



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:15 AM UTC

PDB ID : 5XLD / pdb_00005xld
Title : The structure of hemagglutinin Q226L-G228S mutant from an avian-origin H4N6 influenza virus in complex with human receptor analog LSTc
Authors : Song, H.; Qi, J.; Gao, F.G.
Deposited on : 2017-05-10
Resolution : 2.30 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

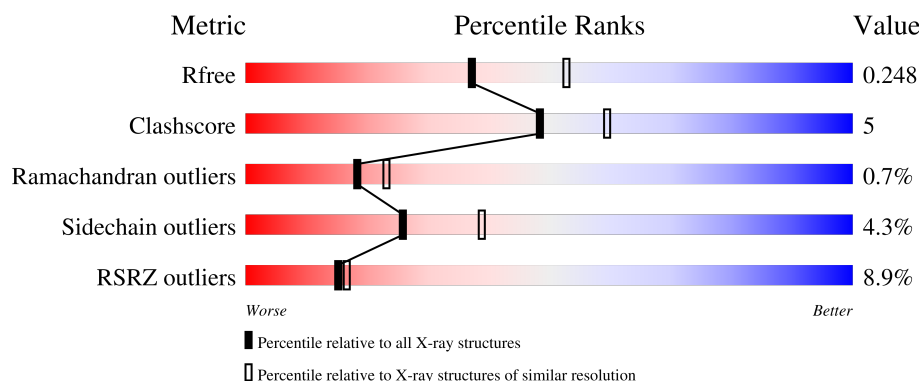
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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.



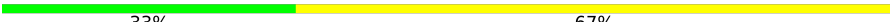
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	6% 85% 10% ...
1	B	327	17% 77% 18% ..
2	C	176	3% 89% 7% ..
2	D	176	2% 91% 5% ..
3	E	3	100%

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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 8217 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
			2460	1542	436	470	12			
1	B	319	Total	C	N	O	S	0	0	0
			2460	1542	436	470	12			

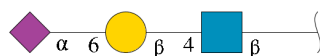
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	223	LEU	GLN	engineered mutation	UNP A3KF09
A	225	SER	GLY	engineered mutation	UNP A3KF09
B	223	LEU	GLN	engineered mutation	UNP A3KF09
B	225	SER	GLY	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.



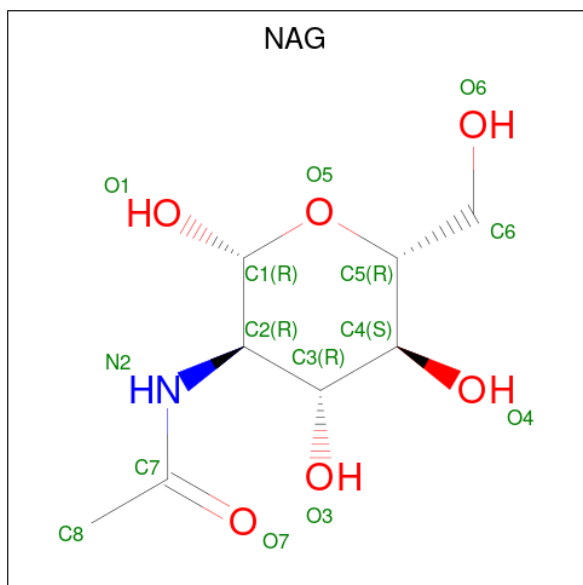
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	3	Total	C	N	O	0	0	0
			46	25	2	19			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
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		

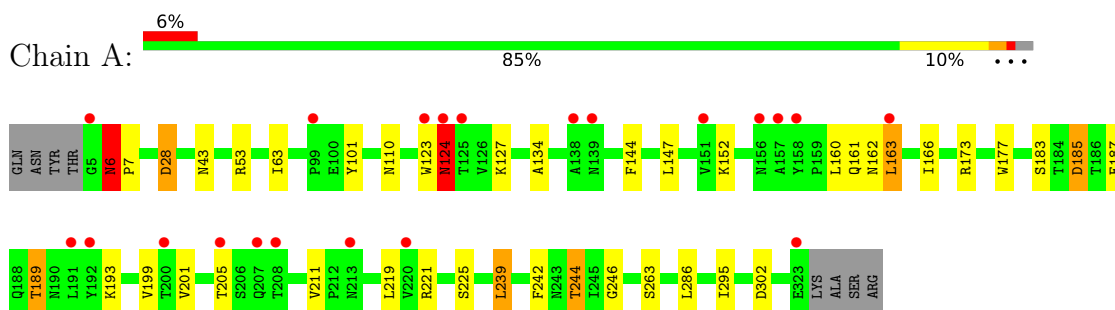
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	97	Total	O	0	0
			97	97		
5	C	100	Total	O	0	0
			100	100		
5	B	63	Total	O	0	0
			63	63		
5	D	81	Total	O	0	0
			81	81		

