



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:01 PM UTC

PDB ID : 6TM0 / pdb_00006tm0
Title : N-Domain P40/P90 Mycoplasma pneumoniae complexed with 6'SL
Authors : Vizarraga, D.; Aparicio, D.; Illanes, R.; Fita, I.; Perez-Luque, R.; Martin, J.
Deposited on : 2019-12-03
Resolution : 2.80 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

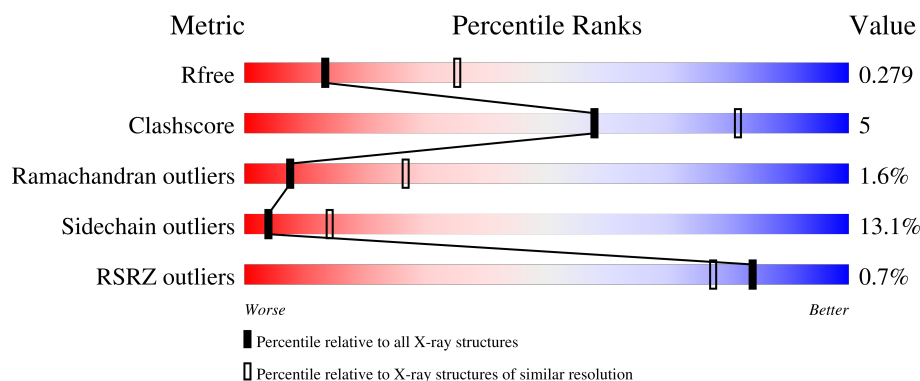
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	976	
1	B	976	
2	C	3	
2	D	3	

2 Entry composition [i](#)

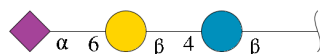
There are 2 unique types of molecules in this entry. The entry contains 12580 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Mgp-operon protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	811	Total	C	N	O	S	0	0	0
			6247	3931	1060	1251	5			
1	B	811	Total	C	N	O	S	0	0	0
			6247	3931	1060	1251	5			

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

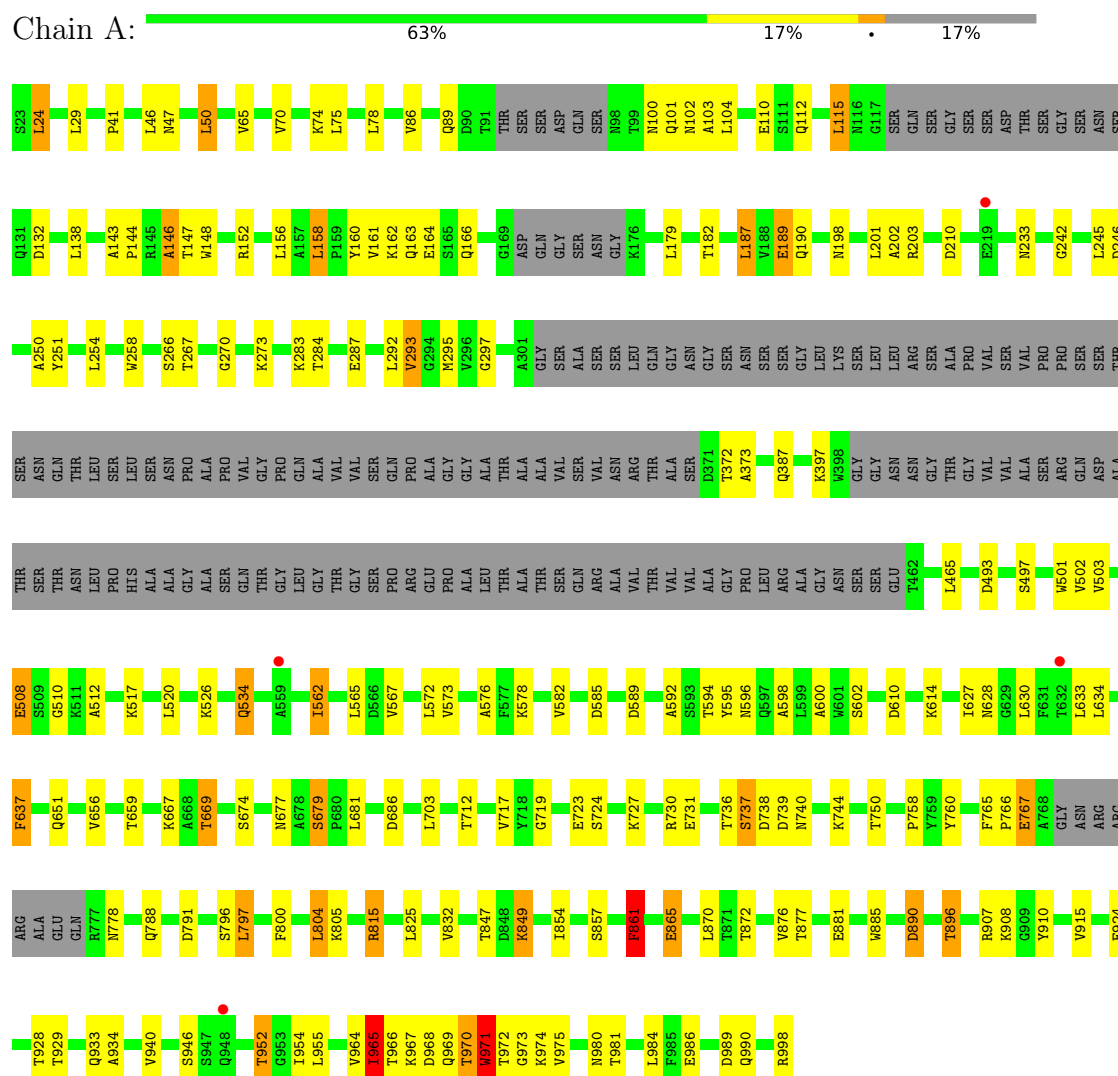


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			43	23	1	19			
2	D	3	Total	C	N	O	0	0	0
			43	23	1	19			

