



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:37 AM UTC

PDB ID : 5LCV / pdb_00005lcv
Title : Structural basis of Zika and Dengue virus potent antibody cross-neutralization
Authors : Barba-Spaeth, G.
Deposited on : 2016-06-22
Resolution : 2.64 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

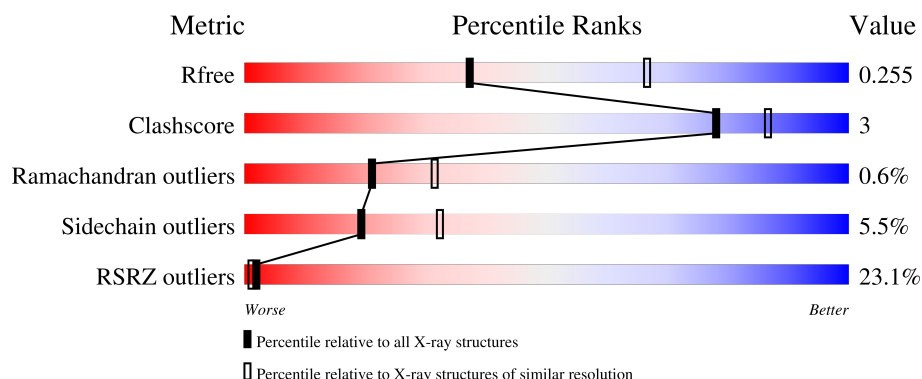
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	447	9% 80% 10% • 9%
1	B	447	14% 81% 8% • 9%
2	H	283	29% 68% 11% • 20%
3	L	216	48% 87% 9% • •
4	C	4	75% 25%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9620 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 Polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	0	0	0
			3100	1939	543	592	26			
1	B	405	Total	C	N	O	S	0	0	0
			3102	1938	543	596	25			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	409	GLY	-	expression tag	UNP A0A120IIH9
A	410	PRO	-	expression tag	UNP A0A120IIH9
A	411	PHE	-	expression tag	UNP A0A120IIH9
A	412	GLU	-	expression tag	UNP A0A120IIH9
A	413	ASP	-	expression tag	UNP A0A120IIH9
A	414	ASP	-	expression tag	UNP A0A120IIH9
A	415	ASP	-	expression tag	UNP A0A120IIH9
A	416	ASP	-	expression tag	UNP A0A120IIH9
A	417	LYS	-	expression tag	UNP A0A120IIH9
A	418	ALA	-	expression tag	UNP A0A120IIH9
A	419	GLY	-	expression tag	UNP A0A120IIH9
A	420	TRP	-	expression tag	UNP A0A120IIH9
A	421	SER	-	expression tag	UNP A0A120IIH9
A	422	HIS	-	expression tag	UNP A0A120IIH9
A	423	PRO	-	expression tag	UNP A0A120IIH9
A	424	GLN	-	expression tag	UNP A0A120IIH9
A	425	PHE	-	expression tag	UNP A0A120IIH9
A	426	GLU	-	expression tag	UNP A0A120IIH9
A	427	LYS	-	expression tag	UNP A0A120IIH9
A	428	GLY	-	expression tag	UNP A0A120IIH9
A	429	GLY	-	expression tag	UNP A0A120IIH9
A	430	GLY	-	expression tag	UNP A0A120IIH9
A	431	SER	-	expression tag	UNP A0A120IIH9
A	432	GLY	-	expression tag	UNP A0A120IIH9
A	433	GLY	-	expression tag	UNP A0A120IIH9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	434	GLY	-	expression tag	UNP A0A120IIH9
A	435	SER	-	expression tag	UNP A0A120IIH9
A	436	GLY	-	expression tag	UNP A0A120IIH9
A	437	GLY	-	expression tag	UNP A0A120IIH9
A	438	GLY	-	expression tag	UNP A0A120IIH9
A	439	SER	-	expression tag	UNP A0A120IIH9
A	440	TRP	-	expression tag	UNP A0A120IIH9
A	441	SER	-	expression tag	UNP A0A120IIH9
A	442	HIS	-	expression tag	UNP A0A120IIH9
A	443	PRO	-	expression tag	UNP A0A120IIH9
A	444	GLN	-	expression tag	UNP A0A120IIH9
A	445	PHE	-	expression tag	UNP A0A120IIH9
A	446	GLU	-	expression tag	UNP A0A120IIH9
A	447	LYS	-	expression tag	UNP A0A120IIH9
B	409	GLY	-	expression tag	UNP A0A120IIH9
B	410	PRO	-	expression tag	UNP A0A120IIH9
B	411	PHE	-	expression tag	UNP A0A120IIH9
B	412	GLU	-	expression tag	UNP A0A120IIH9
B	413	ASP	-	expression tag	UNP A0A120IIH9
B	414	ASP	-	expression tag	UNP A0A120IIH9
B	415	ASP	-	expression tag	UNP A0A120IIH9
B	416	ASP	-	expression tag	UNP A0A120IIH9
B	417	LYS	-	expression tag	UNP A0A120IIH9
B	418	ALA	-	expression tag	UNP A0A120IIH9
B	419	GLY	-	expression tag	UNP A0A120IIH9
B	420	TRP	-	expression tag	UNP A0A120IIH9
B	421	SER	-	expression tag	UNP A0A120IIH9
B	422	HIS	-	expression tag	UNP A0A120IIH9
B	423	PRO	-	expression tag	UNP A0A120IIH9
B	424	GLN	-	expression tag	UNP A0A120IIH9
B	425	PHE	-	expression tag	UNP A0A120IIH9
B	426	GLU	-	expression tag	UNP A0A120IIH9
B	427	LYS	-	expression tag	UNP A0A120IIH9
B	428	GLY	-	expression tag	UNP A0A120IIH9
B	429	GLY	-	expression tag	UNP A0A120IIH9
B	430	GLY	-	expression tag	UNP A0A120IIH9
B	431	SER	-	expression tag	UNP A0A120IIH9
B	432	GLY	-	expression tag	UNP A0A120IIH9
B	433	GLY	-	expression tag	UNP A0A120IIH9
B	434	GLY	-	expression tag	UNP A0A120IIH9
B	435	SER	-	expression tag	UNP A0A120IIH9
B	436	GLY	-	expression tag	UNP A0A120IIH9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	437	GLY	-	expression tag	UNP A0A120IIH9
B	438	GLY	-	expression tag	UNP A0A120IIH9
B	439	SER	-	expression tag	UNP A0A120IIH9
B	440	TRP	-	expression tag	UNP A0A120IIH9
B	441	SER	-	expression tag	UNP A0A120IIH9
B	442	HIS	-	expression tag	UNP A0A120IIH9
B	443	PRO	-	expression tag	UNP A0A120IIH9
B	444	GLN	-	expression tag	UNP A0A120IIH9
B	445	PHE	-	expression tag	UNP A0A120IIH9
B	446	GLU	-	expression tag	UNP A0A120IIH9
B	447	LYS	-	expression tag	UNP A0A120IIH9

