108	LEU	2.2
1	C	369	THR	2.2
1	A	332	SER	2.2
1	B	431	LYS	2.1
1	C	83	GLU	2.1
1	C	435	GLU	2.1
1	A	169	LEU	2.1
1	C	467	MET	2.1
1	C	368	GLU	2.1
1	A	159	LEU	2.1
1	C	332	SER	2.1
1	B	443	ILE	2.1
1	C	463	ASP	2.1
1	C	400	ARG	2.0
1	C	164	GLY	2.0
1	C	171	THR	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)

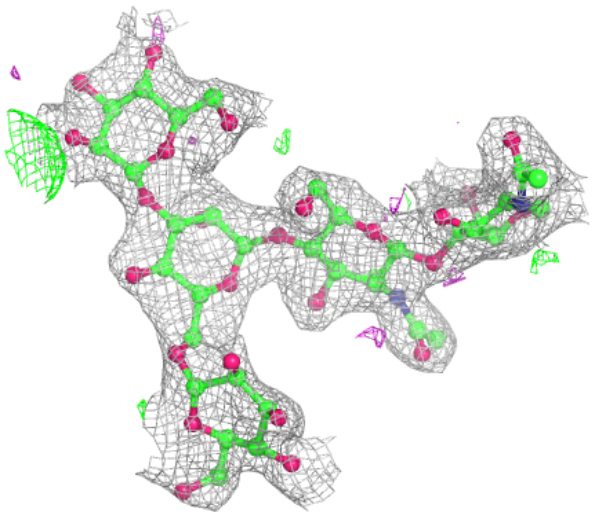
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

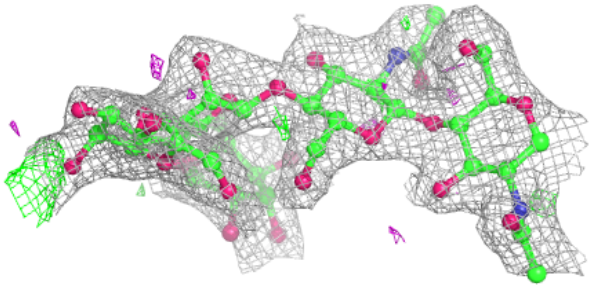
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	L	2	14/15	0.57	0.28	63,64,66,66	0
2	MAN	G	5	11/12	0.69	0.20	47,50,51,52	0
4	NAG	L	1	14/15	0.70	0.22	54,58,61,62	0
3	FUC	J	2	10/11	0.70	0.32	63,64,65,65	0
3	NAG	H	1	14/15	0.72	0.26	58,63,68,71	0
3	NAG	F	1	14/15	0.72	0.21	58,62,65,69	0
3	FUC	F	2	10/11	0.73	0.35	66,67,67,68	0
3	FUC	H	2	10/11	0.74	0.39	70,71,71,72	0
2	MAN	I	4	11/12	0.74	0.23	48,52,54,56	0
2	MAN	K	5	11/12	0.76	0.26	54,54,55,56	0
2	MAN	E	5	11/12	0.76	0.28	52,54,54,55	0
2	MAN	E	4	11/12	0.78	0.22	46,48,50,51	0
2	MAN	G	4	11/12	0.79	0.22	43,46,47,49	0
3	NAG	J	1	14/15	0.81	0.21	52,57,62,63	0
2	BMA	E	3	11/12	0.84	0.16	40,44,47,50	0
2	NAG	K	1	14/15	0.84	0.18	30,36,42,43	0
2	MAN	K	4	11/12	0.84	0.23	49,51,53,55	0
2	BMA	I	3	11/12	0.84	0.19	42,46,48,50	0
2	MAN	I	5	11/12	0.85	0.25	50,51,52,53	0
2	NAG	I	1	14/15	0.88	0.19	27,32,38,39	0
2	NAG	K	2	14/15	0.89	0.13	35,36,39,41	0
2	BMA	K	3	11/12	0.89	0.15	42,46,48,51	0
2	NAG	G	1	14/15	0.89	0.19	22,34,37,38	0
2	NAG	E	2	14/15	0.89	0.18	31,32,35,36	0
2	NAG	E	1	14/15	0.90	0.20	26,32,38,38	0
2	NAG	I	2	14/15	0.90	0.15	29,31,34,37	0
2	NAG	G	2	14/15	0.90	0.14	35,37,40,40	0
2	BMA	G	3	11/12	0.92	0.23	42,44,47,50	0