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: Mgp-operon protein 3



• Molecule 1: Mgp-operon protein 3



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	116.33Å 107.38Å 160.45Å 90.00° 90.07° 90.00°	Depositor
Resolution (Å)	80.22 – 2.80 80.22 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.8 (80.22-2.80) 96.5 (80.22-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.82Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.208 , 0.265 0.225 , 0.279	Depositor DCC
R_{free} test set	2396 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	74.2	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 93.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.457 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12580	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% of the height of the origin peak. No significant pseudotranslation is detected.*

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: BGC, 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	0.85	1/6375 (0.0%)	1.32	27/8668 (0.3%)
1	B	0.84	1/6375 (0.0%)	1.32	27/8668 (0.3%)
All	All	0.84	2/12750 (0.0%)	1.32	54/17336 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	679	SER	C-N	5.33	1.37	1.33
1	A	679	SER	C-N	5.00	1.37	1.33

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	LEU	N-CA-C	-7.89	103.60	113.55
1	B	24	LEU	N-CA-C	-7.70	103.85	113.55
1	B	952	THR	N-CA-C	-6.72	103.99	112.93
1	B	210	ASP	CA-CB-CG	6.48	119.08	112.60
1	A	210	ASP	CA-CB-CG	6.44	119.04	112.60
1	B	637	PHE	CA-CB-CG	6.40	120.20	113.80
1	A	146	ALA	CA-C-N	6.33	133.62	121.54
1	A	146	ALA	C-N-CA	6.33	133.62	121.54
1	A	637	PHE	CA-CB-CG	6.31	120.11	113.80
1	A	952	THR	N-CA-C	-6.27	104.34	112.68
1	A	965	ILE	CB-CA-C	6.04	119.25	110.98
1	B	967	LYS	CB-CA-C	-5.81	108.70	117.07
1	B	283	LYS	CA-C-N	5.71	127.87	120.44
1	B	283	LYS	C-N-CA	5.71	127.87	120.44
1	B	989	ASP	CA-C-N	5.63	127.75	120.44
1	B	989	ASP	C-N-CA	5.63	127.75	120.44
1	B	861	PHE	CA-CB-CG	5.61	119.41	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	GLU	CA-C-N	5.57	127.74	120.28
1	B	287	GLU	C-N-CA	5.57	127.74	120.28
1	A	283	LYS	CA-C-N	5.56	127.67	120.44
1	A	283	LYS	C-N-CA	5.56	127.67	120.44
1	A	989	ASP	CA-C-N	5.53	127.63	120.44
1	A	989	ASP	C-N-CA	5.53	127.63	120.44
1	A	102	ASN	CA-CB-CG	5.51	118.11	112.60
1	B	967	LYS	CA-C-N	5.50	132.05	121.54
1	B	967	LYS	C-N-CA	5.50	132.05	121.54
1	B	731	GLU	CA-C-N	5.43	127.56	120.28
1	B	731	GLU	C-N-CA	5.43	127.56	120.28
1	A	731	GLU	CA-C-N	5.39	127.44	120.44
1	A	731	GLU	C-N-CA	5.39	127.44	120.44
1	B	900	LYS	CA-C-N	5.28	129.85	122.36
1	B	900	LYS	C-N-CA	5.28	129.85	122.36
1	A	270	GLY	CA-C-O	-5.27	118.65	122.45
1	A	890	ASP	CA-CB-CG	5.19	117.79	112.60
1	B	267	THR	N-CA-C	-5.19	105.69	112.23
1	B	862	GLY	CA-C-N	5.18	127.53	120.54
1	B	862	GLY	C-N-CA	5.18	127.53	120.54
1	B	970	THR	CA-C-N	5.17	131.41	121.54
1	B	970	THR	C-N-CA	5.17	131.41	121.54
1	B	890	ASP	CA-CB-CG	5.15	117.75	112.60
1	A	970	THR	CA-C-N	5.15	131.37	121.54
1	A	970	THR	C-N-CA	5.15	131.37	121.54
1	A	738	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	267	THR	N-CA-C	-5.09	105.82	112.23
1	A	182	THR	CA-C-N	5.08	127.09	120.28
1	A	182	THR	C-N-CA	5.08	127.09	120.28
1	A	861	PHE	CA-CB-CG	5.08	118.88	113.80
1	B	738	ASP	CA-CB-CG	5.08	117.68	112.60
1	B	245	LEU	CA-C-N	5.05	127.56	120.28
1	B	245	LEU	C-N-CA	5.05	127.56	120.28
1	A	287	GLU	CA-C-N	5.01	126.99	120.28
1	A	287	GLU	C-N-CA	5.01	126.99	120.28
1	A	669	THR	CA-C-N	5.00	128.21	121.05
1	A	669	THR	C-N-CA	5.00	128.21	121.05

