



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:49 PM UTC

PDB ID : 5W6G / pdb_00005w6g
Title : Human antibody 6649 in complex with influenza hemagglutinin H1 Solomon Islands
Authors : Raymond, D.D.; Harrison, S.C.
Deposited on : 2017-06-16
Resolution : 2.79 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

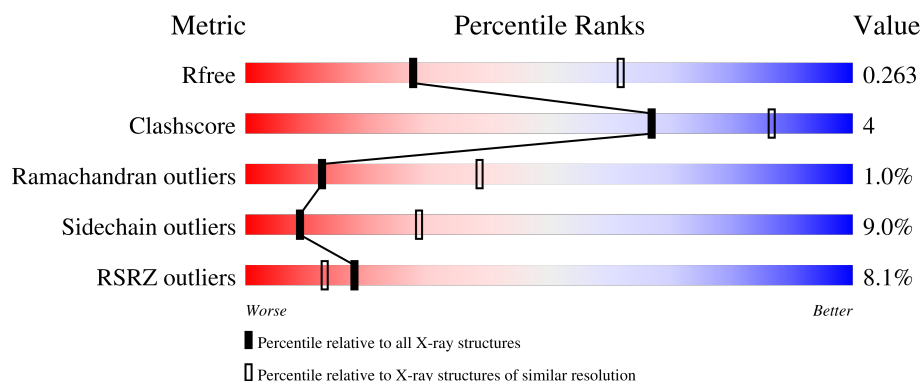
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	334	5% 81% 14% ..
2	B	178	17% 74% 17% .. 6%
3	H	230	7% 77% 18% ..
4	L	218	6% 85% 12% ..
5	C	2	50% 50%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7347 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 HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	326	2563	1618	444	490	11	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ALA	-	expression tag	UNP A7UPX0
A	-2	ASP	-	expression tag	UNP A7UPX0
A	-1	PRO	-	expression tag	UNP A7UPX0
A	0	GLY	-	expression tag	UNP A7UPX0
A	1	TYR	-	expression tag	UNP A7UPX0
A	2	LEU	-	expression tag	UNP A7UPX0
A	3	LEU	-	expression tag	UNP A7UPX0
A	4	GLU	-	expression tag	UNP A7UPX0

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	168	1359	849	233	270	7	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	677	ARG	-	expression tag	UNP A7UPX0
B	678	SER	-	expression tag	UNP A7UPX0

- Molecule 3 is a protein called 6649 antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	225	1708	1087	284	331	6	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	125	GLY	SER	conflict	UNP S6B2B6
H	148	VAL	ALA	conflict	UNP S6B2B6

- Molecule 4 is a protein called 6649 antibody light chain.

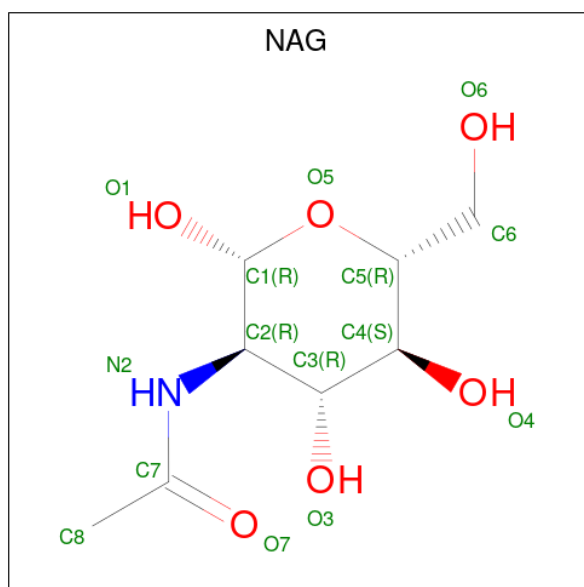
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	214	Total	C	N	O	S	0	0	0
			1580	989	266	321	4			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



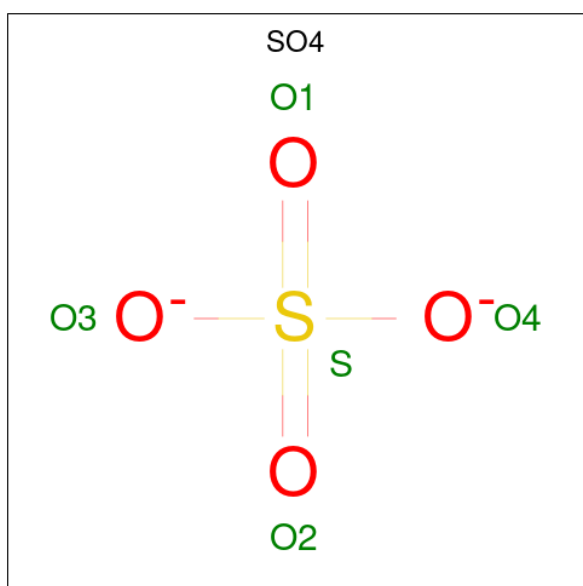
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	2	Total	C	N	O		0	0	0
			28	16	2	10				

