



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 01:30 PM EDT

PDB ID : 8F5I / pdb_00008f5i
Title : SARS-CoV-2 S2 helix epitope scaffold bound by antibody DH1057.1
Authors : Kapingidza, A.B.; Wrapp, D.; Winters, K.; Azoitei, M.L.
Deposited on : 2022-11-14
Resolution : 1.90 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

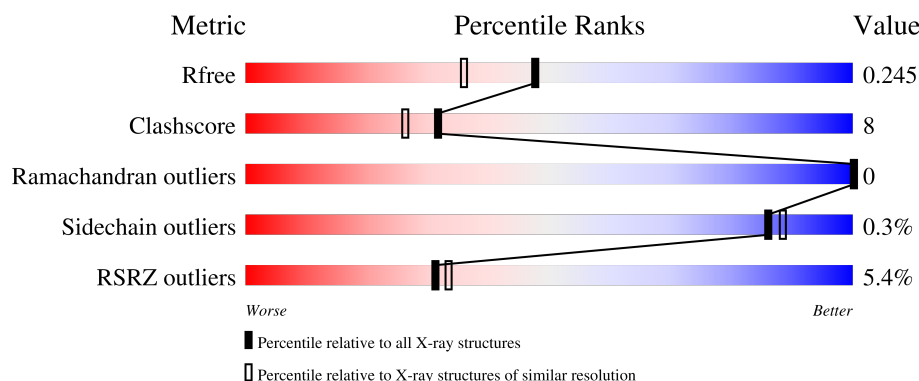
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	101	16% 81% 9% 10%
1	B	101	6% 83% 7% 10%
2	H	227	4% 86% 9% . .
2	X	227	2% 81% 14% . .
3	L	216	5% 86% 12% .

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Mol	Chain	Length	Quality of chain
3	Y	216	 6% 87% 13%
4	C	5	 40% 40% 20%
5	I	4	 25% 75%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9467 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 Specialized acyl carrier protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	91	Total	C	N	O	0	0	0
			711	461	109	141			
1	B	91	Total	C	N	O	0	0	0
			711	461	109	141			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ALA	CYS	conflict	UNP Q6N882
A	37	GLU	SER	conflict	UNP Q6N882
A	54	SER	LYS	conflict	UNP Q6N882
A	58	PHE	GLU	conflict	UNP Q6N882
A	61	GLU	THR	conflict	UNP Q6N882
A	62	LEU	GLN	conflict	UNP Q6N882
A	63	ASP	GLU	conflict	UNP Q6N882
A	65	TYR	ASN	conflict	UNP Q6N882
A	66	PHE	ASP	conflict	UNP Q6N882
A	68	SER	LYS	conflict	UNP Q6N882
A	94	LEU	-	expression tag	UNP Q6N882
A	95	GLU	-	expression tag	UNP Q6N882
A	96	HIS	-	expression tag	UNP Q6N882
A	97	HIS	-	expression tag	UNP Q6N882
A	98	HIS	-	expression tag	UNP Q6N882
A	99	HIS	-	expression tag	UNP Q6N882
A	100	HIS	-	expression tag	UNP Q6N882
A	101	HIS	-	expression tag	UNP Q6N882
B	16	ALA	CYS	conflict	UNP Q6N882
B	37	GLU	SER	conflict	UNP Q6N882
B	54	SER	LYS	conflict	UNP Q6N882
B	58	PHE	GLU	conflict	UNP Q6N882
B	61	GLU	THR	conflict	UNP Q6N882
B	62	LEU	GLN	conflict	UNP Q6N882
B	63	ASP	GLU	conflict	UNP Q6N882

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Chain	Residue	Modelled	Actual	Comment	Reference
B	65	TYR	ASN	conflict	UNP Q6N882
B	66	PHE	ASP	conflict	UNP Q6N882
B	68	SER	LYS	conflict	UNP Q6N882
B	94	LEU	-	expression tag	UNP Q6N882
B	95	GLU	-	expression tag	UNP Q6N882
B	96	HIS	-	expression tag	UNP Q6N882
B	97	HIS	-	expression tag	UNP Q6N882
B	98	HIS	-	expression tag	UNP Q6N882
B	99	HIS	-	expression tag	UNP Q6N882
B	100	HIS	-	expression tag	UNP Q6N882
B	101	HIS	-	expression tag	UNP Q6N882