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	6247	0	6077	58	0
1	B	6247	0	6077	54	0
2	C	43	0	37	0	0
2	D	43	0	37	0	0
All	All	12580	0	12228	112	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 (112) 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:861:PHE:HB2	1:A:865:GLU:HG3	1.54	0.90
1:B:143:ALA:HB1	1:B:144:PRO:HD2	1.55	0.87
1:B:861:PHE:HB2	1:B:865:GLU:HG3	1.57	0.84
1:A:143:ALA:HB1	1:A:144:PRO:HD2	1.61	0.82
1:B:160:TYR:OH	1:B:162:LYS:HG2	1.88	0.74
1:A:47:ASN:HD21	1:A:146:ALA:HB3	1.51	0.73
1:A:861:PHE:HB2	1:A:865:GLU:CG	2.24	0.66
1:B:103:ALA:HB3	1:B:161:VAL:HG13	1.76	0.66
1:A:103:ALA:HB3	1:A:161:VAL:HG13	1.79	0.64
1:A:187:LEU:HD21	1:A:273:LYS:HB2	1.82	0.62
1:B:187:LEU:HD21	1:B:273:LYS:HB2	1.82	0.62
1:B:974:LYS:HG3	1:B:996:LYS:HE2	1.82	0.61
1:A:967:LYS:HB3	1:A:972:THR:HG23	1.86	0.57
1:B:800:PHE:HE2	1:B:870:LEU:HB3	1.69	0.57
1:B:103:ALA:HB2	1:B:163:GLN:HB3	1.89	0.54
1:A:47:ASN:ND2	1:A:146:ALA:HB3	2.22	0.53
1:A:800:PHE:HE1	1:A:870:LEU:HB3	1.73	0.53
1:A:65:VAL:HB	1:A:78:LEU:HD23	1.90	0.53
1:B:143:ALA:HB1	1:B:144:PRO:CD	2.35	0.53
1:B:965:ILE:HD12	1:B:975:VAL:HG22	1.91	0.52
1:A:766:PRO:HB3	1:A:788:GLN:HE22	1.76	0.51
1:A:582:VAL:HG11	1:A:600:ALA:HB2	1.94	0.50
1:B:974:LYS:O	1:B:996:LYS:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:LEU:HD13	1:B:148:TRP:HB2	1.94	0.50
1:B:582:VAL:HG11	1:B:600:ALA:HB2	1.95	0.49
1:B:961:PHE:CE1	1:B:979:LYS:HB2	2.48	0.49
1:A:50:LEU:HD13	1:A:148:TRP:HB2	1.93	0.49
1:A:501:TRP:CE2	1:A:512:ALA:HB2	2.48	0.49
1:B:198:ASN:HD21	1:B:787:SER:HB2	1.77	0.49
1:B:501:TRP:CE2	1:B:512:ALA:HB2	2.48	0.49
1:A:24:LEU:HA	1:A:41:PRO:HG2	1.94	0.48
1:B:24:LEU:HA	1:B:41:PRO:HG2	1.94	0.48
1:A:758:PRO:HB3	1:A:760:TYR:CZ	2.48	0.48
1:A:872:THR:HB	1:A:890:ASP:O	2.12	0.48
1:B:872:THR:HB	1:B:890:ASP:O	2.12	0.48
1:A:242:GLY:HA3	1:A:598:ALA:O	2.14	0.48
1:B:758:PRO:HB3	1:B:760:TYR:CZ	2.49	0.48
1:B:977:ILE:CD1	1:B:995:VAL:HG11	2.43	0.48
1:A:156:LEU:HB3	1:A:501:TRP:CE2	2.49	0.47
1:A:585:ASP:HB3	1:A:594:THR:O	2.15	0.47
1:B:198:ASN:ND2	1:B:787:SER:HB2	2.29	0.47
1:B:242:GLY:HA3	1:B:598:ALA:O	2.15	0.47
1:A:70:VAL:HB	1:A:74:LYS:HB3	1.96	0.47
1:A:896:THR:HA	1:A:907:ARG:NH1	2.30	0.47
1:B:156:LEU:HB3	1:B:501:TRP:CE2	2.50	0.47
1:B:861:PHE:HB2	1:B:865:GLU:CG	2.38	0.46
1:B:766:PRO:HB3	1:B:788:GLN:HE22	1.80	0.46
1:B:997:ARG:HA	1:B:997:ARG:HE	1.80	0.46
1:A:112:GLN:HA	1:A:115:LEU:HD12	1.97	0.45
1:B:719:GLY:HA3	1:B:750:THR:HG22	1.99	0.45
1:A:592:ALA:HB3	1:A:595:TYR:HB2	1.99	0.45
1:A:760:TYR:HB3	1:A:767:GLU:H	1.82	0.44
1:B:592:ALA:HB3	1:B:595:TYR:HB2	1.99	0.44
1:A:189:GLU:HB2	1:A:677:ASN:HA	1.99	0.44
1:B:190:GLN:HB3	1:B:250:ALA:HB3	1.98	0.44
1:A:233:ASN:O	1:A:656:VAL:HG13	2.17	0.44