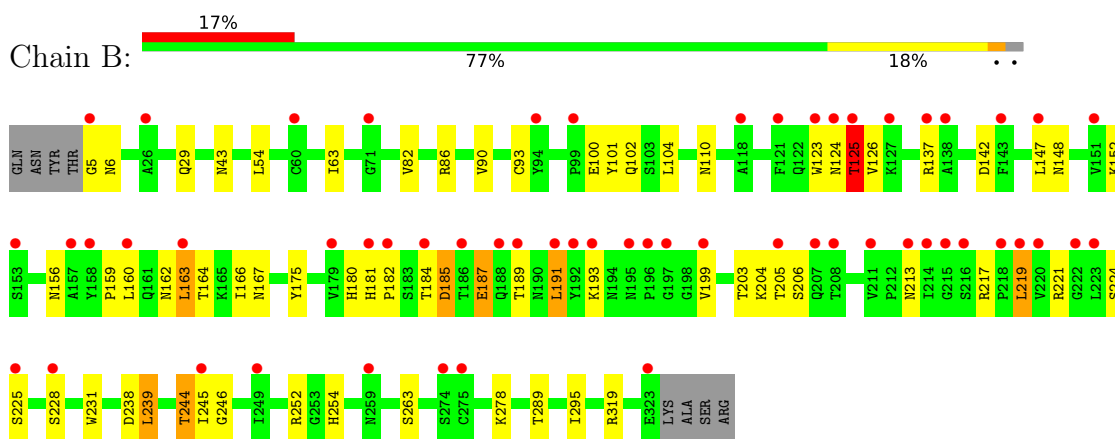
3 Residue-property plots [i](#)

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.

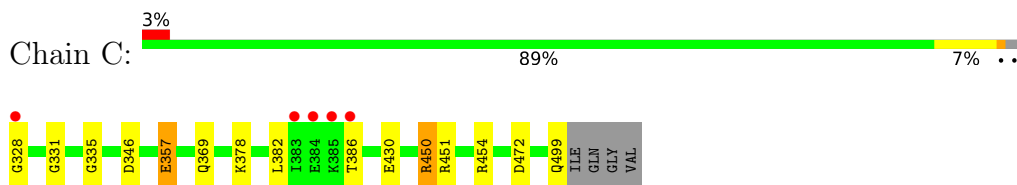
• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin

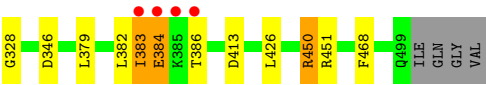


• Molecule 2: Hemagglutinin



• 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	100.41 Å 100.41 Å 686.91 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.73 – 2.30 42.73 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (42.73-2.30) 90.7 (42.73-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 2.29 Å)	Xtriage
Refinement program	PHENIX 1.7.3 _928	Depositor
R, R_{free}	0.214 , 0.251 0.214 , 0.248	Depositor DCC
R_{free} test set	3043 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.587	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.5	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	8217	wwPDB-VP
Average B, all atoms (Å ²)	50.0	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 50.88 % 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 6.0777e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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, 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	0.38	0/2514	0.81	2/3423 (0.1%)
1	B	0.38	0/2514	0.82	0/3423
2	C	0.43	0/1428	0.77	1/1922 (0.1%)
2	D	0.41	0/1428	0.74	0/1922
All	All	0.40	0/7884	0.79	3/10690 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	ASN	CA-C-N	-7.64	111.91	119.78
1	A	6	ASN	C-N-CA	-7.64	111.91	119.78
2	C	454	ARG	CB-CA-C	-6.51	109.06	116.54

