



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:50 PM UTC

PDB ID : 5XL7 / pdb_00005xl7
Title : The structure of hemagglutinin Q226L mutant from an avian-origin H4N6 influenza virus in complex with human receptor analog LSTc
Authors : Song, H.; Qi, J.; Gao, G.F.
Deposited on : 2017-05-10
Resolution : 2.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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

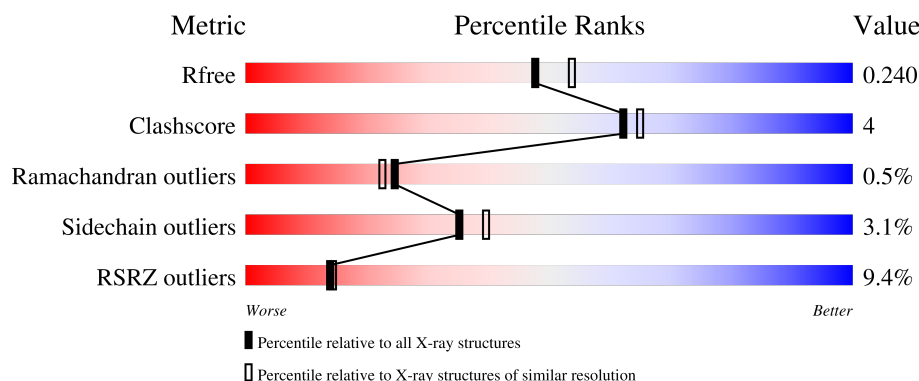
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	327	4% 88% 8% ..
1	B	327	20% 83% 13% ..
2	C	176	3% 91% 7% .
2	D	176	4% 89% 6% ..
3	E	3	33% 33% 33%

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Mol	Chain	Length	Quality of chain
3	F	3	33% 67%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8439 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	319	Total	C	N	O	S	0	0	0
			2458	1541	436	469	12			
1	B	319	Total	C	N	O	S	0	0	0
			2458	1541	436	469	12			

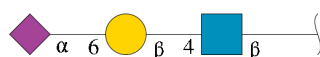
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	223	LEU	GLN	engineered mutation	UNP A3KF09
B	223	LEU	GLN	engineered mutation	UNP A3KF09

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	172	Total	C	N	O	S	0	0	0
			1404	871	250	279	4			
2	D	172	Total	C	N	O	S	0	0	0
			1404	871	250	279	4			

- Molecule 3 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
3	E	3	Total	C	N	O		0	0	0
			46	25	2	19				
3	F	3	Total	C	N	O		0	0	0
			46	25	2	19				

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

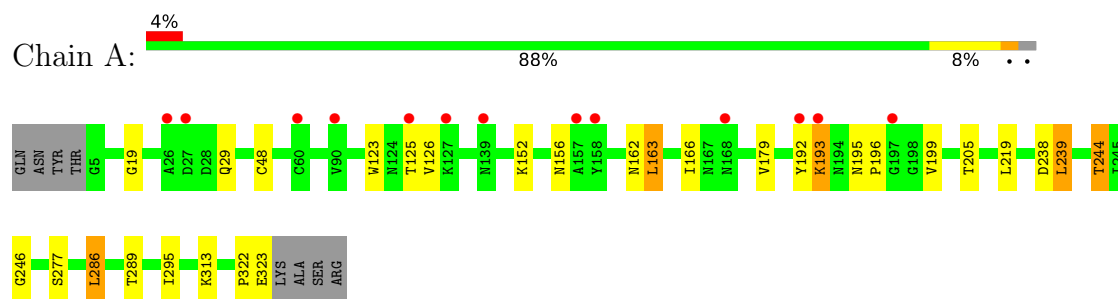
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	173	Total	O	0	0
			173	173		
5	C	165	Total	O	0	0
			165	165		
5	B	90	Total	O	0	0
			90	90		
5	D	139	Total	O	0	0
			139	139		

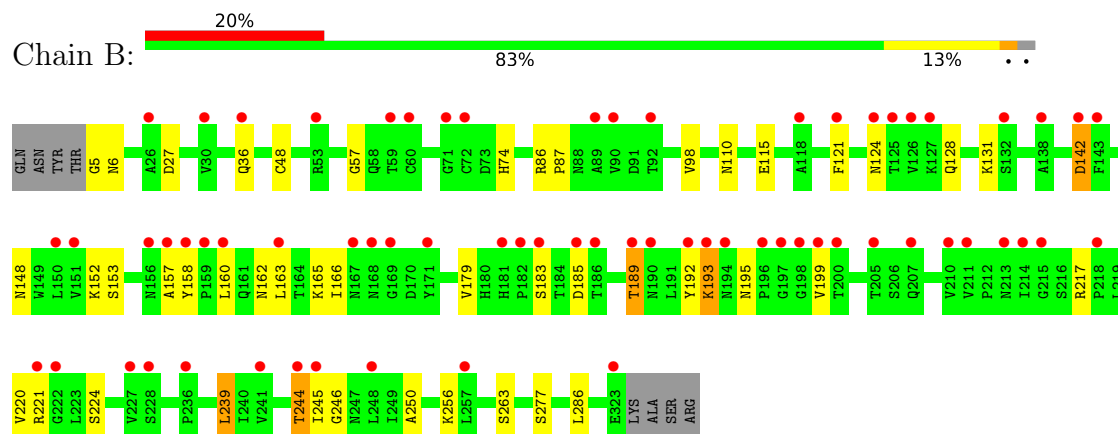
3 Residue-property plots

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.