1:A:952:THR:HB	1:A:965:ILE:HG23	1.99	0.44
1:B:245:LEU:HD21	1:B:598:ALA:HB2	1.98	0.44
1:A:190:GLN:HB3	1:A:250:ALA:HB3	1.98	0.44
1:B:189:GLU:HB2	1:B:677:ASN:HA	2.00	0.44
1:B:202:ALA:O	1:B:266:SER:HB2	2.18	0.44
1:B:681:LEU:HD11	1:B:797:LEU:HD13	2.00	0.44
1:B:681:LEU:HD11	1:B:797:LEU:CD1	2.48	0.44
1:A:202:ALA:O	1:A:266:SER:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:LEU:HD11	1:A:797:LEU:HD13	2.00	0.44
1:A:719:GLY:HA3	1:A:750:THR:HG22	2.00	0.44
1:A:520:LEU:HD13	1:A:717:VAL:HG11	2.00	0.43
1:B:520:LEU:HD13	1:B:717:VAL:HG11	2.00	0.43
1:A:187:LEU:HG	1:A:251:TYR:HB3	1.99	0.43
1:A:245:LEU:HD21	1:A:598:ALA:HB2	1.99	0.43
1:A:152:ARG:NH1	1:A:508:GLU:HA	2.34	0.43
1:A:198:ASN:HD21	1:A:796:SER:H	1.66	0.43
1:B:187:LEU:HG	1:B:251:TYR:HB3	1.99	0.43
1:B:760:TYR:HB3	1:B:767:GLU:H	1.84	0.43
1:A:681:LEU:HD11	1:A:797:LEU:CD1	2.48	0.43
1:B:152:ARG:NH1	1:B:508:GLU:HA	2.34	0.43
1:A:258:TRP:O	1:A:465:LEU:HD12	2.19	0.43
1:B:160:TYR:HE2	1:B:737:SER:HB2	1.82	0.43
1:A:160:TYR:HE2	1:A:737:SER:HB2	1.82	0.43
1:B:854:ILE:HA	1:B:934:ALA:HB2	1.99	0.43
1:A:854:ILE:HA	1:A:934:ALA:HB2	1.99	0.42
1:B:573:VAL:HG23	1:B:804:LEU:HD21	2.01	0.42
1:A:573:VAL:HG23	1:A:804:LEU:HD21	2.01	0.42
1:B:179:LEU:HD13	1:B:517:LYS:HE3	2.01	0.42
1:A:179:LEU:HD13	1:A:517:LYS:HE3	2.01	0.42
1:B:503:VAL:HG12	1:B:510:GLY:HA3	2.01	0.42
1:B:258:TRP:O	1:B:465:LEU:HD12	2.20	0.42
1:B:86:VAL:HG13	1:B:158:LEU:HD21	2.02	0.42
1:A:534:GLN:NE2	1:A:712:THR:HG21	2.34	0.41
1:A:954:ILE:HG12	1:A:964:VAL:HG22	2.01	0.41
1:B:992:SER:O	1:B:996:LYS:HB2	2.20	0.41
1:A:562:ILE:HA	1:A:576:ALA:HB2	2.01	0.41
1:A:86:VAL:HG13	1:A:158:LEU:HD21	2.02	0.41
1:B:562:ILE:HA	1:B:576:ALA:HB2	2.02	0.41
1:A:103:ALA:HA	1:A:163:GLN:HE21	1.86	0.41
1:B:602:SER:HB3	1:B:628:ASN:HB2	2.03	0.41
1:B:885:TRP:HB2	1:B:915:VAL:HB	2.03	0.41
1:A:143:ALA:HB1	1:A:144:PRO:CD	2.40	0.41
1:A:503:VAL:HG12	1:A:510:GLY:HA3	2.02	0.41
1:A:602:SER:HB3	1:A:628:ASN:HB2	2.03	0.41
1:A:885:TRP:HB2	1:A:915:VAL:HB	2.03	0.41
1:A:970:THR:O	1:A:971:TRP:HB3	2.21	0.41
1:A:502:VAL:O	1:A:502:VAL:HG12	2.21	0.41
1:A:614:LYS:HB2	1:A:849:LYS:HB2	2.03	0.41
1:B:194:PRO:HD2	1:B:384:ALA:HB1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:LEU:HD12	1:B:254:LEU:HA	1.96	0.41
1:B:910:TYR:CE2	1:B:946:SER:HB3	2.56	0.41
1:A:254:LEU:HD12	1:A:254:LEU:HA	1.96	0.40
1:A:758:PRO:HB3	1:A:760:TYR:CE2	2.55	0.40
1:A:910:TYR:CE2	1:A:946:SER:HB3	2.56	0.40
1:B:502:VAL:O	1:B:502:VAL:HG12	2.21	0.40
1:B:758:PRO:HB3	1:B:760:TYR:CE2	2.55	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	797/976 (82%)	724 (91%)	57 (7%)	16 (2%)	6	21
1	B	797/976 (82%)	732 (92%)	55 (7%)	10 (1%)	9	31
All	All	1594/1952 (82%)	1456 (91%)	112 (7%)	26 (2%)	7	27

