



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:18 AM UTC

PDB ID : 4K67 / pdb_00004k67
Title : Structure of an airborne transmissible avian influenza H5 hemagglutinin mutant from the influenza virus A/Indonesia/5/2005 complexed with human receptor analog LSTc
Authors : Zhang, W.; Shi, Y.; Lu, X.; Shu, Y.; Gao, G.F.
Deposited on : 2013-04-15
Resolution : 2.70 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 Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

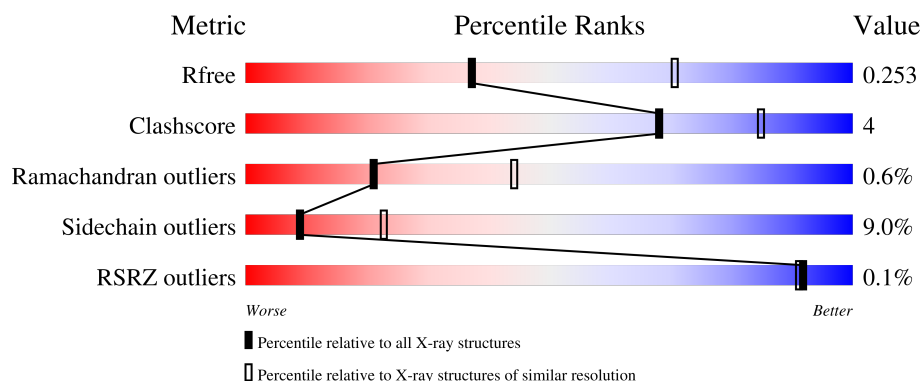
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 $\leq 5\%$. 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	321	 83% 15% .
1	C	321	 83% 15% .
1	E	321	 84% 15% .
1	G	321	 84% 14% .
2	B	164	 80% 18% .

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Mol	Chain	Length	Quality of chain
2	D	164	79%19%
2	F	164	81%17%
2	H	164	%84%13%
3	I	2	50%50%
3	J	2	50%50%
4	K	3	67%33%
4	L	3	33%33%33%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15692 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	321	Total	C	N	O	S	0	0	0
			2542	1609	433	485	15			
1	C	321	Total	C	N	O	S	0	0	0
			2542	1609	433	485	15			
1	E	321	Total	C	N	O	S	0	0	0
			2542	1609	433	485	15			
1	G	321	Total	C	N	O	S	0	0	0
			2542	1609	433	485	15			

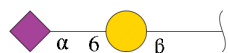
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLN	-	expression tag	UNP A8HWY8
A	107	TYR	HIS	engineered mutation	UNP A8HWY8
A	160	ALA	THR	engineered mutation	UNP A8HWY8
A	226	LEU	GLN	engineered mutation	UNP A8HWY8
A	228	SER	GLY	engineered mutation	UNP A8HWY8
C	4	GLN	-	expression tag	UNP A8HWY8
C	107	TYR	HIS	engineered mutation	UNP A8HWY8
C	160	ALA	THR	engineered mutation	UNP A8HWY8
C	226	LEU	GLN	engineered mutation	UNP A8HWY8
C	228	SER	GLY	engineered mutation	UNP A8HWY8
E	4	GLN	-	expression tag	UNP A8HWY8
E	107	TYR	HIS	engineered mutation	UNP A8HWY8
E	160	ALA	THR	engineered mutation	UNP A8HWY8
E	226	LEU	GLN	engineered mutation	UNP A8HWY8
E	228	SER	GLY	engineered mutation	UNP A8HWY8
G	4	GLN	-	expression tag	UNP A8HWY8
G	107	TYR	HIS	engineered mutation	UNP A8HWY8
G	160	ALA	THR	engineered mutation	UNP A8HWY8
G	226	LEU	GLN	engineered mutation	UNP A8HWY8
G	228	SER	GLY	engineered mutation	UNP A8HWY8

- Molecule 2 is a protein called Hemagglutinin.

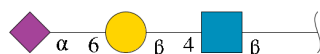
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	164	Total	C	N	O	S	0	0	0
			1328	828	229	263	8			
2	D	164	Total	C	N	O	S	0	0	0
			1328	828	229	263	8			
2	F	164	Total	C	N	O	S	0	0	0
			1328	828	229	263	8			
2	H	164	Total	C	N	O	S	0	0	0
			1328	828	229	263	8			

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose.



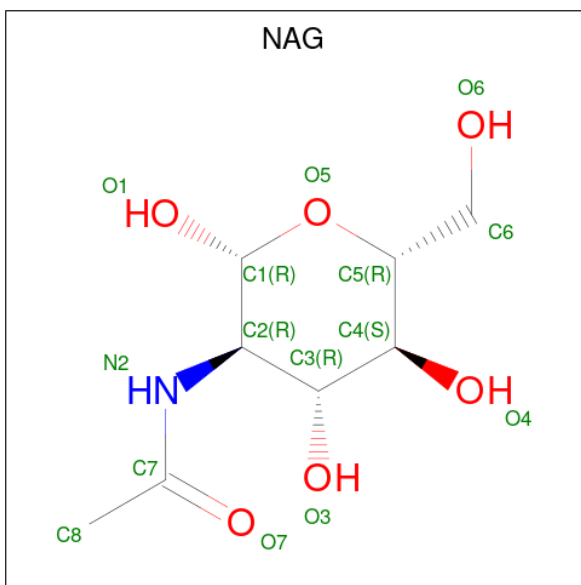
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	2	Total	C	N	O	0	0	0
			32	17	1	14			
3	J	2	Total	C	N	O	0	0	0
			32	17	1	14			

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



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

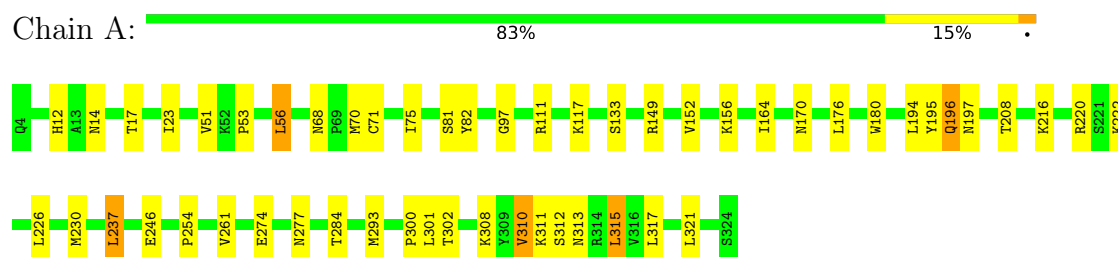


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		

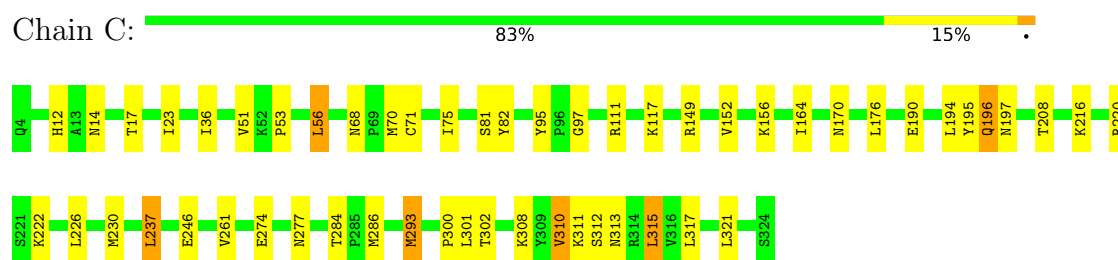
3 Residue-property plots

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.