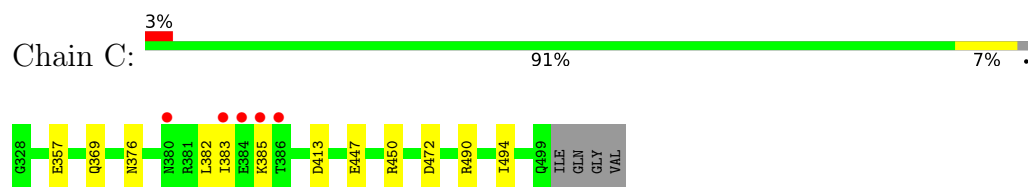
• Molecule 1: Hemagglutinin



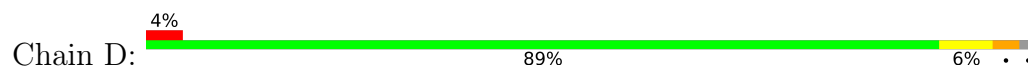
• Molecule 1: Hemagglutinin

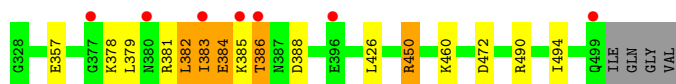


• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin





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



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



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	100.94Å 100.94Å 688.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.84 – 2.10 42.84 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (42.84-2.10) 93.0 (42.84-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.22 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.206 , 0.240 0.210 , 0.240	Depositor DCC
R_{free} test set	4006 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.536	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8439	wwPDB-VP
Average B, all atoms (Å ²)	46.0	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 46.72 % 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 1.1002e-04. 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: NAG, GAL, SIA

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	0.36	0/2512	0.74	0/3420
1	B	0.34	0/2512	0.82	4/3420 (0.1%)
2	C	0.42	0/1428	0.76	1/1922 (0.1%)
2	D	0.38	0/1428	0.75	1/1922 (0.1%)
All	All	0.37	0/7880	0.77	6/10684 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	124	ASN	N-CA-C	9.54	125.49	107.75
1	B	124	ASN	CB-CA-C	-6.63	100.17	111.31
2	C	385	LYS	N-CA-C	-6.15	101.68	110.59
2	D	386	THR	N-CA-C	5.39	117.88	108.76
1	B	98	VAL	CA-C-N	5.05	124.50	119.24
1	B	98	VAL	C-N-CA	5.05	124.50	119.24

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	2458	0	2411	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2458	0	2411	26	0
2	C	1404	0	1320	8	0
2	D	1404	0	1320	10	0
3	E	46	0	40	1	0
3	F	46	0	40	0	0
4	A	28	0	26	2	0
4	B	28	0	26	5	0
5	A	173	0	0	4	1
5	B	90	0	0	2	0
5	C	165	0	0	3	1
5	D	139	0	0	2	0
All	All	8439	0	7594	63	1