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



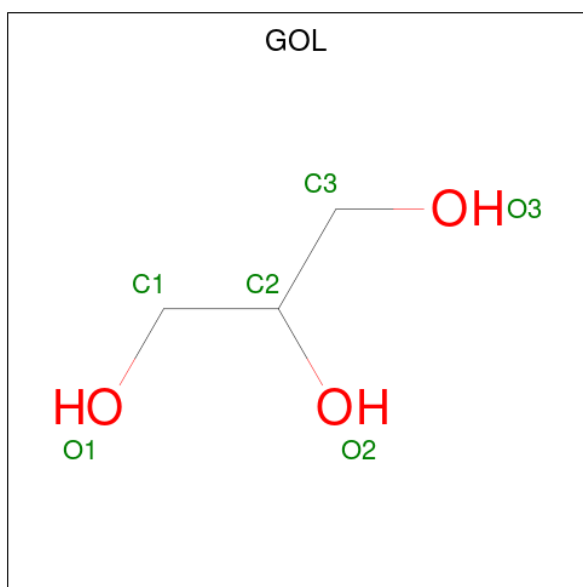
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		

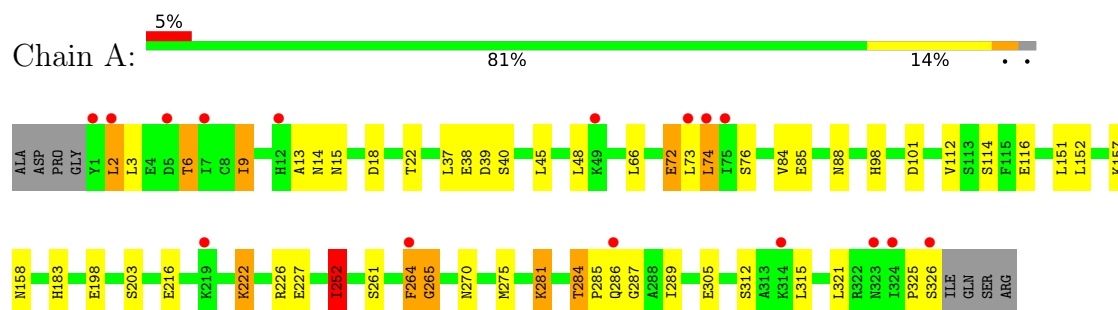
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	7	Total	O	0	0
			7	7		
9	H	2	Total	O	0	0
			2	2		
9	L	2	Total	O	0	0
			2	2		

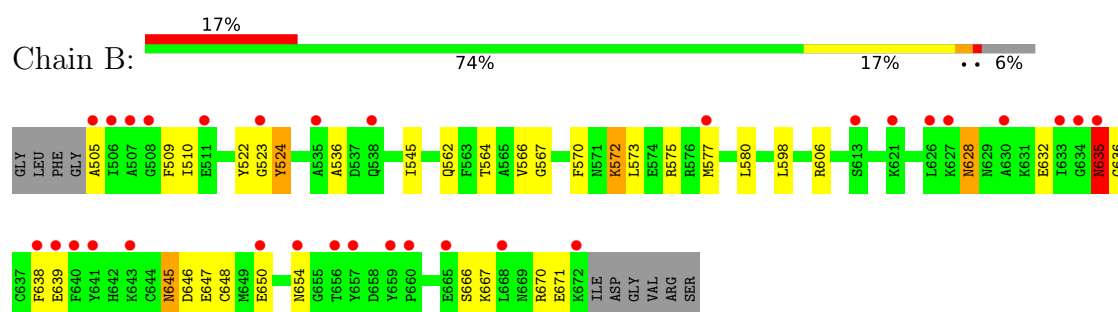
3 Residue-property plots [i](#)

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.