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	2460	0	2413	24	0
1	B	2460	0	2413	45	0
2	C	1404	0	1320	8	0
2	D	1404	0	1320	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	46	0	39	0	0
3	F	46	0	40	0	0
4	A	28	0	26	0	0
4	B	28	0	26	3	0
5	A	97	0	0	4	0
5	B	63	0	0	7	0
5	C	100	0	0	5	0
5	D	81	0	0	5	0
All	All	8217	0	7597	85	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (85) 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:124:ASN:HB2	1:A:161:GLN:HE22	1.39	0.87
2:D:346:ASP:OD1	5:D:701:HOH:O	1.92	0.86
1:A:28:ASP:O	5:A:701:HOH:O	1.93	0.86
1:B:5:GLY:HA2	2:D:468:PHE:HA	1.62	0.82
1:B:152:LYS:NZ	1:B:189:THR:O	2.13	0.82
1:A:124:ASN:CB	1:A:161:GLN:HE22	1.94	0.80
1:B:213:ASN:O	1:B:217:ARG:NH2	2.15	0.79
1:B:244:THR:HG22	1:B:246:GLY:H	1.49	0.75
1:B:187:GLU:O	5:B:701:HOH:O	2.05	0.74
1:A:244:THR:HG22	1:A:246:GLY:H	1.55	0.71
1:B:5:GLY:N	5:B:707:HOH:O	2.25	0.69
2:C:346:ASP:OD2	5:C:601:HOH:O	2.09	0.68
1:A:134:ALA:O	1:A:221:ARG:NH1	2.28	0.67
2:C:369:GLN:OE1	5:C:602:HOH:O	2.11	0.67
1:B:102:GLN:OE1	5:B:703:HOH:O	2.12	0.67
1:B:167:ASN:OD1	5:B:702:HOH:O	2.12	0.67
1:A:302:ASP:OD1	5:A:702:HOH:O	2.14	0.66
2:D:413:ASP:OD1	5:D:702:HOH:O	2.14	0.65
2:D:450:ARG:NH2	5:D:703:HOH:O	2.29	0.64
1:A:166:ILE:HA	1:A:239:LEU:HB3	1.83	0.61
2:D:382:LEU:HD11	2:D:426:LEU:HD21	1.83	0.60
1:B:185:ASP:OD2	1:B:185:ASP:N	2.33	0.60
1:A:124:ASN:HB2	1:A:161:GLN:NE2	2.13	0.59
1:B:319:ARG:NE	5:B:704:HOH:O	2.14	0.57
1:B:199:VAL:HG22	1:B:244:THR:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:SER:N	1:A:187:GLU:OE2	2.27	0.56
2:C:451:ARG:HD2	5:C:606:HOH:O	2.06	0.54
1:B:204:LYS:HE2	1:B:238:ASP:HA	1.88	0.54
1:B:137:ARG:NE	1:B:142:ASP:OD2	2.33	0.54
2:C:450:ARG:NH2	5:C:605:HOH:O	2.42	0.52
1:B:43:ASN:HB3	1:B:295:ILE:HD13	1.90	0.52
1:B:86:ARG:O	5:B:705:HOH:O	2.19	0.51
1:B:182:PRO:HB3	1:B:187:GLU:HB3	1.92	0.51
1:A:152:LYS:NZ	1:A:189:THR:O	2.31	0.51
1:B:181:HIS:HE2	1:B:228:SER:HB2	1.76	0.51
1:B:123:TRP:CH2	1:B:163:LEU:HD11	2.46	0.51
2:C:357:GLU:OE2	2:C:472:ASP:HB2	2.10	0.51
1:B:164:THR:CB	4:B:601:NAG:H81	2.41	0.51
1:A:185:ASP:OD2	1:A:185:ASP:N	2.42	0.50
1:B:124:ASN:O	1:B:126:VAL:N	2.41	0.50
2:C:378:LYS:NZ	2:C:430:GLU:OE1	2.37	0.50
2:D:451:ARG:HD2	5:D:704:HOH:O	2.11	0.50
1:B:289:THR:O	2:D:383:ILE:HG23	2.12	0.50
1:B:63:ILE:HG13	1:B:101:TYR:CE2	2.47	0.49
1:B:100:GLU:HB2	1:B:231:TRP:HH2	1.78	0.49
1:B:184:THR:HG23	1:B:187:GLU:HG3	1.94	0.49
1:B:164:THR:HB	4:B:601:NAG:H81	1.96	0.48
1:B:162:ASN:O	4:B:601:NAG:O7	2.31	0.48
2:D:383:ILE:O	2:D:384:GLU:HB2	2.12	0.48
1:B:100:GLU:HB2	1:B:231:TRP:CH2	2.49	0.48
1:A:173:ARG:NE	5:A:703:HOH:O	2.19	0.48
1:A:110:ASN:HA	1:A:263:SER:O	2.14	0.48
1:B:203:THR:OG1	1:B:206:SER:OG	2.25	0.48
1:A:123:TRP:CH2	1:A:163:LEU:HD11	2.48	0.48
1:B:110:ASN:HA	1:B:263:SER:O	2.15	0.47
2:D:328:GLY:N	5:D:709:HOH:O	2.48	0.46
2:C:328:GLY:N	5:C:609:HOH:O	2.49	0.46
1:B:125:THR:HG23	1:B:159:PRO:HG3	1.97	0.46
1:A:199:VAL:HG22	1:A:244:THR:HG23	1.98	0.46
1:B:175:TYR:HA	5:B:714:HOH:O	2.15	0.46
1:A:6:ASN:HB2	5:A:725:HOH:O	2.16	0.45
2:C:331:GLY:O	2:C:335:GLY:HA3	2.16	0.45
1:B:124:ASN:OD1	1:B:125:THR:HG22	2.17	0.45
1:B:152:LYS:HE3	1:B:191:LEU:C	2.42	0.44
1:B:93:CYS:N	1:B:221:ARG:HH12	2.15	0.44
1:A:162:ASN:HA	1:A:242:PHE:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:THR:HB	1:B:238:ASP:OD1	2.17	0.43
1:A:144:PHE:HB2	1:A:147:LEU:HB2	2.00	0.43
1:B:166:ILE:HA	1:B:239:LEU:HB3	2.00	0.43
1:A:6:ASN:H	1:A:7:PRO:CD	2.31	0.43
1:B:180:HIS:NE2	1:B:225:SER:OG	2.51	0.43
1:B:124:ASN:C	1:B:126:VAL:H	2.26	0.42
1:B:104:LEU:HB2	1:B:231:TRP:CZ3	2.54	0.42
1:A:152:LYS:HE2	1:A:193:LYS:HB2	2.01	0.42
1:A:43:ASN:HB3	1:A:295:ILE:HD13	2.00	0.42
1:B:219:LEU:HD13	1:B:219:LEU:HA	1.91	0.41
1:B:175:TYR:CE2	1:B:254:HIS:HB3	2.55	0.41
1:A:53:ARG:HE	1:A:53:ARG:HB2	1.53	0.41
1:A:177:TRP:CE2	1:A:201:VAL:HG21	2.55	0.41
1:A:63:ILE:HG13	1:A:101:TYR:CE2	2.56	0.41
1:B:54:LEU:HD22	1:B:82:VAL:HB	2.01	0.41
1:B:148:ASN:HB2	1:B:252:ARG:HD2	2.02	0.41
1:B:189:THR:HG22	1:B:193:LYS:O	2.20	0.40
2:D:379:LEU:HD23	2:D:379:LEU:HA	1.93	0.40
1:B:217:ARG:O	1:B:224:SER:OG	2.31	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	301 (95%)	14 (4%)	2 (1%)	21	27
1	B	317/327 (97%)	297 (94%)	17 (5%)	3 (1%)	14	17
2	C	170/176 (97%)	160 (94%)	10 (6%)	0	100	100
2	D	170/176 (97%)	157 (92%)	11 (6%)	2 (1%)	10	12
All	All	974/1006 (97%)	915 (94%)	52 (5%)	7 (1%)	18	23