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 (63) 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:162:ASN:O	4:B:601:NAG:O7	1.85	0.94
2:C:369:GLN:OE1	5:C:701:HOH:O	1.90	0.90
1:A:244:THR:HG22	1:A:246:GLY:H	1.39	0.87
1:B:244:THR:HG22	1:B:246:GLY:H	1.38	0.87
1:A:166:ILE:HA	1:A:239:LEU:HB3	1.67	0.77
1:B:152:LYS:NZ	1:B:189:THR:O	2.18	0.76
2:D:388:ASP:OD2	5:D:701:HOH:O	2.03	0.76
1:B:166:ILE:HG23	1:B:239:LEU:HD12	1.69	0.74
2:C:376:ASN:OD1	5:C:702:HOH:O	2.09	0.69
1:B:163:LEU:HA	4:B:601:NAG:H81	1.76	0.68
1:A:238:ASP:OD2	5:A:701:HOH:O	2.14	0.65
1:B:217:ARG:NH1	1:B:224:SER:O	2.31	0.64
2:D:450:ARG:HH11	2:D:450:ARG:HB3	1.62	0.63
1:B:163:LEU:O	5:B:702:HOH:O	2.16	0.62
1:B:166:ILE:HA	1:B:239:LEU:HB3	1.82	0.61
1:B:162:ASN:ND2	4:B:601:NAG:O7	2.33	0.61
1:B:162:ASN:C	4:B:601:NAG:O7	2.45	0.59
2:D:460:LYS:NZ	5:D:704:HOH:O	2.36	0.59
2:C:413:ASP:OD1	5:C:703:HOH:O	2.16	0.57
2:D:383:ILE:O	2:D:384:GLU:HB2	2.07	0.55
1:B:121:PHE:CD2	1:B:163:LEU:HD11	2.42	0.54
1:A:166:ILE:HG23	1:A:239:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:447:GLU:OE1	2:C:450:ARG:NH2	2.33	0.53
1:A:152:LYS:HD3	1:A:193:LYS:H	1.74	0.53
4:B:602:NAG:O4	5:B:703:HOH:O	2.19	0.51
1:B:185:ASP:O	1:B:189:THR:OG1	2.28	0.51
2:D:379:LEU:HD22	2:D:383:ILE:HD11	1.93	0.50
1:A:162:ASN:O	4:A:601:NAG:H82	2.11	0.50
1:A:205:THR:HG22	5:A:701:HOH:O	2.11	0.50
1:B:220:VAL:HG12	1:B:221:ARG:HG2	1.93	0.49
1:B:128:GLN:HB3	1:B:148:ASN:HD21	1.78	0.49
1:B:185:ASP:OD1	1:B:195:ASN:ND2	2.40	0.48
2:D:382:LEU:HD11	2:D:426:LEU:HD21	1.95	0.48
2:C:357:GLU:OE2	2:C:472:ASP:HB2	2.14	0.48
1:A:162:ASN:O	4:A:601:NAG:C8	2.62	0.47
2:C:490:ARG:O	2:C:494:ILE:HG12	2.15	0.46
1:B:158:TYR:CZ	1:B:246:GLY:HA2	2.50	0.46
2:D:357:GLU:OE2	2:D:472:ASP:HB2	2.15	0.46
1:A:123:TRP:CH2	1:A:163:LEU:HD11	2.51	0.46
1:A:322:PRO:O	1:A:323:GLU:HB2	2.17	0.44
1:B:131:LYS:HD3	1:B:142:ASP:HA	1.99	0.44
1:A:179:VAL:HG22	1:A:199:VAL:HG21	2.00	0.44
1:A:289:THR:O	2:C:383:ILE:HG23	2.17	0.44
2:C:383:ILE:HG22	2:C:383:ILE:O	2.18	0.44
1:A:126:VAL:O	5:A:702:HOH:O	2.21	0.43
1:B:115:GLU:HB3	1:B:256:LYS:HB2	2.00	0.43
2:D:490:ARG:O	2:D:494:ILE:HG12	2.19	0.43
1:A:48:CYS:SG	1:A:277:SER:HB3	2.58	0.43
1:B:148:ASN:N	1:B:250:ALA:O	2.43	0.42
3:E:3:SIA:H113	3:E:3:SIA:O7	2.20	0.42
1:B:48:CYS:SG	1:B:277:SER:HB3	2.60	0.42
1:A:286:LEU:HD11	1:A:295:ILE:HD13	2.01	0.42
1:B:86:ARG:HA	1:B:87:PRO:HD3	1.90	0.42
1:B:110:ASN:HA	1:B:263:SER:O	2.20	0.42
1:B:153:SER:HB3	1:B:157:ALA:H	1.85	0.42
1:B:5:GLY:HA2	1:B:6:ASN:HA	1.65	0.41
2:D:381:ARG:O	2:D:385:LYS:HE3	2.20	0.41
1:A:19:GLY:O	5:A:703:HOH:O	2.22	0.41
1:A:195:ASN:HA	1:A:196:PRO:HA	1.94	0.41
1:B:57:GLY:O	1:B:74:HIS:HE1	2.04	0.41
1:A:244:THR:HG22	1:A:246:GLY:N	2.21	0.40
1:B:179:VAL:HG22	1:B:199:VAL:HG21	2.03	0.40
2:D:378:LYS:O	2:D:382:LEU:HB2	2.21	0.40

All (1) 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)
5:A:803:HOH:O	5:C:862:HOH:O[2_10125]	2.16	0.04

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	317/327 (97%)	304 (96%)	11 (4%)	2 (1%)	21	18
1	B	317/327 (97%)	301 (95%)	15 (5%)	1 (0%)	36	36
2	C	170/176 (97%)	161 (95%)	9 (5%)	0	100	100
2	D	170/176 (97%)	159 (94%)	9 (5%)	2 (1%)	10	7
All	All	974/1006 (97%)	925 (95%)	44 (4%)	5 (0%)	24	22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	THR
2	D	384	GLU
1	B	193	LYS
1	A	193	LYS
2	D	383	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	275/282 (98%)	266 (97%)	9 (3%)	33	37
1	B	275/282 (98%)	262 (95%)	13 (5%)	23	24
2	C	147/150 (98%)	146 (99%)	1 (1%)	76	83
2	D	147/150 (98%)	144 (98%)	3 (2%)	48	56
All	All	844/864 (98%)	818 (97%)	26 (3%)	35	39