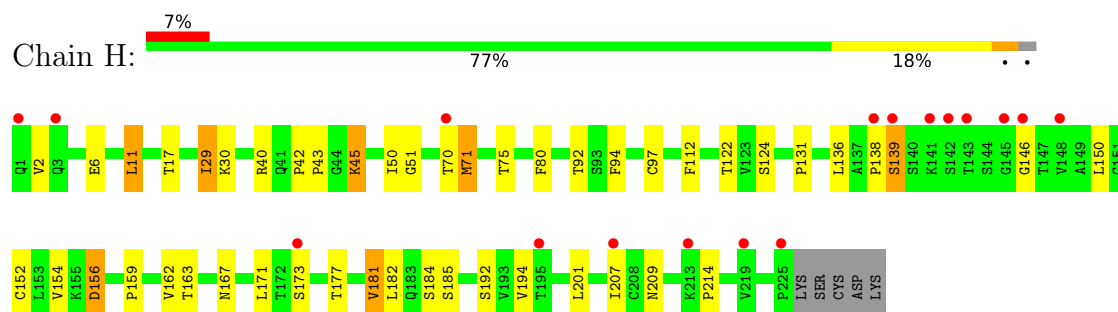
• Molecule 1: Hemagglutinin HA1



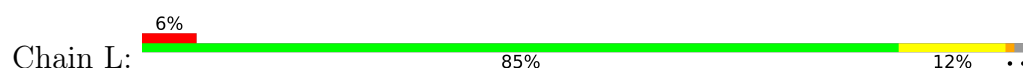
• Molecule 2: Hemagglutinin HA2

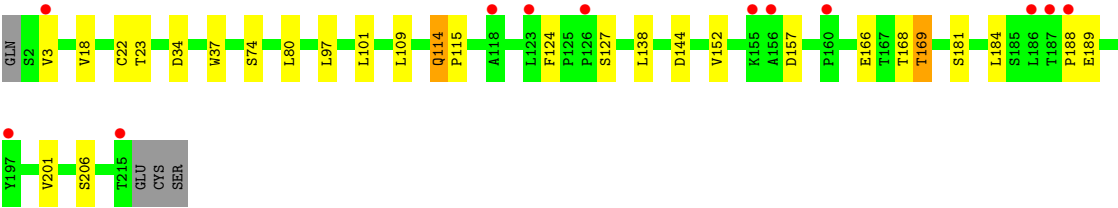


• Molecule 3: 6649 antibody heavy chain



• Molecule 4: 6649 antibody light chain





● Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	177.31Å 177.31Å 177.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.18 – 2.79 49.18 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.18-2.79) 99.6 (49.18-2.79)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.218 , 0.253 0.226 , 0.263	Depositor DCC
R_{free} test set	2291 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	78.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.012 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7347	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% 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: NAG, GOL, SO4

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	0.90	1/2630 (0.0%)	1.30	14/3580 (0.4%)
2	B	0.87	1/1385 (0.1%)	1.47	9/1861 (0.5%)
3	H	0.85	1/1757 (0.1%)	1.25	7/2400 (0.3%)
4	L	0.85	0/1619	1.26	6/2211 (0.3%)
All	All	0.87	3/7391 (0.0%)	1.32	36/10052 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	71	MET	SD-CE	-6.26	1.63	1.79
1	A	252	ILE	CG1-CD1	-5.62	1.29	1.51
2	B	505	ALA	C-N	5.54	1.39	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	654	ASN	CA-CB-CG	6.66	119.26	112.60
2	B	635	ASN	CA-CB-CG	6.38	118.98	112.60
1	A	15	ASN	CA-CB-CG	6.33	118.93	112.60
1	A	227	GLU	N-CA-C	-6.33	104.61	112.90
2	B	566	VAL	CA-C-N	6.01	125.69	119.92
2	B	566	VAL	C-N-CA	6.01	125.69	119.92
1	A	39	ASP	CA-CB-CG	5.98	118.58	112.60
4	L	188	PRO	CA-C-N	5.96	128.18	120.44
4	L	188	PRO	C-N-CA	5.96	128.18	120.44
4	L	34	ASP	CA-CB-CG	5.78	118.38	112.60
1	A	158	ASN	CA-CB-CG	5.74	118.33	112.60
1	A	73	LEU	CA-C-N	5.71	132.44	121.54
1	A	73	LEU	C-N-CA	5.71	132.44	121.54
2	B	628	ASN	CA-CB-CG	5.67	118.27	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	184	SER	CA-C-N	5.65	132.33	121.54
3	H	184	SER	C-N-CA	5.65	132.33	121.54
1	A	281	LYS	N-CA-C	-5.64	107.03	114.31
1	A	198	GLU	N-CA-C	-5.51	106.46	114.12
4	L	169	THR	N-CA-C	-5.50	102.72	109.65
3	H	139	SER	N-CA-C	5.50	117.39	110.24
1	A	14	ASN	CA-CB-CG	5.44	118.04	112.60
4	L	127	SER	CA-C-N	5.36	127.41	120.44
4	L	127	SER	C-N-CA	5.36	127.41	120.44
1	A	18	ASP	CA-CB-CG	5.35	117.95	112.60
3	H	138	PRO	CA-C-N	5.30	128.61	120.82
3	H	138	PRO	C-N-CA	5.30	128.61	120.82
1	A	6	THR	N-CA-C	5.27	117.83	109.50
2	B	650	GLU	CB-CG-CD	5.16	121.36	112.60
1	A	252	ILE	CA-C-N	5.11	127.49	120.39
1	A	252	ILE	C-N-CA	5.11	127.49	120.39
1	A	101	ASP	CA-CB-CG	5.08	117.67	112.60
2	B	567	GLY	N-CA-C	5.03	117.25	111.36
2	B	666	SER	CA-C-N	5.03	127.27	120.38
2	B	666	SER	C-N-CA	5.03	127.27	120.38
3	H	17	THR	CA-C-N	5.00	129.25	122.19
3	H	17	THR	C-N-CA	5.00	129.25	122.19

