Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2025 – 12:25 AM JST

PDB ID	:	8X2D / pdb_00008x2d
Title	:	Crystal structure of H5 hemagglutinin from swan-infecting H5N8 influenza virus complexed with avian receptor analog LSTc
Authors	:	Jin, X.Y.; Han, P.; Song, H.; Qi, J.X.
Deposited on	:	2023-11-09
Resolution	:	2.48 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:

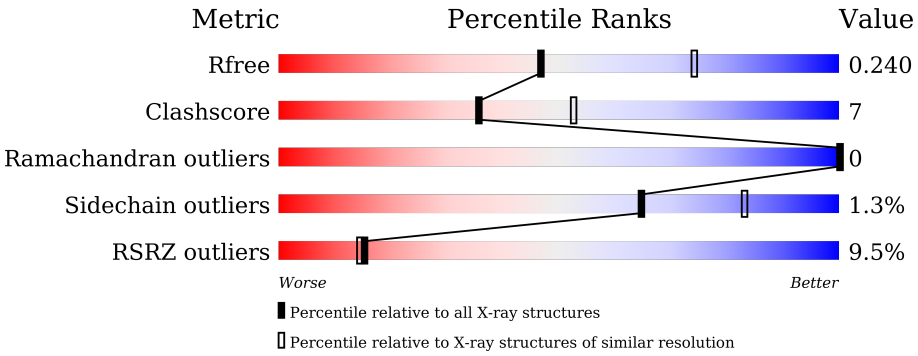
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.48 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}	164625	7106 (2.50-2.46)
Clashscore	180529	7991 (2.50-2.46)
Ramachandran outliers	177936	7888 (2.50-2.46)
Sidechain outliers	177891	7890 (2.50-2.46)
RSRZ outliers	164620	7106 (2.50-2.46)

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	506	6% 80% 16% .
1	B	506	7% 79% 18% .
1	C	506	15% 78% 18% .
2	D	4	25% 50% 25%
3	E	2	100%
3	F	2	100%

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Mol	Chain	Length	Quality of chain
4	G	3	100%
4	H	3	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12327 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	0	0
			3921	2470	680	749	22			
1	B	490	Total	C	N	O	S	0	0	0
			3921	2470	680	749	22			
1	C	490	Total	C	N	O	S	0	0	0
			3921	2470	680	749	22			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	86	VAL	ALA	engineered mutation	UNP A0A8E4ZAK5
A	188	ILE	THR	engineered mutation	UNP A0A8E4ZAK5
A	273	ASN	HIS	engineered mutation	UNP A0A8E4ZAK5
B	86	VAL	ALA	engineered mutation	UNP A0A8E4ZAK5
B	188	ILE	THR	engineered mutation	UNP A0A8E4ZAK5
B	273	ASN	HIS	engineered mutation	UNP A0A8E4ZAK5
C	86	VAL	ALA	engineered mutation	UNP A0A8E4ZAK5
C	188	ILE	THR	engineered mutation	UNP A0A8E4ZAK5
C	273	ASN	HIS	engineered mutation	UNP A0A8E4ZAK5

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galacto pyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose.

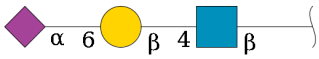
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	4	Total	C	N	O	0	0	0
			57	31	2	24			

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

cetamido-2-deoxy-beta-D-glucopyranose.

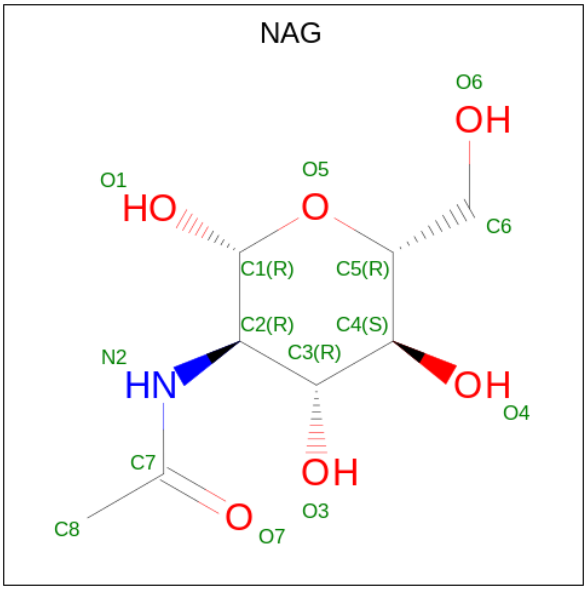
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	E	2	Total C N O 28 16 2 10	0	0	0
3	F	2	Total C N O 28 16 2 10	0	0	0

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galacto pyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	G	3	Total C N O 46 25 2 19	0	0	0
4	H	3	Total C N O 46 25 2 19	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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	B	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

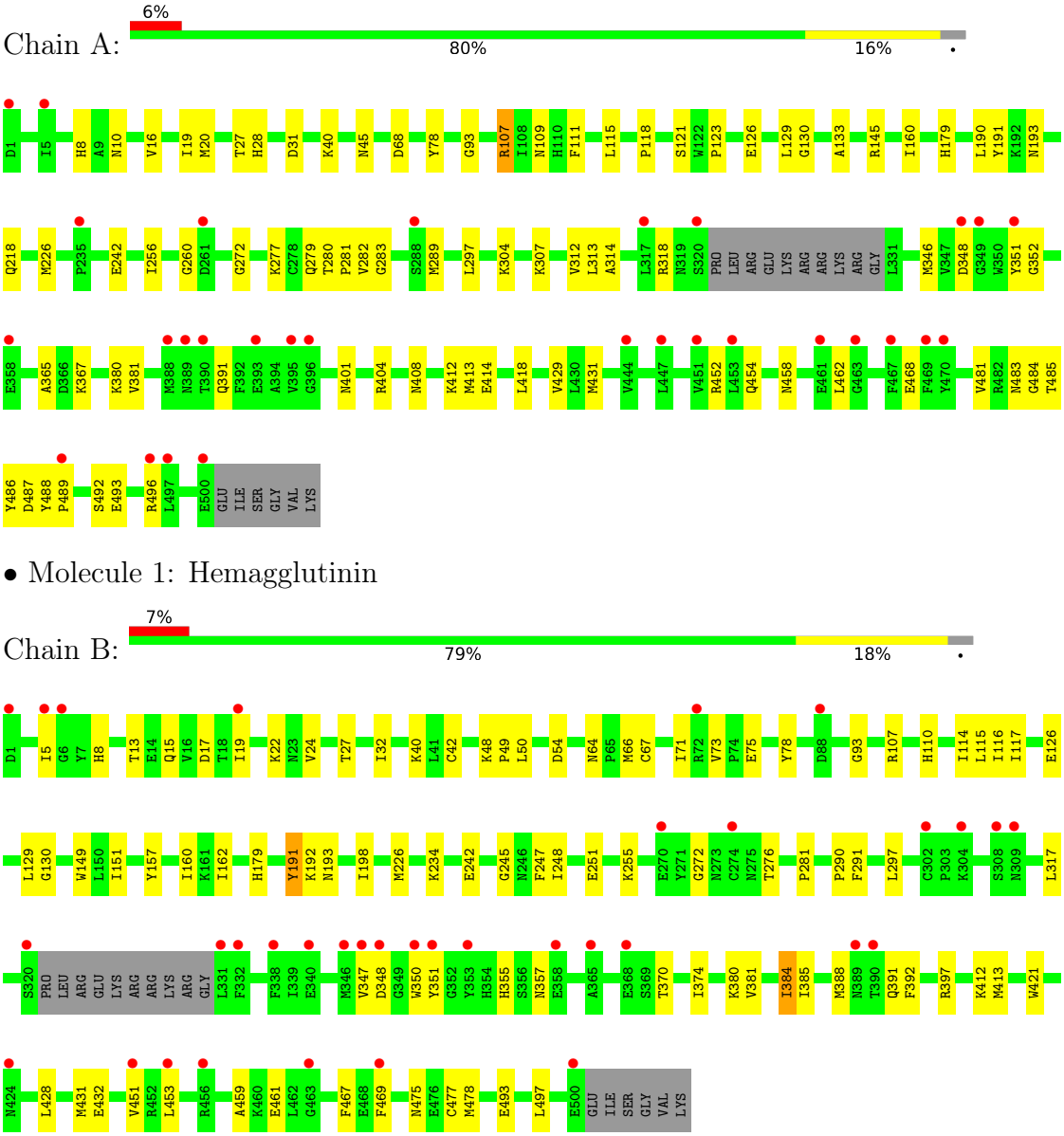
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	123	Total O 123 123	0	0
6	B	97	Total O 97 97	0	0
6	C	55	Total O 55 55	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.

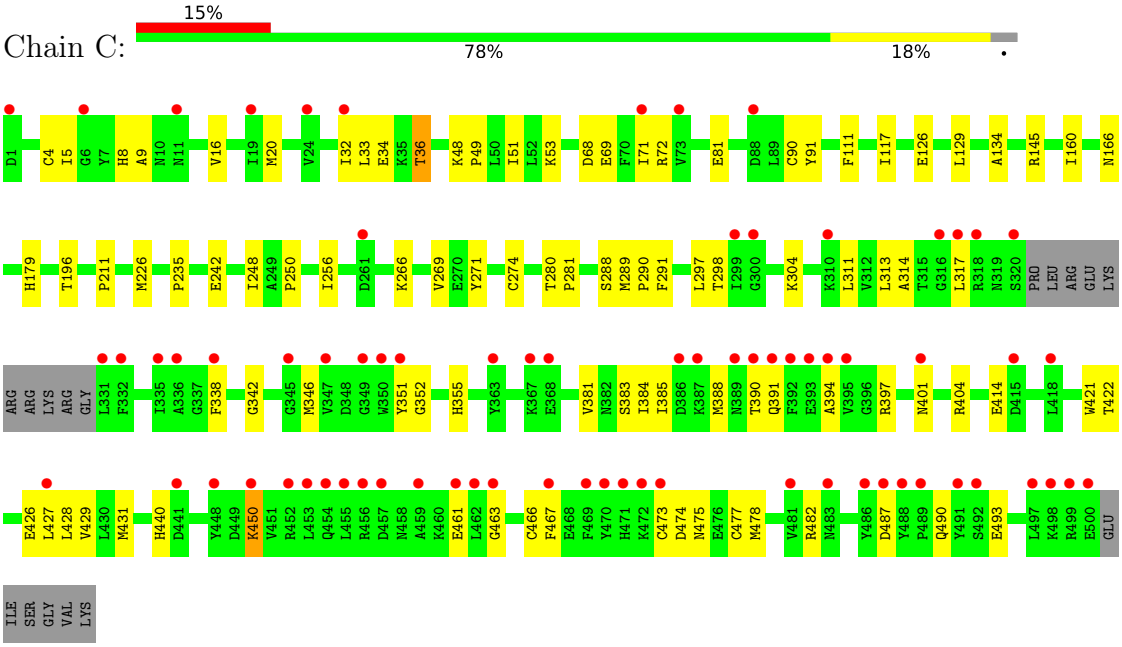
• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin

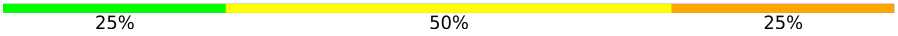
• Molecule 1: Hemagglutinin

Chain C:



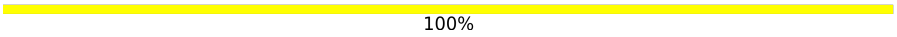
• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose

Chain D:



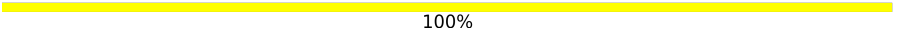
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



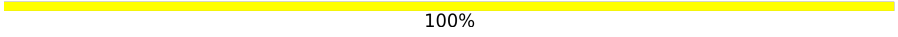
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



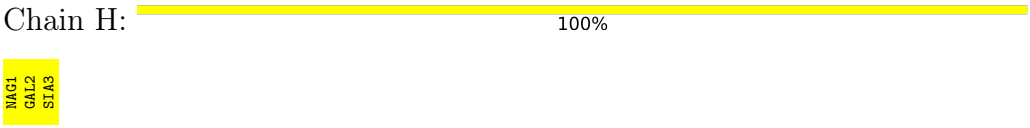
• Molecule 4: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



• Molecule 4: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	80.68Å 107.03Å 134.33Å 90.00° 100.47° 90.00°	Depositor
Resolution (Å)	49.63 – 2.48 49.63 – 2.48	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.63-2.48) 92.2 (49.63-2.48)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.234 , 0.252 0.234 , 0.240	Depositor DCC
R_{free} test set	76660 reflections (2.57%)	wwPDB-VP
Wilson B-factor (Å^2)	46.1	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 46.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12327	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% 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: SIA, NAG, GAL

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	0.44	0/4010	0.61	0/5431
1	B	0.41	0/4010	0.59	1/5431 (0.0%)
1	C	0.35	0/4010	0.52	0/5431
All	All	0.40	0/12030	0.57	1/16293 (0.0%)

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

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

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	B	347	VAL	N-CA-CB	-5.01	105.44	112.35