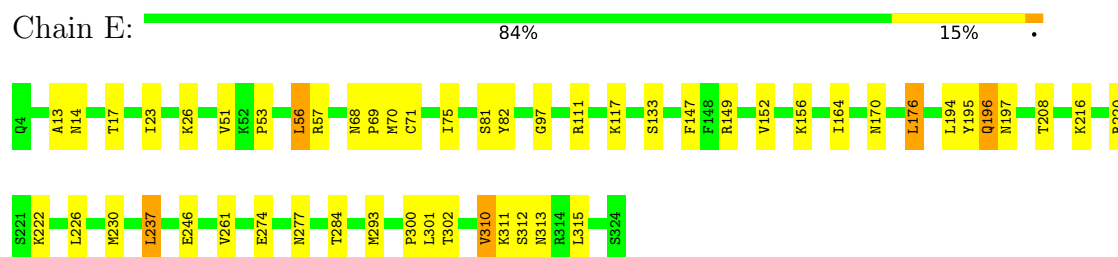
• Molecule 1: Hemagglutinin



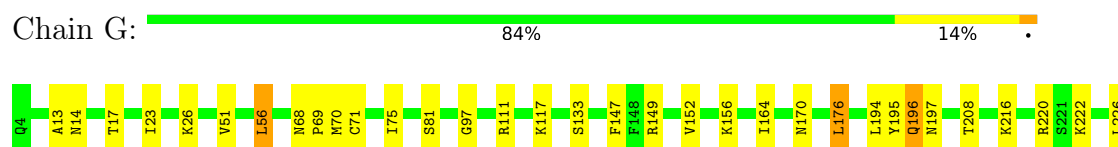
• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin

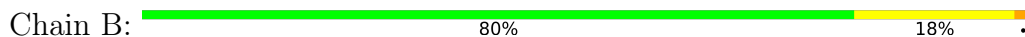


• Molecule 1: Hemagglutinin

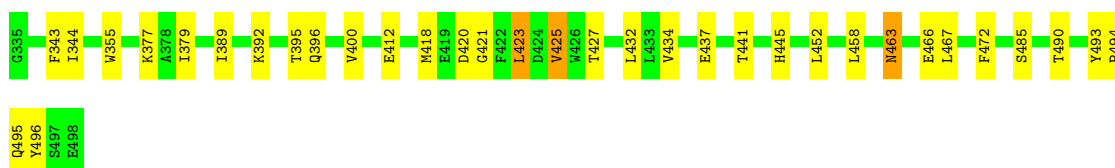
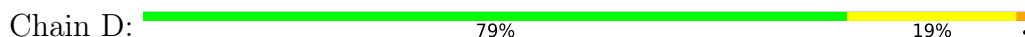




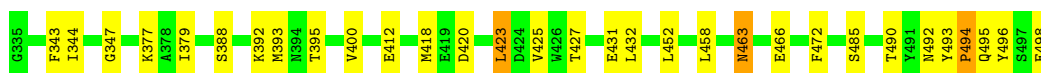
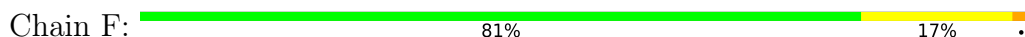
• Molecule 2: Hemagglutinin



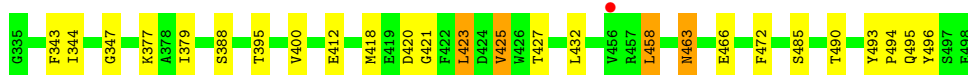
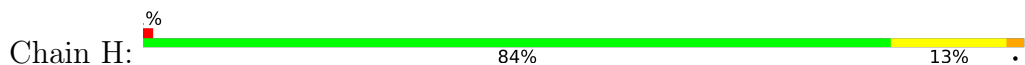
• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



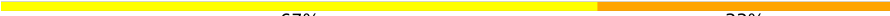
• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose



• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose



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

Chain K:  67% 33%

HA01
GAL2
SIA3

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

Chain L:  33% 33% 33%

HA01
GAL2
SIA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	70.63Å 70.63Å 494.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.12 – 2.70 49.12 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.2 (49.12-2.70) 95.3 (49.12-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.227 , 0.255 0.225 , 0.253	Depositor DCC
R_{free} test set	3634 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.437 for -h,-k,l 0.069 for h,-h-k,-l 0.062 for -k,-h,-l	Xtriage
Reported twinning fraction	0.221 for -h,-k,l	Depositor
Outliers	0 of 72276 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15692	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.5285e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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, GAL, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.39	0/2604	0.79	2/3539 (0.1%)
1	C	0.39	0/2604	0.79	2/3539 (0.1%)
1	E	0.40	0/2604	0.83	5/3539 (0.1%)
1	G	0.39	0/2604	0.79	2/3539 (0.1%)
2	B	0.33	0/1355	0.71	0/1823
2	D	0.32	0/1355	0.71	0/1823
2	F	0.33	0/1355	0.71	0/1823
2	H	0.32	0/1355	0.72	0/1823
All	All	0.37	0/15836	0.77	11/21448 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	57	ARG	NE-CZ-NH1	-10.88	110.61	121.50
1	E	57	ARG	NE-CZ-NH2	9.89	128.10	119.20
1	E	57	ARG	CD-NE-CZ	9.62	137.88	124.40
1	G	56	LEU	N-CA-C	-5.65	102.03	110.23
1	G	14	ASN	N-CA-C	5.59	114.92	108.49
1	E	14	ASN	N-CA-C	5.49	114.81	108.49
1	A	14	ASN	N-CA-C	5.48	114.79	108.49
1	C	14	ASN	N-CA-C	5.43	114.73	108.49
1	C	56	LEU	N-CA-C	-5.32	102.52	110.23
1	A	56	LEU	N-CA-C	-5.28	102.57	110.23
1	E	56	LEU	N-CA-C	-5.15	102.77	110.23

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	2542	0	2483	22	0
1	C	2542	0	2483	25	0
1	E	2542	0	2483	18	1
1	G	2542	0	2483	18	1
2	B	1328	0	1231	13	0
2	D	1328	0	1231	14	0
2	F	1328	0	1231	10	1
2	H	1328	0	1231	8	1
3	I	32	0	27	1	0
3	J	32	0	27	2	0
4	K	46	0	39	1	0
4	L	46	0	39	1	0
5	A	14	0	13	0	0
5	C	14	0	13	0	0
5	E	14	0	13	0	0
5	G	14	0	13	0	0
All	All	15692	0	15040	109	2

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 4.