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	2563	0	2474	18	0
2	B	1359	0	1286	11	0
3	H	1708	0	1657	21	0
4	L	1580	0	1530	8	0
5	C	28	0	25	0	0
6	A	56	0	52	0	0
7	A	30	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	12	0	16	1	0
9	A	7	0	0	0	0
9	H	2	0	0	0	0
9	L	2	0	0	0	0
All	All	7347	0	7040	53	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 4.

All (53) 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:85:GLU:O	1:A:270:ASN:HA	1.85	0.77
1:A:284:THR:HB	1:A:287:GLY:O	1.84	0.77
3:H:51:GLY:HA3	3:H:71:MET:HE1	1.75	0.68
3:H:40:ARG:HB3	3:H:50:ILE:HD11	1.82	0.61
1:A:284:THR:HG22	1:A:286:GLN:H	1.68	0.59
3:H:167:ASN:HD22	3:H:207:ILE:HG13	1.67	0.59
3:H:167:ASN:ND2	3:H:207:ILE:H	2.00	0.58
3:H:51:GLY:CA	3:H:71:MET:HE1	2.34	0.56
3:H:92:THR:HG23	3:H:122:THR:HA	1.87	0.56
1:A:2:LEU:H	1:A:2:LEU:HD13	1.70	0.56
1:A:114:SER:HB3	1:A:261:SER:HB2	1.90	0.53
3:H:167:ASN:HA	3:H:207:ILE:HG13	1.91	0.52
3:H:11:LEU:HD21	3:H:124:SER:HB3	1.93	0.51
1:A:98:HIS:HA	8:A:414:GOL:H32	1.92	0.50
4:L:152:VAL:HG22	4:L:201:VAL:HG22	1.94	0.50
1:A:13:ALA:HB1	1:A:325:PRO:HB3	1.94	0.49
1:A:264:PHE:HD1	1:A:265:GLY:H	1.61	0.49
1:A:66:LEU:HD22	1:A:151:LEU:HD11	1.93	0.49
3:H:42:PRO:HB2	3:H:45:LYS:HD3	1.94	0.48
3:H:131:PRO:HB2	3:H:154:VAL:HG13	1.95	0.48
1:A:183:HIS:HB2	1:A:252:ILE:HD11	1.94	0.48
1:A:284:THR:HG23	1:A:285:PRO:HD2	1.97	0.47
2:B:510:ILE:HA	2:B:635:ASN:HB2	1.96	0.47
2:B:570:PHE:CE1	2:B:577:MET:HB3	2.50	0.47
1:A:38:GLU:HG2	1:A:289:ILE:HG23	1.95	0.47
3:H:136:LEU:HB3	4:L:124:PHE:CD2	2.50	0.47
4:L:80:LEU:HD11	4:L:109:LEU:HD21	1.96	0.46
1:A:37:LEU:HB2	1:A:315:LEU:HB2	1.97	0.46
2:B:635:ASN:HD22	2:B:636:GLY:H	1.64	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:523:GLY:HA3	2:B:536:ALA:HA	1.98	0.46
1:A:222:LYS:HA	1:A:226:ARG:O	2.17	0.45
1:A:6:THR:HG23	2:B:639:GLU:OE1	2.16	0.45
4:L:114:GLN:HA	4:L:115:PRO:HD2	1.89	0.44
3:H:159:PRO:HD2	3:H:214:PRO:CB	2.48	0.44
1:A:2:LEU:H	1:A:2:LEU:CD1	2.31	0.44
3:H:177:THR:HA	3:H:192:SER:HA	2.00	0.44
2:B:632:GLU:HG2	2:B:638:PHE:HE1	1.83	0.43
2:B:667:LYS:HG2	2:B:670:ARG:CZ	2.47	0.43
2:B:645:ASN:HD22	2:B:647:GLU:HB2	1.83	0.43
3:H:29:ILE:HD11	3:H:80:PHE:HB3	2.01	0.43
1:A:9:ILE:HG22	2:B:524:TYR:HD1	1.84	0.42
4:L:138:LEU:HD12	4:L:184:LEU:HD23	2.00	0.42
3:H:131:PRO:CB	3:H:154:VAL:HG13	2.50	0.42
2:B:509:PHE:O	2:B:635:ASN:HB3	2.20	0.41
3:H:6:GLU:HG3	3:H:97:CYS:SG	2.61	0.41
3:H:43:PRO:HG3	3:H:94:PHE:CE2	2.55	0.41
3:H:30:LYS:HD2	3:H:75:THR:HG21	2.03	0.41
2:B:572:LYS:H	2:B:572:LYS:HE2	1.85	0.41
1:A:45:LEU:HD13	1:A:84:VAL:HG11	2.03	0.40
3:H:112:PHE:CZ	4:L:101:LEU:HD13	2.56	0.40
4:L:22:CYS:HB2	4:L:37:TRP:CH2	2.57	0.40
3:H:159:PRO:HD2	3:H:214:PRO:HB3	2.02	0.40
3:H:181:VAL:CG1	4:L:168:THR:HG22	2.52	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	324/334 (97%)	299 (92%)	21 (6%)	4 (1%)	10 34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	166/178 (93%)	154 (93%)	11 (7%)	1 (1%)	21	51
3	H	223/230 (97%)	200 (90%)	20 (9%)	3 (1%)	9	31
4	L	212/218 (97%)	200 (94%)	11 (5%)	1 (0%)	24	55
All	All	925/960 (96%)	853 (92%)	63 (7%)	9 (1%)	12	38