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	124	ASN
1	B	125	THR
2	D	384	GLU
1	B	6	ASN
1	B	156	ASN
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	276/283 (98%)	262 (95%)	14 (5%)	21	32
1	B	276/283 (98%)	261 (95%)	15 (5%)	20	29
2	C	147/150 (98%)	142 (97%)	5 (3%)	32	49
2	D	147/150 (98%)	145 (99%)	2 (1%)	59	76
All	All	846/866 (98%)	810 (96%)	36 (4%)	26	39

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASP
1	A	124	ASN
1	A	127	LYS
1	A	160	LEU
1	A	163	LEU
1	A	185	ASP
1	A	189	THR
1	A	205	THR
1	A	211	VAL
1	A	219	LEU
1	A	225	SER
1	A	239	LEU
1	A	244	THR

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Mol	Chain	Res	Type
1	A	286	LEU
2	C	357	GLU
2	C	382	LEU
2	C	386	THR
2	C	450	ARG
2	C	499	GLN
1	B	29	GLN
1	B	90	VAL
1	B	125	THR
1	B	147	LEU
1	B	160	LEU
1	B	163	LEU
1	B	185	ASP
1	B	187	GLU
1	B	191	LEU
1	B	205	THR
1	B	219	LEU
1	B	239	LEU
1	B	244	THR
1	B	245	ILE
1	B	278	LYS
2	D	386	THR
2	D	450	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	124	ASN
1	A	161	GLN
1	A	243	ASN
2	C	387	ASN
2	C	452	GLN
1	B	14	HIS
2	D	387	ASN
2	D	443	ASN
2	D	499	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 ⓘ

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	0.52	0	21,21,21	1.54	3 (14%)
3	GAL	E	2	3	11,11,12	1.51	1 (9%)	15,15,17	1.52	4 (26%)
3	SIA	E	3	3	20,20,21	0.65	0	21,28,31	3.65	3 (14%)
3	NAG	F	1	3	15,15,15	0.48	0	21,21,21	1.42	3 (14%)
3	GAL	F	2	3	11,11,12	0.25	0	15,15,17	0.52	0
3	SIA	F	3	3	20,20,21	0.74	0	21,28,31	3.66	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	-	2/2/19/22	0/1/1/1
3	SIA	E	3	3	-	3/18/34/38	0/1/1/1
3	NAG	F	1	3	-	0/6/26/26	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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	GAL	O4-C4	-4.53	1.31	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	3	SIA	O6-C2-C3	-13.81	91.99	110.56
3	E	3	SIA	O6-C2-C3	-13.80	92.00	110.56
3	E	3	SIA	O6-C2-C1	8.51	123.78	107.72
3	F	3	SIA	O6-C2-C1	8.46	123.68	107.72
3	E	1	NAG	C4-C3-C2	4.22	116.55	110.40
3	F	1	NAG	C4-C3-C2	4.18	116.49	110.40
3	E	1	NAG	C1-C2-C3	3.52	115.35	110.54
3	F	1	NAG	C1-C2-C3	2.91	114.51	110.54
3	E	2	GAL	C3-C4-C5	-2.83	105.11	110.23
3	E	2	GAL	C1-O5-C5	-2.79	108.45	112.19
3	E	2	GAL	O5-C5-C6	2.63	112.78	107.66
3	E	2	GAL	C1-C2-C3	2.57	113.39	109.64
3	E	3	SIA	O1B-C1-C2	2.57	119.40	112.71
3	F	3	SIA	O1B-C1-C2	2.50	119.21	112.71
3	F	1	NAG	C3-C4-C5	2.23	114.28	110.23
3	E	1	NAG	C1-C2-N2	-2.19	108.19	110.73
3	F	3	SIA	C8-C7-C6	-2.02	109.26	113.05

There are no chirality outliers.