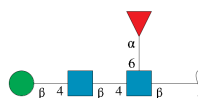
- Molecule 2 is a protein called BROADLY NEUTRALIZING HUMAN ANTIBODY EDE2 A11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	226	Total	C	N	O	S	0	0	0
			1722	1091	292	332	7			

- Molecule 3 is a protein called BROADLY NEUTRALIZING HUMAN ANTIBODY EDE2 A11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	212	Total	C	N	O	S	0	0	0
			1572	982	263	321	6			

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	4	Total	C	N	O	0	0	0
			49	28	2	19			

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



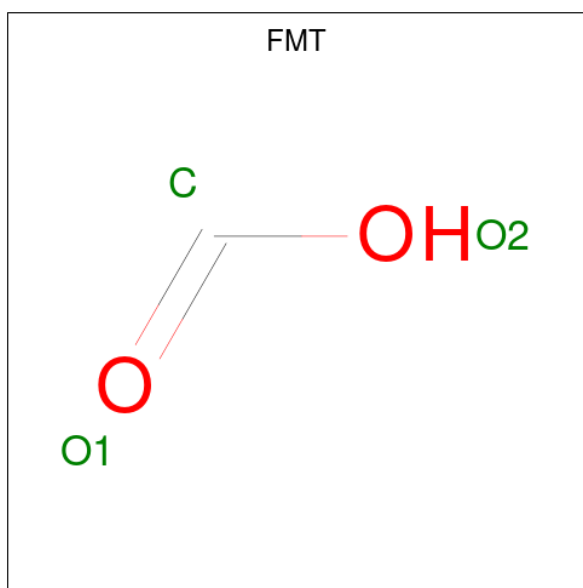
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).

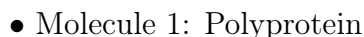


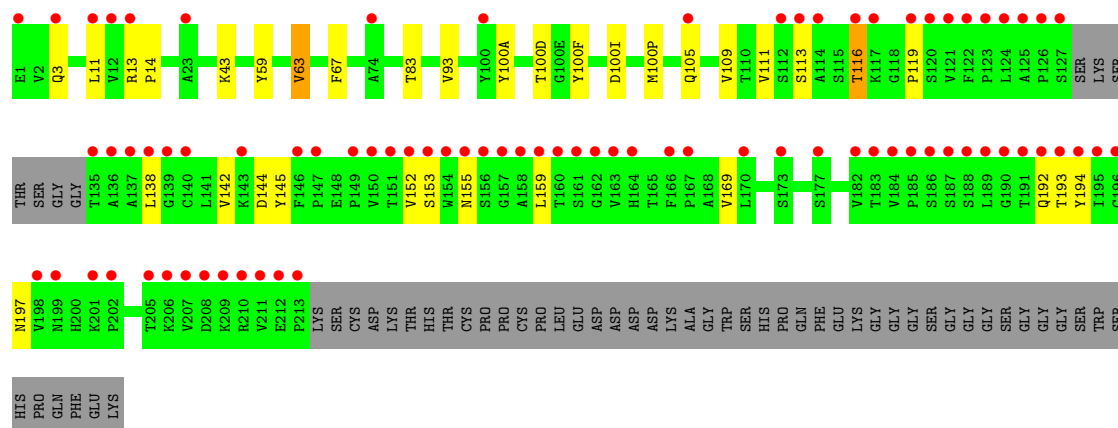
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			3	1	2		

- Molecule 8 is water.