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	PHE
2	B	635	ASN
3	H	146	GLY
1	A	74	LEU
3	H	156	ASP
3	H	185	SER
4	L	157	ASP
1	A	72	GLU
1	A	265	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	286/292 (98%)	261 (91%)	25 (9%)	9	30
2	B	146/153 (95%)	129 (88%)	17 (12%)	5	18
3	H	193/198 (98%)	175 (91%)	18 (9%)	8	27
4	L	177/181 (98%)	165 (93%)	12 (7%)	14	42
All	All	802/824 (97%)	730 (91%)	72 (9%)	9	28

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	3	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	9	ILE
1	A	22	THR
1	A	40	SER
1	A	48	LEU
1	A	72	GLU
1	A	74	LEU
1	A	76	SER
1	A	88	ASN
1	A	112	VAL
1	A	116	GLU
1	A	152	LEU
1	A	157	LYS
1	A	203	SER
1	A	216	GLU
1	A	222	LYS
1	A	252	ILE
1	A	275	MET
1	A	281	LYS
1	A	284	THR
1	A	305	GLU
1	A	312	SER
1	A	321	LEU
1	A	326	SER
2	B	522	TYR
2	B	524	TYR
2	B	545	ILE
2	B	562	GLN
2	B	564	THR
2	B	572	LYS
2	B	573	LEU
2	B	575	ARG
2	B	580	LEU
2	B	598	LEU
2	B	606	ARG
2	B	628	ASN
2	B	635	ASN
2	B	645	ASN
2	B	646	ASP
2	B	648	CYS
2	B	671	GLU
3	H	2	VAL
3	H	11	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	29	ILE
3	H	45	LYS
3	H	70	THR
3	H	139	SER
3	H	150	LEU
3	H	152	CYS
3	H	156	ASP
3	H	162	VAL
3	H	163	THR
3	H	171	LEU
3	H	173	SER
3	H	181	VAL
3	H	182	LEU
3	H	194	VAL
3	H	201	LEU
3	H	209	ASN
4	L	3	VAL
4	L	18	VAL
4	L	23	THR
4	L	74	SER
4	L	97	LEU
4	L	114	GLN
4	L	144	ASP
4	L	166	GLU
4	L	169	THR
4	L	181	SER
4	L	189	GLU
4	L	206	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	35	ASN
1	A	142	ASN
1	A	158	ASN
2	B	538	GLN
2	B	542	GLN
2	B	546	ASN
2	B	625	GLN
2	B	635	ASN
2	B	669	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	167	ASN
4	L	39	GLN
4	L	114	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 ⓘ

2 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	$\# Z > 2$
5	NAG	C	1	5,1	14,14,15	0.34	0	17,19,21	0.94	1 (5%)
5	NAG	C	2	5	14,14,15	0.33	0	17,19,21	0.68	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
5	NAG	C	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	C	2	5	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1	NAG	O5-C1-C2	-2.26	107.79	111.29

There are no chirality outliers.