All (109) 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:E:216:LYS:O	1:E:220:ARG:NH2	2.22	0.73
1:A:216:LYS:O	1:A:220:ARG:NH2	2.23	0.72
1:C:216:LYS:O	1:C:220:ARG:NH2	2.24	0.71
1:G:216:LYS:O	1:G:220:ARG:NH2	2.25	0.70
1:C:95:TYR:OH	3:J:2:SIA:H91	2.00	0.62
1:G:51:VAL:HG13	1:G:81:SER:HB3	1.83	0.61
1:A:51:VAL:HG13	1:A:81:SER:HB3	1.83	0.60
1:E:51:VAL:HG13	1:E:81:SER:HB3	1.84	0.59
1:C:51:VAL:HG13	1:C:81:SER:HB3	1.84	0.58
1:C:12:HIS:HB2	2:D:355:TRP:HA	1.86	0.57
1:C:317:LEU:HD21	2:D:389:ILE:HD12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LEU:HD21	2:B:389:ILE:HD12	1.88	0.55
1:C:321:LEU:HB3	2:D:445:HIS:CD2	2.43	0.54
1:G:310:VAL:HG12	1:G:312:SER:H	1.75	0.52
1:A:12:HIS:HB2	2:B:355:TRP:HA	1.91	0.52
1:G:170:ASN:HB2	1:G:237:LEU:HD13	1.92	0.52
1:G:195:TYR:O	1:G:197:ASN:N	2.41	0.52
1:E:312:SER:OG	2:F:431:GLU:OE2	2.19	0.52
1:C:170:ASN:HB2	1:C:237:LEU:HD13	1.92	0.51
1:A:97:GLY:HA3	1:A:230:MET:O	2.11	0.51
1:E:170:ASN:HB2	1:E:237:LEU:HD13	1.93	0.51
1:A:321:LEU:HB3	2:B:445:HIS:CD2	2.46	0.51
1:E:310:VAL:HG12	1:E:312:SER:H	1.75	0.50
1:A:310:VAL:HG12	1:A:312:SER:H	1.75	0.50
1:G:97:GLY:HA3	1:G:230:MET:O	2.12	0.50
1:C:195:TYR:O	1:C:197:ASN:N	2.43	0.49
1:E:133:SER:O	4:K:3:SIA:H113	2.13	0.49
1:C:310:VAL:HG12	1:C:312:SER:H	1.75	0.49
1:E:164:ILE:O	1:E:246:GLU:HA	2.12	0.49
2:B:343:PHE:CD1	2:B:344:ILE:HG13	2.48	0.49
1:C:311:LYS:HE3	2:D:423:LEU:HD11	1.92	0.49
1:E:156:LYS:HD2	1:E:196:GLN:HG2	1.94	0.49
1:A:311:LYS:HE3	2:B:423:LEU:HD11	1.93	0.48
1:C:97:GLY:HA3	1:C:230:MET:O	2.13	0.48
1:A:222:LYS:HA	1:A:226:LEU:O	2.14	0.48
2:F:343:PHE:CD1	2:F:344:ILE:HG13	2.49	0.48
1:E:97:GLY:HA3	1:E:230:MET:O	2.14	0.48
2:B:463:ASN:N	2:B:463:ASN:OD1	2.47	0.48
1:C:164:ILE:O	1:C:246:GLU:HA	2.13	0.48
2:D:343:PHE:CD1	2:D:344:ILE:HG13	2.48	0.48
1:G:164:ILE:O	1:G:246:GLU:HA	2.13	0.48
1:A:170:ASN:HB2	1:A:237:LEU:HD13	1.96	0.48
1:C:68:ASN:HB3	1:C:71:CYS:SG	2.53	0.47
1:A:300:PRO:HG2	1:A:301:LEU:HD12	1.96	0.47
2:F:463:ASN:N	2:F:463:ASN:OD1	2.47	0.47
1:G:156:LYS:HD2	1:G:196:GLN:HG2	1.96	0.47
1:G:68:ASN:HB3	1:G:71:CYS:SG	2.54	0.47
1:A:164:ILE:O	1:A:246:GLU:HA	2.13	0.47
1:G:311:LYS:HE3	2:H:423:LEU:HD11	1.97	0.47
1:C:300:PRO:HG2	1:C:301:LEU:HD12	1.97	0.47
2:H:343:PHE:CD1	2:H:344:ILE:HG13	2.49	0.47
1:C:317:LEU:HD13	2:D:434:VAL:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:311:LYS:HE3	2:F:423:LEU:HD11	1.97	0.47
2:D:463:ASN:N	2:D:463:ASN:OD1	2.47	0.47
1:G:133:SER:O	4:L:3:SIA:H113	2.14	0.47
1:C:315:LEU:HD22	2:D:434:VAL:HG21	1.98	0.46
1:E:68:ASN:HB3	1:E:71:CYS:SG	2.56	0.46
1:G:300:PRO:HG2	1:G:301:LEU:HD12	1.97	0.46
1:A:156:LYS:HD2	1:A:196:GLN:HG2	1.97	0.46
1:E:300:PRO:HG2	1:E:301:LEU:HD12	1.97	0.46
2:H:463:ASN:OD1	2:H:463:ASN:N	2.47	0.46
1:C:156:LYS:HD2	1:C:196:GLN:HG2	1.97	0.46
1:E:195:TYR:O	1:E:197:ASN:N	2.44	0.45
1:E:13:ALA:HB2	2:F:347:GLY:HA3	1.99	0.45
1:C:222:LYS:HA	1:C:226:LEU:O	2.16	0.45
1:C:315:LEU:HD23	1:C:315:LEU:HA	1.82	0.45
1:A:315:LEU:HD22	2:B:434:VAL:HG21	1.99	0.45
1:A:308:LYS:HB3	2:B:396:GLN:NE2	2.31	0.45
1:C:190:GLU:OE2	3:J:2:SIA:O9	2.35	0.45
1:G:222:LYS:HA	1:G:226:LEU:O	2.16	0.45
1:A:317:LEU:HD13	2:B:434:VAL:HG22	1.98	0.44
1:A:68:ASN:HB3	1:A:71:CYS:SG	2.56	0.44
1:E:222:LYS:HA	1:E:226:LEU:O	2.18	0.44
2:B:493:TYR:O	2:B:495:GLN:N	2.51	0.43
2:D:452:LEU:HD12	2:D:452:LEU:HA	1.89	0.43
1:G:317:LEU:HD12	1:G:317:LEU:HA	1.87	0.43
1:E:176:LEU:HD23	1:E:176:LEU:HA	1.86	0.43
1:C:308:LYS:HB3	2:D:396:GLN:NE2	2.32	0.43
1:A:195:TYR:O	1:A:197:ASN:N	2.44	0.43
2:D:493:TYR:O	2:D:495:GLN:N	2.51	0.42
2:D:466:GLU:HA	2:D:472:PHE:HD2	1.84	0.42
2:F:452:LEU:HD12	2:F:452:LEU:HA	1.90	0.42
1:G:176:LEU:HD23	1:G:176:LEU:HA	1.86	0.42
1:A:317:LEU:HD12	1:A:317:LEU:HA	1.85	0.42
2:B:466:GLU:HA	2:B:472:PHE:HD2	1.84	0.42
2:H:493:TYR:O	2:H:495:GLN:N	2.53	0.42
2:F:493:TYR:O	2:F:495:GLN:N	2.53	0.42
1:A:133:SER:O	3:I:2:SIA:H113	2.19	0.42
2:F:393:MET:HE2	2:F:393:MET:HB3	1.94	0.42
2:F:466:GLU:HA	2:F:472:PHE:HD2	1.85	0.42
2:D:421:GLY:O	2:D:425:VAL:HG13	2.20	0.41
2:B:421:GLY:O	2:B:425:VAL:HG13	2.20	0.41
1:G:69:PRO:HG3	1:G:147:PHE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:MET:HE2	2:B:393:MET:HB3	1.94	0.41
1:C:53:PRO:HB3	1:C:82:TYR:CZ	2.55	0.41
1:G:315:LEU:HD23	1:G:315:LEU:HA	1.82	0.41
1:C:286:MET:HE2	1:C:286:MET:HB3	1.92	0.41
1:G:13:ALA:HB2	2:H:347:GLY:HA3	2.02	0.41
2:H:421:GLY:O	2:H:425:VAL:HG13	2.21	0.41
2:H:466:GLU:HA	2:H:472:PHE:HD2	1.85	0.41
1:C:237:LEU:HD23	1:C:237:LEU:HA	1.93	0.41
1:A:53:PRO:HB3	1:A:82:TYR:CZ	2.56	0.40
1:A:180:TRP:HB3	1:A:254:PRO:HG3	2.03	0.40
2:D:437:GLU:O	2:D:441:THR:OG1	2.33	0.40
1:E:53:PRO:HB3	1:E:82:TYR:CZ	2.57	0.40
1:E:69:PRO:HG3	1:E:147:PHE:O	2.21	0.40
2:H:458:LEU:HD13	2:H:458:LEU:HA	1.94	0.40
1:C:36:ILE:C	1:C:293:MET:HG3	2.46	0.40
2:F:492:ASN:OD1	2:F:494:PRO:HD2	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:LYS:NZ	2:F:388:SER:OG[3_655]	2.06	0.14
1:G:26:LYS:NZ	2:H:388:SER:OG[3_665]	2.06	0.14

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	319/321 (99%)	305 (96%)	13 (4%)	1 (0%)	36 60
1	C	319/321 (99%)	306 (96%)	12 (4%)	1 (0%)	36 60
1	E	319/321 (99%)	307 (96%)	11 (3%)	1 (0%)	36 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	319/321 (99%)	306 (96%)	12 (4%)	1 (0%)	36	60
2	B	162/164 (99%)	150 (93%)	10 (6%)	2 (1%)	10	27
2	D	162/164 (99%)	149 (92%)	11 (7%)	2 (1%)	10	27
2	F	162/164 (99%)	149 (92%)	11 (7%)	2 (1%)	10	27
2	H	162/164 (99%)	150 (93%)	10 (6%)	2 (1%)	10	27
All	All	1924/1940 (99%)	1822 (95%)	90 (5%)	12 (1%)	21	44

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	496	TYR
2	D	496	TYR
2	F	496	TYR
2	H	496	TYR
2	B	494	PRO
2	D	494	PRO
2	F	494	PRO
2	H	494	PRO
1	A	196	GLN
1	C	196	GLN
1	G	196	GLN
1	E	196	GLN