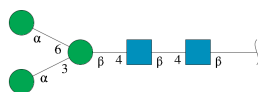
- Molecule 2 is a protein called DH1057.1 HC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	0	0	0
			1632	1026	274	325	7			
2	X	219	Total	C	N	O	S	0	0	0
			1635	1029	275	324	7			

- Molecule 3 is a protein called DH1057.1 LC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	215	Total	C	N	O	S	0	0	0
			1657	1039	285	329	4			
3	Y	215	Total	C	N	O	S	0	0	0
			1657	1039	285	329	4			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

pyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	4	Total	C	N	O	0	0	0
			50	28	2	20			

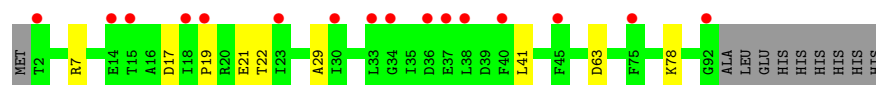
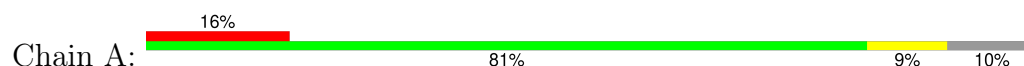
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	70	Total	O	0	0
			70	70		
6	B	110	Total	O	0	0
			110	110		
6	H	312	Total	O	0	0
			312	312		
6	L	266	Total	O	0	0
			266	266		
6	X	322	Total	O	0	0
			322	322		
6	Y	273	Total	O	0	0
			273	273		

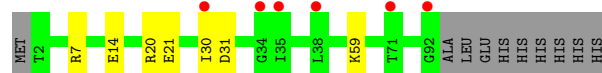
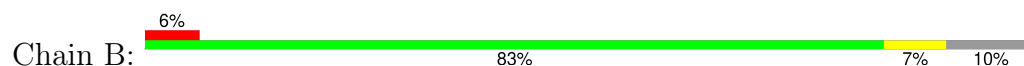
3 Residue-property plots [i](#)

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.

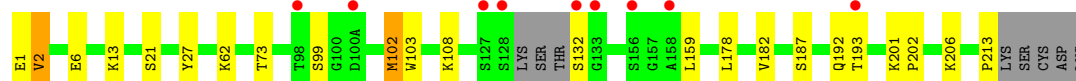
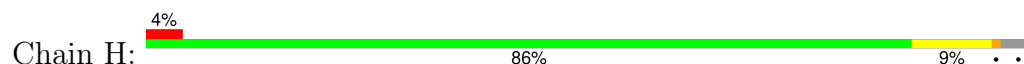
- Molecule 1: Specialized acyl carrier protein



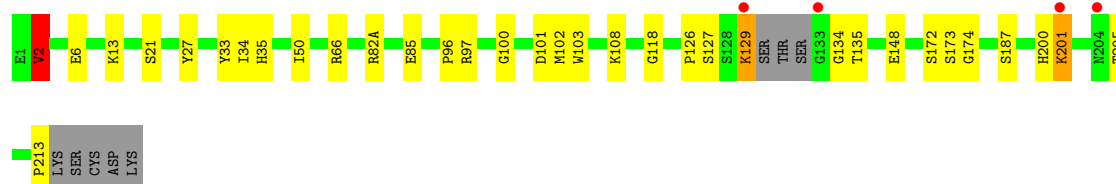
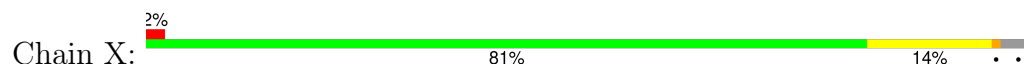
- Molecule 1: Specialized acyl carrier protein