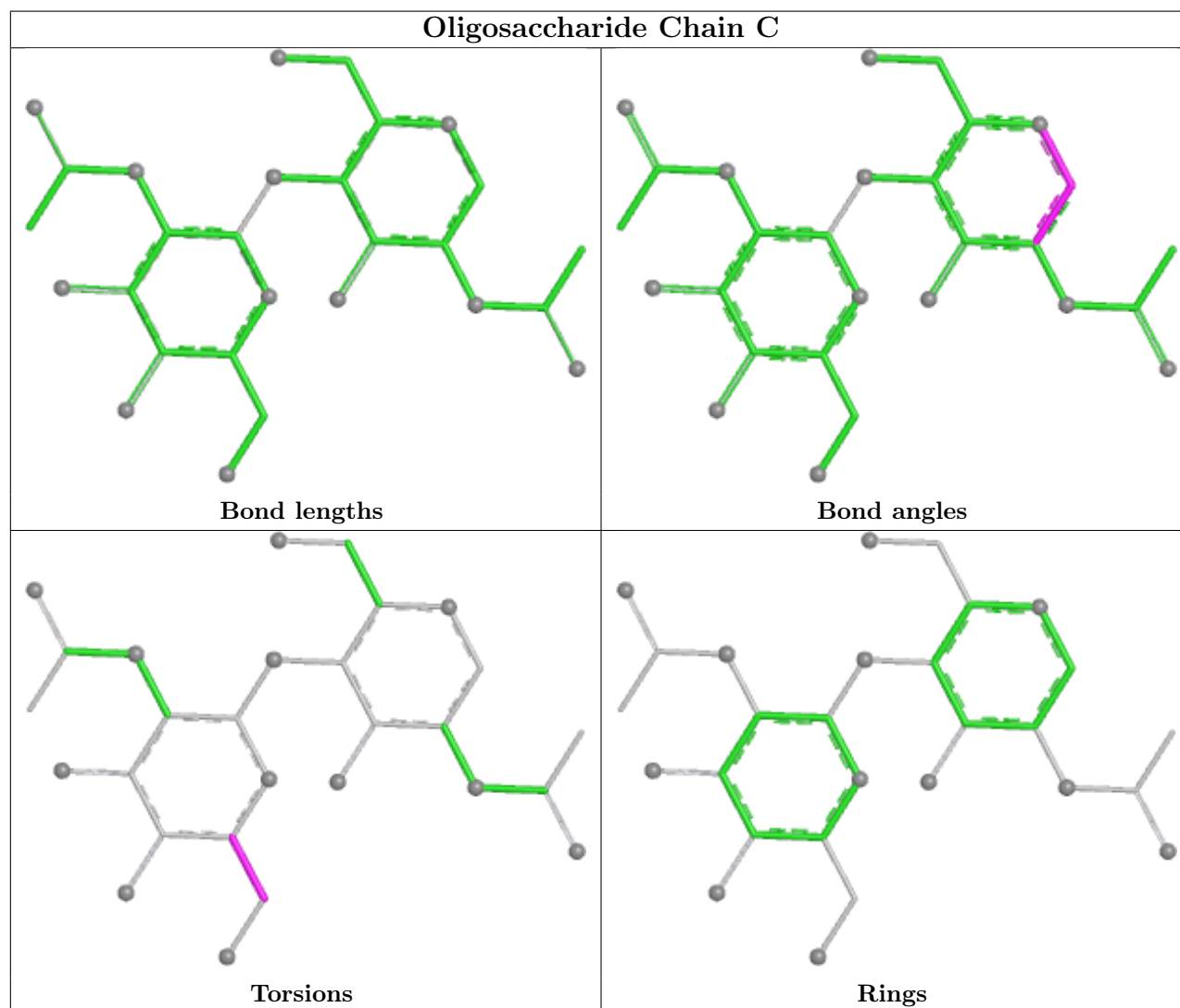
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	2	NAG	O5-C5-C6-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.



5.6 Ligand geometry

12 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
6	NAG	A	404	1	14,14,15	0.33	0	17,19,21	1.24	2 (11%)
7	SO4	A	412	-	4,4,4	0.34	0	6,6,6	0.27	0
7	SO4	A	408	-	4,4,4	0.26	0	6,6,6	0.24	0
8	GOL	A	413	-	5,5,5	0.14	0	5,5,5	0.47	0
6	NAG	A	403	1	14,14,15	0.38	0	17,19,21	1.40	2 (11%)
6	NAG	A	405	1	14,14,15	0.36	0	17,19,21	0.90	1 (5%)
7	SO4	A	410	-	4,4,4	0.27	0	6,6,6	0.21	0
8	GOL	A	414	-	5,5,5	0.09	0	5,5,5	0.26	0
7	SO4	A	411	-	4,4,4	0.30	0	6,6,6	0.76	0
6	NAG	A	406	1	14,14,15	0.38	0	17,19,21	0.84	2 (11%)
7	SO4	A	407	-	4,4,4	0.32	0	6,6,6	0.24	0
7	SO4	A	409	-	4,4,4	0.31	0	6,6,6	0.21	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
6	NAG	A	404	1	-	2/6/23/26	0/1/1/1
8	GOL	A	413	-	-	0/4/4/4	-
6	NAG	A	403	1	-	1/6/23/26	0/1/1/1
6	NAG	A	405	1	-	2/6/23/26	0/1/1/1
8	GOL	A	414	-	-	2/4/4/4	-
6	NAG	A	406	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	403	NAG	C1-C2-N2	4.20	117.06	110.43
6	A	404	NAG	C1-O5-C5	3.61	117.02	112.19
6	A	405	NAG	C1-O5-C5	3.26	116.56	112.19
6	A	403	NAG	C2-N2-C7	2.97	126.88	122.90
6	A	404	NAG	C2-N2-C7	2.18	125.83	122.90
6	A	406	NAG	C1-O5-C5	2.15	115.07	112.19
6	A	406	NAG	O5-C1-C2	-2.00	108.19	111.29