5.3.2 Protein sidechains ⓘ

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	288/288 (100%)	266 (92%)	22 (8%)	12	30
1	C	288/288 (100%)	266 (92%)	22 (8%)	12	30
1	E	288/288 (100%)	266 (92%)	22 (8%)	12	30
1	G	288/288 (100%)	266 (92%)	22 (8%)	12	30
2	B	140/140 (100%)	123 (88%)	17 (12%)	5	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	140/140 (100%)	123 (88%)	17 (12%)	5	12
2	F	140/140 (100%)	123 (88%)	17 (12%)	5	12
2	H	140/140 (100%)	125 (89%)	15 (11%)	6	16
All	All	1712/1712 (100%)	1558 (91%)	154 (9%)	9	23

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	23	ILE
1	A	56	LEU
1	A	70	MET
1	A	75	ILE
1	A	111	ARG
1	A	117	LYS
1	A	149	ARG
1	A	152	VAL
1	A	176	LEU
1	A	194	LEU
1	A	208	THR
1	A	237	LEU
1	A	261	VAL
1	A	274	GLU
1	A	277	ASN
1	A	284	THR
1	A	293	MET
1	A	302	THR
1	A	310	VAL
1	A	313	ASN
1	A	315	LEU
2	B	377	LYS
2	B	379	ILE
2	B	392	LYS
2	B	395	THR
2	B	400	VAL
2	B	412	GLU
2	B	418	MET
2	B	420	ASP
2	B	423	LEU
2	B	425	VAL
2	B	427	THR

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Mol	Chain	Res	Type
2	B	432	LEU
2	B	458	LEU
2	B	463	ASN
2	B	485	SER
2	B	490	THR
2	B	498	GLU
1	C	17	THR
1	C	23	ILE
1	C	56	LEU
1	C	70	MET
1	C	75	ILE
1	C	111	ARG
1	C	117	LYS
1	C	149	ARG
1	C	152	VAL
1	C	176	LEU
1	C	194	LEU
1	C	208	THR
1	C	237	LEU
1	C	261	VAL
1	C	274	GLU
1	C	277	ASN
1	C	284	THR
1	C	293	MET
1	C	302	THR
1	C	310	VAL
1	C	313	ASN
1	C	315	LEU
2	D	377	LYS
2	D	379	ILE
2	D	392	LYS
2	D	395	THR
2	D	400	VAL
2	D	412	GLU
2	D	418	MET
2	D	420	ASP
2	D	423	LEU
2	D	425	VAL
2	D	427	THR
2	D	432	LEU
2	D	458	LEU
2	D	463	ASN

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Mol	Chain	Res	Type
2	D	467	LEU
2	D	485	SER
2	D	490	THR
1	E	17	THR
1	E	23	ILE
1	E	56	LEU
1	E	70	MET
1	E	75	ILE
1	E	111	ARG
1	E	117	LYS
1	E	149	ARG
1	E	152	VAL
1	E	176	LEU
1	E	194	LEU
1	E	208	THR
1	E	237	LEU
1	E	261	VAL
1	E	274	GLU
1	E	277	ASN
1	E	284	THR
1	E	293	MET
1	E	302	THR
1	E	310	VAL
1	E	313	ASN
1	E	315	LEU
2	F	377	LYS
2	F	379	ILE
2	F	392	LYS
2	F	395	THR
2	F	400	VAL
2	F	412	GLU
2	F	418	MET
2	F	420	ASP
2	F	423	LEU
2	F	425	VAL
2	F	427	THR
2	F	432	LEU
2	F	458	LEU
2	F	463	ASN
2	F	485	SER
2	F	490	THR
2	F	498	GLU

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Mol	Chain	Res	Type
1	G	17	THR
1	G	23	ILE
1	G	56	LEU
1	G	70	MET
1	G	75	ILE
1	G	111	ARG
1	G	117	LYS
1	G	149	ARG
1	G	152	VAL
1	G	176	LEU
1	G	194	LEU
1	G	208	THR
1	G	237	LEU
1	G	261	VAL
1	G	274	GLU
1	G	277	ASN
1	G	284	THR
1	G	293	MET
1	G	302	THR
1	G	310	VAL
1	G	313	ASN
1	G	315	LEU
2	H	377	LYS
2	H	379	ILE
2	H	395	THR
2	H	400	VAL
2	H	412	GLU
2	H	418	MET
2	H	420	ASP
2	H	423	LEU
2	H	425	VAL
2	H	427	THR
2	H	432	LEU
2	H	458	LEU
2	H	463	ASN
2	H	485	SER
2	H	490	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN

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Mol	Chain	Res	Type
1	A	119	GLN
1	A	173	GLN
1	A	196	GLN
2	B	396	GLN
2	B	413	ASN
2	B	459	GLN
1	C	19	GLN
1	C	173	GLN
1	C	196	GLN
1	C	240	ASN
2	D	396	GLN
2	D	413	ASN
2	D	459	GLN
1	E	12	HIS
1	E	32	HIS
1	E	173	GLN
1	E	196	GLN
2	F	396	GLN
2	F	413	ASN
2	F	459	GLN
1	G	12	HIS
1	G	19	GLN
1	G	32	HIS
1	G	172	ASN
1	G	173	GLN
1	G	196	GLN
2	H	396	GLN
2	H	413	ASN
2	H	459	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 ⓘ

10 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GAL	I	1	3	12,12,12	0.49	0	17,17,17	1.22	1 (5%)
3	SIA	I	2	3	20,20,21	3.72	7 (35%)	21,28,31	3.24	4 (19%)
3	GAL	J	1	3	12,12,12	0.47	0	17,17,17	0.92	1 (5%)
3	SIA	J	2	3	20,20,21	3.63	10 (50%)	21,28,31	3.03	5 (23%)
4	NAG	K	1	4	15,15,15	0.41	0	21,21,21	1.21	2 (9%)
4	GAL	K	2	4	11,11,12	0.62	0	15,15,17	1.59	1 (6%)
4	SIA	K	3	4	20,20,21	3.59	9 (45%)	21,28,31	3.20	4 (19%)
4	NAG	L	1	4	15,15,15	0.42	0	21,21,21	0.78	0
4	GAL	L	2	4	11,11,12	0.67	0	15,15,17	1.53	1 (6%)
4	SIA	L	3	4	20,20,21	3.59	9 (45%)	21,28,31	3.39	6 (28%)