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	156	ASN
1	A	163	LEU
1	A	192	TYR
1	A	219	LEU
1	A	239	LEU
1	A	244	THR
1	A	286	LEU
1	A	313	LYS
2	C	382	LEU
1	B	27	ASP
1	B	36	GLN
1	B	142	ASP
1	B	160	LEU
1	B	165	LYS
1	B	183	SER
1	B	189	THR
1	B	192	TYR
1	B	193	LYS
1	B	239	LEU
1	B	244	THR
1	B	245	ILE
1	B	286	LEU
2	D	382	LEU
2	D	386	THR
2	D	450	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN

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Mol	Chain	Res	Type
1	A	58	GLN
1	A	64	ASN
1	A	124	ASN
1	A	243	ASN
2	C	387	ASN
2	C	452	GLN
1	B	42	GLN
1	B	74	HIS
2	D	387	ASN
2	D	486	HIS

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 ⓘ

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	E	1	3	15,15,15	0.57	0	21,21,21	0.96	1 (4%)
3	GAL	E	2	3	11,11,12	0.53	0	15,15,17	0.78	0
3	SIA	E	3	3	20,20,21	0.68	0	21,28,31	3.57	5 (23%)
3	NAG	F	1	3	15,15,15	0.48	0	21,21,21	1.55	1 (4%)
3	GAL	F	2	3	11,11,12	0.67	0	15,15,17	0.87	0
3	SIA	F	3	3	20,20,21	0.72	0	21,28,31	3.67	4 (19%)

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

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

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	3	SIA	O6-C2-C3	-13.91	91.86	110.56
3	E	3	SIA	O6-C2-C3	-13.42	92.51	110.56
3	F	3	SIA	O6-C2-C1	8.41	123.59	107.72
3	E	3	SIA	O6-C2-C1	8.11	123.03	107.72
3	F	1	NAG	O5-C1-C2	5.77	115.32	109.52
3	F	3	SIA	C8-C7-C6	-2.79	107.81	113.05
3	E	3	SIA	O1B-C1-C2	2.72	119.79	112.71
3	F	3	SIA	O1B-C1-C2	2.35	118.83	112.71
3	E	1	NAG	C1-C2-C3	2.27	113.64	110.54
3	E	3	SIA	C8-C7-C6	-2.25	108.83	113.05
3	E	3	SIA	O1A-C1-C2	-2.03	118.46	122.85

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	E	3	SIA	O1A-C1-C2-O6
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	F	3	SIA	C11-C10-N5-C5
3	F	3	SIA	O10-C10-N5-C5
3	F	1	NAG	O5-C5-C6-O6
3	E	3	SIA	C11-C10-N5-C5
3	E	3	SIA	O10-C10-N5-C5