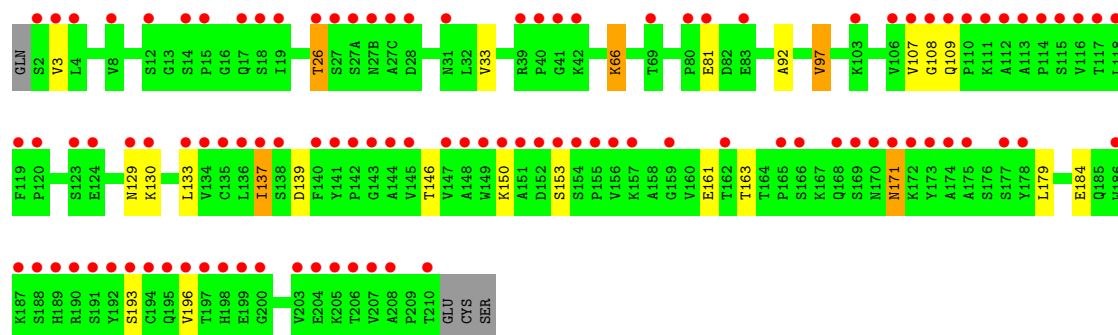
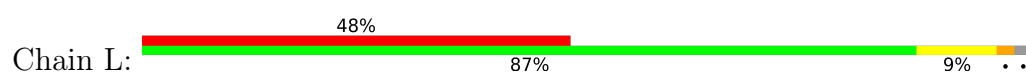
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	16	Total	O	0	0
			16	16		
8	B	15	Total	O	0	0
			15	15		
8	H	8	Total	O	0	0
			8	8		
8	L	1	Total	O	0	0
			1	1		

- Molecule 1: Polyprotein





• Molecule 3: BROADLY NEUTRALIZING HUMAN ANTIBODY EDE2 A11



• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	204.29Å 207.32Å 124.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.64 40.00 – 2.64	Depositor EDS
% Data completeness (in resolution range)	61.9 (40.00-2.64) 61.8 (40.00-2.64)	Depositor EDS
R_{merge}	0.50	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.224 , 0.237 0.243 , 0.255	Depositor DCC
R_{free} test set	2436 reflections (3.14%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.028 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	9620	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, FUC, FMT, NAG, GOL

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	0.69	0/3167	1.13	4/4289 (0.1%)
1	B	0.70	0/3169	1.11	4/4294 (0.1%)
2	H	0.67	0/1768	1.08	1/2412 (0.0%)
3	L	0.68	0/1608	1.06	0/2196
All	All	0.69	0/9712	1.11	9/13191 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	67	PHE	CA-CB-CG	6.48	120.28	113.80
1	A	266	HIS	CA-CB-CG	5.78	119.58	113.80
1	A	359	ILE	N-CA-C	-5.58	105.41	110.82
1	A	17	GLY	CA-C-N	5.51	125.34	120.10
1	A	17	GLY	C-N-CA	5.51	125.34	120.10
1	B	230	ASP	CA-CB-CG	5.41	118.00	112.60
1	B	359	ILE	N-CA-C	-5.24	105.74	110.82
1	B	392	GLY	CA-C-N	5.18	127.22	120.28
1	B	392	GLY	C-N-CA	5.18	127.22	120.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3100	0	3017	19	0
1	B	3102	0	3020	14	0
2	H	1722	0	1646	16	0
3	L	1572	0	1539	10	0
4	C	49	0	43	0	0
5	A	14	0	13	0	0
6	A	12	0	16	0	0
6	B	6	0	8	0	0
7	A	3	0	1	0	0
8	A	16	0	0	0	0
8	B	15	0	0	0	0
8	H	8	0	0	0	0
8	L	1	0	0	0	0
All	All	9620	0	9303	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 3.