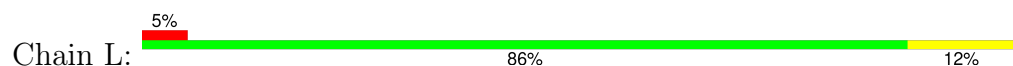
- Molecule 2: DH1057.1 HC



- Molecule 2: DH1057.1 HC

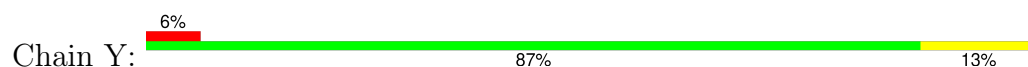


- Molecule 3: DH1057.1 LC

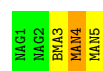




• Molecule 3: DH1057.1 LC



• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-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 1	Depositor
Cell constants a, b, c, α , β , γ	56.68Å 76.36Å 79.02Å 71.60° 69.99° 88.30°	Depositor
Resolution (Å)	45.68 – 1.90 45.68 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.9 (45.68-1.90) 93.9 (45.68-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 1.89Å)	Xtriage
Refinement program	PHENIX dev-3758	Depositor
R, R_{free}	0.211 , 0.244 0.211 , 0.245	Depositor DCC
R_{free} test set	4327 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for h,-k,h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9467	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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 45.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2576e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.16	0/725	0.34	0/987
1	B	0.20	0/725	0.41	0/987
2	H	0.50	1/1671 (0.1%)	0.52	1/2276 (0.0%)
2	X	0.67	6/1674 (0.4%)	0.61	2/2279 (0.1%)
3	L	0.33	0/1695	0.58	6/2303 (0.3%)
3	Y	0.39	1/1695 (0.1%)	0.49	0/2303
All	All	0.45	8/8185 (0.1%)	0.52	9/11135 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	129	LYS	CD-CE	-5.78	1.35	1.52
2	X	2	VAL	C-O	-5.72	1.18	1.24
2	H	102	MET	C-O	-5.60	1.17	1.23
3	Y	30	TYR	C-O	-5.27	1.18	1.24
2	X	96	PRO	C-O	-5.08	1.17	1.23
2	X	135	THR	C-O	-5.04	1.17	1.24
2	X	187	SER	C-O	-5.03	1.17	1.24
2	X	201	LYS	CD-CE	-5.00	1.37	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	134	GLY	N-CA-C	7.79	125.80	110.77
3	L	27(B)	LEU	CA-C-N	6.50	129.64	120.28
3	L	27(B)	LEU	C-N-CA	6.50	129.64	120.28
2	H	2	VAL	N-CA-C	-5.20	102.87	109.58
3	L	25	ALA	CA-C-N	5.12	127.14	120.28
3	L	25	ALA	C-N-CA	5.12	127.14	120.28
2	X	101	ASP	N-CA-C	5.10	119.49	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	28	SER	CA-C-N	5.04	129.67	122.21
3	L	28	SER	C-N-CA	5.04	129.67	122.21

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	711	0	698	12	0
1	B	711	0	698	10	0
2	H	1632	0	1585	21	0
2	X	1635	0	1593	28	0
3	L	1657	0	1616	29	0
3	Y	1657	0	1616	29	0
4	C	61	0	52	1	0
5	I	50	0	43	2	1
6	A	70	0	0	9	1
6	B	110	0	0	8	1
6	H	312	0	0	16	1
6	L	266	0	0	20	0
6	X	322	0	0	15	0
6	Y	273	0	0	23	0
All	All	9467	0	7901	130	2

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 8.