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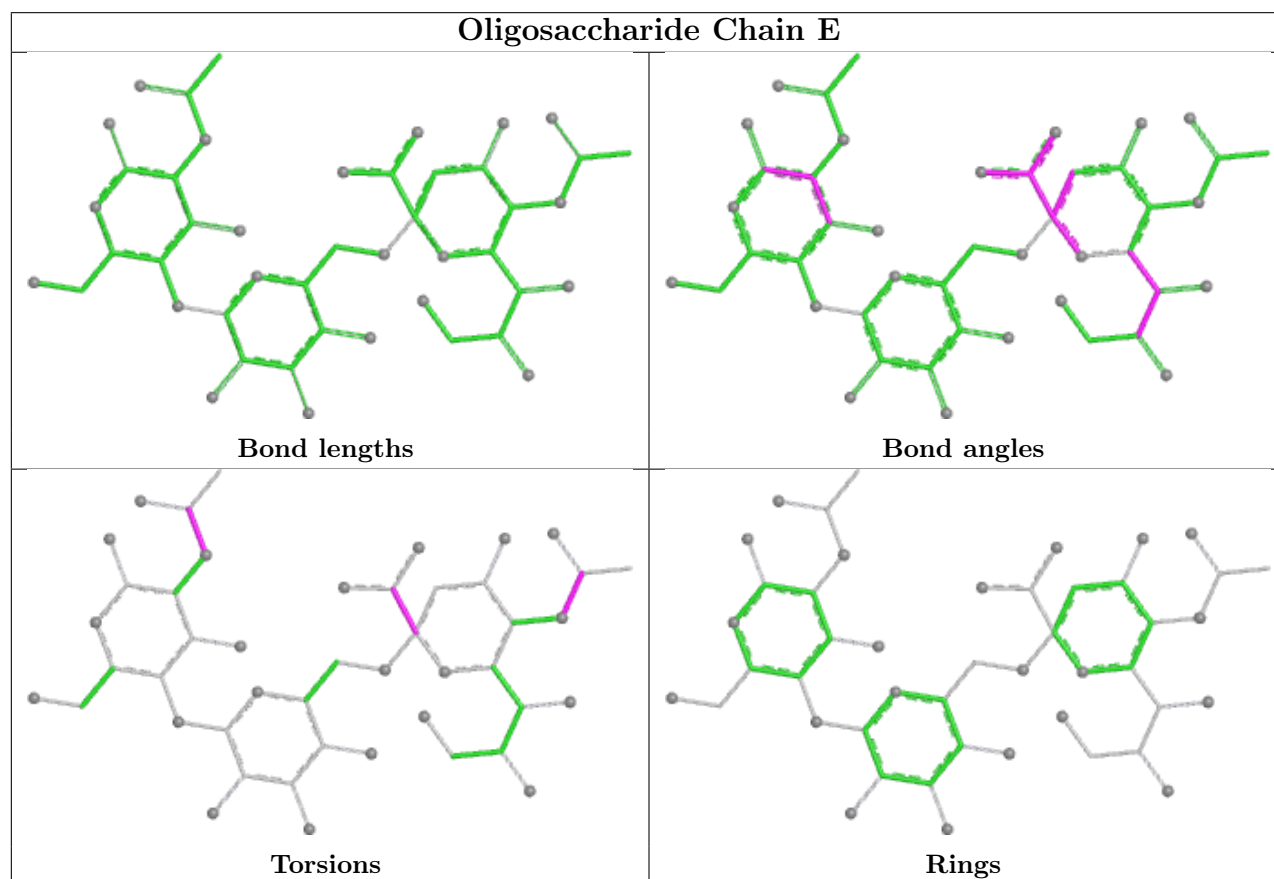
Mol	Chain	Res	Type	Atoms
3	F	1	NAG	C4-C5-C6-O6
3	F	3	SIA	O1A-C1-C2-O6

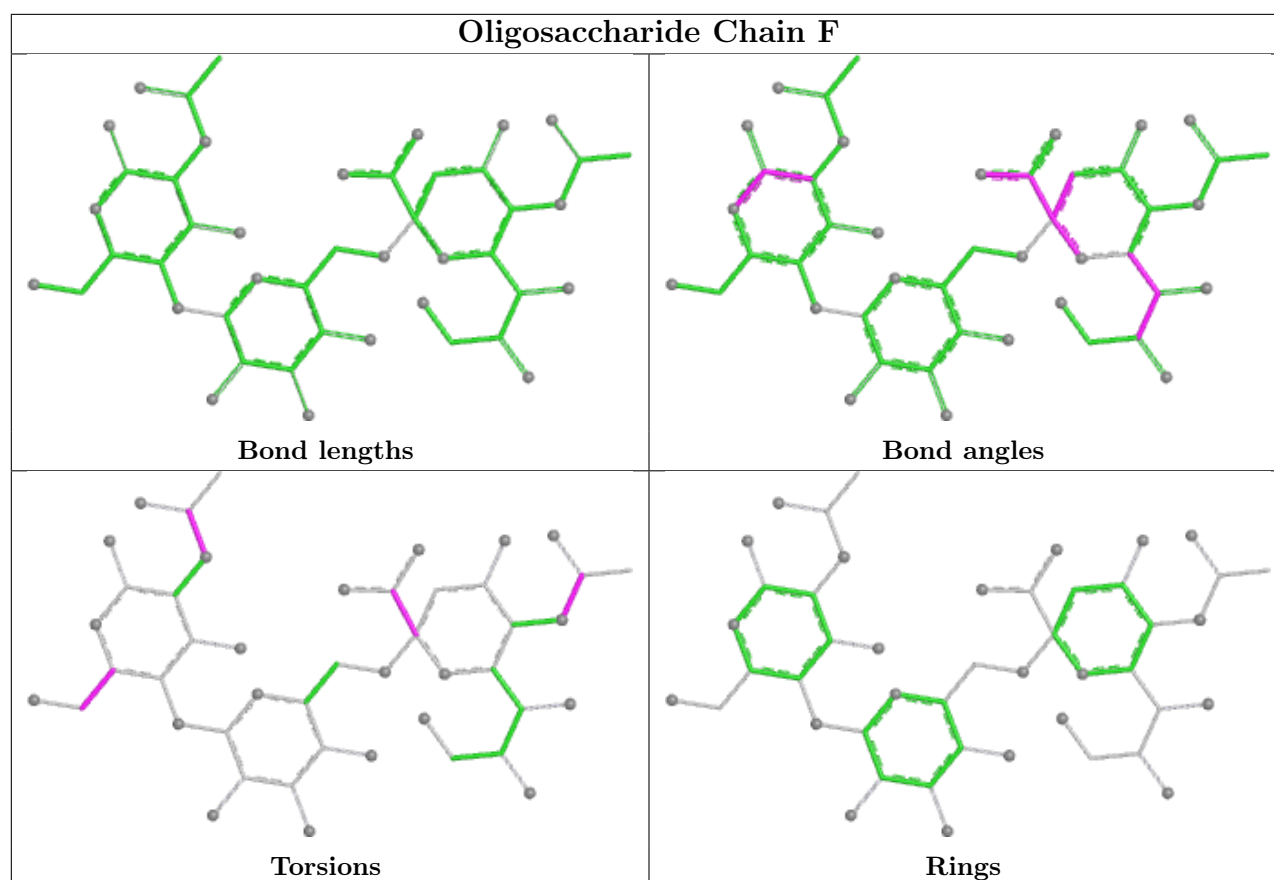
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	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.