All (10) torsion outliers are listed below:

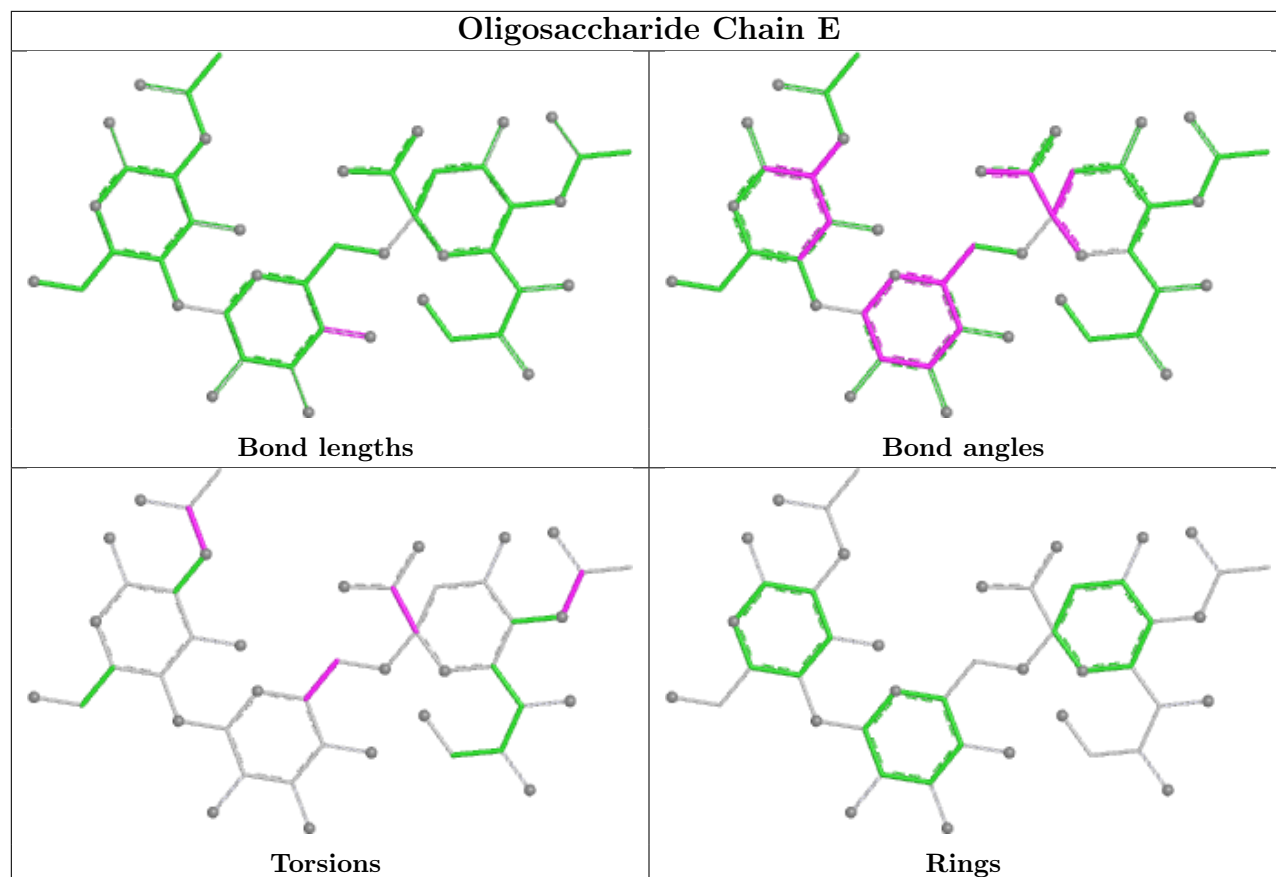
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	E	3	SIA	O1A-C1-C2-O6
3	F	3	SIA	C11-C10-N5-C5
3	F	3	SIA	O10-C10-N5-C5
3	E	2	GAL	O5-C5-C6-O6
3	E	2	GAL	C4-C5-C6-O6
3	E	3	SIA	C11-C10-N5-C5
3	E	3	SIA	O10-C10-N5-C5
3	F	3	SIA	O1A-C1-C2-O6

There are no ring outliers.