All (130) 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:7:ARG:NH2	6:A:201:HOH:O	1.83	1.10
3:Y:54:ARG:NE	6:Y:301:HOH:O	1.84	1.09
2:H:132:SER:N	6:H:301:HOH:O	1.85	1.09
3:L:24:ARG:NH2	6:L:301:HOH:O	1.86	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:81:GLU:CD	6:L:302:HOH:O	2.06	0.98
2:H:192:GLN:OE1	6:H:302:HOH:O	1.86	0.92
3:L:81:GLU:OE2	6:L:302:HOH:O	1.86	0.91
1:A:17:ASP:O	6:A:202:HOH:O	1.88	0.91
2:X:148:GLU:OE2	6:X:302:HOH:O	1.88	0.90
3:Y:107:LYS:O	6:Y:302:HOH:O	1.91	0.87
2:H:13:LYS:NZ	6:H:304:HOH:O	1.93	0.87
3:Y:40:PRO:HD3	6:Y:392:HOH:O	1.74	0.87
2:H:193:THR:OG1	6:H:303:HOH:O	1.92	0.87
1:B:21:GLU:OE1	6:B:202:HOH:O	1.92	0.86
3:Y:39:LYS:NZ	6:Y:304:HOH:O	2.05	0.86
3:Y:199:GLN:NE2	6:Y:303:HOH:O	1.99	0.84
2:H:62:LYS:HD2	6:H:456:HOH:O	1.77	0.84
3:Y:160:GLN:HG3	6:Y:494:HOH:O	1.77	0.84
2:H:73:THR:HG21	6:H:460:HOH:O	1.77	0.82
2:H:99:SER:N	6:H:305:HOH:O	2.14	0.80
3:L:25:ALA:C	6:L:304:HOH:O	2.24	0.80
2:H:99:SER:C	6:H:305:HOH:O	2.25	0.79
2:X:100:GLY:O	6:X:304:HOH:O	2.01	0.78
3:L:25:ALA:O	6:L:304:HOH:O	2.01	0.78
3:Y:54:ARG:CZ	6:Y:301:HOH:O	2.28	0.77
1:A:29:ALA:O	6:A:203:HOH:O	2.03	0.77
1:B:20:ARG:NH1	6:B:201:HOH:O	1.91	0.76
3:L:107:LYS:O	6:L:305:HOH:O	2.04	0.75
3:L:27(B):LEU:HD12	3:L:71:PHE:CE1	2.22	0.74
2:X:173:SER:O	6:X:305:HOH:O	2.05	0.74
3:L:27(B):LEU:HD12	3:L:71:PHE:CZ	2.23	0.73
3:L:25:ALA:HB3	6:L:304:HOH:O	1.91	0.69
3:Y:161:GLU:OE2	6:Y:306:HOH:O	2.11	0.69
2:X:2:VAL:HG12	2:X:102:MET:HG2	1.75	0.68
2:H:201:LYS:HG3	6:H:390:HOH:O	1.95	0.67
1:A:7:ARG:CD	6:A:201:HOH:O	2.42	0.66
2:X:85:GLU:OE1	6:X:306:HOH:O	2.14	0.66
2:X:34:ILE:HD11	6:X:316:HOH:O	1.96	0.66
3:Y:160:GLN:HG3	6:Y:556:HOH:O	1.97	0.64
1:A:7:ARG:NE	6:A:206:HOH:O	2.32	0.63
3:Y:142:ARG:NH2	6:Y:308:HOH:O	2.27	0.63
3:L:142:ARG:NH1	3:L:163:VAL:HG21	2.14	0.62
2:H:206:LYS:HD2	6:H:445:HOH:O	1.99	0.62
1:A:41:LEU:HD11	3:Y:29:SER:HB2	1.82	0.62
3:Y:54:ARG:NH1	6:Y:301:HOH:O	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:34:ILE:CD1	6:X:316:HOH:O	2.48	0.61
3:L:54:ARG:NH2	6:L:311:HOH:O	2.30	0.60
3:L:110:VAL:HG23	6:L:514:HOH:O	2.01	0.60
3:Y:37:GLN:HB2	3:Y:47:LEU:HD11	1.84	0.60
1:B:31:ASP:OD1	6:B:205:HOH:O	2.16	0.60
2:X:129:LYS:O	6:X:307:HOH:O	2.17	0.59
1:A:19:PRO:O	1:A:22:THR:HG22	2.02	0.59
1:B:21:GLU:HB2	6:B:202:HOH:O	2.02	0.59
3:Y:50:ALA:HB3	3:Y:53:LYS:HD3	1.84	0.59
2:H:187:SER:HB2	6:Y:321:HOH:O	2.02	0.59
3:Y:184:ALA:O	3:Y:188:LYS:HG3	2.03	0.58
3:L:53:LYS:HD3	6:L:317:HOH:O	2.04	0.58
2:X:108:LYS:HG3	6:X:557:HOH:O	2.03	0.57
1:A:41:LEU:CD1	3:Y:29:SER:HB2	2.35	0.57
2:X:13:LYS:NZ	6:X:303:HOH:O	2.00	0.56
2:H:99:SER:CA	6:H:305:HOH:O	2.50	0.56
3:Y:143:GLU:HG3	6:Y:303:HOH:O	2.06	0.55
3:L:100:GLN:HG3	6:L:527:HOH:O	2.06	0.55
3:L:105:GLU:OE1	3:L:173:TYR:OH	2.18	0.54
6:X:610:HOH:O	5:I:1:NAG:C6	2.54	0.54
2:X:200:HIS:HB3	2:X:205:THR:OG1	2.05	0.54