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)
2:H:11:LEU:HD23	2:H:116:THR:OG1	1.58	1.01
2:H:83:THR:C	2:H:111:VAL:HG11	2.10	0.77
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.73	0.70
2:H:169:VAL:HB	3:L:163:THR:HG22	1.75	0.68
2:H:11:LEU:CD2	2:H:116:THR:OG1	2.41	0.67
3:L:150:LYS:HB2	3:L:193:SER:HB3	1.76	0.66
1:B:214:HIS:H	1:B:422:HIS:HE1	1.45	0.64
3:L:3:VAL:HB	3:L:26:THR:HG23	1.85	0.58
2:H:93:VAL:HG11	2:H:100(P):MET:HB3	1.89	0.55
1:A:82:LEU:H	1:A:85:GLN:HE21	1.55	0.53
2:H:155:ASN:HD21	2:H:194:TYR:HB3	1.73	0.53
2:H:153:SER:HB3	2:H:197:ASN:HB2	1.90	0.53
1:A:125:MET:HE1	1:A:265:VAL:HG21	1.91	0.52
1:A:357:ARG:HD2	1:A:379:ASP:HB3	1.91	0.52
1:B:82:LEU:H	1:B:85:GLN:HE21	1.56	0.52
1:A:214:HIS:H	1:A:422:HIS:HE1	1.58	0.52
1:A:340:LYS:HE2	1:A:362:ASN:HD21	1.75	0.52
3:L:137:ILE:HD12	3:L:196:VAL:HG21	1.92	0.51
1:A:345:MET:HE1	1:A:378:LEU:HB3	1.92	0.51
1:B:125:MET:HE1	1:B:265:VAL:HG21	1.94	0.50
2:H:59:TYR:HB3	2:H:63:VAL:HG13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:MET:HE1	1:B:378:LEU:HB3	1.93	0.49
3:L:133:LEU:HD13	3:L:179:LEU:HD23	1.94	0.49
1:A:345:MET:HE2	1:A:345:MET:HB2	1.84	0.48
3:L:92:ALA:HB2	3:L:97:VAL:HG22	1.97	0.47
2:H:83:THR:CA	2:H:111:VAL:HG11	2.45	0.47
1:A:72:SER:O	2:H:100(I):ASP:HA	2.15	0.46
2:H:14:PRO:HD3	2:H:113:SER:HA	1.97	0.46
1:A:104:GLY:HA2	2:H:100(A):TYR:C	2.40	0.46
1:B:374:MET:HE1	1:B:376:LEU:HB3	1.98	0.46
1:B:380:PRO:HG2	1:B:402:ARG:HG3	1.98	0.46
1:B:153:VAL:HG11	2:H:100(D):THR:HG22	1.98	0.45
1:A:380:PRO:HG2	1:A:402:ARG:HG3	1.98	0.45
1:A:311:ALA:HB2	1:A:394:LYS:HD2	1.99	0.45
1:B:226:HIS:HD2	1:B:230:ASP:HB3	1.82	0.44
1:A:109:GLY:HA2	1:B:322:LEU:HD12	2.00	0.44
1:A:91:VAL:HG11	1:A:243:VAL:HG21	2.00	0.44
3:L:133:LEU:HB2	3:L:179:LEU:HB3	2.00	0.44
1:B:311:ALA:HB2	1:B:394:LYS:HD2	2.00	0.43
1:A:144:HIS:HB3	1:A:360:THR:HG23	2.00	0.43
1:B:344:GLN:HG3	1:B:388:VAL:HG13	2.00	0.43
2:H:111:VAL:O	2:H:111:VAL:HG12	2.19	0.43
3:L:66:LYS:C	3:L:66:LYS:HE3	2.44	0.43
1:A:344:GLN:HG3	1:A:388:VAL:HG13	2.00	0.42
1:A:374:MET:HE1	1:A:376:LEU:HB3	2.00	0.42
1:B:340:LYS:HA	1:B:364:VAL:HG12	2.02	0.42
1:B:91:VAL:HG11	1:B:243:VAL:HG21	2.02	0.42
3:L:109:GLN:HE22	3:L:171:ASN:HB3	1.85	0.42
1:A:252:ARG:HG2	2:H:100(F):TYR:CZ	2.56	0.41
1:A:265:VAL:HG22	1:A:420:TRP:HH2	1.84	0.41
1:B:144:HIS:HB3	1:B:360:THR:HG23	2.02	0.40
1:A:53:MET:HB3	1:A:128:LYS:HB3	2.03	0.40
3:L:107:VAL:HG12	3:L:108:GLY:N	2.36	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	400/447 (90%)	384 (96%)	14 (4%)	2 (0%)	24	36
1	B	399/447 (89%)	382 (96%)	15 (4%)	2 (0%)	24	36
2	H	222/283 (78%)	210 (95%)	10 (4%)	2 (1%)	14	21
3	L	210/216 (97%)	202 (96%)	6 (3%)	2 (1%)	12	18
All	All	1231/1393 (88%)	1178 (96%)	45 (4%)	8 (1%)	21	31

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	GLN
1	B	147	GLN
2	H	144	ASP
3	L	153	SER
2	H	116	THR
3	L	139	ASP
1	B	197	ASP
1	A	228	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	337/367 (92%)	320 (95%)	17 (5%)	22	36
1	B	339/367 (92%)	323 (95%)	16 (5%)	23	38
2	H	189/236 (80%)	177 (94%)	12 (6%)	16	27
3	L	178/183 (97%)	166 (93%)	12 (7%)	15	24
All	All	1043/1153 (90%)	986 (94%)	57 (6%)	19	32

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	A	103	ASN
1	A	179	THR
1	A	186	LEU
1	A	257	VAL
1	A	258	LEU
1	A	276	GLU
1	A	322	LEU
1	A	326	VAL
1	A	329	GLU
1	A	345	MET
1	A	357	ARG
1	A	358	LEU
1	A	365	ILE
1	A	376	LEU
1	A	389	ILE
1	A	402	ARG
1	B	68	MET
1	B	83	ASP
1	B	186	LEU
1	B	199	SER
1	B	253	GLN
1	B	258	LEU
1	B	322	LEU
1	B	326	VAL
1	B	329	GLU
1	B	345	MET
1	B	357	ARG
1	B	358	LEU
1	B	365	ILE
1	B	376	LEU
1	B	389	ILE
1	B	402	ARG
2	H	3	GLN
2	H	13	ARG
2	H	43	LYS
2	H	63	VAL
2	H	105	GLN
2	H	109	VAL
2	H	138	LEU
2	H	142	VAL
2	H	152	VAL
2	H	159	LEU