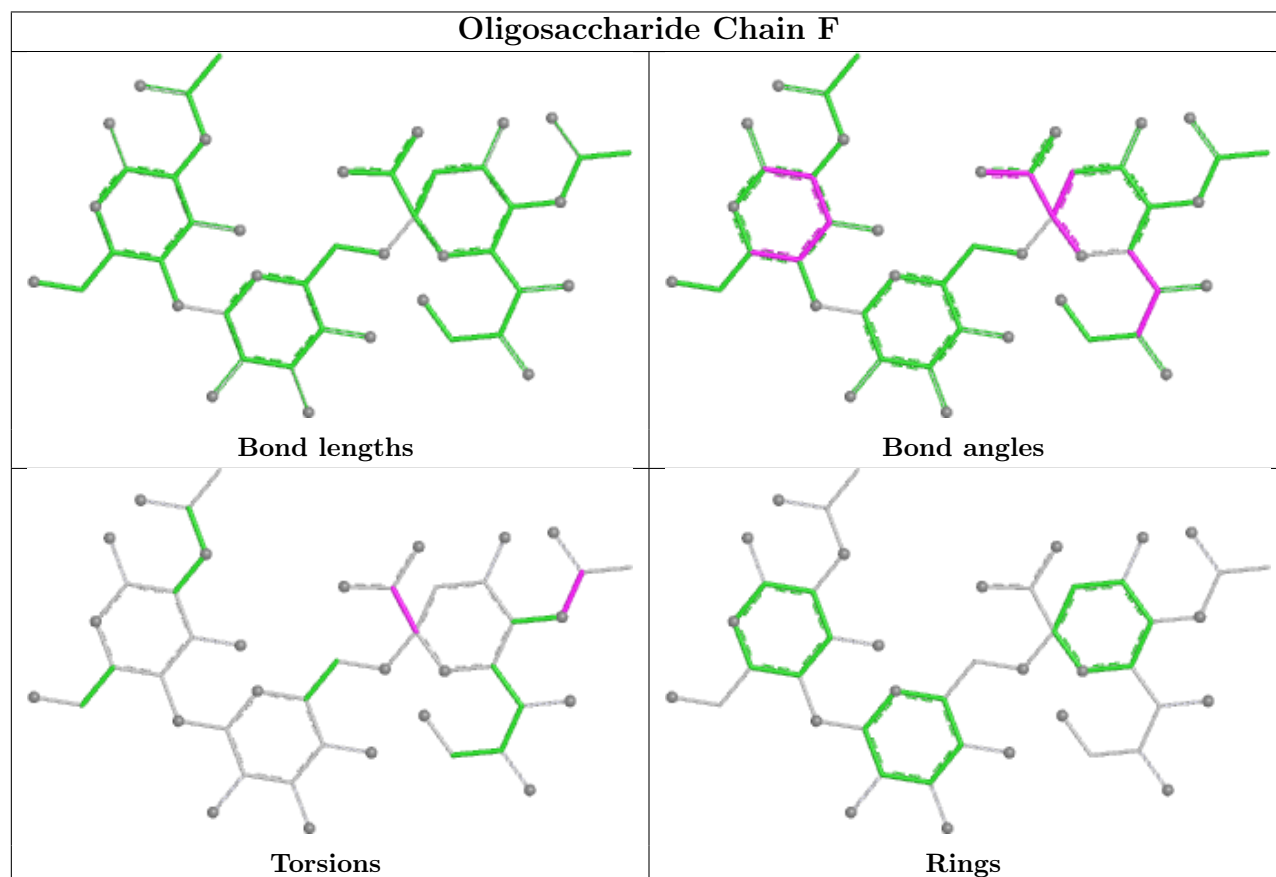
No monomer is involved in short contacts.

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

Oligosaccharide Chain E



Oligosaccharide Chain F



5.6 Ligand geometry

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	601	1	14,14,15	0.51	0	17,19,21	1.03	1 (5%)
4	NAG	A	602	1	14,14,15	0.44	0	17,19,21	1.03	1 (5%)
4	NAG	B	602	1	14,14,15	0.45	0	17,19,21	1.09	1 (5%)
4	NAG	B	601	1	14,14,15	0.30	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	601	1	-	1/6/23/26	0/1/1/1
4	NAG	A	602	1	-	0/6/23/26	0/1/1/1
4	NAG	B	602	1	-	0/6/23/26	0/1/1/1
4	NAG	B	601	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	602	NAG	C1-O5-C5	3.64	117.06	112.19
4	A	602	NAG	C1-O5-C5	3.15	116.40	112.19
4	A	601	NAG	O5-C1-C2	2.75	115.54	111.29

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	601	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	B	601	NAG	O7-C7-N2-C2
4	B	601	NAG	C4-C5-C6-O6
4	B	601	NAG	O5-C5-C6-O6
4	A	601	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	601	NAG	3	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%)	0.31	21 (6%) 24 26	21, 45, 82, 120	0
1	B	319/327 (97%)	0.97	57 (17%) 3 4	24, 64, 115, 139	0
2	C	172/176 (97%)	-0.14	5 (2%) 53 56	19, 33, 52, 114	0
2	D	172/176 (97%)	-0.09	4 (2%) 61 63	24, 35, 62, 123	0
All	All	982/1006 (97%)	0.37	87 (8%) 15 17	19, 43, 97, 139	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	383	ILE	6.3
2	C	383	ILE	6.2
1	B	157	ALA	5.2
1	B	192	TYR	4.8
1	B	245	ILE	4.2
1	B	191	LEU	4.2
1	B	5	GLY	4.1
1	A	124	ASN	4.1
2	C	385	LYS	4.1
2	D	385	LYS	4.1
1	B	138	ALA	3.8
1	B	205	THR	3.8
1	B	214	ILE	3.8
1	B	193	LYS	3.7
1	B	158	TYR	3.7
2	C	386	THR	3.7
1	B	197	GLY	3.6
1	B	225	SER	3.5
1	A	5	GLY	3.5
1	B	216	SER	3.4
1	A	157	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	163	LEU	3.3
1	A	138	ALA	3.3
1	B	125	THR	3.2
1	B	123	TRP	3.2
1	B	211	VAL	3.1
1	B	196	PRO	3.1
1	B	215	GLY	3.1
1	B	222	GLY	3.1
1	B	207	GLN	2.9
1	B	160	LEU	2.8
1	B	220	VAL	2.8
1	A	151	VAL	2.8
1	B	60	CYS	2.8
1	B	219	LEU	2.8
1	B	99	PRO	2.7
1	B	179	VAL	2.7
1	B	213	ASN	2.7
1	A	323	GLU	2.7
1	B	26	ALA	2.7
1	A	125	THR	2.7
1	B	121	PHE	2.6
2	D	386	THR	2.6
1	B	274	SER	2.6
1	B	127	LYS	2.6
1	A	213	ASN	2.6
1	B	151	VAL	2.6
1	B	275	CYS	2.6
1	B	94	TYR	2.6
1	B	259	ASN	2.5
1	B	208	THR	2.5
1	A	192	TYR	2.5
1	A	158	TYR	2.5
1	B	181	HIS	2.5
1	A	191	LEU	2.5
1	A	139	ASN	2.5
1	A	208	THR	2.4
1	B	199	VAL	2.4
1	A	123	TRP	2.4
1	A	99	PRO	2.4
1	B	323	GLU	2.4
1	B	189	THR	2.4
1	A	163	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	195	ASN	2.3
1	B	228	SER	2.3
1	B	188	GLN	2.3
2	D	384	GLU	2.3
2	C	384	GLU	2.3
1	A	200	THR	2.3
1	B	186	THR	2.3
1	B	147	LEU	2.2
1	B	218	PRO	2.2
2	C	328	GLY	2.2
1	A	205	THR	2.2
1	B	143	PHE	2.2
1	B	184	THR	2.2
1	B	249	ILE	2.2
1	A	156	ASN	2.2
1	B	182	PRO	2.2
1	A	207	GLN	2.2
1	B	118	ALA	2.2
1	B	153	SER	2.1
1	B	124	ASN	2.1
1	A	220	VAL	2.1
1	B	71	GLY	2.1
1	B	223	LEU	2.0
1	B	137	ARG	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, 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.