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

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

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	2	SIA	C4-C5	-11.62	1.42	1.53
3	J	2	SIA	C4-C5	-11.06	1.43	1.53
4	K	3	SIA	C4-C5	-10.63	1.43	1.53
4	L	3	SIA	C4-C5	-10.38	1.44	1.53
4	L	3	SIA	C7-C6	-8.53	1.42	1.52
4	K	3	SIA	C7-C6	-8.46	1.42	1.52
3	J	2	SIA	C7-C6	-8.13	1.42	1.52
3	I	2	SIA	C7-C6	-8.04	1.43	1.52
4	L	3	SIA	C10-N5	4.87	1.50	1.34
4	K	3	SIA	C10-N5	4.76	1.49	1.34
3	I	2	SIA	C10-N5	4.75	1.49	1.34
3	J	2	SIA	C10-N5	4.58	1.49	1.34
4	L	3	SIA	O6-C6	3.86	1.49	1.44
4	K	3	SIA	O6-C6	3.77	1.49	1.44
3	I	2	SIA	O6-C6	3.69	1.49	1.44
3	J	2	SIA	O6-C6	3.64	1.49	1.44
3	I	2	SIA	C2-C1	-3.05	1.48	1.52
3	J	2	SIA	O6-C2	-2.70	1.38	1.43
4	L	3	SIA	C3-C2	2.60	1.56	1.52
3	I	2	SIA	O6-C2	-2.59	1.38	1.43
4	K	3	SIA	O6-C2	-2.56	1.38	1.43
3	J	2	SIA	C2-C1	-2.50	1.49	1.52
4	L	3	SIA	O6-C2	-2.48	1.38	1.43
4	L	3	SIA	C5-N5	2.43	1.49	1.45
3	I	2	SIA	O8-C8	-2.41	1.38	1.43
3	J	2	SIA	C5-N5	2.30	1.49	1.45
4	K	3	SIA	C3-C2	2.29	1.56	1.52
3	J	2	SIA	O8-C8	-2.27	1.38	1.43
4	L	3	SIA	C2-C1	-2.27	1.49	1.52
4	L	3	SIA	O7-C7	-2.19	1.37	1.43
4	K	3	SIA	C5-N5	2.17	1.49	1.45
4	K	3	SIA	O8-C8	-2.08	1.39	1.43
4	K	3	SIA	C2-C1	-2.06	1.49	1.52
3	J	2	SIA	C3-C2	2.06	1.55	1.52
3	J	2	SIA	O7-C7	-2.00	1.38	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	3	SIA	O6-C2-C3	-10.85	95.97	110.56
3	I	2	SIA	O6-C2-C3	-10.62	96.27	110.56
4	K	3	SIA	O6-C2-C3	-10.36	96.63	110.56
3	J	2	SIA	O6-C2-C3	-9.70	97.51	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	3	SIA	O6-C2-C1	8.23	123.26	107.72
3	I	2	SIA	O6-C2-C1	8.07	122.96	107.72
4	K	3	SIA	O6-C2-C1	7.33	121.56	107.72
3	J	2	SIA	O6-C2-C1	7.32	121.53	107.72
4	K	2	GAL	C1-O5-C5	-5.38	104.98	112.19
4	L	2	GAL	C1-O5-C5	-5.25	105.16	112.19
4	K	3	SIA	C8-C7-C6	-4.26	105.05	113.05
3	I	2	SIA	C8-C7-C6	-3.45	106.58	113.05
3	J	2	SIA	O1B-C1-C2	3.28	121.24	112.71
4	K	3	SIA	O1B-C1-C2	3.20	121.03	112.71
4	L	3	SIA	O9-C9-C8	3.18	117.83	111.16
4	K	1	NAG	C1-C2-C3	3.10	114.78	110.54
4	L	3	SIA	O1B-C1-C2	2.96	120.40	112.71
4	L	3	SIA	C8-C7-C6	-2.91	107.59	113.05
3	I	2	SIA	O1B-C1-C2	2.81	120.03	112.71
3	J	2	SIA	C8-C7-C6	-2.77	107.84	113.05
3	I	1	GAL	C6-C5-C4	-2.48	106.93	113.02
3	J	1	GAL	C6-C5-C4	-2.36	107.22	113.02
4	L	3	SIA	C11-C10-N5	2.16	119.70	116.12
3	J	2	SIA	C11-C10-N5	2.12	119.63	116.12
4	K	1	NAG	O5-C1-C2	2.03	111.56	109.52

There are no chirality outliers.

All (13) torsion outliers are listed below:

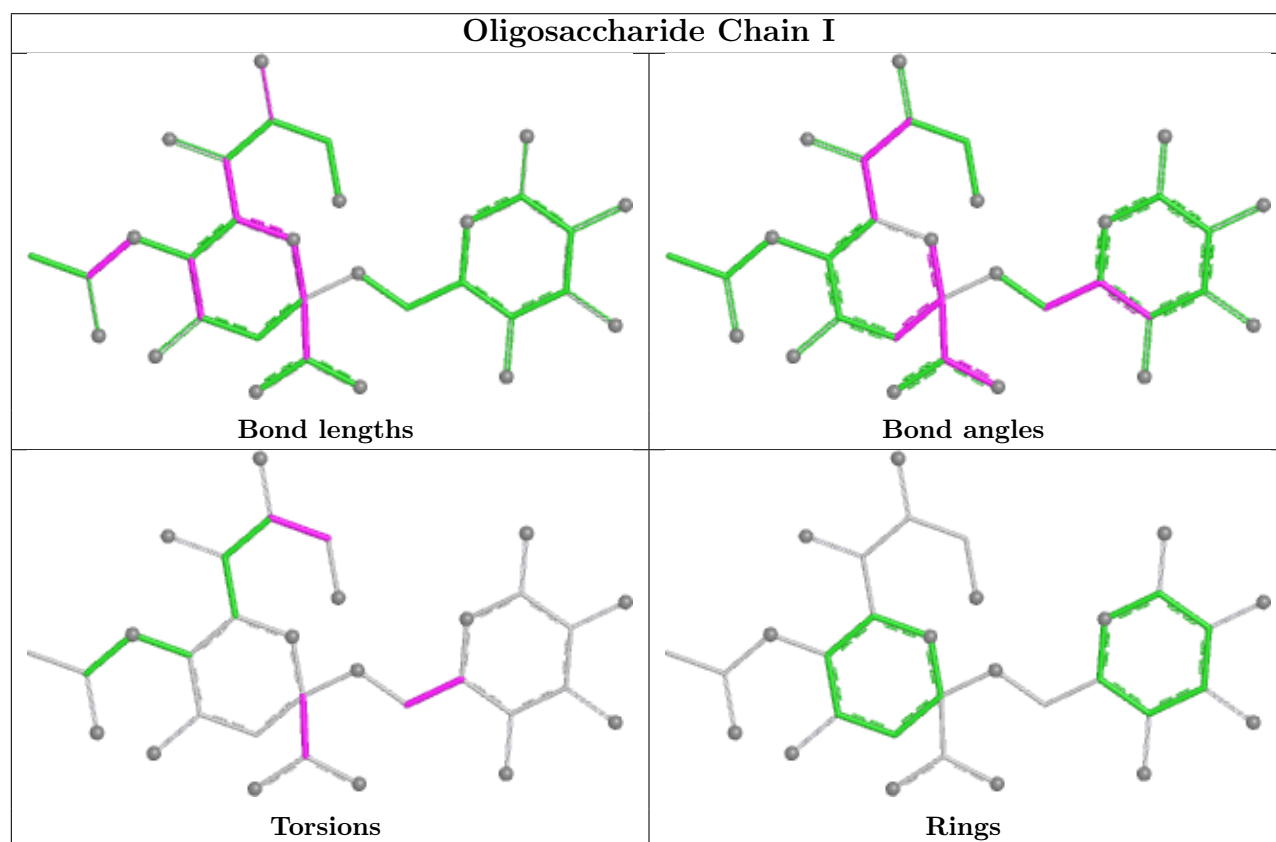
Mol	Chain	Res	Type	Atoms
3	I	2	SIA	O8-C8-C9-O9
3	J	2	SIA	C7-C8-C9-O9
4	K	3	SIA	O1A-C1-C2-O6
4	K	3	SIA	O8-C8-C9-O9
3	J	2	SIA	O8-C8-C9-O9
3	I	2	SIA	C7-C8-C9-O9
3	I	1	GAL	C4-C5-C6-O6
3	I	1	GAL	O5-C5-C6-O6
4	K	3	SIA	C7-C8-C9-O9
4	L	3	SIA	O8-C8-C9-O9
3	J	2	SIA	O1A-C1-C2-O6
3	I	2	SIA	O1A-C1-C2-O6
4	L	3	SIA	O1A-C1-C2-O6

There are no ring outliers.