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	THR
1	A	815	ARG
1	A	737	SER
1	A	778	ASN
1	A	929	THR
1	A	971	TRP
1	B	737	SER
1	B	929	THR
1	B	971	TRP
1	A	373	ALA
1	A	589	ASP

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Mol	Chain	Res	Type
1	A	791	ASP
1	A	975	VAL
1	B	589	ASP
1	B	791	ASP
1	B	815	ARG
1	A	627	ILE
1	A	686	ASP
1	B	627	ILE
1	B	686	ASP
1	B	975	VAL
1	A	100	ASN
1	B	973	GLY
1	A	293	VAL
1	A	297	GLY
1	A	973	GLY

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	677/800 (85%)	584 (86%)	93 (14%)	3	13
1	B	677/800 (85%)	593 (88%)	84 (12%)	4	16
All	All	1354/1600 (85%)	1177 (87%)	177 (13%)	4	14

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	46	LEU
1	A	50	LEU
1	A	75	LEU
1	A	89	GLN
1	A	101	GLN
1	A	104	LEU
1	A	110	GLU

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Mol	Chain	Res	Type
1	A	115	LEU
1	A	132	ASP
1	A	138	LEU
1	A	158	LEU
1	A	162	LYS
1	A	164	GLU
1	A	166	GLN
1	A	187	LEU
1	A	189	GLU
1	A	201	LEU
1	A	203	ARG
1	A	246	ASP
1	A	284	THR
1	A	292	LEU
1	A	293	VAL
1	A	295	MET
1	A	372	THR
1	A	387	GLN
1	A	397	LYS
1	A	493	ASP
1	A	497	SER
1	A	508	GLU
1	A	526	LYS
1	A	534	GLN
1	A	562	ILE
1	A	565	LEU
1	A	567	VAL
1	A	572	LEU
1	A	578	LYS
1	A	596	ASN
1	A	610	ASP
1	A	630	LEU
1	A	633	LEU
1	A	634	LEU
1	A	637	PHE
1	A	651	GLN
1	A	659	THR
1	A	667	LYS
1	A	669	THR
1	A	674	SER
1	A	679	SER
1	A	703	LEU

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Mol	Chain	Res	Type
1	A	723	GLU
1	A	724	SER
1	A	727	LYS
1	A	730	ARG
1	A	736	THR
1	A	739	ASP
1	A	740	ASN
1	A	744	LYS
1	A	765	PHE
1	A	767	GLU
1	A	797	LEU
1	A	804	LEU
1	A	805	LYS
1	A	815	ARG
1	A	825	LEU
1	A	832	VAL
1	A	847	THR
1	A	849	LYS
1	A	857	SER
1	A	861	PHE
1	A	865	GLU
1	A	876	VAL
1	A	877	THR
1	A	881	GLU
1	A	896	THR
1	A	908	LYS
1	A	924	GLU
1	A	928	THR
1	A	933	GLN
1	A	940	VAL
1	A	955	LEU
1	A	965	ILE
1	A	966	THR
1	A	968	ASP
1	A	969	GLN
1	A	971	TRP
1	A	974	LYS
1	A	980	ASN
1	A	981	THR
1	A	984	LEU
1	A	986	GLU
1	A	990	GLN

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Mol	Chain	Res	Type
1	A	998	ARG
1	B	29	LEU
1	B	46	LEU
1	B	50	LEU
1	B	65	VAL
1	B	75	LEU
1	B	89	GLN
1	B	90	ASP
1	B	101	GLN
1	B	104	LEU
1	B	110	GLU
1	B	115	LEU
1	B	145	ARG
1	B	158	LEU
1	B	162	LYS
1	B	164	GLU
1	B	187	LEU
1	B	189	GLU
1	B	201	LEU
1	B	203	ARG
1	B	232	LYS
1	B	246	ASP
1	B	284	THR
1	B	292	LEU
1	B	293	VAL
1	B	295	MET
1	B	387	GLN
1	B	395	LEU
1	B	493	ASP
1	B	497	SER
1	B	508	GLU
1	B	526	LYS
1	B	534	GLN
1	B	562	ILE
1	B	565	LEU
1	B	567	VAL
1	B	572	LEU
1	B	578	LYS
1	B	596	ASN
1	B	610	ASP
1	B	630	LEU
1	B	633	LEU

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Mol	Chain	Res	Type
1	B	637	PHE
1	B	651	GLN
1	B	659	THR
1	B	669	THR
1	B	674	SER
1	B	679	SER
1	B	703	LEU
1	B	723	GLU
1	B	724	SER
1	B	727	LYS
1	B	736	THR
1	B	739	ASP
1	B	740	ASN
1	B	744	LYS
1	B	765	PHE
1	B	767	GLU
1	B	797	LEU
1	B	804	LEU
1	B	805	LYS
1	B	825	LEU
1	B	832	VAL
1	B	846	SER
1	B	847	THR
1	B	849	LYS
1	B	857	SER
1	B	861	PHE
1	B	865	GLU
1	B	876	VAL
1	B	877	THR
1	B	881	GLU
1	B	896	THR
1	B	908	LYS
1	B	924	GLU
1	B	928	THR
1	B	933	GLN
1	B	940	VAL
1	B	966	THR
1	B	971	TRP
1	B	980	ASN
1	B	981	THR
1	B	990	GLN
1	B	996	LYS

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Mol	Chain	Res	Type
1	B	997	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	47	ASN
1	A	101	GLN
1	A	163	GLN
1	A	198	ASN
1	A	233	ASN
1	A	288	ASN
1	A	386	HIS
1	A	471	GLN
1	A	652	ASN
1	A	682	ASN
1	A	732	ASN
1	A	788	GLN
1	A	835	ASN
1	A	901	GLN
1	A	902	GLN
1	A	942	ASN
1	A	948	GLN
1	A	969	GLN
1	B	26	ASN
1	B	98	ASN
1	B	112	GLN
1	B	386	HIS
1	B	471	GLN
1	B	652	ASN
1	B	682	ASN
1	B	698	ASN
1	B	732	ASN
1	B	788	GLN
1	B	835	ASN
1	B	901	GLN
1	B	941	GLN
1	B	942	ASN
1	B	948	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$
2	BGC	C	1	2	12,12,12	0.28	0	17,17,17	0.48	0
2	GAL	C	2	2	11,11,12	0.37	0	15,15,17	0.47	0
2	SIA	C	3	2	20,20,21	0.53	1 (5%)	21,28,31	0.64	0
2	BGC	D	1	2	12,12,12	0.35	0	17,17,17	0.97	1 (5%)
2	GAL	D	2	2	11,11,12	0.38	0	15,15,17	0.66	0
2	SIA	D	3	2	20,20,21	1.06	3 (15%)	21,28,31	1.31	2 (9%)

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	BGC	C	1	2	-	0/2/22/22	0/1/1/1
2	GAL	C	2	2	-	0/2/19/22	0/1/1/1
2	SIA	C	3	2	-	2/18/34/38	0/1/1/1
2	BGC	D	1	2	-	0/2/22/22	0/1/1/1
2	GAL	D	2	2	-	0/2/19/22	0/1/1/1
2	SIA	D	3	2	-	2/18/34/38	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	SIA	O1A-C1	3.24	1.31	1.22
2	D	3	SIA	O1B-C1	-2.53	1.22	1.30
2	D	3	SIA	C2-C1	2.13	1.54	1.52
2	C	3	SIA	C2-C1	2.10	1.54	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	SIA	O1B-C1-C2	4.00	123.11	112.71
2	D	3	SIA	O1A-C1-C2	-3.62	115.03	122.85
2	D	1	BGC	C1-O5-C5	3.18	119.80	113.65

There are no chirality outliers.