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	ARG	Sidechain

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	3921	0	3787	60	0
1	B	3921	0	3787	60	0
1	C	3921	0	3788	59	0
2	D	57	0	49	6	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
4	G	46	0	40	0	0
4	H	46	0	40	0	0
5	A	42	0	39	1	0
5	B	14	0	13	0	0
5	C	28	0	26	0	0
6	A	123	0	0	2	0
6	B	97	0	0	0	0
6	C	55	0	0	0	0
All	All	12327	0	11619	171	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 (171) 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:190:LEU:HD11	2:D:2:NAG:H83	1.64	0.78
1:C:401:ASN:OD1	1:C:404:ARG:NH1	2.17	0.77
1:A:280:THR:HB	1:A:283:GLY:O	1.89	0.73
1:A:190:LEU:CD1	2:D:2:NAG:H83	2.22	0.70
1:B:412:LYS:NZ	1:C:414:GLU:OE2	2.24	0.70
1:A:280:THR:HG22	1:A:282:VAL:H	1.56	0.69
1:B:19:ILE:HD11	1:B:431:MET:HA	1.74	0.69
1:B:355:HIS:HB2	1:B:478:MET:HE3	1.73	0.69
1:C:474:ASP:OD1	1:C:475:ASN:N	2.27	0.68
1:B:357:ASN:HD21	1:B:475:ASN:HD22	1.41	0.67
1:A:19:ILE:HD11	1:A:431:MET:HA	1.77	0.67
1:C:71:ILE:HD12	1:C:72:ARG:HB2	1.78	0.66
1:A:380:LYS:HE3	1:C:20:MET:HE2	1.77	0.65
1:B:291:PHE:HZ	1:B:388:MET:HG3	1.61	0.65
1:C:280:THR:HG22	1:C:298:THR:HG22	1.78	0.64
1:A:458:ASN:HD21	1:A:492:SER:HA	1.61	0.64
1:B:107:ARG:O	1:B:107:ARG:HG3	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:ILE:HD11	1:B:432:GLU:HG3	1.80	0.64
1:B:40:LYS:HD3	1:B:272:GLY:HA3	1.81	0.62
1:B:357:ASN:HD21	1:B:475:ASN:ND2	1.97	0.61
1:A:462:LEU:HD11	1:A:468:GLU:HB2	1.81	0.61
1:C:16:VAL:HG21	1:C:314:ALA:HB2	1.83	0.61
1:C:33:LEU:HB2	1:C:311:LEU:HB2	1.81	0.60
1:A:160:ILE:O	1:A:242:GLU:HA	2.01	0.60
1:B:412:LYS:HE2	1:C:397:ARG:HH12	1.67	0.60
1:C:49:PRO:HG2	1:C:51:ILE:HD11	1.84	0.60
1:A:307:LYS:HD2	1:A:418:LEU:HG	1.84	0.59
1:A:493:GLU:HA	1:A:496:ARG:HG2	1.84	0.59
1:A:20:MET:HE2	1:B:380:LYS:HE3	1.85	0.58
1:C:351:TYR:OH	1:C:440:HIS:HD2	1.85	0.58
1:C:111:PHE:HE1	1:C:256:ILE:HG12	1.67	0.58
1:A:313:LEU:HD23	1:A:381:VAL:HG22	1.84	0.58
1:A:401:ASN:OD1	1:A:404:ARG:NH2	2.37	0.57
1:A:16:VAL:HG21	1:A:314:ALA:HB2	1.85	0.57
1:A:27:THR:C	1:A:28:HIS:HD1	2.11	0.57
1:B:391:GLN:HG2	1:B:421:TRP:CD2	2.39	0.57
1:A:126:GLU:HG2	1:A:129:LEU:HD12	1.87	0.57
1:B:126:GLU:HG2	1:B:129:LEU:HD12	1.86	0.56
1:A:31:ASP:HB3	1:A:289:MET:HE1	1.87	0.56
1:A:109:ASN:ND2	1:A:260:GLY:HA3	2.20	0.56
1:C:68:ASP:OD2	1:C:145:ARG:NH1	2.39	0.56
1:C:391:GLN:HG2	1:C:421:TRP:CD2	2.41	0.56
1:C:34:GLU:OE2	1:C:36:THR:HG22	2.07	0.55
1:C:355:HIS:HB2	1:C:478:MET:HE3	1.89	0.55
1:A:452:ARG:C	1:A:454:GLN:H	2.16	0.54
1:A:408:ASN:OD1	1:B:397:ARG:NH1	2.38	0.54
1:A:115:LEU:HD11	1:A:118:PRO:HB3	1.88	0.54
1:B:157:TYR:CZ	1:B:245:GLY:HA2	2.42	0.54
1:B:493:GLU:O	1:B:497:LEU:HG	2.08	0.54
1:C:422:THR:O	1:C:426:GLU:HG3	2.07	0.54
1:C:313:LEU:HD23	1:C:429:VAL:HG13	1.90	0.54
1:B:93:GLY:HA3	1:B:226:MET:O	2.07	0.53
1:A:129:LEU:O	2:D:4:SIA:H113	2.09	0.53
1:B:290:PRO:HB3	1:B:385:ILE:HG23	1.90	0.53
1:A:481:VAL:HG22	1:A:486:TYR:HD2	1.74	0.52
1:B:130:GLY:HA3	1:B:149:TRP:HB3	1.92	0.52
1:A:191:TYR:O	1:A:193:ASN:N	2.39	0.52
1:A:483:ASN:HB3	1:A:485:THR:HG23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:GLY:HA2	6:A:796:HOH:O	2.09	0.52
1:A:20:MET:HE2	1:B:380:LYS:CE	2.40	0.52
1:A:179:HIS:HB2	1:A:226:MET:HE2	1.93	0.51
1:C:390:THR:O	1:C:390:THR:OG1	2.28	0.51
1:B:116:ILE:HG13	1:B:117:ILE:HG13	1.93	0.51
1:A:346:MET:HE1	1:A:352:GLY:HA3	1.93	0.50
1:C:338:PHE:HB2	1:C:463:GLY:O	2.11	0.50
1:A:454:GLN:HE22	1:A:484:GLY:HA2	1.76	0.50
1:B:431:MET:HE1	1:C:431:MET:HE3	1.93	0.49
1:B:48:LYS:HG2	1:B:49:PRO:HD2	1.94	0.49
1:B:381:VAL:O	1:B:385:ILE:HG13	2.13	0.49
1:B:160:ILE:O	1:B:242:GLU:HA	2.13	0.48
1:C:493:GLU:H	1:C:493:GLU:CD	2.21	0.48
1:A:348:ASP:OD1	1:A:348:ASP:N	2.42	0.48
1:A:346:MET:CE	1:A:365:ALA:HA	2.44	0.48
1:A:280:THR:CG2	1:A:282:VAL:HG22	2.44	0.47
1:A:111:PHE:HE1	1:A:256:ILE:HG13	1.80	0.46
1:C:450:LYS:HA	1:C:450:LYS:HD3	1.57	0.46
1:A:93:GLY:HA3	1:A:226:MET:O	2.15	0.46
1:A:313:LEU:HD13	1:A:429:VAL:HG22	1.96	0.46
1:B:459:ALA:HB2	1:B:469:PHE:CD1	2.50	0.46
1:C:32:ILE:HG13	1:C:311:LEU:HB3	1.97	0.46
1:B:179:HIS:HB2	1:B:248:ILE:HD11	1.97	0.46
1:B:461:GLU:HG2	1:B:467:PHE:CE1	2.51	0.46
1:B:5:ILE:HD11	1:B:451:VAL:HG21	1.97	0.45
1:B:19:ILE:HD12	1:B:19:ILE:H	1.82	0.45
1:B:66:MET:HA	1:B:66:MET:HE2	1.97	0.45
1:B:32:ILE:O	1:B:290:PRO:HD2	2.16	0.45
1:A:45:ASN:OD1	1:A:277:LYS:HE2	2.16	0.45
1:C:427:LEU:HG	1:C:431:MET:HE2	1.99	0.44
1:A:130:GLY:HA2	2:D:4:SIA:H113	1.99	0.44
1:C:346:MET:HE1	1:C:352:GLY:HA3	1.99	0.44
1:C:384:ILE:HG12	1:C:428:LEU:HD21	1.99	0.44
1:C:311:LEU:HD22	1:C:429:VAL:HG21	1.98	0.44
1:A:304:LYS:HD2	1:A:391:GLN:HB3	2.00	0.44
1:B:459:ALA:HB2	1:B:469:PHE:HD1	1.83	0.44
1:A:78:TYR:CZ	1:A:279:GLN:HG2	2.53	0.44
1:B:50:LEU:HD22	1:B:73:VAL:HG11	2.00	0.44
1:C:68:ASP:O	1:C:71:ILE:HG23	2.17	0.44
1:C:288:SER:O	1:C:288:SER:OG	2.35	0.44
1:C:313:LEU:HD23	1:C:313:LEU:HA	1.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:GLU:CD	1:A:493:GLU:H	2.25	0.44
1:B:75:GLU:HG2	1:B:110:HIS:HB2	1.99	0.44
1:C:166:ASN:O	1:C:235:PRO:O	2.35	0.44
1:B:15:GLN:HA	1:B:24:VAL:O	2.17	0.43
1:C:196:THR:OG1	1:C:211:PRO:HG2	2.18	0.43
1:B:42:CYS:HB2	1:B:276:THR:HG22	2.01	0.43
1:C:5:ILE:HD12	1:C:5:ILE:N	2.33	0.43
1:C:281:PRO:HD3	1:C:297:LEU:O	2.18	0.43
1:A:16:VAL:HG12	1:A:312:VAL:HG12	2.01	0.43
1:A:281:PRO:HD3	1:A:297:LEU:O	2.18	0.43
1:C:461:GLU:HB3	1:C:467:PHE:CE2	2.53	0.43
1:A:454:GLN:HE22	1:A:484:GLY:C	2.27	0.43
1:B:384:ILE:HG12	1:B:428:LEU:HD21	1.99	0.43
1:B:191:TYR:O	1:B:192:LYS:C	2.61	0.43
1:B:380:LYS:NZ	1:B:432:GLU:OE1	2.50	0.43
1:C:487:ASP:OD2	1:C:490:GLN:HB2	2.19	0.43
1:A:412:LYS:HA	1:A:412:LYS:HD3	1.78	0.43
1:C:90:CYS:HB2	1:C:134:ALA:O	2.19	0.43
1:C:289:MET:HG3	1:C:290:PRO:HD2	2.01	0.43
1:C:317:LEU:H	1:C:317:LEU:HD12	1.83	0.43
1:C:346:MET:HE1	1:C:351:TYR:C	2.43	0.43
1:A:367:LYS:HE3	1:A:367:LYS:HB3	1.84	0.42
5:A:601:NAG:O6	5:A:601:NAG:O4	2.25	0.42
1:C:9:ALA:HB2	1:C:342:GLY:HA3	2.01	0.42
1:C:126:GLU:HG2	1:C:129:LEU:HD12	2.01	0.42
1:B:191:TYR:O	1:B:193:ASN:N	2.52	0.42
1:B:392:PHE:HZ	1:B:413:MET:HE3	1.85	0.42
1:C:4:CYS:HA	1:C:466:CYS:HA	2.00	0.42
1:B:351:TYR:H	1:B:370:THR:CG2	2.33	0.42
1:A:133:ALA:N	2:D:4:SIA:O1A	2.33	0.42
1:A:121:SER:C	1:A:123:PRO:HD3	2.45	0.42
1:B:22:LYS:NZ	1:C:383:SER:OG	2.30	0.42
1:C:291:PHE:HZ	1:C:388:MET:HE3	1.85	0.42
1:B:115:LEU:CD1	1:B:251:GLU:HG2	2.50	0.42
1:B:126:GLU:HB3	1:B:151:ILE:HB	2.02	0.41
1:C:304:LYS:HA	1:C:304:LYS:HD3	1.74	0.41
1:A:346:MET:HE1	1:A:352:GLY:CA	2.49	0.41
1:A:413:MET:CE	1:A:414:GLU:HG2	2.50	0.41
1:A:486:TYR:HE1	1:A:488:TYR:HA	1.85	0.41
1:C:160:ILE:O	1:C:242:GLU:HA	2.20	0.41
1:B:392:PHE:CZ	1:B:413:MET:HE3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:HIS:ND1	1:C:9:ALA:N	2.69	0.41
1:B:49:PRO:HB3	1:B:78:TYR:CE1	2.54	0.41
1:C:81:GLU:O	1:C:266:LYS:HA	2.19	0.41
1:B:49:PRO:HB3	1:B:78:TYR:CZ	2.55	0.41
1:C:48:LYS:HE2	1:C:271:TYR:CE2	2.56	0.41
1:C:53:LYS:NZ	1:C:69:GLU:OE1	2.46	0.41
1:A:40:LYS:HG2	1:A:272:GLY:HA3	2.02	0.41
1:B:281:PRO:HD3	1:B:297:LEU:O	2.20	0.41
1:C:478:MET:O	1:C:482:ARG:HG3	2.21	0.41
1:A:129:LEU:O	2:D:4:SIA:C11	2.69	0.41
1:B:453:LEU:HA	1:B:453:LEU:HD12	1.88	0.41
1:C:117:ILE:HD12	1:C:250:PRO:HG2	2.02	0.41
1:C:381:VAL:O	1:C:385:ILE:HG13	2.20	0.41
1:C:474:ASP:O	1:C:477:CYS:HB3	2.21	0.41
1:A:68:ASP:CG	1:A:145:ARG:HE	2.29	0.41
1:B:234:LYS:HA	1:B:234:LYS:HD2	1.84	0.41
1:C:179:HIS:HB2	1:C:248:ILE:HD11	2.02	0.41
1:B:22:LYS:HA	1:B:22:LYS:HD3	1.78	0.41
1:B:64:ASN:HB3	1:B:67:CYS:SG	2.61	0.41
1:B:27:THR:HG23	1:B:317:LEU:O	2.20	0.40
1:A:8:HIS:HE1	1:A:10:ASN:HB3	1.85	0.40
1:A:487:ASP:OD1	1:A:489:PRO:HD2	2.21	0.40
1:A:218:GLN:O	6:A:701:HOH:O	2.22	0.40
1:B:370:THR:O	1:B:374:ILE:HG13	2.21	0.40
1:C:91:TYR:CE1	1:C:226:MET:HE3	2.56	0.40
1:A:313:LEU:CD1	1:A:429:VAL:HG22	2.51	0.40
1:A:452:ARG:C	1:A:454:GLN:N	2.80	0.40
1:B:8:HIS:HB2	1:B:350:TRP:HA	2.03	0.40
1:B:114:ILE:HG21	1:B:255:LYS:HE2	2.03	0.40
1:B:198:ILE:HD13	1:B:247:PHE:HD1	1.86	0.40
1:B:412:LYS:NZ	1:C:394:ALA:HA	2.36	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	486/506 (96%)	470 (97%)	16 (3%)	0	100	100
1	B	486/506 (96%)	474 (98%)	12 (2%)	0	100	100
1	C	486/506 (96%)	471 (97%)	15 (3%)	0	100	100
All	All	1458/1518 (96%)	1415 (97%)	43 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	432/446 (97%)	429 (99%)	3 (1%)	81	92
1	B	432/446 (97%)	423 (98%)	9 (2%)	48	72
1	C	432/446 (97%)	427 (99%)	5 (1%)	67	84
All	All	1296/1338 (97%)	1279 (99%)	17 (1%)	65	83

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	ARG
1	A	318	ARG
1	A	351	TYR
1	B	13	THR
1	B	17	ASP
1	B	54	ASP
1	B	71	ILE
1	B	162	ILE
1	B	191	TYR
1	B	348	ASP
1	B	384	ILE
1	B	477	CYS
1	C	36	THR

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Mol	Chain	Res	Type
1	C	269	VAL
1	C	274	CYS
1	C	450	LYS
1	C	473	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	103	HIS
1	A	109	ASN
1	A	354	HIS
1	A	391	GLN
1	A	454	GLN
1	A	458	ASN
1	A	483	ASN
1	B	15	GLN
1	B	45	ASN
1	B	96	ASN
1	B	146	ASN
1	B	371	GLN
1	B	401	ASN
1	B	475	ASN
1	C	15	GLN
1	C	109	ASN
1	C	189	ASN
1	C	440	HIS
1	C	454	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

14 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	GAL	D	1	2	12,12,12	0.17	0	17,17,17	0.37	0
2	NAG	D	2	2	14,14,15	0.38	0	17,19,21	1.02	0
2	GAL	D	3	2	11,11,12	0.77	0	15,15,17	1.12	1 (6%)
2	SIA	D	4	2	20,20,21	1.93	2 (10%)	24,28,31	1.85	6 (25%)
3	NAG	E	1	1,3	14,14,15	2.01	3 (21%)	17,19,21	1.72	5 (29%)
3	NAG	E	2	3	14,14,15	1.96	4 (28%)	17,19,21	0.95	0
3	NAG	F	1	1,3	14,14,15	2.01	4 (28%)	17,19,21	1.29	2 (11%)
3	NAG	F	2	3	14,14,15	2.43	4 (28%)	17,19,21	1.88	5 (29%)
4	NAG	G	1	4	15,15,15	1.87	5 (33%)	21,21,21	2.96	12 (57%)
4	GAL	G	2	4	11,11,12	1.70	3 (27%)	15,15,17	2.10	5 (33%)
4	SIA	G	3	4	20,20,21	1.81	4 (20%)	24,28,31	2.76	13 (54%)
4	NAG	H	1	4	15,15,15	1.76	3 (20%)	21,21,21	2.77	12 (57%)
4	GAL	H	2	4	11,11,12	1.67	2 (18%)	15,15,17	1.83	3 (20%)
4	SIA	H	3	4	20,20,21	1.64	3 (15%)	24,28,31	2.52	8 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	D	1	2	-	0/2/22/22	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	GAL	D	3	2	-	0/2/19/22	0/1/1/1
2	SIA	D	4	2	-	3/18/34/38	0/1/1/1
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
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	3/6/23/26	0/1/1/1
4	NAG	G	1	4	-	4/6/26/26	0/1/1/1
4	GAL	G	2	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SIA	G	3	4	-	0/18/34/38	0/1/1/1
4	NAG	H	1	4	-	2/6/26/26	0/1/1/1
4	GAL	H	2	4	-	0/2/19/22	0/1/1/1
4	SIA	H	3	4	-	0/18/34/38	0/1/1/1