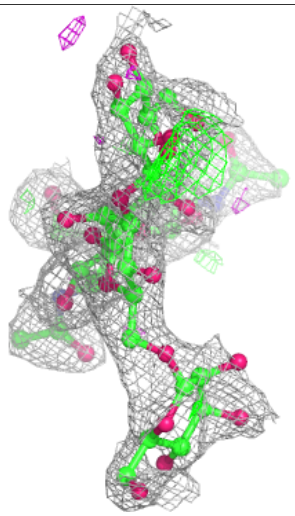
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

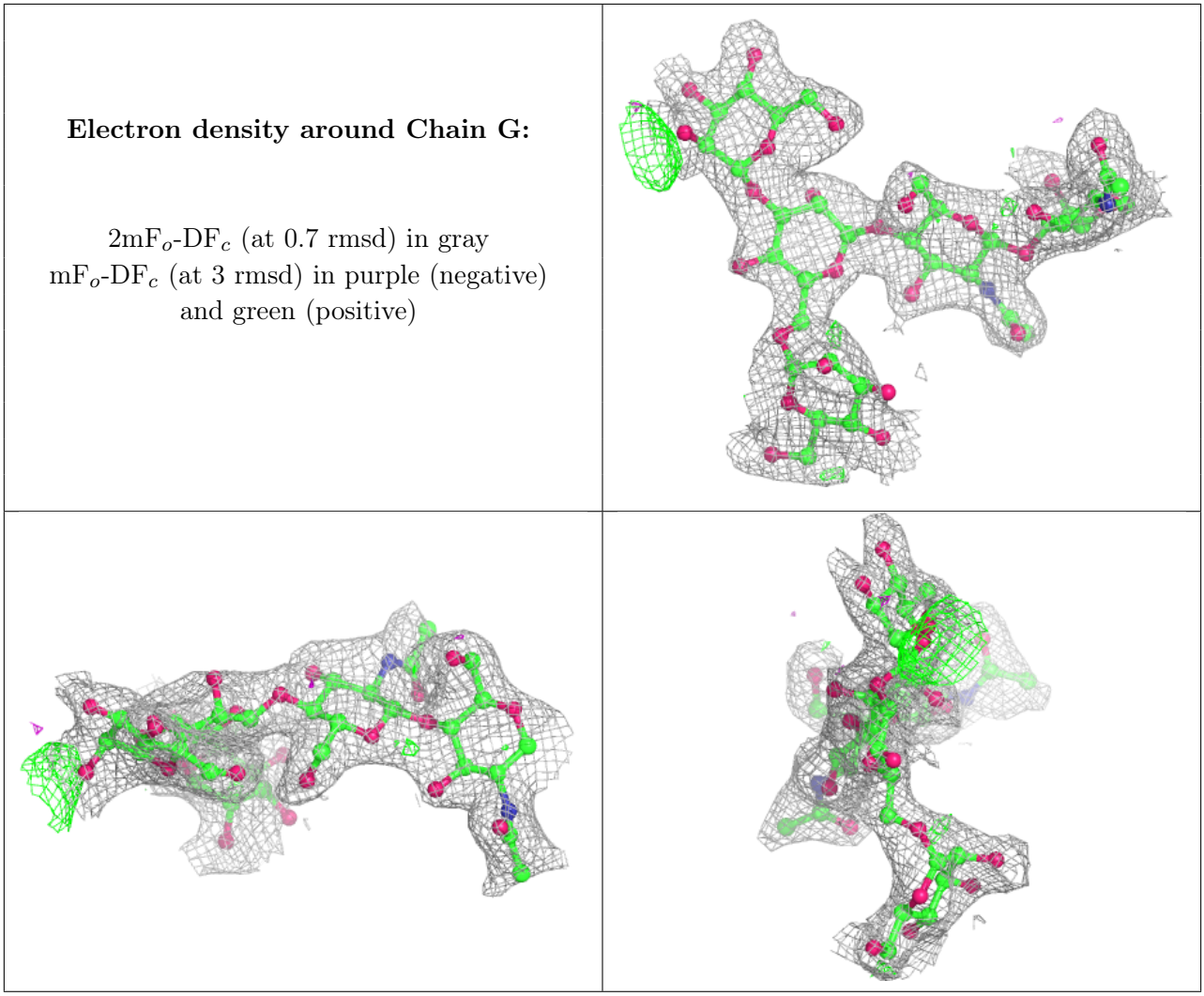






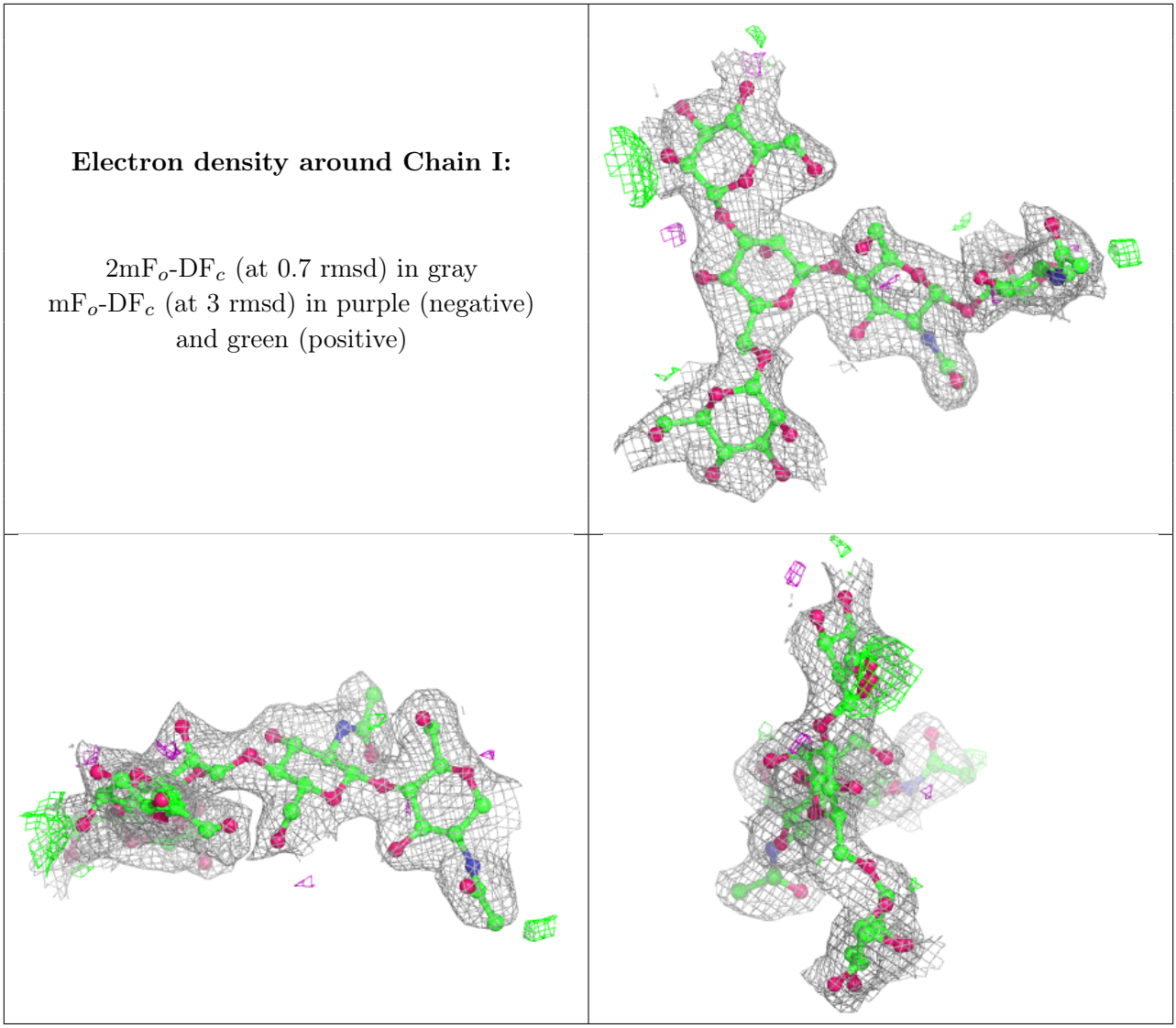
Electron density around Chain G:

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



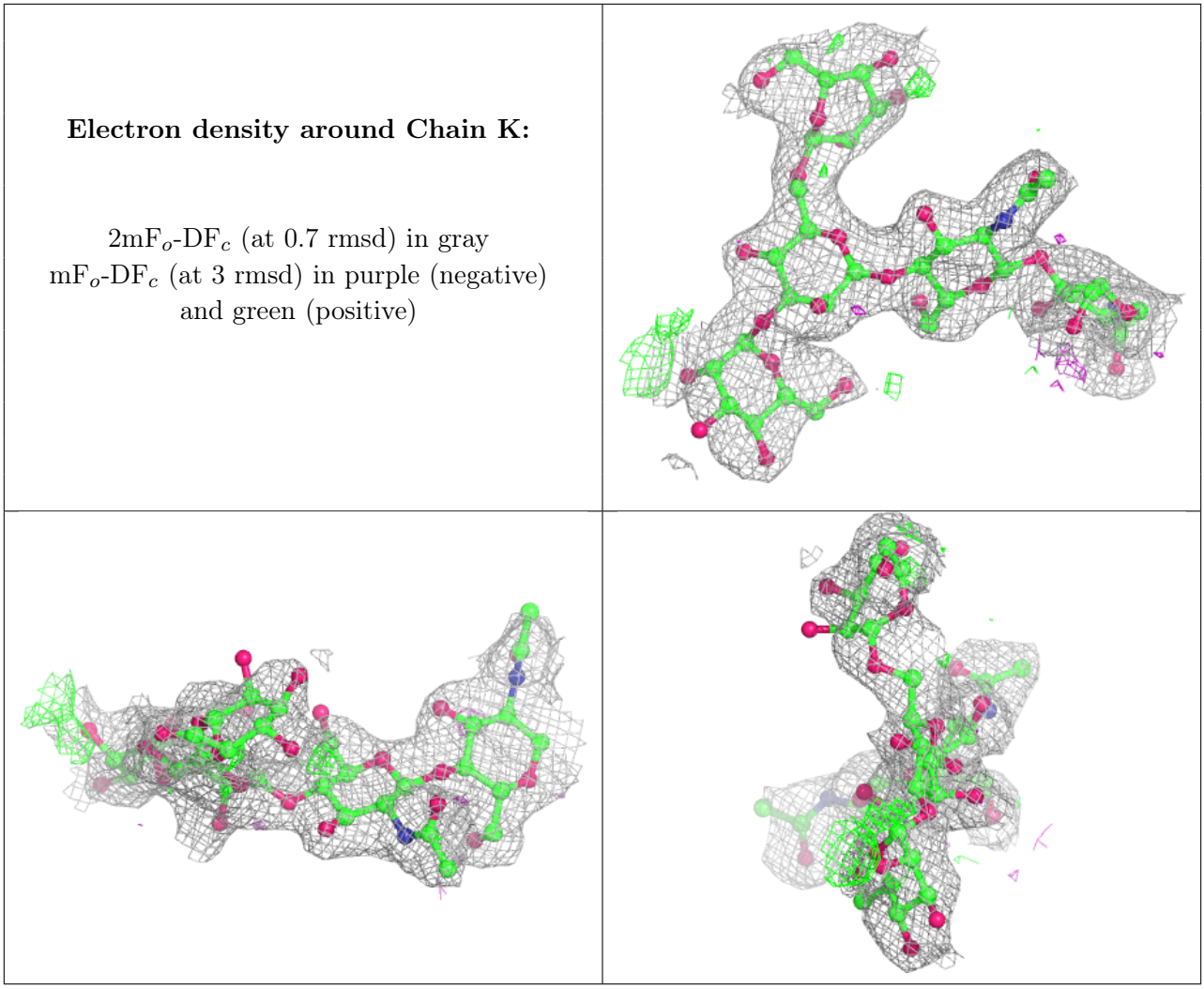
Electron density around Chain I:

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



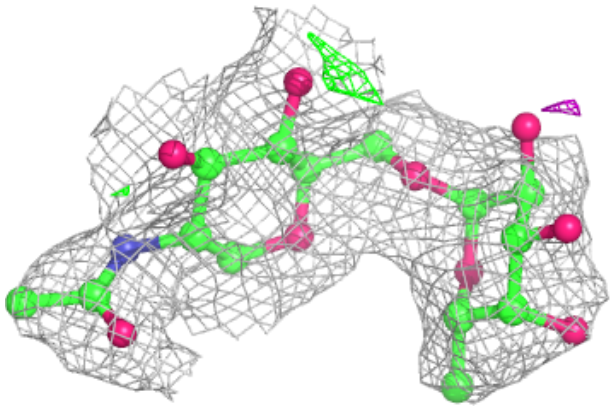
Electron density around Chain K:

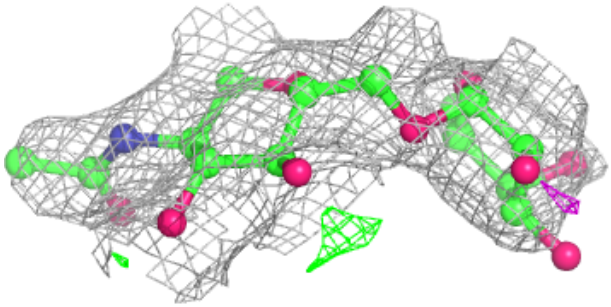
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

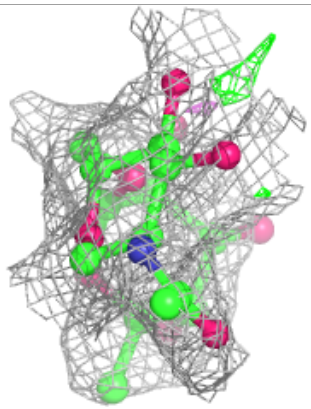


Electron density around Chain F:

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

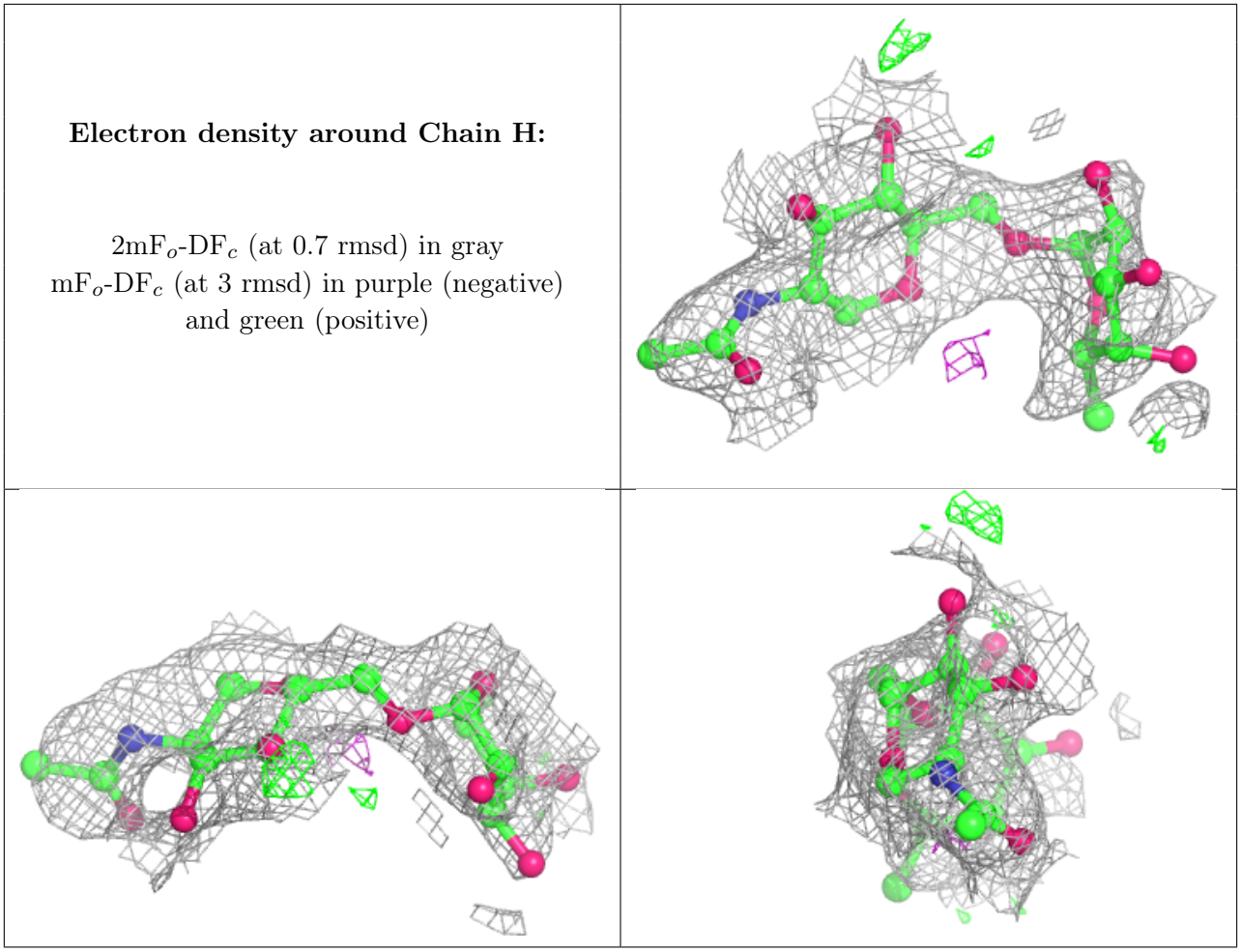