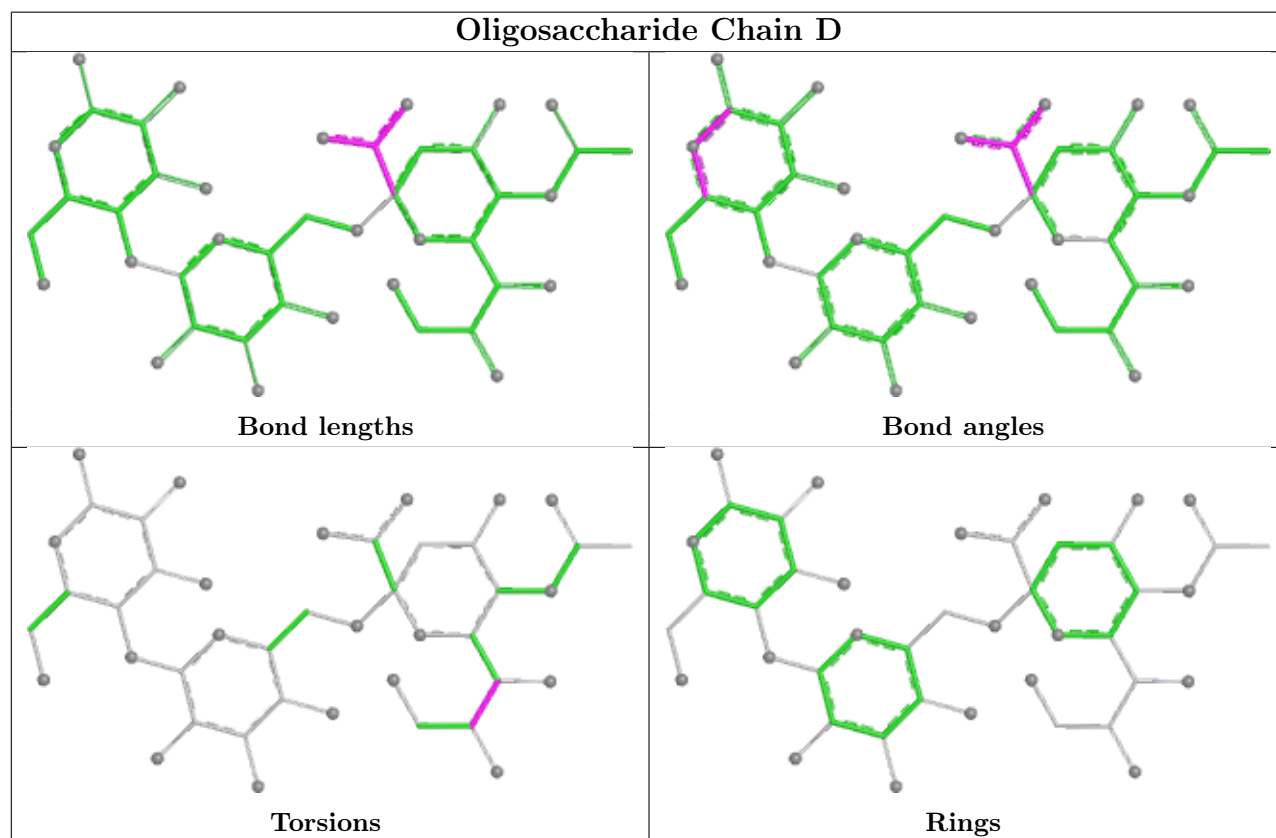
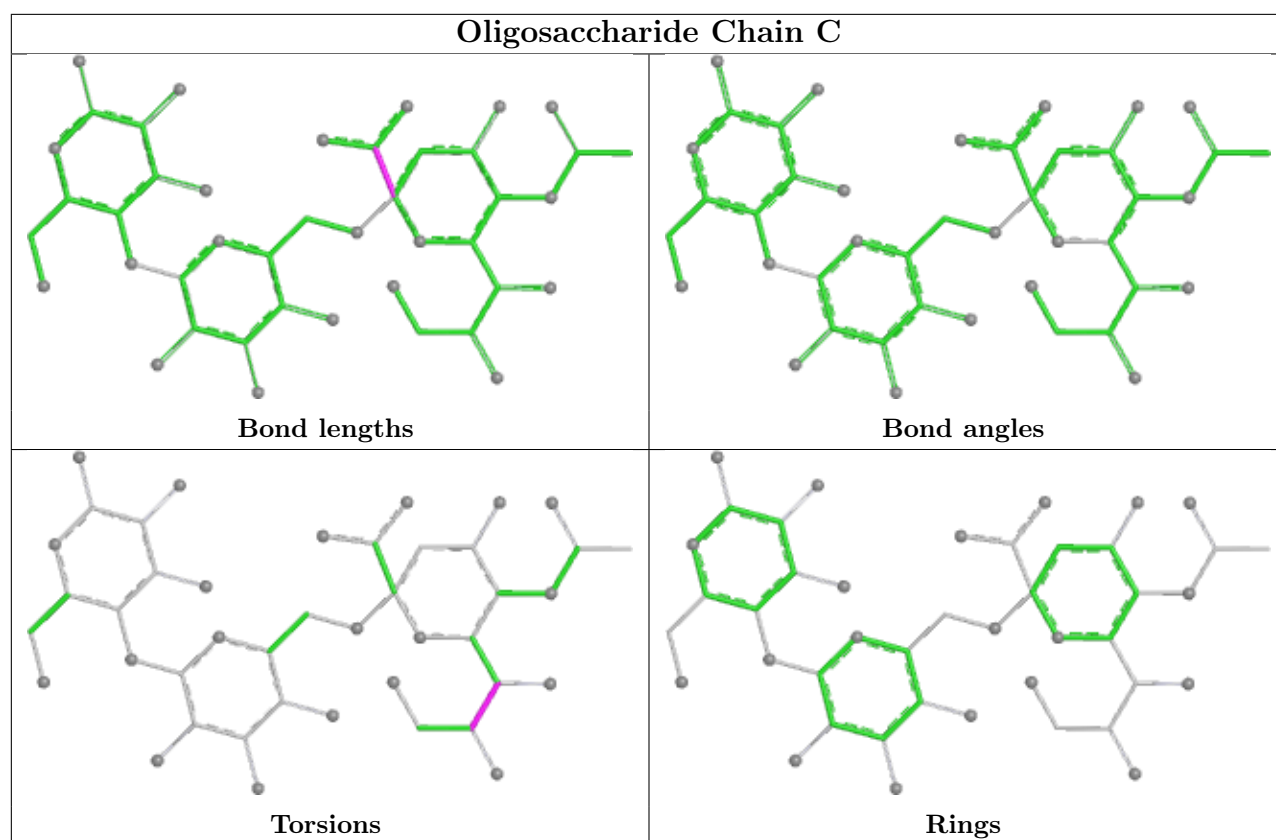
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3	SIA	C6-C7-C8-O8
2	D	3	SIA	C6-C7-C8-O8
2	C	3	SIA	O7-C7-C8-O8
2	D	3	SIA	O7-C7-C8-O8