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	$\# Z > 2$
4	NAG	A	602	1	14,14,15	0.49	0	17,19,21	0.99	1 (5%)
4	NAG	B	601	1	14,14,15	0.29	0	17,19,21	0.55	0
4	NAG	B	602	1	14,14,15	0.55	0	17,19,21	1.19	1 (5%)
4	NAG	A	601	1	14,14,15	0.28	0	17,19,21	0.56	0

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	602	1	-	0/6/23/26	0/1/1/1
4	NAG	B	601	1	-	2/6/23/26	0/1/1/1
4	NAG	B	602	1	-	0/6/23/26	0/1/1/1
4	NAG	A	601	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	602	NAG	C1-O5-C5	4.43	118.12	112.19
4	A	602	NAG	C1-O5-C5	3.28	116.58	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	NAG	C8-C7-N2-C2
4	A	601	NAG	O7-C7-N2-C2
4	B	601	NAG	C8-C7-N2-C2
4	B	601	NAG	O7-C7-N2-C2
4	A	601	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	601	NAG	4	0
4	B	602	NAG	1	0
4	A	601	NAG	2	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, 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	319/327 (97%)	0.40	13 (4%) 41 43	19, 39, 61, 90	0
1	B	319/327 (97%)	1.26	67 (21%) 2 2	24, 62, 98, 118	0
2	C	172/176 (97%)	0.05	5 (2%) 53 56	21, 29, 47, 108	0
2	D	172/176 (97%)	0.22	7 (4%) 41 43	23, 33, 60, 118	0
All	All	982/1006 (97%)	0.59	92 (9%) 14 14	19, 40, 88, 118	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	383	ILE	9.6
2	D	383	ILE	4.8
1	B	214	ILE	4.6
1	A	158	TYR	4.1
1	B	90	VAL	4.0
1	B	158	TYR	4.0
1	A	193	LYS	3.9
1	B	157	ALA	3.8
1	B	151	VAL	3.8
1	B	213	ASN	3.7
1	A	192	TYR	3.7
1	B	181	HIS	3.7
1	B	160	LEU	3.7
1	B	143	PHE	3.7
1	A	125	THR	3.7
1	B	192	TYR	3.6
1	B	169	GLY	3.6
1	B	183	SER	3.6
1	A	26	ALA	3.5
2	D	385	LYS	3.5
1	B	126	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	182	PRO	3.3
1	B	218	PRO	3.3
1	B	205	THR	3.3
1	A	157	ALA	3.3
1	A	139	ASN	3.2
1	B	245	ILE	3.2
1	A	27	ASP	3.2
1	B	60	CYS	3.2
1	B	211	VAL	3.2
1	B	138	ALA	3.1
1	B	221	ARG	3.1
1	B	132	SER	3.1
1	B	222	GLY	3.0
1	B	59	THR	3.0
1	B	207	GLN	3.0
1	B	163	LEU	2.9
2	D	380	ASN	2.9
1	A	127	LYS	2.9
2	C	384	GLU	2.9
1	B	121	PHE	2.9
1	B	189	THR	2.8
1	A	90	VAL	2.8
1	B	199	VAL	2.8
1	B	168	ASN	2.7
1	B	92	THR	2.7
2	C	380	ASN	2.7
1	B	197	GLY	2.7
1	B	71	GLY	2.6
1	A	168	ASN	2.6
1	B	89	ALA	2.6
1	A	60	CYS	2.6
1	B	26	ALA	2.6
1	B	186	THR	2.6
1	B	36	GLN	2.5
1	B	228	SER	2.5
2	D	386	THR	2.5
1	B	257	LEU	2.5
1	B	127	LYS	2.5
2	C	385	LYS	2.5
1	B	210	VAL	2.4
1	B	142	ASP	2.4
1	B	196	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	185	ASP	2.4
1	B	244	THR	2.4
1	B	227	VAL	2.4
1	B	72	CYS	2.4
1	B	118	ALA	2.3
1	B	193	LYS	2.3
1	B	241	VAL	2.3
1	B	150	LEU	2.3
1	B	124	ASN	2.3
1	B	198	GLY	2.3
2	D	377	GLY	2.3
2	D	499	GLN	2.2
1	B	159	PRO	2.2
1	B	215	GLY	2.2
2	C	386	THR	2.2
1	B	248	LEU	2.1
1	B	194	ASN	2.1
1	B	323	GLU	2.1
1	B	156	ASN	2.1
1	B	167	ASN	2.1
1	B	125	THR	2.1
1	B	236	PRO	2.1
1	B	30	VAL	2.1
2	D	396	GLU	2.0
1	B	53	ARG	2.0
1	B	200	THR	2.0
1	B	190	ASN	2.0
1	A	197	GLY	2.0
1	B	171	TYR	2.0