3:Y:142:ARG:NH2	6:Y:316:HOH:O	2.37	0.54
1:A:21:GLU:OE1	6:A:204:HOH:O	2.18	0.53
2:H:178:LEU:HA	6:H:384:HOH:O	2.08	0.53
6:H:483:HOH:O	2:X:174:GLY:HA2	2.08	0.53
2:H:108:LYS:HD3	6:H:541:HOH:O	2.09	0.53
2:X:2:VAL:CG1	2:X:102:MET:HG2	2.38	0.52
3:L:126:LYS:HD3	6:L:533:HOH:O	2.08	0.52
2:H:213:PRO:C	6:H:310:HOH:O	2.52	0.52
3:Y:90:GLN:NE2	6:Y:314:HOH:O	2.36	0.51
2:X:127:SER:OG	2:X:129:LYS:HG3	2.10	0.51
2:H:102:MET:HE3	2:H:103:TRP:H	1.75	0.51
3:L:213:GLU:HB2	6:L:512:HOH:O	2.09	0.50
1:A:63:ASP:OD1	6:A:205:HOH:O	2.20	0.50
2:X:102:MET:HE3	2:X:103:TRP:H	1.75	0.50
3:Y:18:ARG:NH1	6:Y:319:HOH:O	2.45	0.50
3:Y:160:GLN:OE1	6:Y:307:HOH:O	2.19	0.50
3:L:27(B):LEU:HD13	3:L:32:TYR:O	2.11	0.50
2:H:2:VAL:HG13	2:H:27:TYR:CD1	2.47	0.50
2:X:2:VAL:HG22	2:X:27:TYR:HB3	1.94	0.50
3:L:18:ARG:NH2	6:L:316:HOH:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:201:LYS:HD2	2:H:202:PRO:CD	2.43	0.49
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.94	0.49
1:A:17:ASP:HB3	6:A:202:HOH:O	2.13	0.48
2:X:13:LYS:HE2	6:X:342:HOH:O	2.13	0.48
3:L:129:THR:OG1	6:L:306:HOH:O	2.11	0.48
1:A:78:LYS:HD2	6:A:251:HOH:O	2.11	0.48
1:B:14:GLU:OE1	6:B:206:HOH:O	2.20	0.48
3:L:25:ALA:CB	6:L:304:HOH:O	2.56	0.48
3:L:31:ASN:HB3	6:L:409:HOH:O	2.13	0.47
2:X:6:GLU:HA	2:X:21:SER:O	2.15	0.47
2:X:33:TYR:CG	2:X:50:ILE:HD11	2.49	0.47
3:Y:24:ARG:NH2	6:Y:322:HOH:O	2.48	0.47
1:B:7:ARG:NH1	6:B:204:HOH:O	2.16	0.46
2:H:201:LYS:HD2	2:H:202:PRO:HD3	1.96	0.46
6:X:610:HOH:O	5:I:1:NAG:O6	2.21	0.46
3:Y:158:ASN:HB2	6:Y:370:HOH:O	2.16	0.46
2:X:33:TYR:CE2	2:X:97:ARG:HG2	2.52	0.45
2:X:126:PRO:HG2	2:X:213:PRO:HA	1.99	0.45
6:H:607:HOH:O	4:C:4:MAN:O2	2.21	0.45
3:L:54:ARG:HG2	3:L:58:ILE:HB	1.99	0.45
3:L:81:GLU:CG	6:L:302:HOH:O	2.57	0.44
2:X:201:LYS:NZ	6:X:325:HOH:O	2.47	0.44
2:X:66:ARG:HD2	2:X:82(A):ARG:O	2.17	0.44
3:Y:109:THR:HG23	6:Y:415:HOH:O	2.18	0.44
1:B:14:GLU:HG3	6:B:216:HOH:O	2.18	0.44
2:X:172:SER:CB	6:X:329:HOH:O	2.66	0.43
1:B:59:LYS:HD3	1:B:59:LYS:HA	1.88	0.43
1:B:20:ARG:NE	6:B:201:HOH:O	2.50	0.43
2:H:159:LEU:HD21	2:H:182:VAL:HG21	2.00	0.42
3:Y:147:GLN:HG2	6:Y:518:HOH:O	2.18	0.42
3:Y:123:GLU:HB2	6:Y:315:HOH:O	2.17	0.42
1:B:30:ILE:HG22	1:B:31:ASP:OD1	2.20	0.42
3:L:25:ALA:CA	6:L:304:HOH:O	2.65	0.42
2:H:6:GLU:HA	2:H:21:SER:O	2.20	0.42
3:L:10:THR:OG1	6:L:308:HOH:O	2.21	0.42
2:X:35:HIS:CE1	2:X:50:ILE:HD12	2.55	0.42
3:L:184:ALA:O	3:L:188:LYS:HD3	2.20	0.41
2:X:201:LYS:HG2	6:X:481:HOH:O	2.20	0.41
3:L:163:VAL:HG22	3:L:175:LEU:HD12	2.01	0.41
3:Y:140:TYR:CG	3:Y:141:PRO:HA	2.55	0.41
3:Y:126:LYS:H	3:Y:126:LYS:HG2	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:201:LYS:HA	2:X:201:LYS:HD2	1.79	0.41
3:Y:94:ARG:NH2	6:Y:333:HOH:O	2.54	0.40
2:X:118:GLY:HA3	2:X:205:THR:HG21	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:270:HOH:O	6:H:505:HOH:O[1_455]	1.95	0.25
5:I:3:BMA:O3	6:A:263:HOH:O[1_655]	1.99	0.21