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.



5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	811/976 (83%)	-0.48	4 (0%) 87 82	55, 91, 139, 201	0
1	B	811/976 (83%)	-0.44	7 (0%) 81 74	59, 91, 137, 200	0
All	All	1622/1952 (83%)	-0.46	11 (0%) 84 77	55, 91, 139, 201	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	662	VAL	3.3
1	B	109	GLN	2.7
1	A	219	GLU	2.6
1	A	559	ALA	2.4
1	B	207	VAL	2.3
1	A	632	THR	2.1
1	B	145	ARG	2.1
1	A	948	GLN	2.1
1	B	211	THR	2.0
1	B	972	THR	2.0
1	B	610	ASP	2.0

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

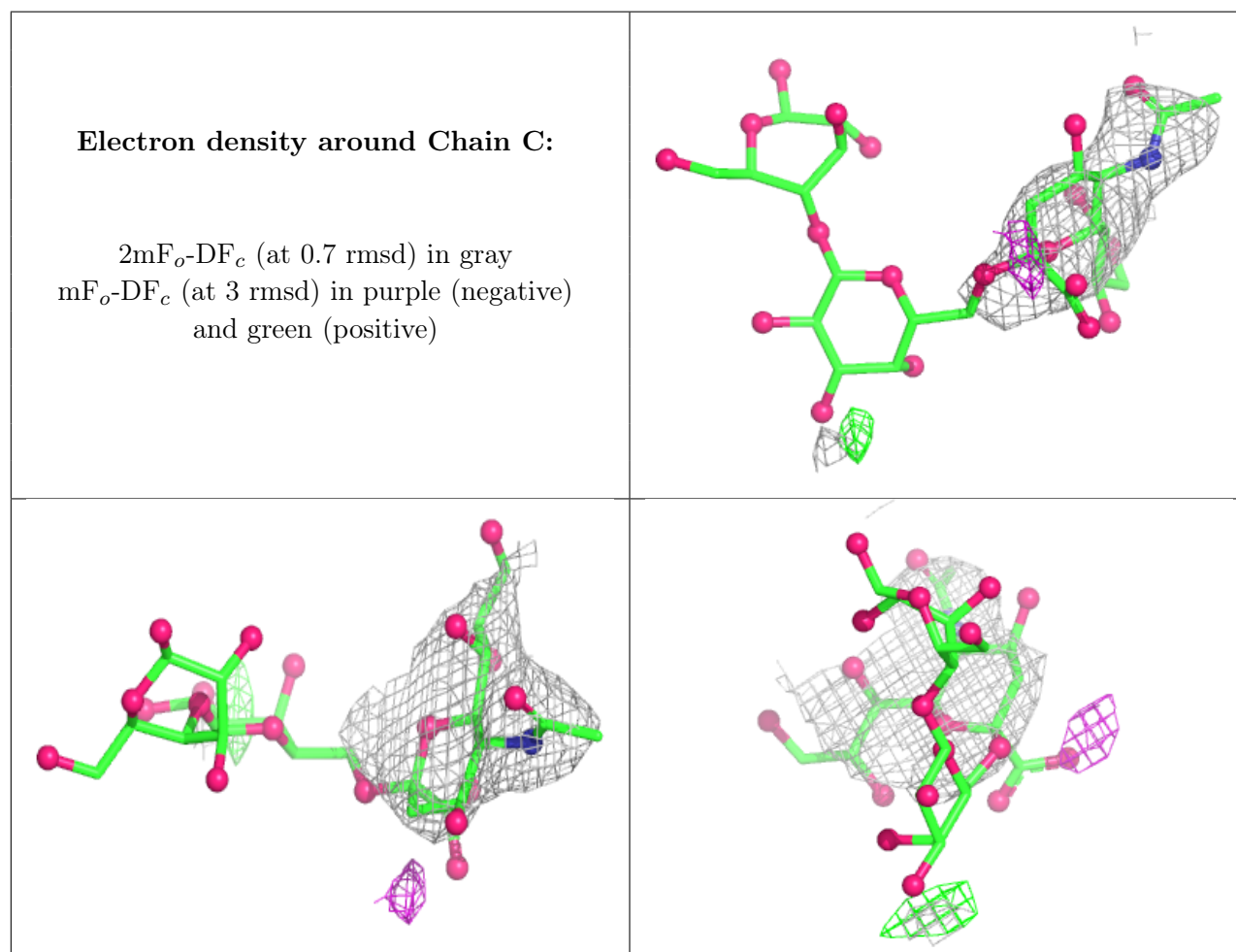
There are no non-standard protein/DNA/RNA residues in this entry.