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

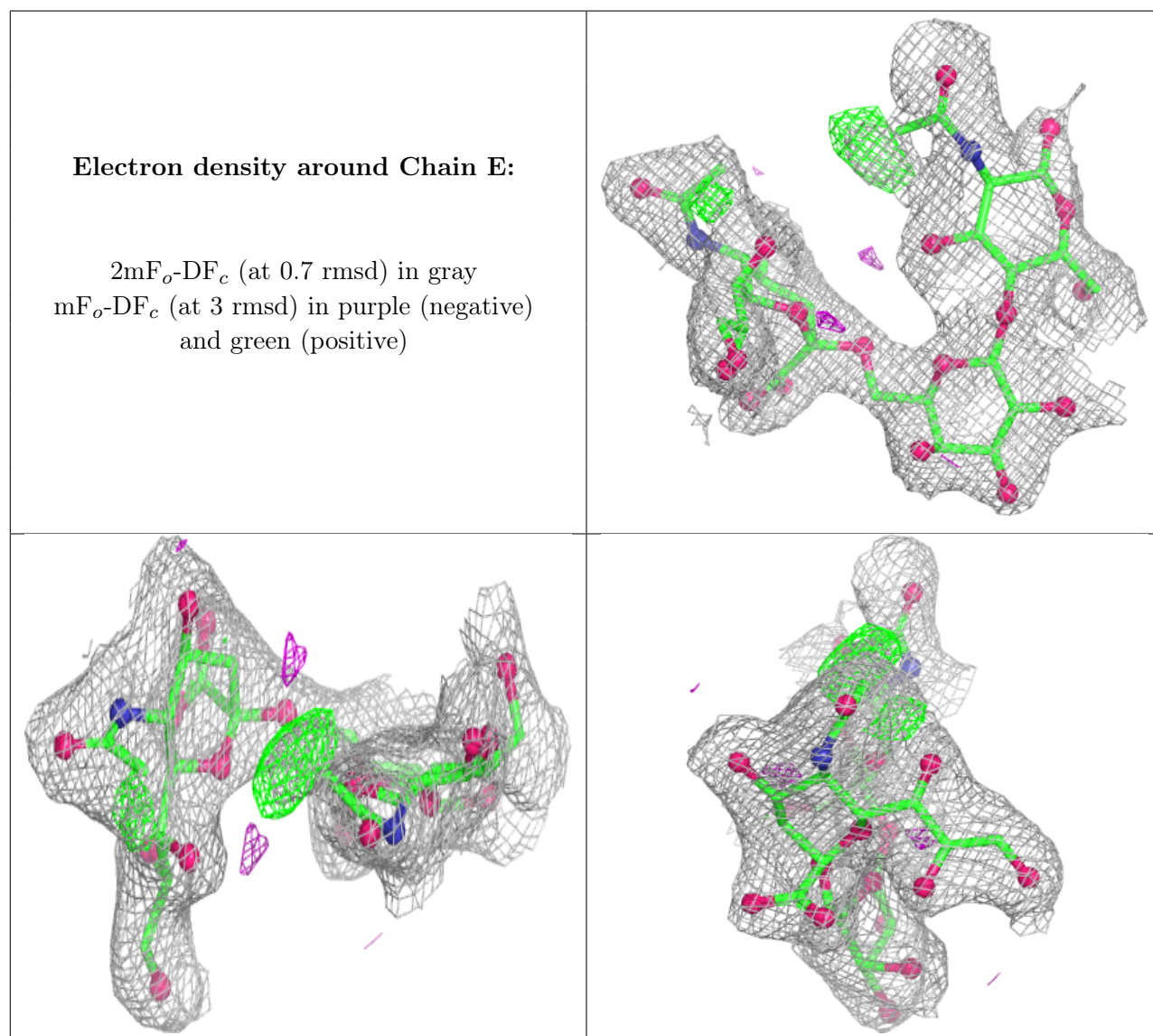
There are no non-standard protein/DNA/RNA residues in this entry.