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	403	NAG	C1-C2-N2-C7
6	A	404	NAG	C1-C2-N2-C7
8	A	414	GOL	C1-C2-C3-O3
8	A	414	GOL	O2-C2-C3-O3
6	A	405	NAG	C4-C5-C6-O6
6	A	405	NAG	O5-C5-C6-O6
6	A	404	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	414	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	326/334 (97%)	0.37	16 (4%) 35 27	54, 72, 106, 135	0
2	B	168/178 (94%)	1.03	31 (18%) 3 2	54, 99, 137, 148	0
3	H	225/230 (97%)	0.52	17 (7%) 20 14	53, 84, 121, 171	0
4	L	214/218 (98%)	0.53	12 (5%) 30 23	57, 85, 135, 152	0
All	All	933/960 (97%)	0.56	76 (8%) 18 13	53, 80, 131, 171	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	75	ILE	7.4
2	B	668	LEU	6.7
2	B	506	ILE	6.6
4	L	215	THR	5.5
2	B	643	LYS	4.8
3	H	148	VAL	4.3
1	A	73	LEU	4.3
1	A	74	LEU	4.3
3	H	145	GLY	4.2
2	B	672	LYS	4.1
3	H	138	PRO	4.1
1	A	2	LEU	4.0
3	H	141	LYS	3.9
3	H	225	PRO	3.8
3	H	146	GLY	3.6
1	A	326	SER	3.4
2	B	505	ALA	3.4
1	A	1	TYR	3.3
2	B	665	GLU	3.2
3	H	195	THR	3.2
2	B	507	ALA	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	L	3	VAL	3.1
1	A	286	GLN	3.1
3	H	213	LYS	3.1
4	L	156	ALA	3.0
1	A	324	ILE	3.0
2	B	627	LYS	2.9
2	B	654	ASN	2.8
1	A	5	ASP	2.8
2	B	535	ALA	2.8
2	B	508	GLY	2.8
2	B	630	ALA	2.8
1	A	264	PHE	2.8
2	B	657	TYR	2.7
2	B	639	GLU	2.7
3	H	1	GLN	2.6
2	B	659	TYR	2.5
2	B	660	PRO	2.5
3	H	173	SER	2.5
1	A	314	LYS	2.5
4	L	160	PRO	2.5
1	A	219	LYS	2.5
2	B	511	GLU	2.5
3	H	143	THR	2.4
4	L	123	LEU	2.4
2	B	656	THR	2.3
4	L	155	LYS	2.3
1	A	12	HIS	2.3
1	A	49	LYS	2.3
2	B	650	GLU	2.3
3	H	139	SER	2.3
3	H	3	GLN	2.3
2	B	577	MET	2.3
2	B	613	SER	2.3
2	B	638	PHE	2.3
2	B	633	ILE	2.3
4	L	197	TYR	2.3
2	B	634	GLY	2.3
2	B	621	LYS	2.2
2	B	635	ASN	2.2
2	B	640	PHE	2.2
4	L	186	LEU	2.2
4	L	187	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	H	219	VAL	2.2
4	L	126	PRO	2.2
2	B	523	GLY	2.1
2	B	641	TYR	2.1
4	L	118	ALA	2.1
4	L	188	PRO	2.1
3	H	207	ILE	2.1
3	H	142	SER	2.1
3	H	70	THR	2.1
2	B	538	GLN	2.0
2	B	626	LEU	2.0
1	A	7	ILE	2.0
1	A	323	ASN	2.0