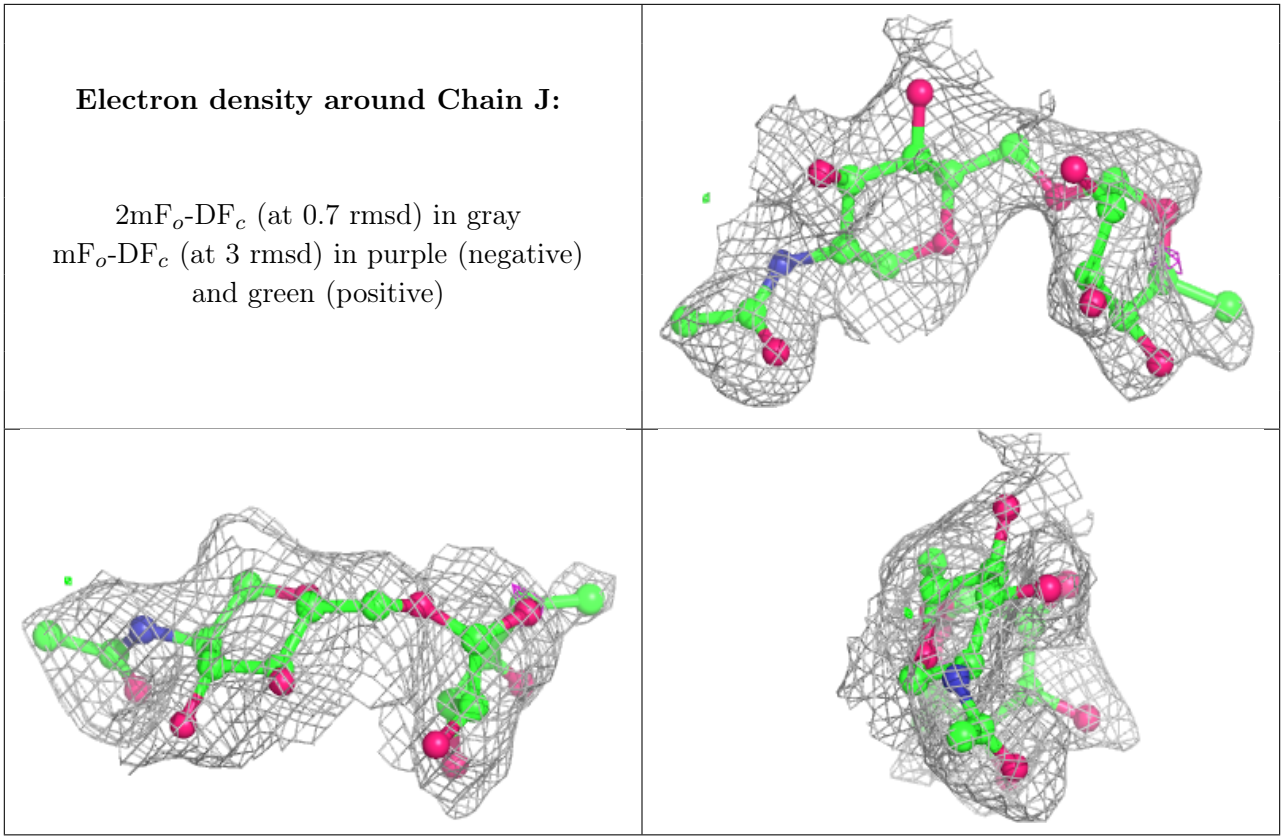
Electron density around Chain H:

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



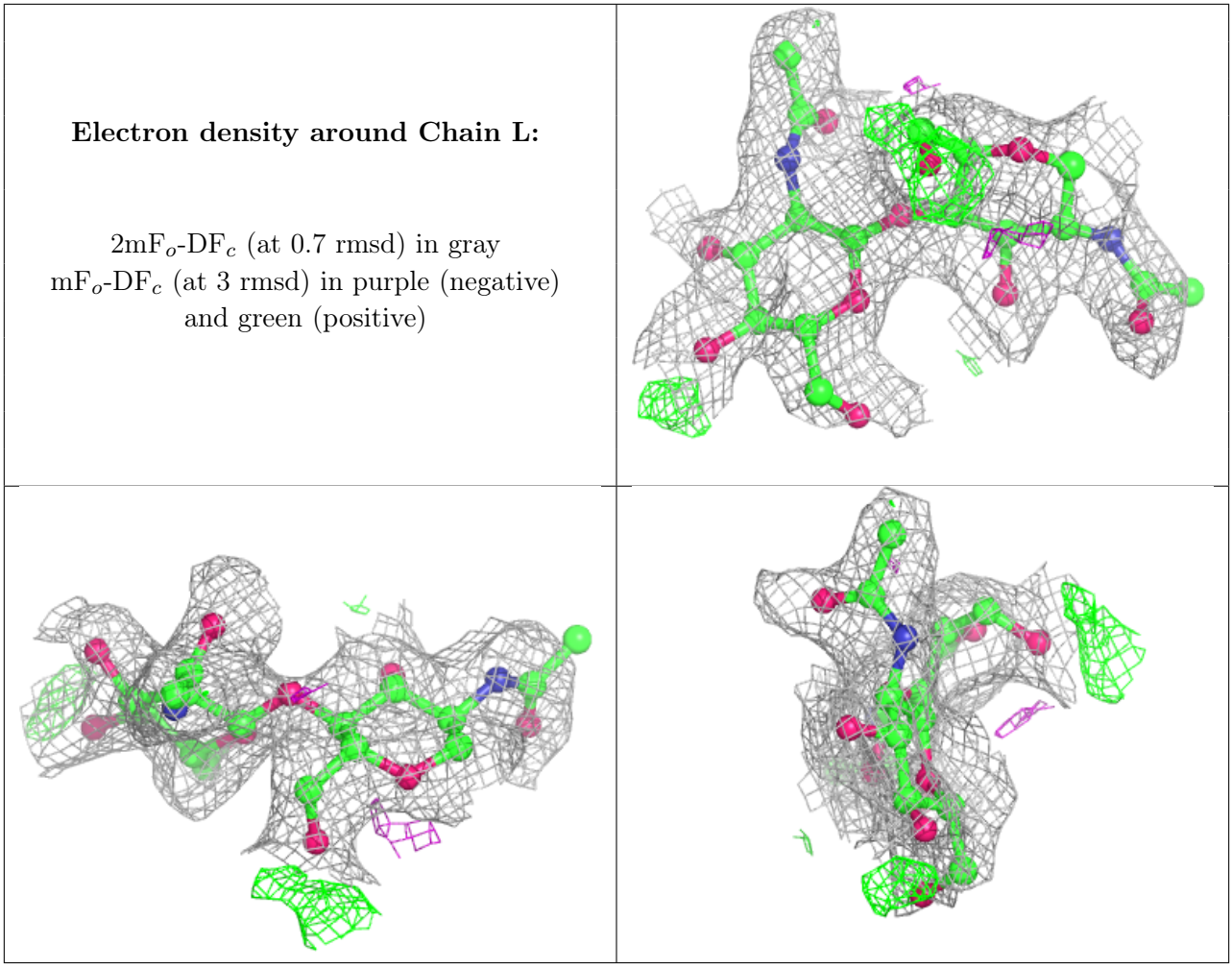
Electron density around Chain J:

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



Electron density around Chain L:

$2mF_o$-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
7	NAG	C	509	14/15	0.68	0.32	60,64,64,64	0
7	NAG	D	508	14/15	0.69	0.31	59,63,65,65	0
7	NAG	C	512	14/15	0.71	0.31	54,56,59,59	0
7	NAG	B	508	14/15	0.71	0.29	50,53,55,55	0
7	NAG	B	511	14/15	0.76	0.33	50,53,54,54	0
7	NAG	D	511	14/15	0.76	0.25	53,56,57,58	0
7	NAG	A	510	14/15	0.79	0.28	50,54,55,56	0
6	EPE	D	502	15/15	0.83	0.25	38,41,45,45	0
5	CA	C	502	1/1	0.86	0.09	34,34,34,34	0
6	EPE	C	503	15/15	0.86	0.26	42,48,51,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CA	C	501	1/1	0.87	0.15	64,64,64,64	0
6	EPE	A	502	15/15	0.91	0.20	37,43,45,46	0
6	EPE	B	502	15/15	0.92	0.17	35,38,39,40	0
5	CA	A	501	1/1	0.94	0.08	34,34,34,34	0
5	CA	B	501	1/1	0.97	0.07	30,30,30,30	0
5	CA	D	501	1/1	1.00	0.03	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.