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Mol	Chain	Res	Type
2	H	192	GLN
2	H	193	THR
3	L	26	THR
3	L	33	VAL
3	L	66	LYS
3	L	81	GLU
3	L	97	VAL
3	L	129	ASN
3	L	130	LYS
3	L	137	ILE
3	L	146	THR
3	L	161	GLU
3	L	171	ASN
3	L	184	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	27	HIS
1	A	85	GLN
1	A	103	ASN
1	A	144	HIS
1	A	148	HIS
1	A	253	GLN
1	A	362	ASN
1	B	8	ASN
1	B	85	GLN
1	B	131	GLN
1	B	144	HIS
1	B	172	ASN
1	B	226	HIS
1	B	249	HIS
1	B	266	HIS
1	B	362	ASN
2	H	39	GLN
2	H	155	ASN
2	H	171	GLN
2	H	192	GLN
3	L	38	GLN
3	L	79	GLN
3	L	109	GLN

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Mol	Chain	Res	Type
3	L	127	GLN
3	L	168	GLN
3	L	170	ASN
3	L	171	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

4 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	$\# Z > 2$
4	NAG	C	1	4,1	14,14,15	0.36	0	17,19,21	0.65	0
4	NAG	C	2	4	14,14,15	0.34	0	17,19,21	0.63	0
4	BMA	C	3	4	11,11,12	0.50	0	15,15,17	1.66	1 (6%)
4	FUC	C	4	4	10,10,11	0.41	0	14,14,16	0.79	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	C	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	C	2	4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	C	3	4	-	0/2/19/22	1/1/1/1
4	FUC	C	4	4	-	-	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(°)
4	C	3	BMA	C1-O5-C5	6.13	120.40	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

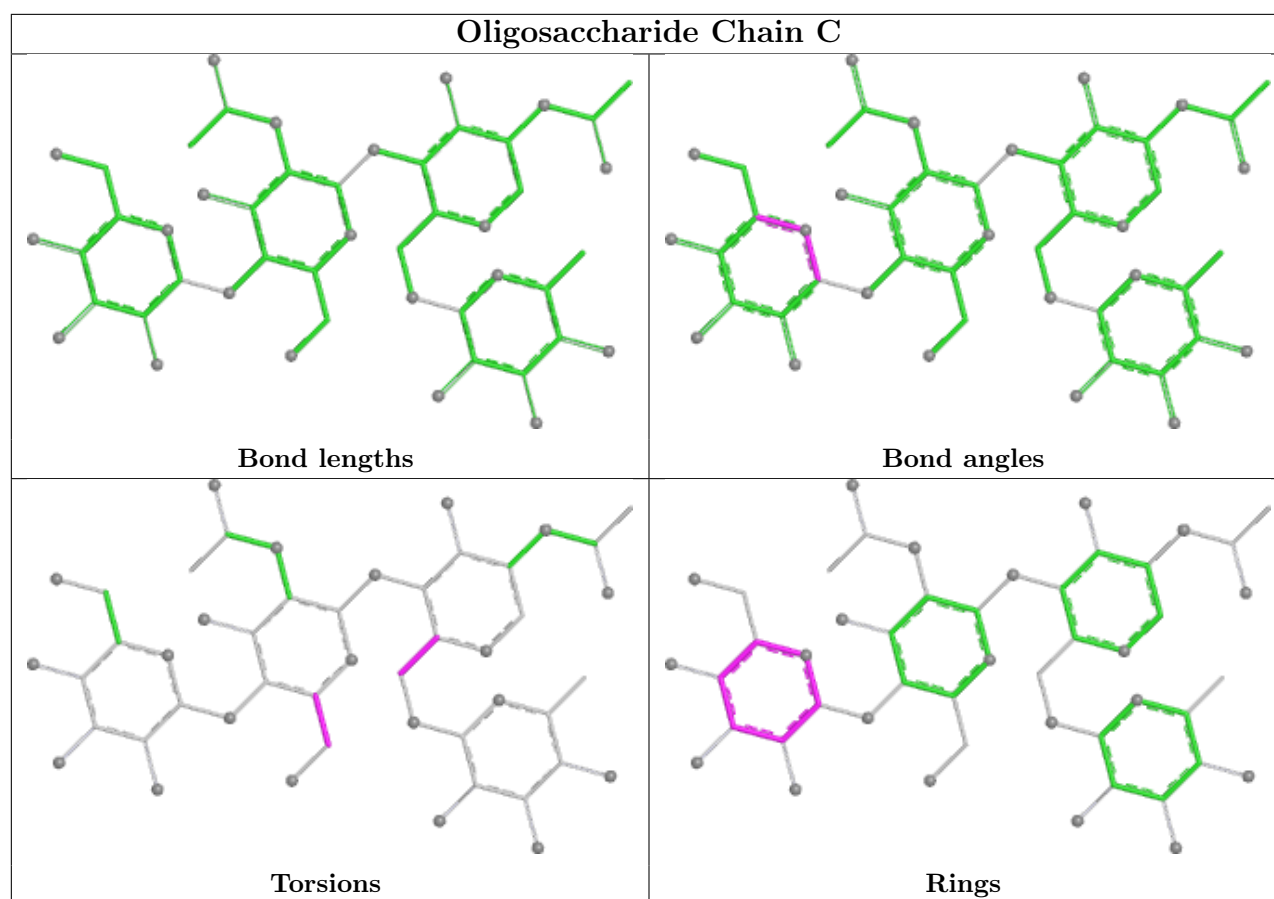
Mol	Chain	Res	Type	Atoms
4	C	2	NAG	O5-C5-C6-O6
4	C	2	NAG	C4-C5-C6-O6
4	C	1	NAG	O5-C5-C6-O6
4	C	1	NAG	C4-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	3	BMA	C1-C2-C3-C4-C5-O5