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	SIA	C2-C1	7.29	1.58	1.52
3	F	2	NAG	O5-C1	5.94	1.53	1.43
4	G	3	SIA	O6-C2	4.98	1.50	1.43
4	H	3	SIA	O6-C2	4.79	1.50	1.43
3	F	1	NAG	O5-C1	4.59	1.51	1.43
4	H	2	GAL	O5-C1	4.58	1.51	1.43
3	E	1	NAG	O5-C1	4.50	1.50	1.43
4	G	2	GAL	O5-C1	4.24	1.50	1.43
3	E	2	NAG	O5-C1	4.20	1.50	1.43
3	F	2	NAG	C7-N2	4.01	1.48	1.34
4	G	1	NAG	C7-N2	3.88	1.47	1.34
3	E	1	NAG	C7-N2	3.75	1.47	1.34
4	H	1	NAG	C2-N2	3.69	1.51	1.45
3	E	2	NAG	C7-N2	3.66	1.46	1.34
3	F	1	NAG	C7-N2	3.60	1.46	1.34
4	G	1	NAG	C2-N2	3.40	1.51	1.45
4	H	1	NAG	C7-N2	3.38	1.46	1.34
3	F	2	NAG	C2-N2	3.16	1.51	1.46
4	H	3	SIA	C10-N5	3.12	1.45	1.34
4	G	3	SIA	C3-C4	-3.03	1.47	1.52
4	H	3	SIA	C3-C4	-2.98	1.47	1.52
3	E	1	NAG	C2-N2	2.91	1.51	1.46
4	G	3	SIA	C10-N5	2.90	1.44	1.34
2	D	4	SIA	O6-C2	2.81	1.47	1.43
4	G	1	NAG	O5-C1	2.63	1.49	1.42
3	E	2	NAG	C2-N2	2.60	1.50	1.46
3	F	2	NAG	O5-C5	2.58	1.48	1.43
4	H	1	NAG	O5-C1	2.49	1.49	1.42
3	F	1	NAG	C2-N2	2.47	1.50	1.46
4	G	1	NAG	O7-C7	-2.47	1.17	1.23
4	G	3	SIA	C4-C5	-2.41	1.51	1.53
3	E	2	NAG	O5-C5	2.24	1.48	1.43
4	G	1	NAG	O5-C5	2.20	1.49	1.44
4	G	2	GAL	O5-C5	2.20	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	2	GAL	O3-C3	2.12	1.48	1.43
3	F	1	NAG	O5-C5	2.06	1.47	1.43
4	H	2	GAL	O5-C5	2.05	1.47	1.43

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	1	NAG	C8-C7-N2	7.05	128.04	116.10
4	H	1	NAG	C1-C2-N2	-6.26	103.47	110.73
4	H	3	SIA	C6-C5-N5	-6.02	100.91	110.91
4	G	3	SIA	C6-C5-N5	-5.19	102.28	110.91
4	H	1	NAG	C8-C7-N2	5.19	124.89	116.10
4	H	3	SIA	O6-C2-C3	5.13	117.52	110.46
3	F	2	NAG	C8-C7-N2	5.12	124.77	116.10
4	H	3	SIA	C4-C3-C2	5.07	118.89	109.81
4	G	3	SIA	O6-C2-C3	5.02	117.36	110.46
2	D	4	SIA	O1A-C1-C2	-4.76	111.33	122.57
4	H	3	SIA	C8-C7-C6	-4.56	104.39	113.03
4	G	2	GAL	O6-C6-C5	-4.47	95.95	111.29
4	G	3	SIA	O8-C8-C9	-4.45	98.70	109.14
4	G	3	SIA	O1A-C1-C2	-4.19	112.67	122.57
4	G	1	NAG	C2-N2-C7	4.09	133.12	123.18
4	G	1	NAG	O7-C7-C8	-4.05	114.53	122.06
4	H	1	NAG	O5-C1-C2	4.04	113.57	109.52
4	G	1	NAG	O3-C3-C2	-3.91	101.75	109.66
4	H	2	GAL	C1-C2-C3	3.90	114.47	109.67
4	H	2	GAL	O6-C6-C5	-3.83	98.16	111.29
4	G	2	GAL	C1-C2-C3	3.79	114.33	109.67
4	G	3	SIA	O1B-C1-C2	3.77	123.80	113.03
4	G	1	NAG	O1-C1-C2	3.70	116.91	109.22
4	G	1	NAG	O4-C4-C3	-3.66	101.89	110.35
2	D	4	SIA	C6-C5-N5	-3.63	104.88	110.91
4	G	3	SIA	O8-C8-C7	3.50	117.61	109.10
4	H	1	NAG	C1-O5-C5	-3.45	107.16	113.66
3	F	2	NAG	C2-N2-C7	3.41	127.76	122.90
4	G	3	SIA	C11-C10-N5	-3.38	110.37	116.10
3	E	1	NAG	C2-N2-C7	-3.26	118.25	122.90
4	H	1	NAG	O5-C5-C4	3.24	115.58	109.69
3	E	1	NAG	C8-C7-N2	3.21	121.54	116.10
4	H	1	NAG	C4-C3-C2	3.17	114.98	110.34
4	H	2	GAL	O5-C1-C2	3.04	115.46	110.77
4	H	1	NAG	C1-C2-C3	3.01	114.65	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	1	NAG	C3-C4-C5	-2.95	104.98	110.24
2	D	4	SIA	C6-O6-C2	2.87	117.48	111.34
4	G	3	SIA	C4-C5-N5	-2.86	104.72	110.38
4	G	1	NAG	C4-C3-C2	2.83	114.49	110.34
3	E	1	NAG	C4-C3-C2	2.82	115.16	111.02
3	F	1	NAG	C1-O5-C5	2.78	115.96	112.19
4	G	3	SIA	C6-O6-C2	-2.75	105.45	111.34
4	G	1	NAG	O3-C3-C4	2.71	116.61	110.35
4	G	3	SIA	C4-C3-C2	2.63	114.52	109.81
3	F	2	NAG	O7-C7-C8	-2.59	117.25	122.06
4	G	3	SIA	O9-C9-C8	-2.58	105.46	111.07
4	H	3	SIA	O1B-C1-C2	2.54	120.27	113.03
4	G	2	GAL	O4-C4-C3	-2.51	104.54	110.35
2	D	4	SIA	O1B-C1-O1A	2.48	129.72	124.09
4	G	1	NAG	O7-C7-N2	-2.47	117.41	121.95
4	H	1	NAG	O7-C7-C8	-2.47	117.48	122.06
4	H	3	SIA	C4-C5-C6	2.44	115.27	109.10
2	D	3	GAL	C1-O5-C5	2.36	115.39	112.19
4	H	1	NAG	O7-C7-N2	-2.35	117.64	121.95
4	G	3	SIA	C3-C4-C5	-2.31	108.67	111.46
4	H	1	NAG	O4-C4-C3	2.29	115.64	110.35
3	E	1	NAG	C1-O5-C5	2.23	115.22	112.19
4	G	1	NAG	O5-C5-C4	2.23	113.75	109.69
4	H	1	NAG	O4-C4-C5	-2.23	103.77	109.30
4	G	2	GAL	C1-O5-C5	-2.19	109.22	112.19
4	H	3	SIA	C5-N5-C10	-2.18	117.89	123.18
3	F	2	NAG	O7-C7-N2	-2.16	117.97	121.95
4	G	1	NAG	C6-C5-C4	-2.15	107.96	113.00
2	D	4	SIA	C4-C3-C2	2.14	113.65	109.81
3	F	1	NAG	C8-C7-N2	2.13	119.71	116.10
3	F	2	NAG	C6-C5-C4	-2.09	108.10	113.00
2	D	4	SIA	O1B-C1-C2	2.07	118.95	113.03
4	G	2	GAL	O5-C5-C6	-2.07	103.96	107.20
4	G	3	SIA	O6-C2-C1	2.05	111.72	107.70
4	H	3	SIA	O1A-C1-C2	-2.04	117.74	122.57
4	H	1	NAG	C6-C5-C4	-2.01	108.31	113.00
3	E	1	NAG	O5-C1-C2	2.00	114.45	111.29

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1	NAG	C1-C2-N2-C7
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
3	E	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
2	D	4	SIA	C6-C7-C8-O8
4	G	1	NAG	C1-C2-N2-C7
2	D	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C3-C2-N2-C7
4	G	1	NAG	C3-C2-N2-C7
4	H	1	NAG	C3-C2-N2-C7
2	D	4	SIA	C7-C8-C9-O9
2	D	4	SIA	O7-C7-C8-O8

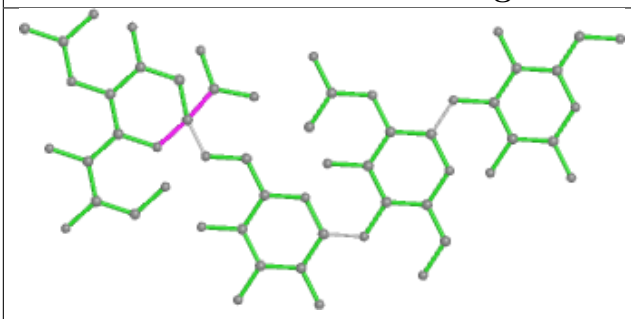
There are no ring outliers.