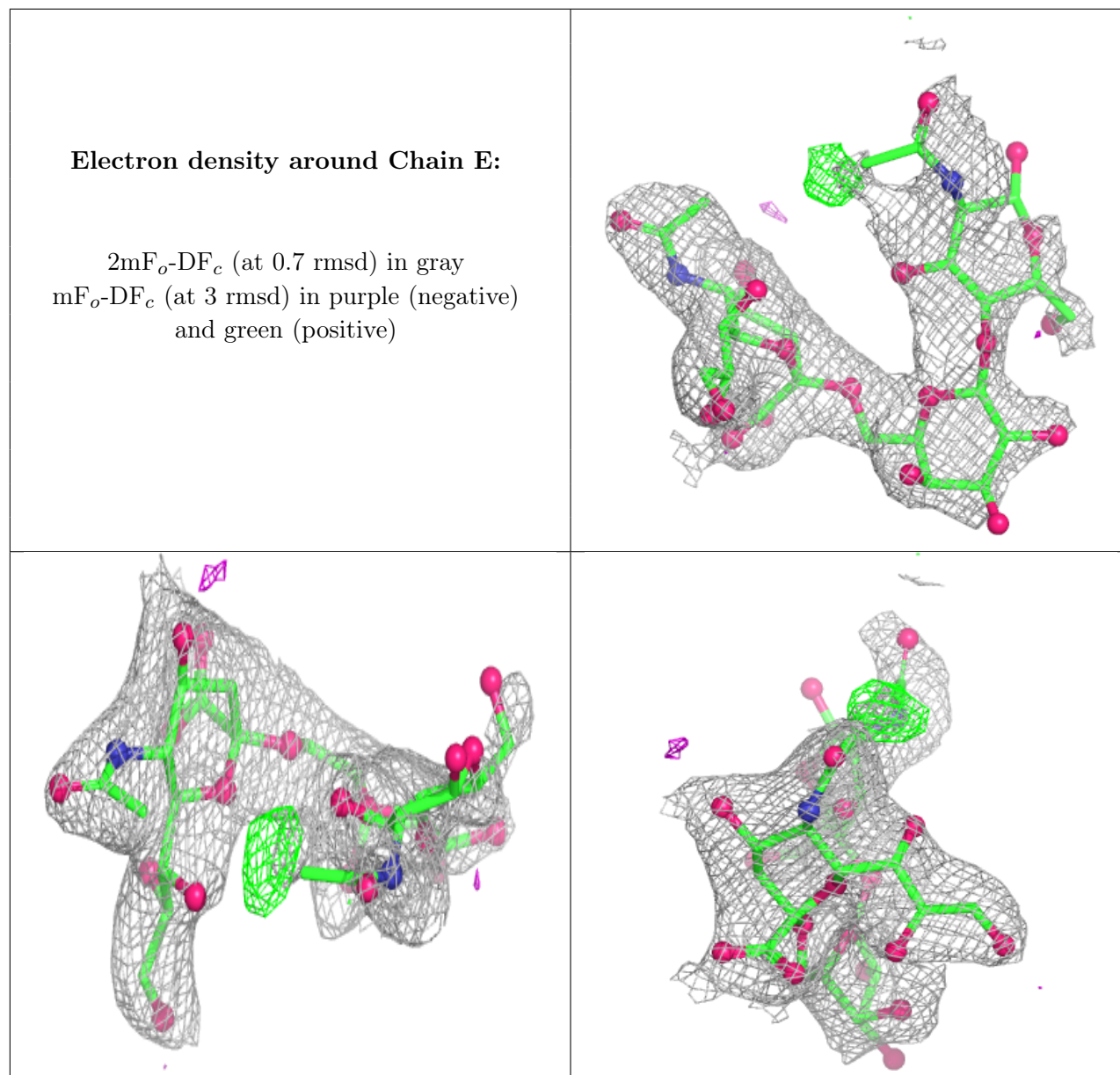
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	F	1	15/15	0.34	0.22	149,164,169,171	0
3	NAG	E	1	15/15	0.42	0.19	126,135,142,144	0
3	GAL	F	2	11/12	0.72	0.16	116,134,143,147	0
3	GAL	E	2	11/12	0.73	0.15	98,112,122,123	0