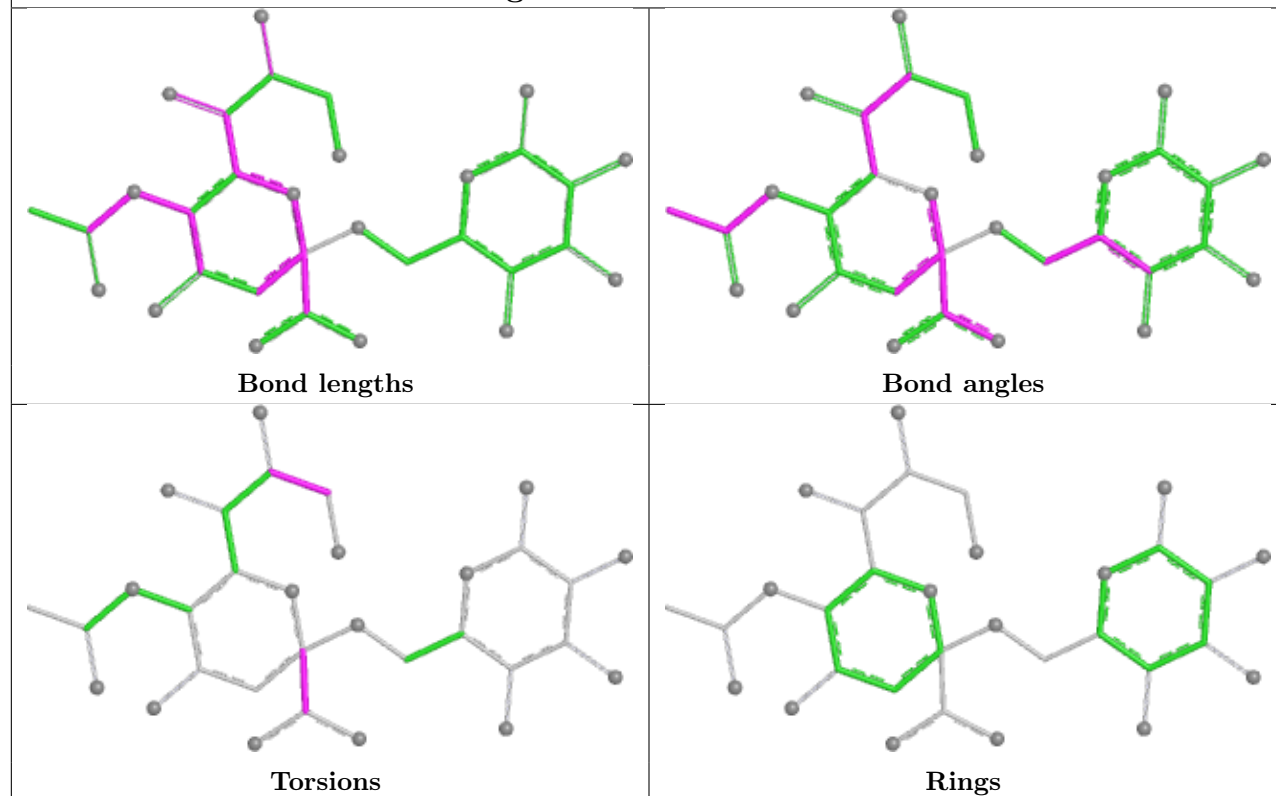
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	3	SIA	1	0
3	I	2	SIA	1	0
3	J	2	SIA	2	0
4	L	3	SIA	1	0

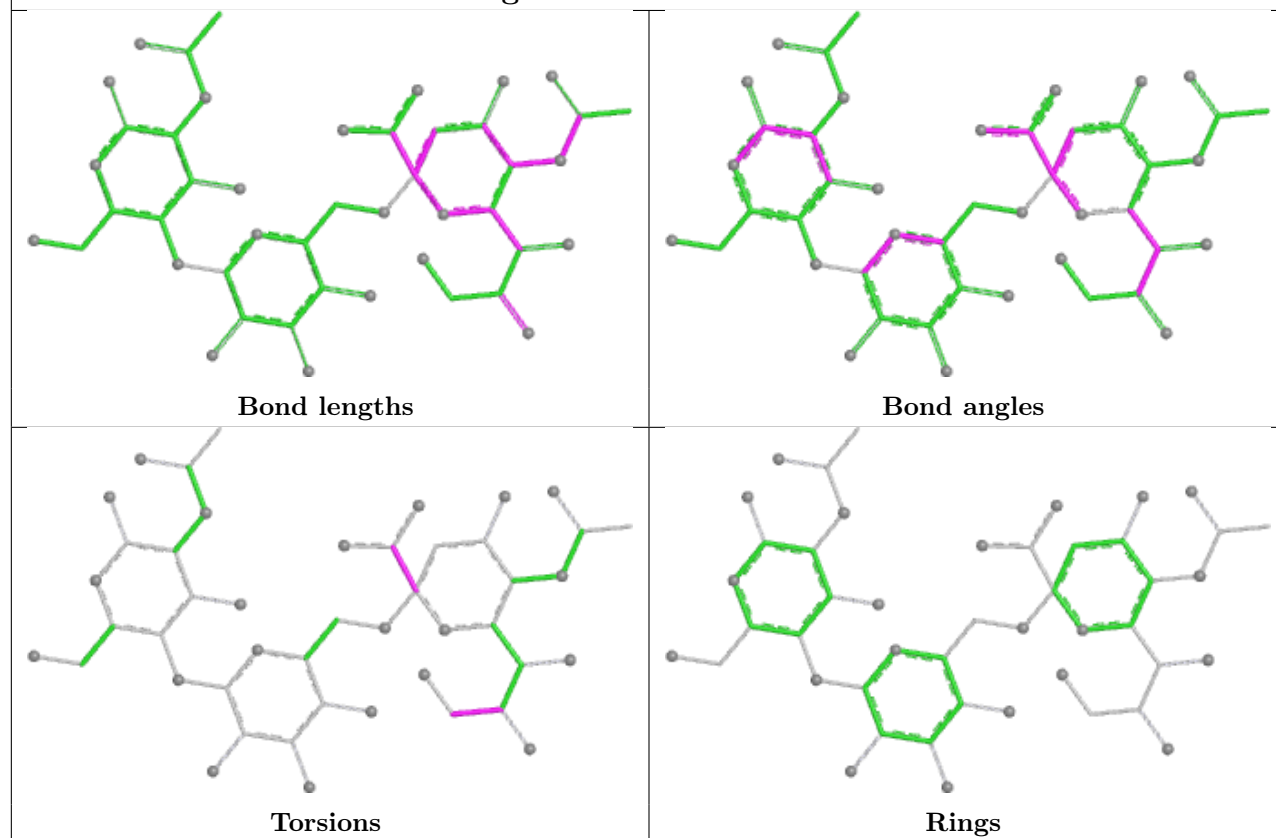
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