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 [i](#)

5 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	$\# Z > 2$
7	FMT	A	504	-	2,2,2	1.10	0	1,1,1	1.12	0
5	NAG	A	501	1	14,14,15	0.35	0	17,19,21	0.85	1 (5%)
6	GOL	A	502	-	5,5,5	0.06	0	5,5,5	0.22	0
6	GOL	B	505	-	5,5,5	0.06	0	5,5,5	0.14	0
6	GOL	A	503	-	5,5,5	0.05	0	5,5,5	0.13	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	GOL	B	505	-	-	1/4/4/4	-
6	GOL	A	503	-	-	0/4/4/4	-
5	NAG	A	501	1	-	0/6/23/26	0/1/1/1
6	GOL	A	502	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	NAG	C1-O5-C5	2.99	116.19	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	505	GOL	C1-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	406/447 (90%)	0.80	41 (10%)	12 10	23, 46, 71, 100	0
1	B	405/447 (90%)	0.89	63 (15%)	5 4	23, 50, 77, 90	0
2	H	226/283 (79%)	1.54	81 (35%)	1 0	26, 64, 111, 136	0
3	L	212/216 (98%)	1.99	104 (49%)	0 0	31, 75, 100, 142	0
All	All	1249/1393 (89%)	1.16	289 (23%)	2 1	23, 53, 99, 142	0