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

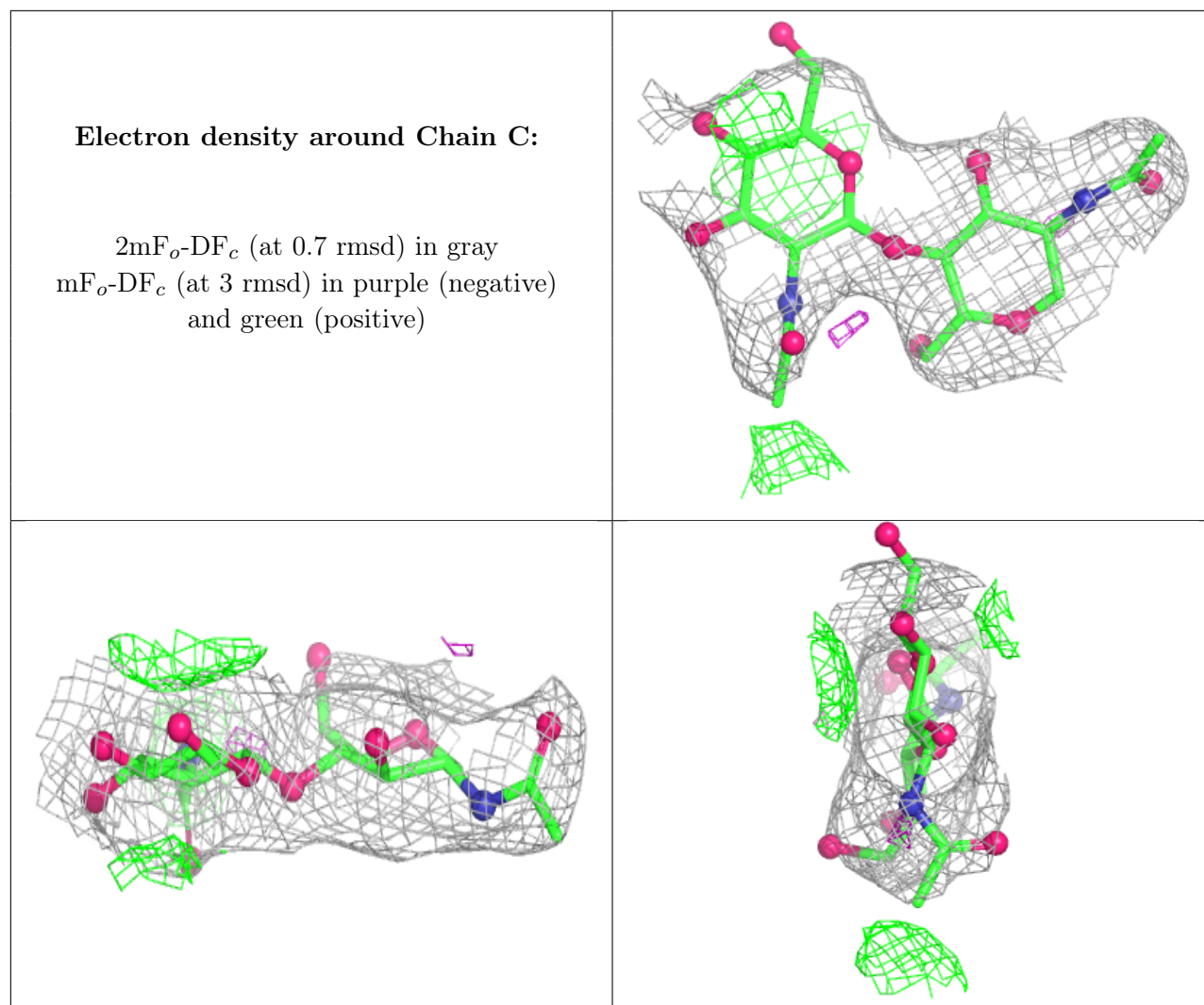
There are no non-standard protein/DNA/RNA residues in this entry.

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(Å ²)	Q<0.9
5	NAG	C	1	14/15	-	-	84,95,101,109	0
5	NAG	C	2	14/15	-	-	116,121,126,127	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
6	NAG	A	406	14/15	0.56	0.17	130,133,134,135	0
6	NAG	A	403	14/15	0.59	0.18	133,136,137,138	0
6	NAG	A	405	14/15	0.69	0.17	122,128,131,131	0
8	GOL	A	414	6/6	0.71	0.31	103,106,108,108	0
7	SO4	A	412	5/5	0.75	0.11	139,139,139,139	0
7	SO4	A	407	5/5	0.78	0.12	116,118,120,120	0
7	SO4	A	409	5/5	0.82	0.09	139,139,141,142	0
7	SO4	A	411	5/5	0.84	0.13	106,107,108,109	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	GOL	A	413	6/6	0.85	0.21	88,99,101,102	0
6	NAG	A	404	14/15	0.87	0.13	100,102,105,108	0
7	SO4	A	410	5/5	0.88	0.08	145,146,146,147	0
7	SO4	A	408	5/5	0.95	0.08	75,79,81,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.