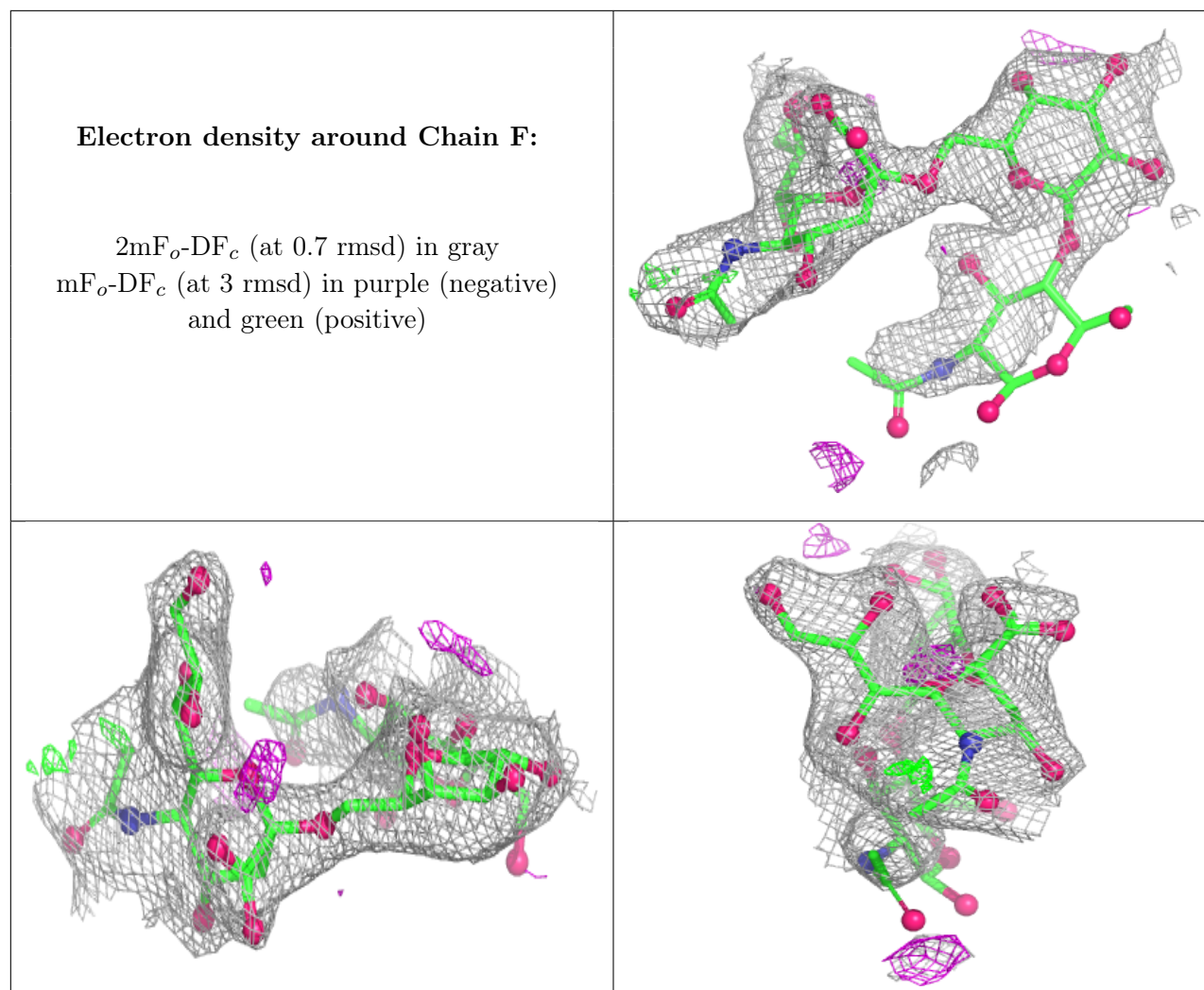
6.3 Carbohydrates ⓘ

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
3	NAG	E	1	15/15	0.59	0.15	92,98,102,102	0
3	NAG	F	1	15/15	0.68	0.19	146,158,166,168	0
3	GAL	F	2	11/12	0.81	0.10	90,99,108,109	0
3	GAL	E	2	11/12	0.82	0.12	53,66,76,79	0
3	SIA	F	3	20/21	0.84	0.14	72,77,82,83	0
3	SIA	E	3	20/21	0.89	0.10	36,47,51,52	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.





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	B	601	14/15	0.61	0.21	101,108,110,114	0
4	NAG	A	601	14/15	0.62	0.18	91,95,97,99	0
4	NAG	A	602	14/15	0.91	0.08	30,37,41,46	0
4	NAG	B	602	14/15	0.91	0.09	44,48,52,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.