All (289) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	213	PRO	8.7
1	B	14	GLY	8.3
3	L	108	GLY	8.1
3	L	2	SER	7.8
2	H	195	ILE	6.1
1	A	193	ARG	6.0
1	A	419	GLY	5.8
3	L	210	THR	5.7
1	A	425	PHE	5.6
3	L	3	VAL	5.5
1	A	229	ALA	5.3
2	H	127	SER	5.3
2	H	209	LYS	5.3
3	L	169	SER	5.3
2	H	184	VAL	5.2
1	B	18	GLY	4.9
3	L	107	VAL	4.9
2	H	185	PRO	4.9
1	A	196	LEU	4.8
1	A	155	ASP	4.8
2	H	136	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
3	L	144	ALA	4.7
2	H	205	THR	4.6
2	H	137	ALA	4.6
3	L	190	ARG	4.5
2	H	122	PHE	4.5
2	H	194	TYR	4.5
2	H	158	ALA	4.5
2	H	206	LYS	4.4
3	L	199	GLU	4.4
2	H	156	SER	4.3
2	H	192	GLN	4.3
3	L	172	LYS	4.2
1	B	20	TRP	4.2
1	B	403	SER	4.1
2	H	211	VAL	4.1
3	L	205	LYS	4.0
1	A	192	PRO	4.0
3	L	27(B)	ASN	4.0
1	B	252	ARG	4.0
2	H	162	GLY	4.0
1	B	200	ASP	4.0
2	H	135	THR	3.9
2	H	159	LEU	3.9
3	L	157	LYS	3.9
3	L	145	VAL	3.9
3	L	42	LYS	3.9
3	L	27	SER	3.9
2	H	189	LEU	3.9
1	A	403	SER	3.8
2	H	151	THR	3.8
3	L	147	VAL	3.8
3	L	12	SER	3.8
1	B	304	SER	3.7
2	H	121	VAL	3.7
3	L	112	ALA	3.7
2	H	193	THR	3.7
3	L	28	ASP	3.7
2	H	188	SER	3.7
3	L	119	PHE	3.6
2	H	164	HIS	3.6
3	L	206	THR	3.5
1	A	296	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
2	H	149	PRO	3.5
3	L	140	PHE	3.5
1	B	214	HIS	3.5
3	L	203	VAL	3.5
3	L	193	SER	3.5
2	H	212	GLU	3.5
2	H	146	PHE	3.5
1	A	199	SER	3.4
1	A	103	ASN	3.4
1	A	247	ASP	3.4
2	H	117	LYS	3.4
2	H	138	LEU	3.4
3	L	133	LEU	3.4
2	H	160	THR	3.4
3	L	195	GLN	3.4
2	H	154	TRP	3.3
2	H	100	TYR	3.3
2	H	191	THR	3.3
3	L	196	VAL	3.3
3	L	153	SER	3.3
3	L	124	GLU	3.3
1	B	156	THR	3.3
3	L	69	THR	3.3
3	L	141	TYR	3.3
1	A	195	GLY	3.3
3	L	155	PRO	3.3
3	L	191	SER	3.3
1	B	56	VAL	3.3
3	L	116	VAL	3.3
3	L	186	TRP	3.2
2	H	124	LEU	3.2
1	B	422	HIS	3.2
2	H	116	THR	3.2
1	B	423	PRO	3.2
3	L	109	GLN	3.2
3	L	14	SER	3.2
1	A	194	THR	3.2
1	B	233	THR	3.2
2	H	207	VAL	3.2
1	B	247	ASP	3.1
2	H	140	CYS	3.1
2	H	143	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
3	L	170	ASN	3.1
3	L	152	ASP	3.1
3	L	143	GLY	3.1
3	L	192	TYR	3.1
1	B	258	LEU	3.1
3	L	168	GLN	3.1
1	B	127	GLY	3.1
3	L	150	LYS	3.1
2	H	201	LYS	3.1
2	H	150	VAL	3.1
1	B	199	SER	3.1
3	L	31	ASN	3.0
3	L	103	LYS	3.0
1	B	283	ARG	3.0
1	B	394	LYS	3.0
3	L	136	LEU	3.0
2	H	210	ARG	3.0
2	H	157	GLY	3.0
2	H	139	GLY	3.0
3	L	111	LYS	2.9
1	A	68	MET	2.9
2	H	198	VAL	2.9
2	H	167	PRO	2.9
2	H	161	SER	2.9
1	A	154	ASN	2.9
3	L	200	GLY	2.9
3	L	207	VAL	2.9
3	L	154	SER	2.9
1	B	302	GLY	2.9
2	H	166	PHE	2.9
1	A	131	GLN	2.8
3	L	188	SER	2.8
2	H	199	ASN	2.8
3	L	117	THR	2.8
1	B	249	HIS	2.8
2	H	152	VAL	2.8
3	L	198	HIS	2.8
3	L	40	PRO	2.8
1	A	215	LYS	2.8
1	B	348	ASP	2.8
3	L	113	ALA	2.8
3	L	208	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
3	L	134	VAL	2.8
1	B	154	ASN	2.8
3	L	156	VAL	2.8
3	L	15	PRO	2.7
1	A	421	SER	2.7
1	B	286	SER	2.7
2	H	183	THR	2.7
1	A	251	LYS	2.7
3	L	149	TRP	2.7
3	L	166	SER	2.7
1	A	234	PRO	2.7
1	A	424	GLN	2.7
2	H	105	GLN	2.7
1	B	303	VAL	2.7
1	B	273	LEU	2.7
1	B	259	GLY	2.7
3	L	39	ARG	2.7
1	B	270	ALA	2.7
3	L	130	LYS	2.7
1	A	197	ASP	2.7
3	L	135	CYS	2.6
1	B	215	LYS	2.6
3	L	151	ALA	2.6
1	B	19	THR	2.6
2	H	147	PRO	2.6
2	H	11	LEU	2.6
3	L	81	GLU	2.6
3	L	27(A)	SER	2.6
3	L	177	SER	2.6
3	L	137	ILE	2.6
3	L	175	ALA	2.6
1	A	350	GLN	2.6
2	H	186	SER	2.5
3	L	123	SER	2.5
3	L	138	SER	2.5
1	B	271	GLY	2.5
1	B	291	CYS	2.5
1	A	207	ASN	2.5
1	A	267	THR	2.5
3	L	204	GLU	2.5
1	A	394	LYS	2.5
1	B	132	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	15	MET	2.5
2	H	3	GLN	2.5
2	H	125	ALA	2.5
1	B	246	LYS	2.5
3	L	80	PRO	2.5
3	L	17	GLN	2.5
1	B	248	ALA	2.5
1	B	272	ALA	2.5
3	L	187	LYS	2.4
1	A	18	GLY	2.4
2	H	202	PRO	2.4
3	L	41	GLY	2.4
1	B	267	THR	2.4
1	B	146	SER	2.4
2	H	196	CYS	2.4
1	B	68	MET	2.4
1	B	386	TYR	2.4
3	L	106	VAL	2.4
3	L	26	THR	2.4
1	A	219	HIS	2.4
1	A	86	SER	2.4
2	H	153	SER	2.4
2	H	177	SER	2.4
1	A	83	ASP	2.4
1	B	301	LYS	2.4
2	H	163	VAL	2.4
2	H	182	VAL	2.4
2	H	74	ALA	2.4
1	A	284	LEU	2.4
2	H	170	LEU	2.4
1	B	207	ASN	2.4
1	A	278	ASP	2.4
2	H	208	ASP	2.4
3	L	114	PRO	2.4
2	H	12	VAL	2.4
2	H	13	ARG	2.4
3	L	148	ALA	2.4
3	L	4	LEU	2.3
2	H	112	SER	2.3
3	L	115	SER	2.3
1	B	81	TYR	2.3
3	L	162	THR	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	155	ASN	2.3
1	B	294	LYS	2.3
2	H	113	SER	2.3
2	H	123	PRO	2.3
3	L	165	PRO	2.3
1	B	5	GLY	2.3
1	B	145	GLY	2.3
1	B	108	PHE	2.3
3	L	178	TYR	2.3
1	B	373	LYS	2.3
1	A	132	PRO	2.3
3	L	142	PRO	2.3
1	B	107	LEU	2.3
1	B	284	LEU	2.3
1	B	266	HIS	2.3
1	B	196	LEU	2.3
1	B	250	ALA	2.2
2	H	23	ALA	2.2
1	A	393	GLU	2.2
3	L	83	GLU	2.2
3	L	173	TYR	2.2
3	L	18	SER	2.2
1	B	279	GLY	2.2
3	L	27(C)	ALA	2.2
1	B	159	GLU	2.2
1	B	94	ARG	2.2
2	H	190	GLY	2.2
3	L	118	LEU	2.2
1	B	419	GLY	2.2
3	L	159	GLY	2.2
2	H	187	SER	2.2
1	A	158	HIS	2.2
1	B	420	TRP	2.2
3	L	19	ILE	2.2
2	H	114	ALA	2.2
2	H	1	GLU	2.2
1	B	296	ASP	2.2
3	L	194	CYS	2.1
2	H	119	PRO	2.1
3	L	110	PRO	2.1
3	L	120	PRO	2.1
1	A	102	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	120	SER	2.1
2	H	173	SER	2.1
3	L	129	ASN	2.1
3	L	171	ASN	2.1
3	L	174	ALA	2.1
3	L	197	THR	2.1
2	H	126	PRO	2.1
3	L	189	HIS	2.1
3	L	8	VAL	2.1
1	A	283	ARG	2.0
1	A	250	ALA	2.0
1	B	276	GLU	2.0
1	B	305	TYR	2.0
1	B	73	ARG	2.0
1	B	281	LYS	2.0
1	A	259	GLY	2.0