2 monomers are involved in 6 short contacts:

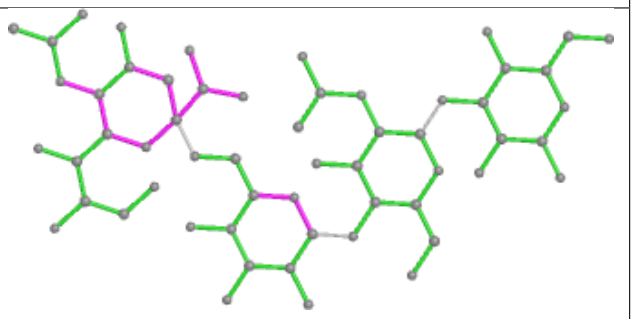
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	NAG	2	0
2	D	4	SIA	4	0

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

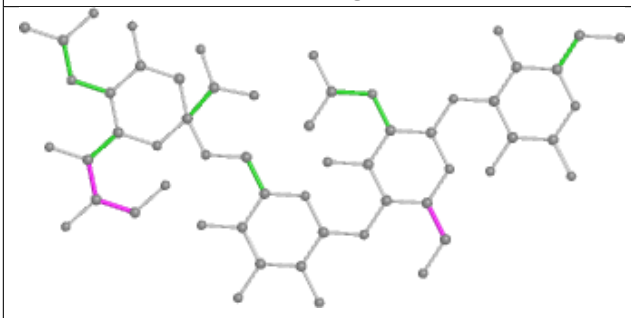
Oligosaccharide Chain D



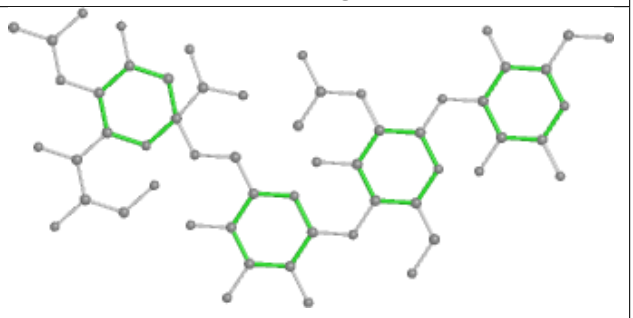
Bond lengths



Bond angles

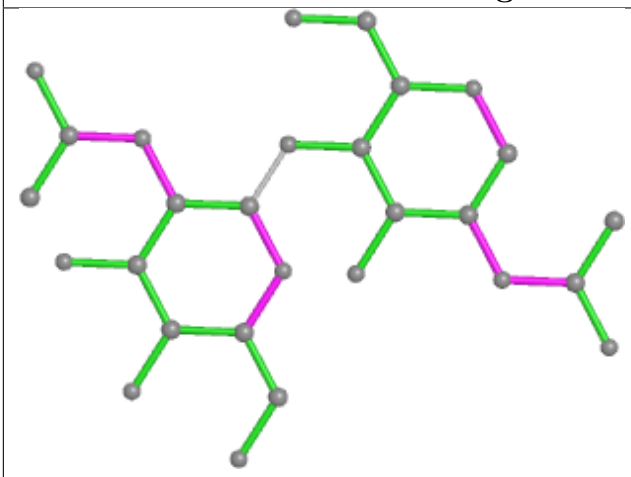


Torsions

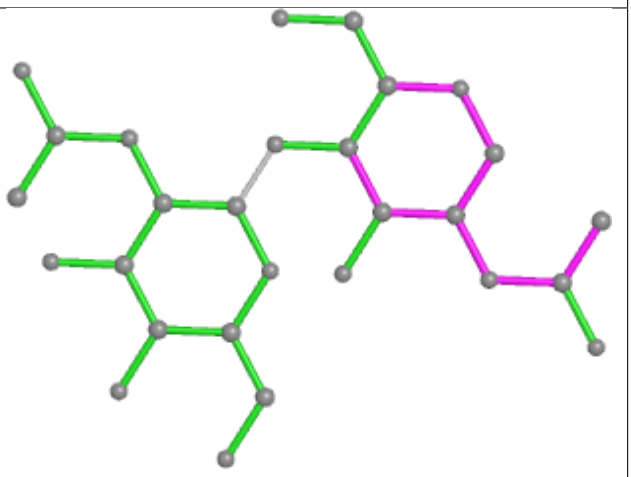


Rings

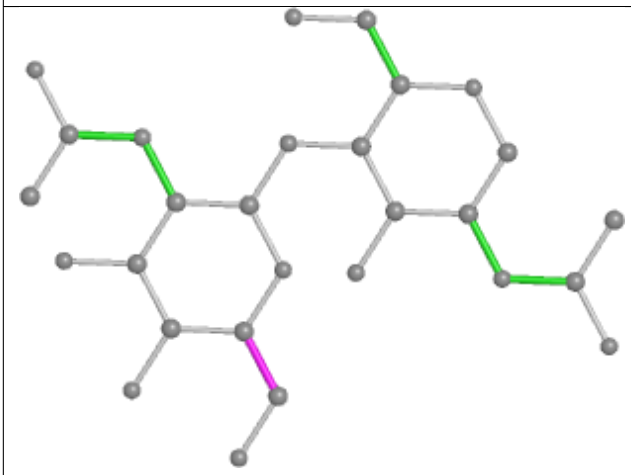
Oligosaccharide Chain E



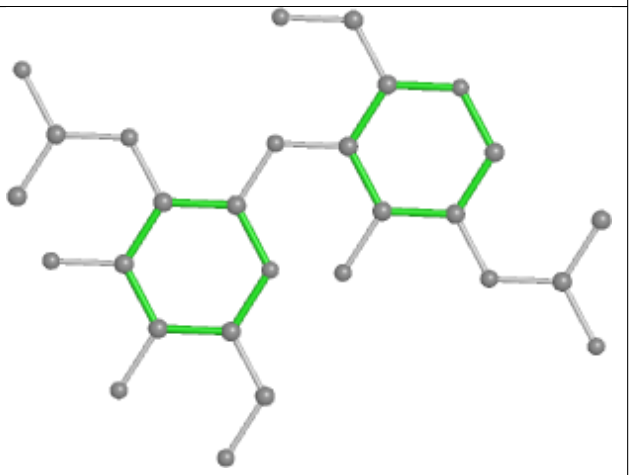
Bond lengths



Bond angles

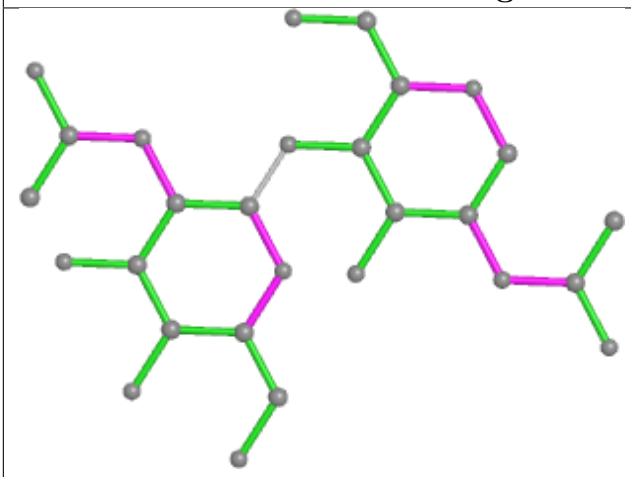


Torsions

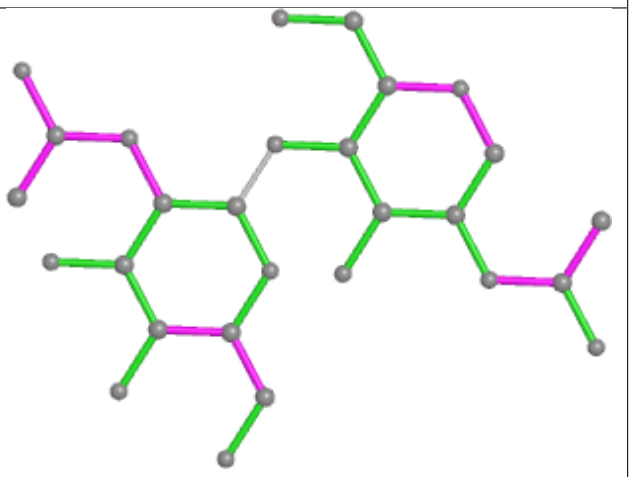


Rings

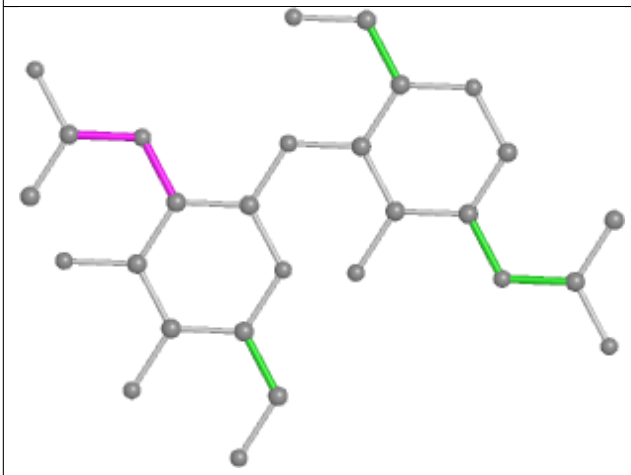
Oligosaccharide Chain F



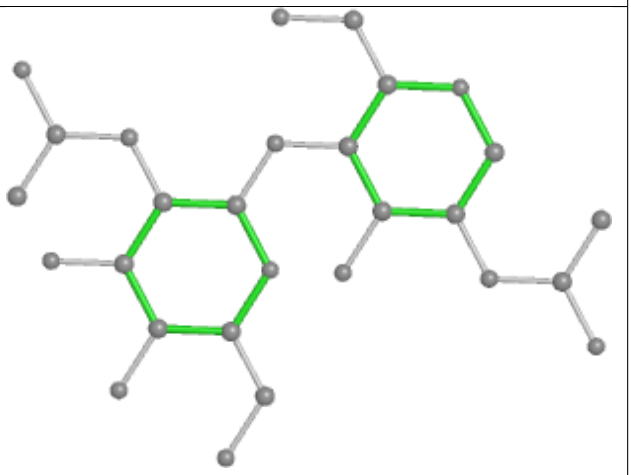
Bond lengths



Bond angles

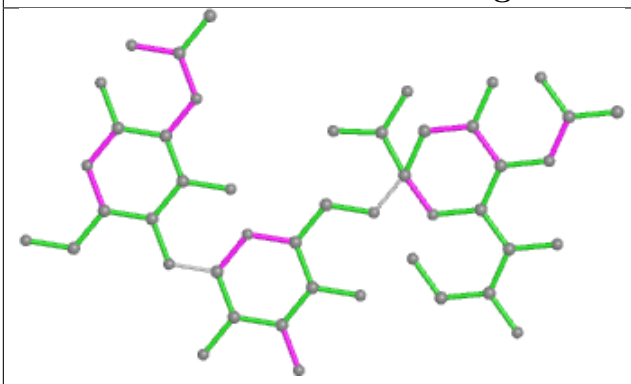


Torsions

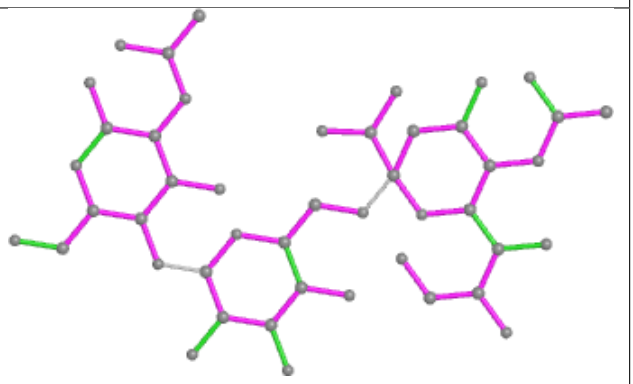


Rings

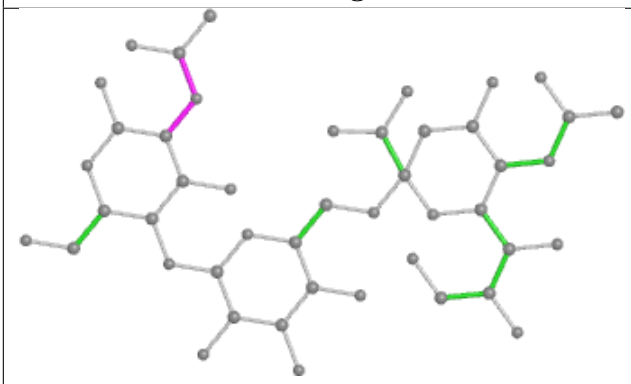
Oligosaccharide Chain G



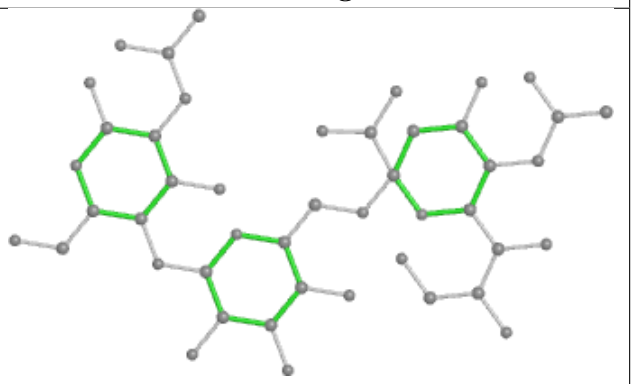
Bond lengths



Bond angles

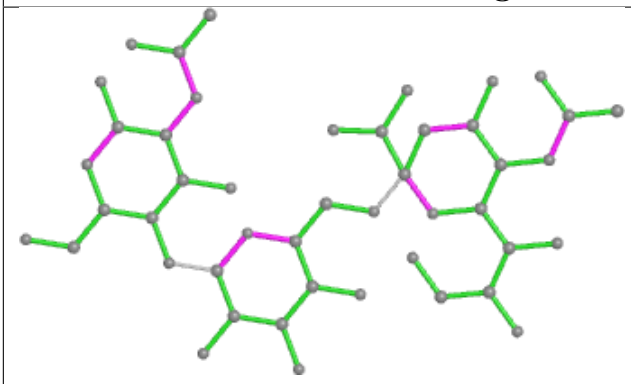


Torsions

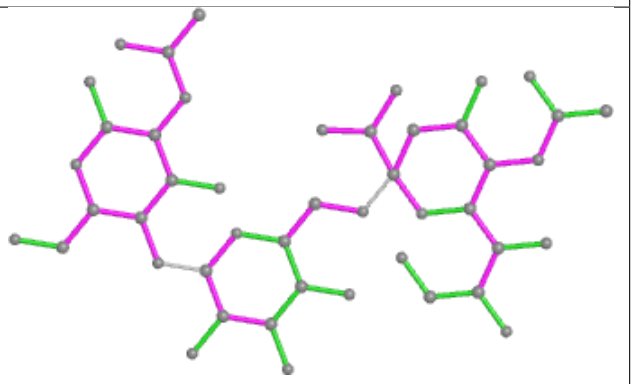


Rings

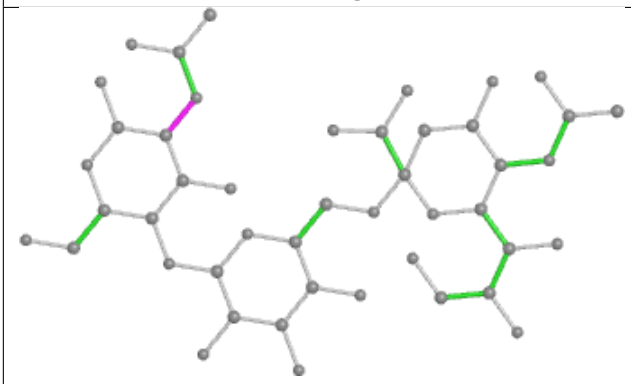
Oligosaccharide Chain H



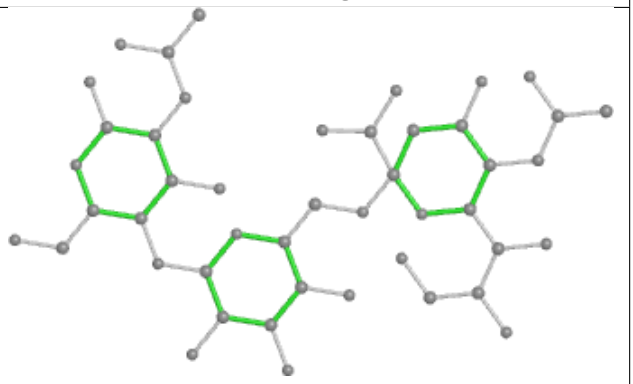
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	A	602	1	14,14,15	2.06	4 (28%)	17,19,21	0.99	1 (5%)
5	NAG	C	601	1	14,14,15	2.00	4 (28%)	17,19,21	0.89	0
5	NAG	C	602	1	14,14,15	2.04	4 (28%)	17,19,21	1.19	3 (17%)
5	NAG	A	601	1	14,14,15	2.10	4 (28%)	17,19,21	1.30	2 (11%)
5	NAG	B	601	1	14,14,15	2.11	4 (28%)	17,19,21	1.27	3 (17%)
5	NAG	A	603	1	14,14,15	2.06	4 (28%)	17,19,21	1.20	3 (17%)