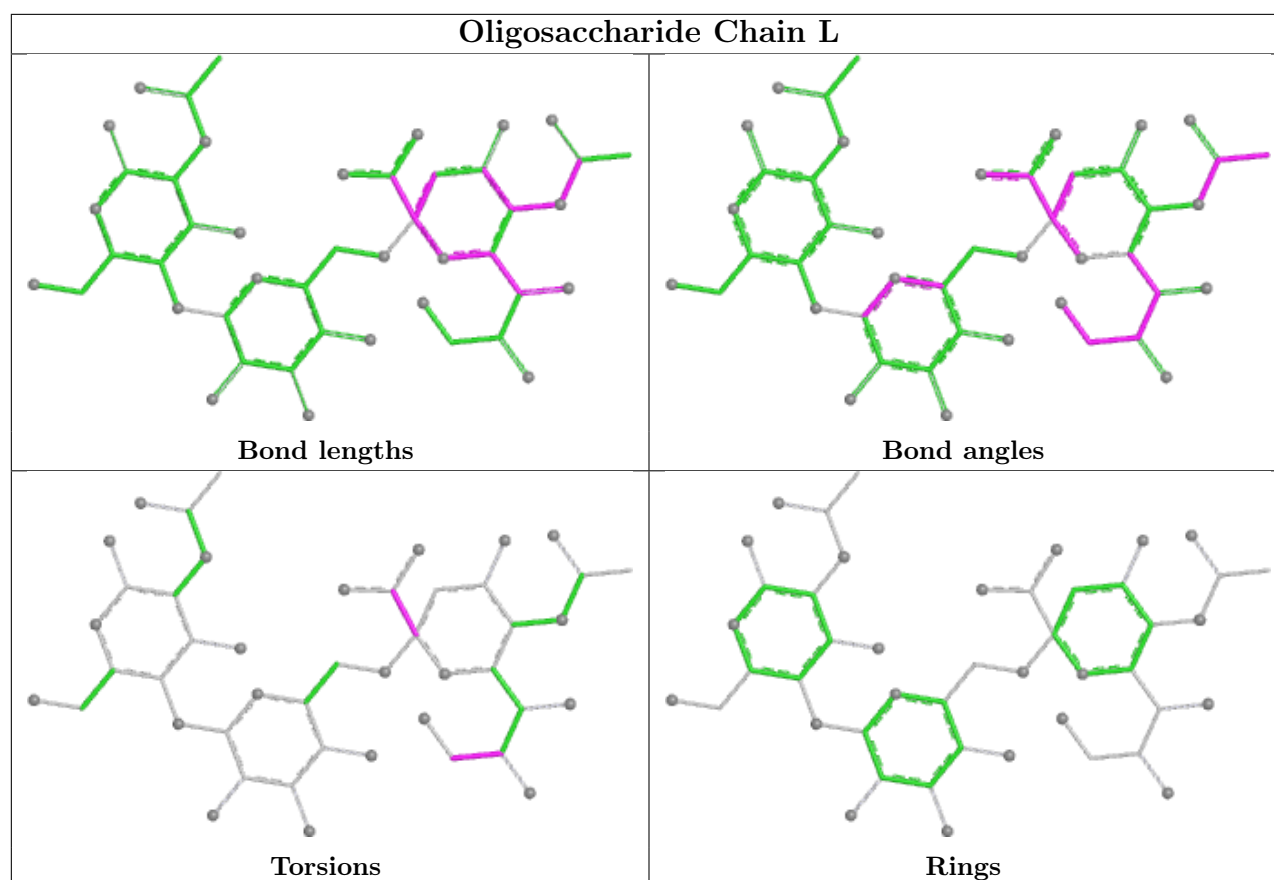


Oligosaccharide Chain J



Oligosaccharide Chain K





5.6 Ligand geometry [i](#)

4 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	E	601	1	14,14,15	0.55	0	17,19,21	1.10	1 (5%)
5	NAG	G	601	1	14,14,15	0.56	0	17,19,21	0.86	1 (5%)
5	NAG	A	601	1	14,14,15	0.50	0	17,19,21	1.32	2 (11%)
5	NAG	C	601	1	14,14,15	0.46	0	17,19,21	1.33	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
5	NAG	E	601	1	-	0/6/23/26	0/1/1/1
5	NAG	G	601	1	-	2/6/23/26	0/1/1/1
5	NAG	A	601	1	-	2/6/23/26	0/1/1/1
5	NAG	C	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	NAG	C1-O5-C5	3.48	116.84	112.19
5	C	601	NAG	C1-O5-C5	3.28	116.58	112.19
5	A	601	NAG	C2-N2-C7	-2.63	119.38	122.90
5	C	601	NAG	C2-N2-C7	-2.62	119.39	122.90
5	E	601	NAG	C1-C2-N2	-2.26	106.87	110.43
5	G	601	NAG	C1-C2-N2	-2.09	107.15	110.43

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	321/321 (100%)	-1.63	0 100 100	19, 46, 102, 171	0
1	C	321/321 (100%)	-1.64	0 100 100	18, 46, 99, 165	0
1	E	321/321 (100%)	-1.51	0 100 100	18, 48, 130, 244	0
1	G	321/321 (100%)	-1.53	0 100 100	22, 46, 124, 234	0
2	B	164/164 (100%)	-1.04	0 100 100	27, 103, 164, 204	0
2	D	164/164 (100%)	-1.02	0 100 100	28, 103, 167, 189	0
2	F	164/164 (100%)	-0.62	0 100 100	26, 144, 214, 255	0
2	H	164/164 (100%)	-0.53	1 (0%) 85 85	28, 147, 223, 253	0
All	All	1940/1940 (100%)	-1.31	1 (0%) 92 91	18, 58, 177, 255	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	456	VAL	3.1

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

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

6.3 Carbohydrates [i](#)

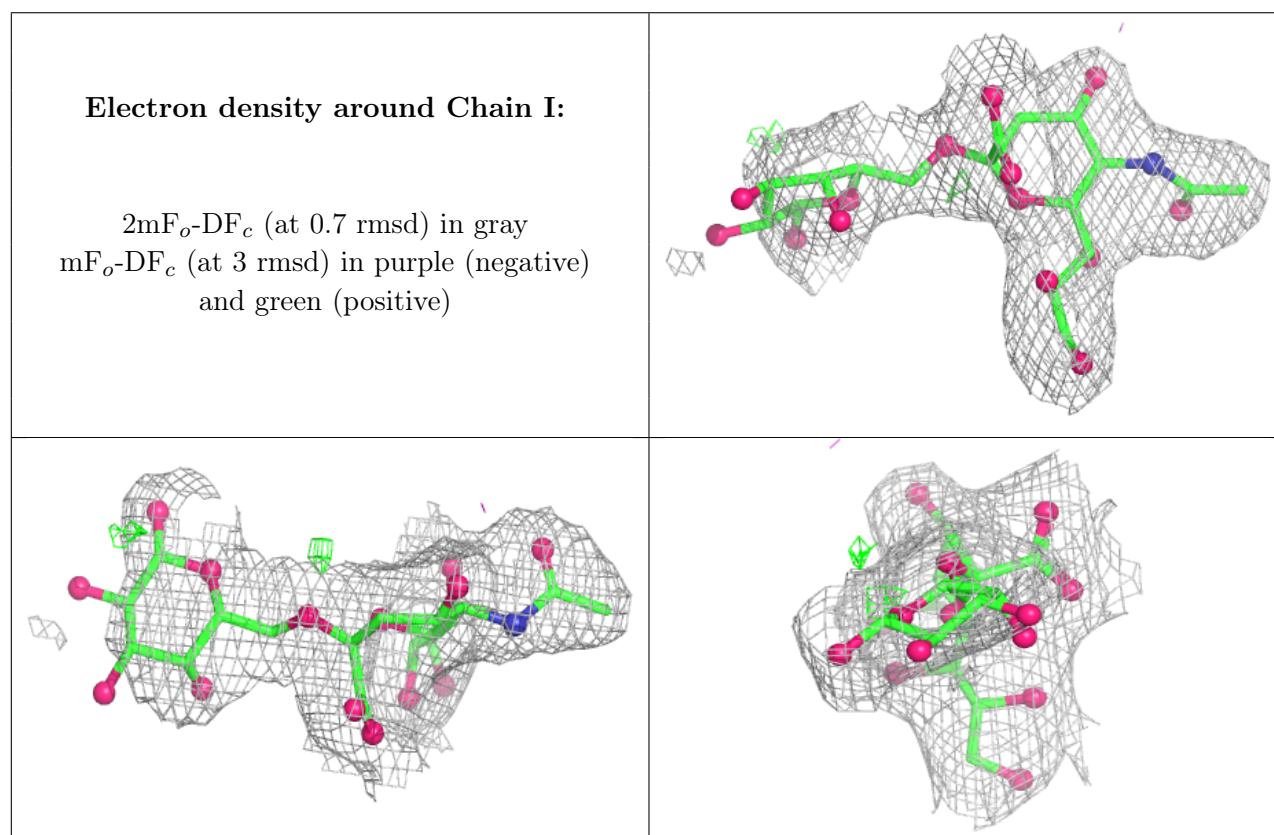
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

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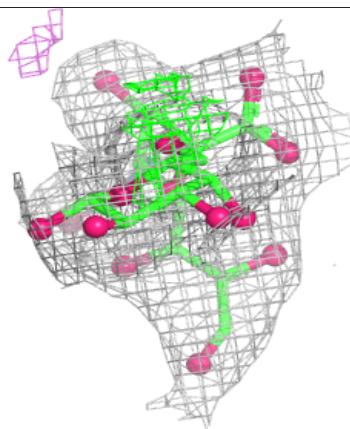
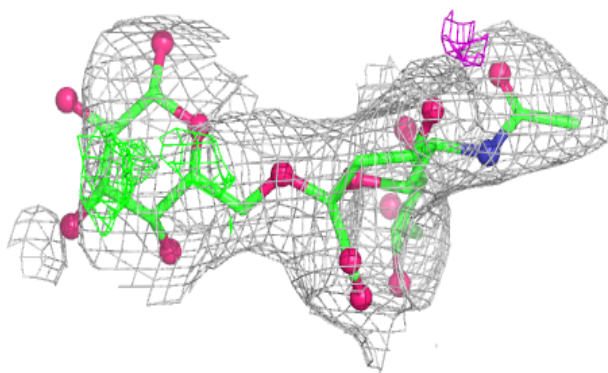
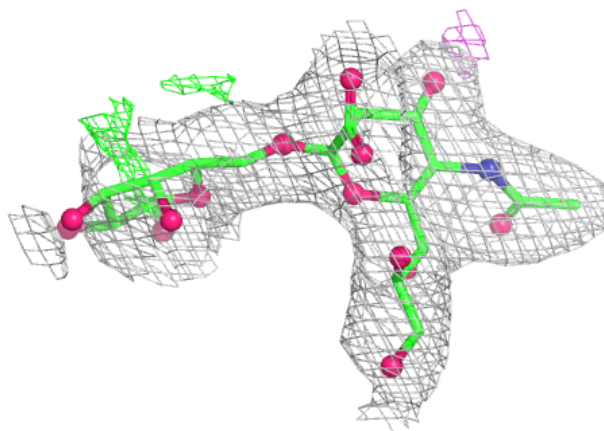
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GAL	J	1	12/12	0.97	0.07	71,111,126,129	0
4	NAG	K	1	15/15	0.97	0.06	110,121,137,139	0
4	NAG	L	1	15/15	0.97	0.05	95,118,133,134	0
3	GAL	I	1	12/12	0.98	0.07	87,101,125,135	0
4	GAL	K	2	11/12	0.99	0.05	61,88,126,129	0
4	GAL	L	2	11/12	0.99	0.05	60,92,113,123	0
4	SIA	K	3	20/21	1.00	0.02	31,47,59,61	0
3	SIA	I	2	20/21	1.00	0.02	30,43,49,53	0
3	SIA	J	2	20/21	1.00	0.03	26,46,56,58	0
4	SIA	L	3	20/21	1.00	0.03	35,47,57,60	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.