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

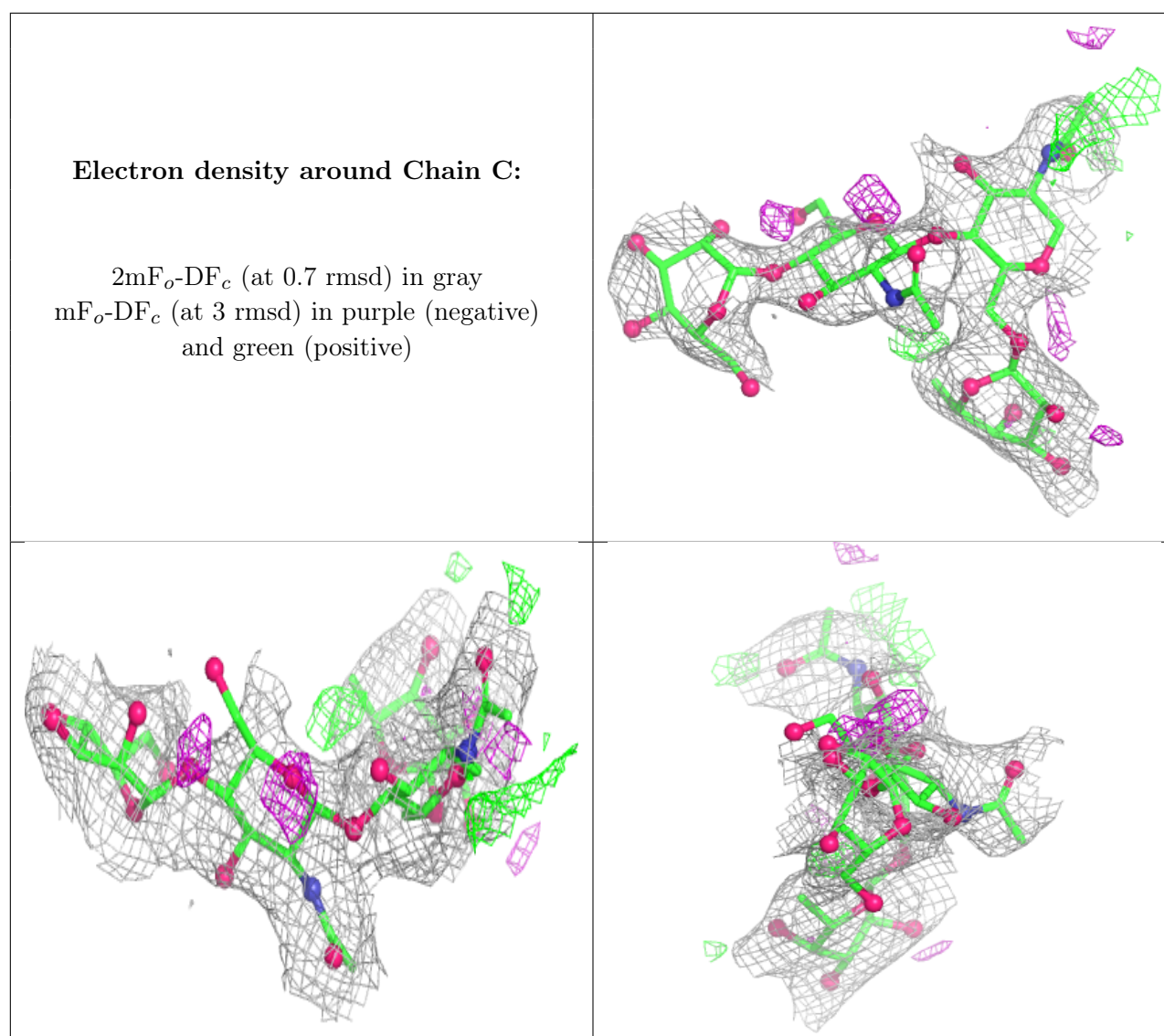
There are no non-standard protein/DNA/RNA residues in this entry.

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
4	NAG	C	1	14/15	-	-	71,77,81,85	0
4	NAG	C	2	14/15	-	-	89,92,94,95	0
4	BMA	C	3	11/12	-	-	97,99,100,102	0
4	FUC	C	4	10/11	-	-	79,80,82,82	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
5	NAG	A	501	14/15	0.67	0.19	66,70,71,72	0
6	GOL	B	505	6/6	0.69	0.29	76,76,77,77	0
6	GOL	A	502	6/6	0.87	0.19	43,44,44,45	0
6	GOL	A	503	6/6	0.91	0.13	44,45,45,46	0
7	FMT	A	504	3/3	0.94	0.15	45,45,45,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.