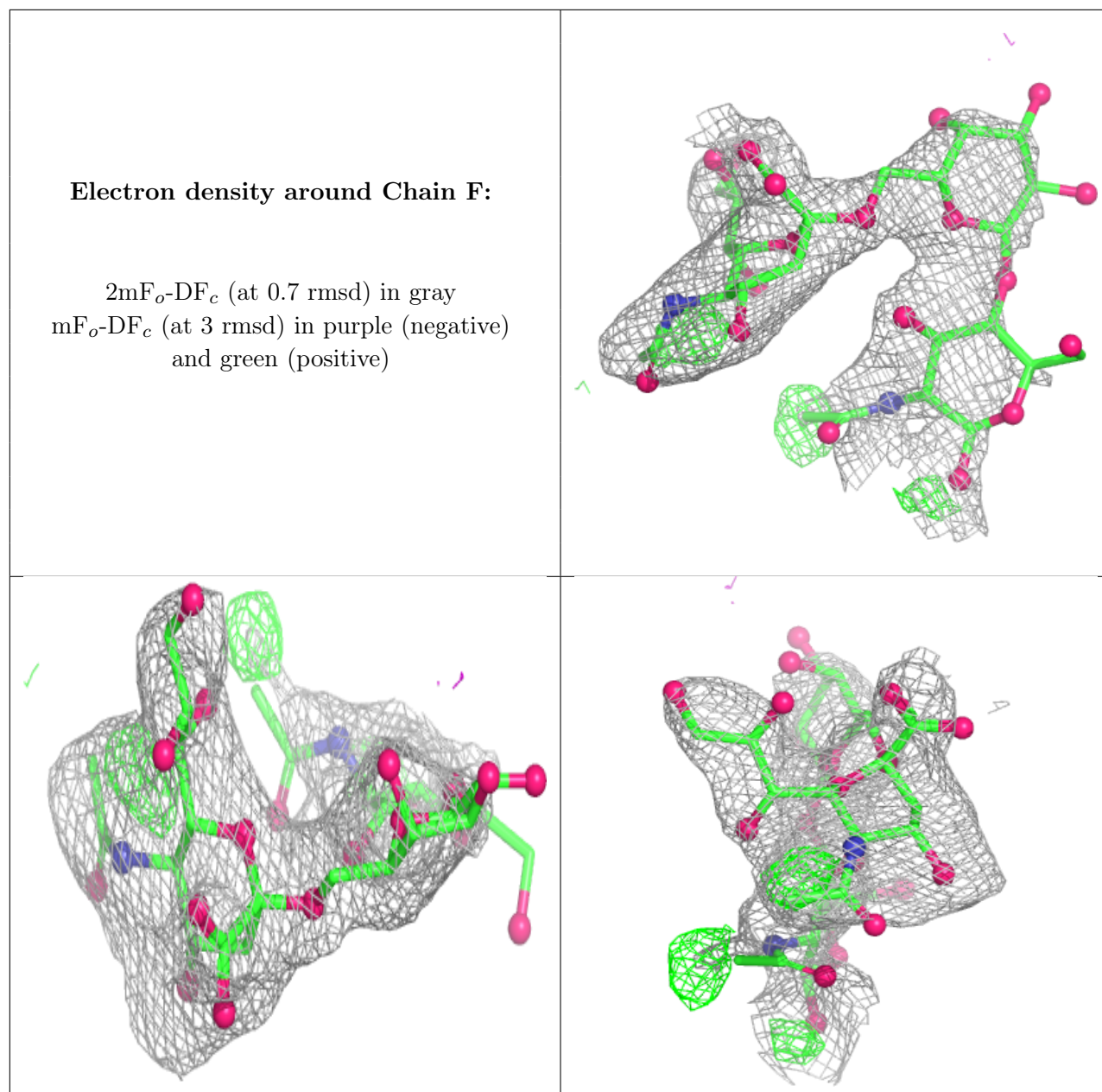
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SIA	F	3	20/21	0.79	0.15	82,88,93,95	0
3	SIA	E	3	20/21	0.88	0.12	63,69,76,76	0

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 ⓘ

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	A	601	14/15	0.66	0.17	90,96,100,101	0
4	NAG	B	601	14/15	0.70	0.18	101,106,113,113	0
4	NAG	A	602	14/15	0.89	0.09	29,36,42,44	0
4	NAG	B	602	14/15	0.90	0.09	39,43,48,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.