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	A	602	1	-	2/6/23/26	0/1/1/1
5	NAG	C	601	1	-	0/6/23/26	0/1/1/1
5	NAG	C	602	1	-	2/6/23/26	0/1/1/1
5	NAG	A	601	1	-	1/6/23/26	0/1/1/1
5	NAG	B	601	1	-	2/6/23/26	0/1/1/1
5	NAG	A	603	1	-	2/6/23/26	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	NAG	O5-C1	5.13	1.51	1.43
5	B	601	NAG	O5-C1	4.83	1.51	1.43
5	A	603	NAG	O5-C1	4.80	1.51	1.43
5	C	602	NAG	O5-C1	4.72	1.51	1.43
5	C	601	NAG	O5-C1	4.55	1.51	1.43
5	A	602	NAG	O5-C1	4.52	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	601	NAG	C7-N2	3.78	1.47	1.34
5	A	603	NAG	C7-N2	3.76	1.47	1.34
5	A	602	NAG	C7-N2	3.72	1.47	1.34
5	C	602	NAG	C7-N2	3.58	1.46	1.34
5	A	601	NAG	C7-N2	3.54	1.46	1.34
5	C	601	NAG	C7-N2	3.46	1.46	1.34
5	B	601	NAG	C2-N2	2.81	1.51	1.46
5	A	602	NAG	C2-N2	2.75	1.51	1.46
5	A	603	NAG	C2-N2	2.48	1.50	1.46
5	C	602	NAG	O5-C5	2.43	1.48	1.43
5	A	601	NAG	O5-C5	2.42	1.48	1.43
5	B	601	NAG	O5-C5	2.33	1.48	1.43
5	A	602	NAG	O5-C5	2.24	1.48	1.43
5	C	601	NAG	O5-C5	2.24	1.48	1.43
5	C	601	NAG	C2-N2	2.16	1.50	1.46
5	C	602	NAG	C2-N2	2.15	1.50	1.46
5	A	603	NAG	O5-C5	2.14	1.47	1.43
5	A	601	NAG	C2-N2	2.10	1.49	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	601	NAG	C6-C5-C4	-2.83	106.37	113.00
5	B	601	NAG	C8-C7-N2	2.66	120.60	116.10
5	A	601	NAG	O5-C5-C6	2.56	111.22	107.20
5	C	602	NAG	C1-C2-N2	-2.26	106.62	110.49
5	C	602	NAG	C8-C7-N2	2.26	119.93	116.10
5	A	603	NAG	O5-C5-C6	2.25	110.73	107.20
5	A	603	NAG	C8-C7-N2	2.20	119.82	116.10
5	B	601	NAG	O5-C5-C6	2.15	110.57	107.20
5	C	602	NAG	C2-N2-C7	-2.13	119.88	122.90
5	B	601	NAG	C6-C5-C4	-2.10	108.07	113.00
5	A	602	NAG	C8-C7-N2	2.01	119.50	116.10
5	A	603	NAG	C1-C2-N2	-2.01	107.06	110.49