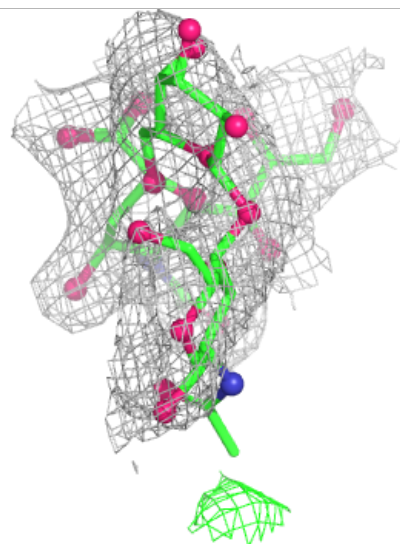
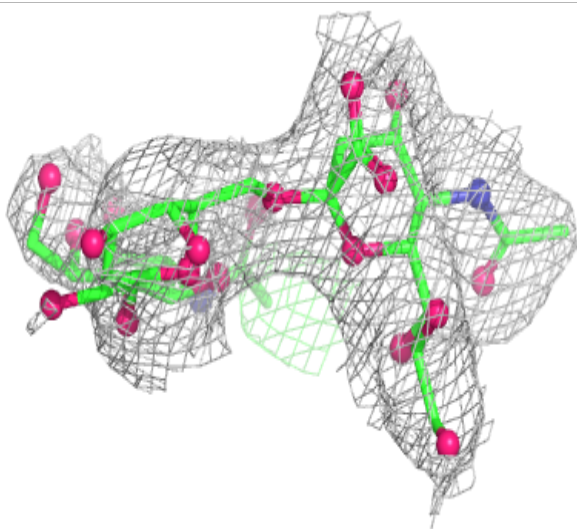
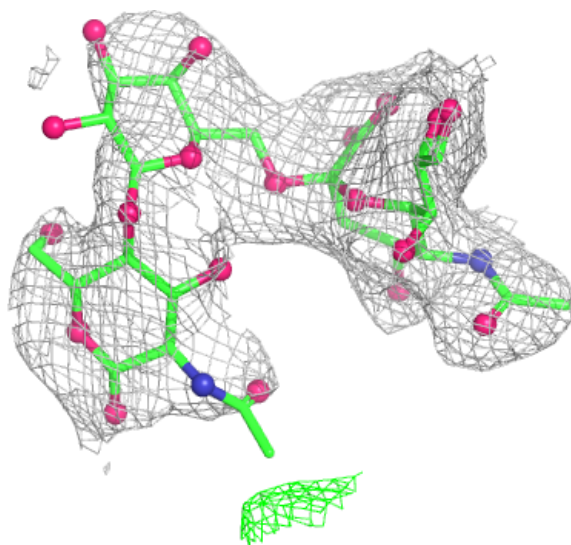
Electron density around Chain J:

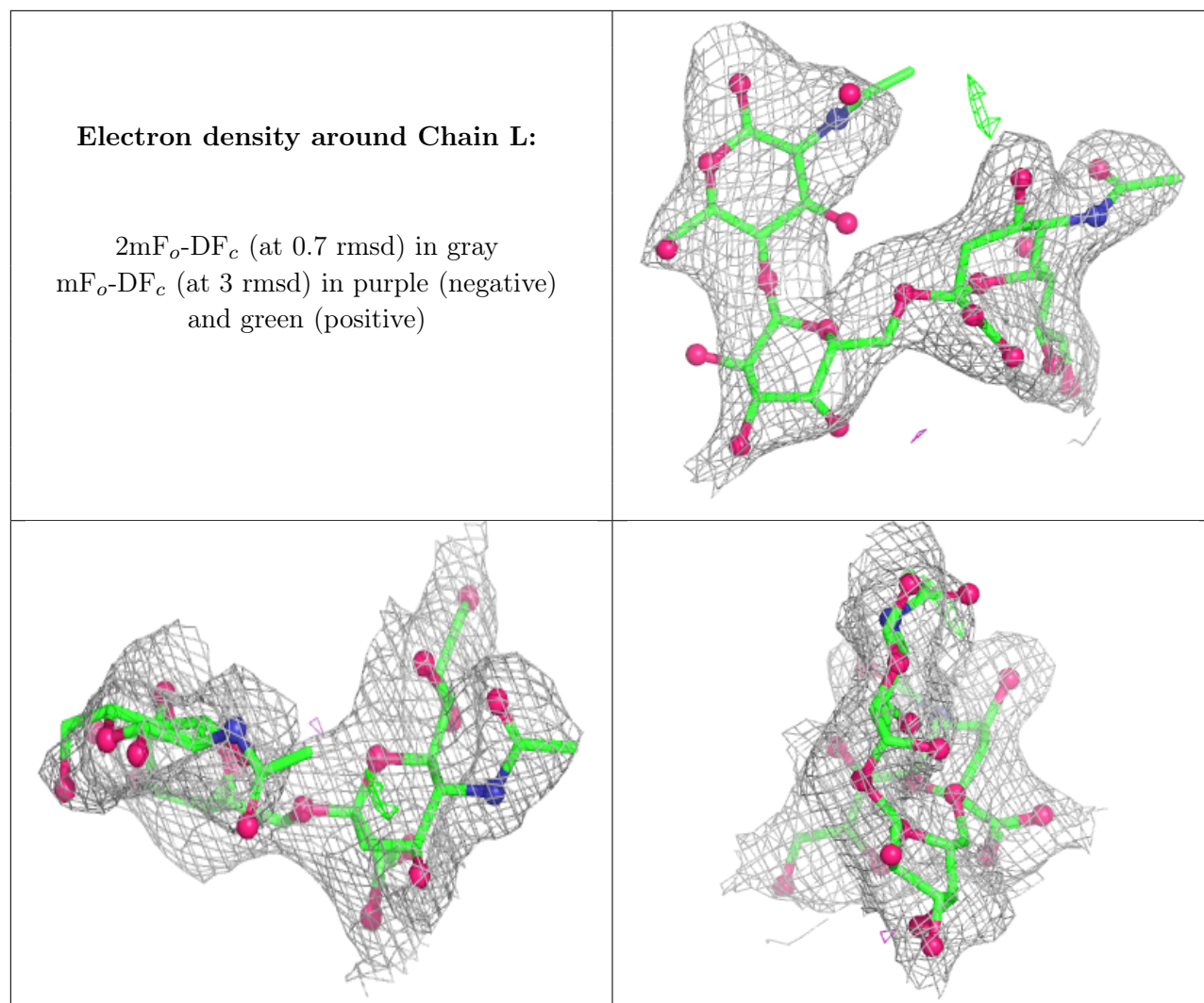
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain K:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	C	601	14/15	0.98	0.04	50,64,83,96	0
5	NAG	A	601	14/15	0.99	0.04	49,75,89,98	0
5	NAG	E	601	14/15	0.99	0.04	44,68,84,85	0
5	NAG	G	601	14/15	0.99	0.04	40,68,80,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.