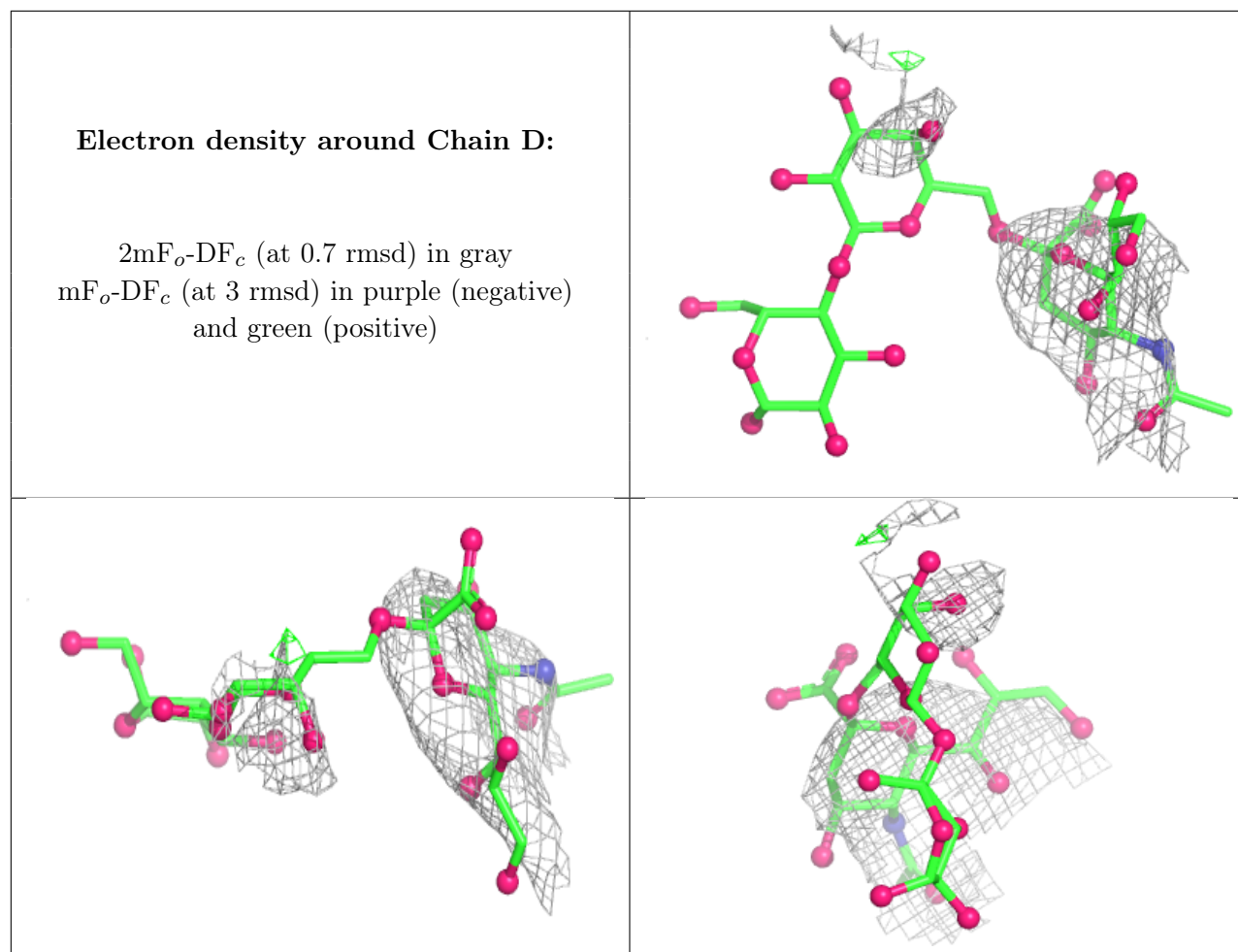
6.3 Carbohydrates [i](#)

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($\text{\AA}^2$)	Q<0.9
2	GAL	C	2	11/12	0.89	0.25	116,117,118,119	11
2	GAL	D	2	11/12	0.90	0.18	116,118,118,119	11
2	BGC	D	1	12/12	0.96	0.23	118,121,121,122	12
2	BGC	C	1	12/12	0.96	0.21	115,117,119,119	12
2	SIA	C	3	20/21	0.97	0.13	105,114,119,121	20
2	SIA	D	3	20/21	0.98	0.12	104,113,119,120	20

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.