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	602	NAG	C4-C5-C6-O6
5	B	601	NAG	O5-C5-C6-O6
5	B	601	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	602	NAG	O5-C5-C6-O6
5	C	602	NAG	C4-C5-C6-O6
5	A	603	NAG	C4-C5-C6-O6
5	A	601	NAG	O5-C5-C6-O6
5	C	602	NAG	O5-C5-C6-O6
5	A	603	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	490/506 (96%)	0.64	30 (6%)	28	26	36, 60, 103, 136	0
1	B	490/506 (96%)	0.73	35 (7%)	23	22	41, 72, 100, 123	0
1	C	490/506 (96%)	0.99	74 (15%)	6	6	31, 75, 155, 177	0
All	All	1470/1518 (96%)	0.79	139 (9%)	15	14	31, 69, 119, 177	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	348	ASP	5.9
1	C	331	LEU	5.1
1	C	455	LEU	5.1
1	B	331	LEU	5.1
1	C	453	LEU	5.1
1	C	497	LEU	4.4
1	A	390	THR	4.2
1	A	453	LEU	4.1
1	A	317	LEU	3.9
1	C	481	VAL	3.7
1	A	500	GLU	3.7
1	C	349	GLY	3.7
1	C	456	ARG	3.6
1	A	320	SER	3.6
1	C	500	GLU	3.5
1	A	288	SER	3.5
1	A	1	ASP	3.5
1	B	347	VAL	3.5
1	A	467	PHE	3.5
1	A	497	LEU	3.4
1	B	320	SER	3.3
1	C	450	LYS	3.2
1	C	401	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	320	SER	3.1
1	C	394	ALA	3.1
1	C	351	TYR	3.1
1	A	461	GLU	3.1
1	C	486	TYR	3.1
1	B	346	MET	3.1
1	B	500	GLU	3.0
1	C	473	CYS	3.0
1	C	386	ASP	3.0
1	C	462	LEU	2.9
1	C	489	PRO	2.9
1	C	461	GLU	2.9
1	C	492	SER	2.9
1	B	358	GLU	2.9
1	C	345	GLY	2.8
1	C	472	LYS	2.8
1	C	363	TYR	2.8
1	A	395	VAL	2.8
1	C	499	ARG	2.8
1	B	308	SER	2.8
1	C	488	TYR	2.8
1	B	365	ALA	2.8
1	C	467	PHE	2.8
1	C	389	ASN	2.7
1	A	469	PHE	2.7
1	C	498	LYS	2.7
1	A	388	MET	2.7
1	A	489	PRO	2.7
1	B	274	CYS	2.7
1	A	348	ASP	2.7
1	A	463	GLY	2.7
1	A	451	VAL	2.7
1	C	395	VAL	2.7
1	B	6	GLY	2.6
1	C	350	TRP	2.6
1	C	390	THR	2.6
1	C	317	LEU	2.6
1	C	88	ASP	2.6
1	C	261	ASP	2.6
1	C	332	PHE	2.5
1	B	270	GLU	2.5
1	C	457	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	418	LEU	2.5
1	C	471	HIS	2.5
1	C	452	ARG	2.5
1	C	463	GLY	2.5
1	C	310	LYS	2.5
1	C	470	TYR	2.5
1	A	393	GLU	2.5
1	B	1	ASP	2.5
1	C	483	ASN	2.5
1	B	350	TRP	2.4
1	B	390	THR	2.4
1	A	261	ASP	2.4
1	C	392	PHE	2.4
1	C	24	VAL	2.4
1	C	71	ILE	2.4
1	B	72	ARG	2.4
1	C	1	ASP	2.4
1	B	469	PHE	2.4
1	C	338	PHE	2.4
1	B	451	VAL	2.4
1	C	347	VAL	2.4
1	C	19	ILE	2.4
1	C	454	GLN	2.4
1	C	300	GLY	2.4
1	B	338	PHE	2.3
1	A	235	PRO	2.3
1	C	318	ARG	2.3
1	C	393	GLU	2.3
1	B	5	ILE	2.3
1	C	459	ALA	2.3
1	B	351	TYR	2.3
1	C	491	TYR	2.3
1	B	389	ASN	2.2
1	B	19	ILE	2.2
1	B	463	GLY	2.2
1	C	316	GLY	2.2
1	C	415	ASP	2.2
1	C	441	ASP	2.2
1	B	309	ASN	2.2
1	C	335	ILE	2.2
1	B	453	LEU	2.2
1	A	349	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	456	ARG	2.2
1	C	427	LEU	2.2
1	B	332	PHE	2.2
1	C	469	PHE	2.2
1	A	389	ASN	2.2
1	B	368	GLU	2.2
1	A	396	GLY	2.1
1	B	302	CYS	2.1
1	B	88	ASP	2.1
1	C	11	ASN	2.1
1	C	487	ASP	2.1
1	A	447	LEU	2.1
1	B	304	LYS	2.1
1	C	299	ILE	2.1
1	C	73	VAL	2.1
1	C	336	ALA	2.1
1	A	470	TYR	2.1
1	A	358	GLU	2.1
1	A	444	VAL	2.1
1	C	367	LYS	2.1
1	C	391	GLN	2.1
1	C	32	ILE	2.1
1	C	6	GLY	2.0
1	B	353	TYR	2.0
1	B	340	GLU	2.0
1	C	368	GLU	2.0
1	A	496	ARG	2.0
1	C	387	LYS	2.0
1	A	351	TYR	2.0
1	C	448	TYR	2.0
1	A	5	ILE	2.0
1	B	424	ASN	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,

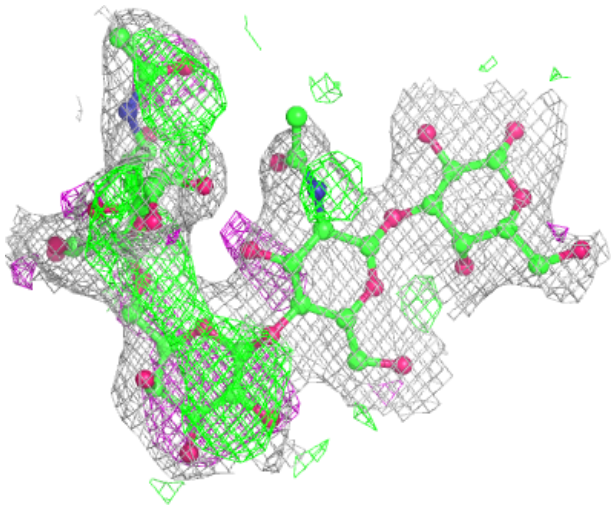
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

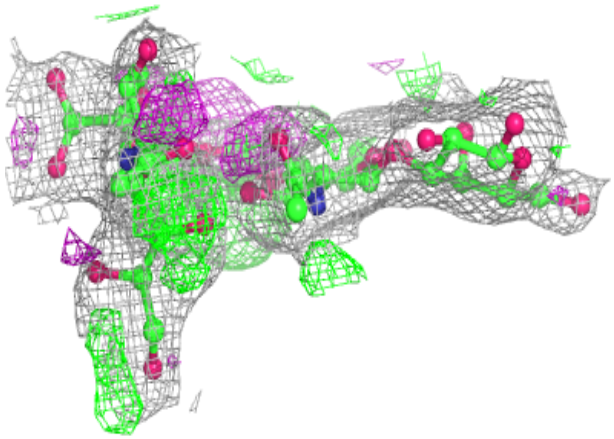
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	F	2	14/15	0.33	0.18	112,117,122,122	0
2	GAL	D	3	11/12	0.41	0.29	57,63,69,69	0
4	NAG	G	1	15/15	0.48	0.24	70,79,89,89	0
4	NAG	H	1	15/15	0.51	0.19	81,96,99,104	0
4	GAL	G	2	11/12	0.63	0.24	68,73,83,91	0
4	GAL	H	2	11/12	0.68	0.15	76,87,92,92	0
3	NAG	E	2	14/15	0.70	0.13	88,95,102,102	0
2	NAG	D	2	14/15	0.73	0.20	67,72,76,78	0
2	SIA	D	4	20/21	0.76	0.19	44,57,65,67	0
2	GAL	D	1	12/12	0.77	0.17	63,78,83,87	0
3	NAG	F	1	14/15	0.79	0.13	81,98,105,112	0
3	NAG	E	1	14/15	0.85	0.10	60,75,87,93	0
4	SIA	G	3	20/21	0.88	0.12	33,54,65,70	0
4	SIA	H	3	20/21	0.89	0.12	54,62,74,77	0

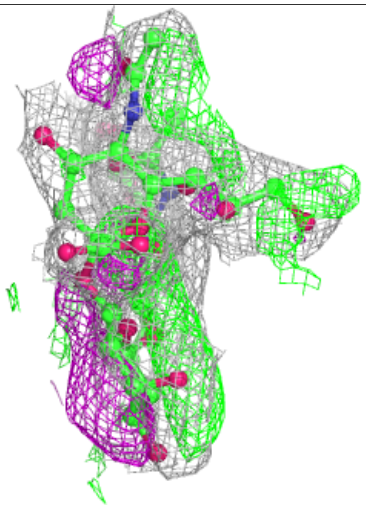
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain D:

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

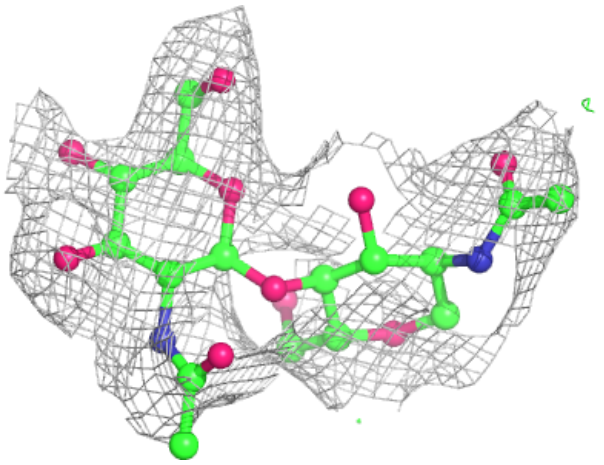


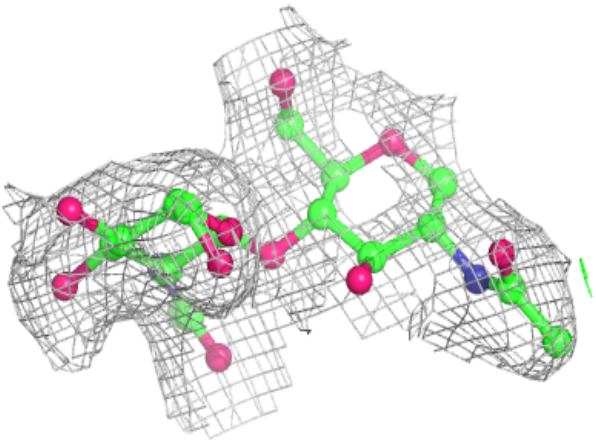


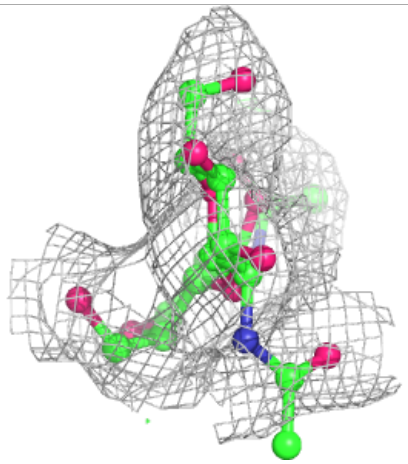


Electron density around Chain E:

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

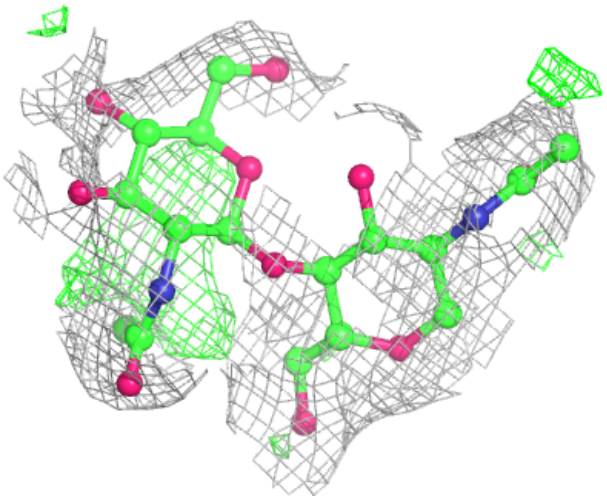


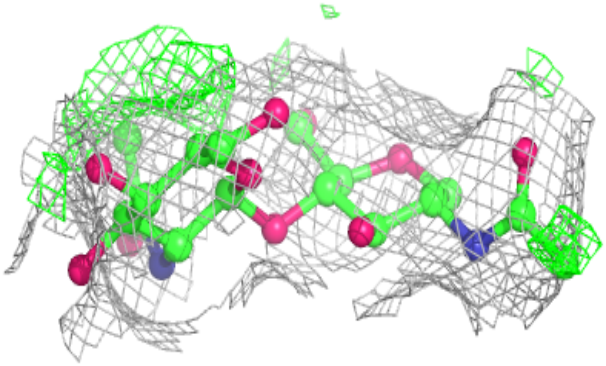


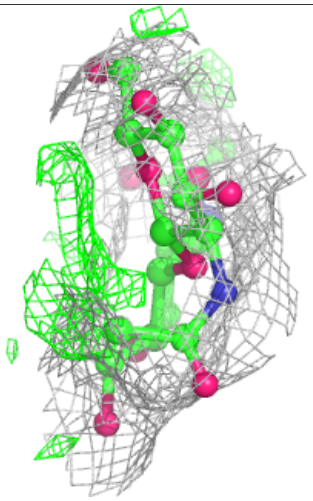


Electron density around Chain F:

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

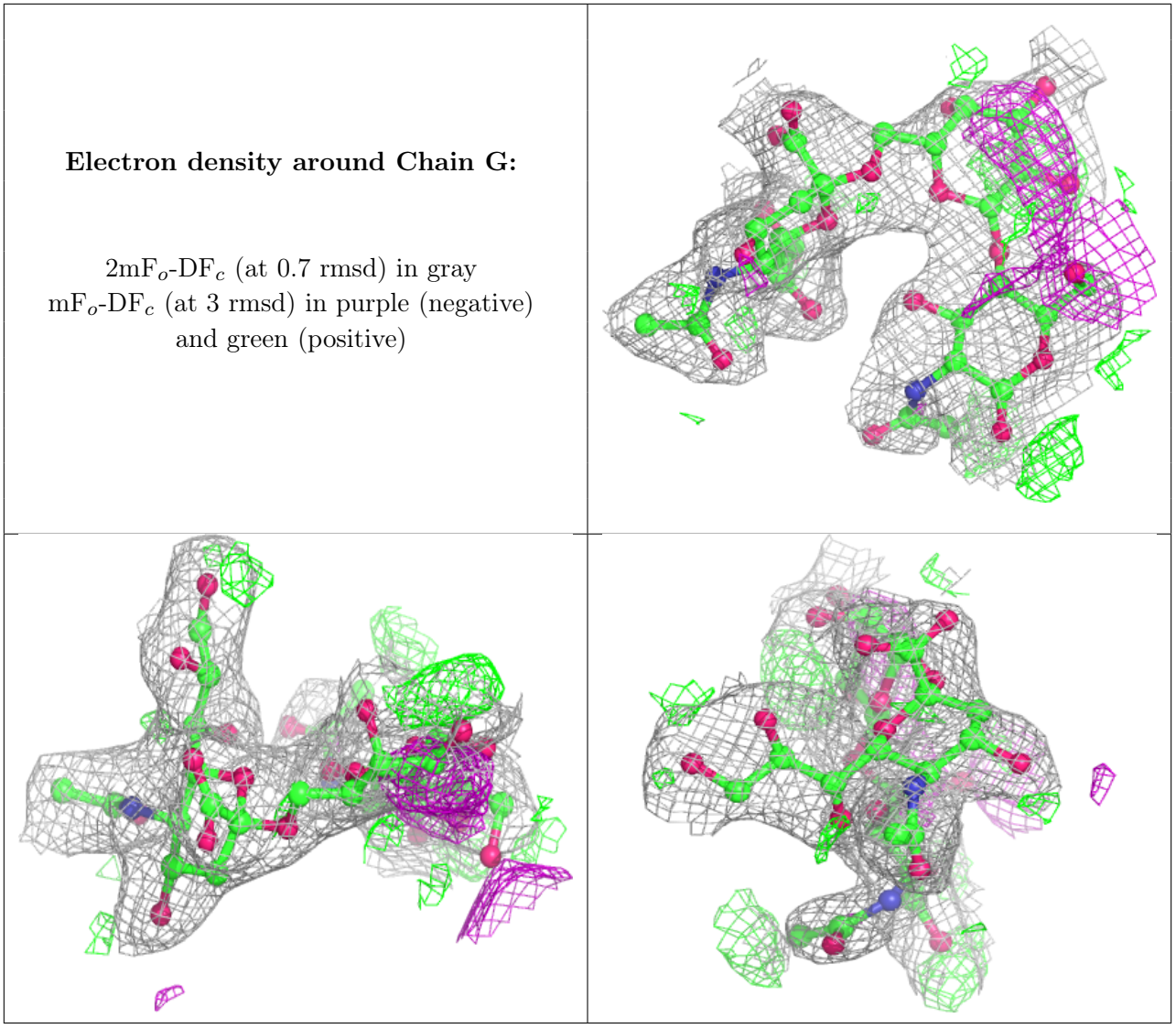






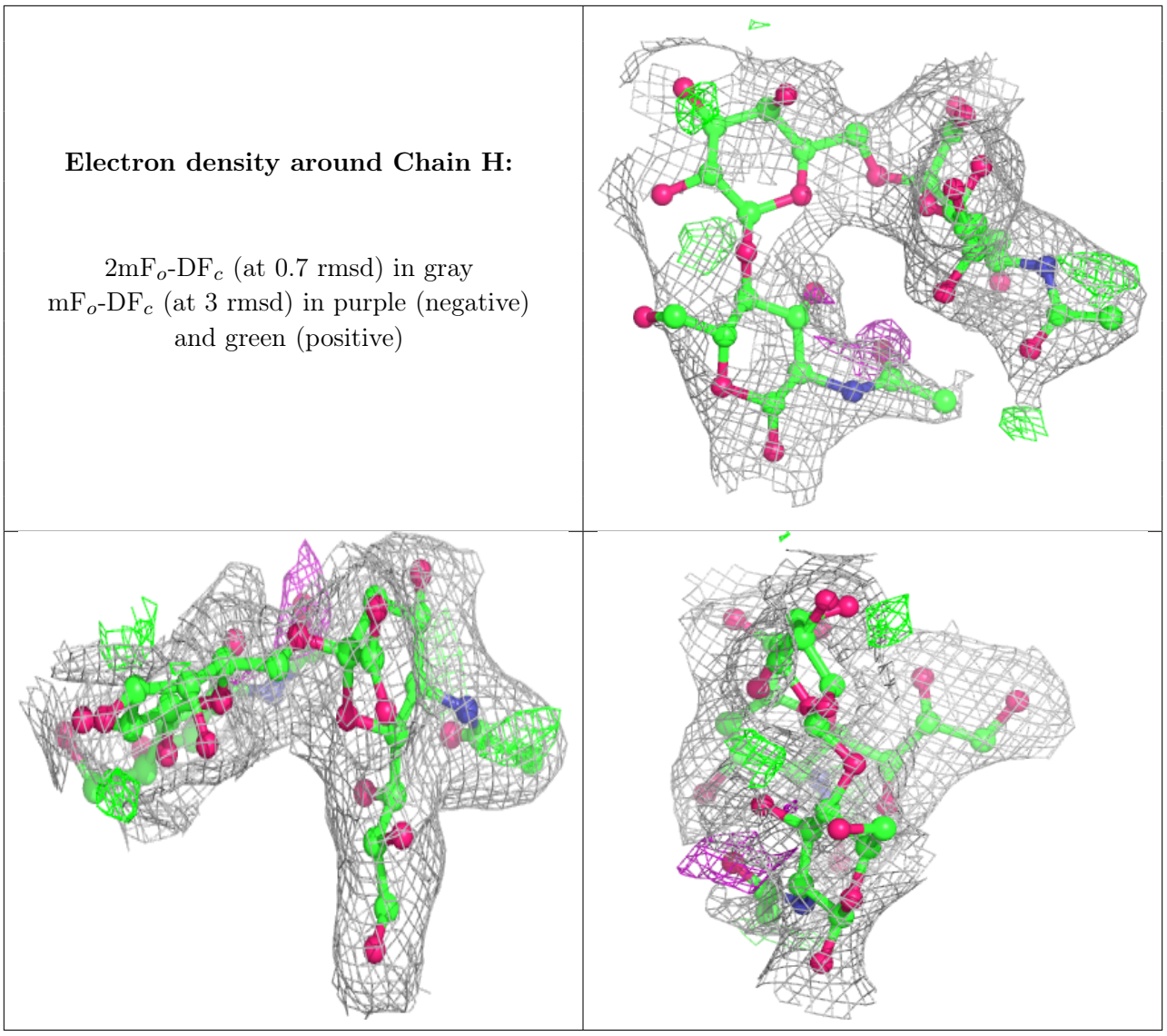
Electron density around Chain G:

$2mF_o$-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)



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	603	14/15	0.56	0.17	82,95,100,103	0
5	NAG	A	602	14/15	0.68	0.17	86,93,98,102	0
5	NAG	C	602	14/15	0.71	0.16	105,111,113,116	0
5	NAG	B	601	14/15	0.75	0.18	99,104,109,109	0
5	NAG	C	601	14/15	0.76	0.13	66,82,90,92	0
5	NAG	A	601	14/15	0.83	0.13	70,77,90,93	0

6.5 Other polymers (i)

There are no such residues in this entry.