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	89/101 (88%)	88 (99%)	1 (1%)	0	100	100
1	B	89/101 (88%)	86 (97%)	3 (3%)	0	100	100
2	H	215/227 (95%)	212 (99%)	3 (1%)	0	100	100
2	X	215/227 (95%)	212 (99%)	3 (1%)	0	100	100
3	L	213/216 (99%)	209 (98%)	4 (2%)	0	100	100
3	Y	213/216 (99%)	211 (99%)	2 (1%)	0	100	100
All	All	1034/1088 (95%)	1018 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	75/84 (89%)	75 (100%)	0	100	100
1	B	75/84 (89%)	75 (100%)	0	100	100
2	H	183/191 (96%)	182 (100%)	1 (0%)	81	84
2	X	183/191 (96%)	182 (100%)	1 (0%)	81	84
3	L	185/186 (100%)	184 (100%)	1 (0%)	81	84
3	Y	185/186 (100%)	185 (100%)	0	100	100
All	All	886/922 (96%)	883 (100%)	3 (0%)	86	88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	1	GLU
3	L	29	SER
2	X	2	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	3	GLN
2	H	61	GLN
2	H	64	GLN
2	H	171	GLN
3	L	210	ASN
2	X	39	GLN
3	Y	38	GLN
3	Y	42	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 ⓘ

9 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	4,2	14,14,15	0.46	0	17,19,21	0.46	0
4	NAG	C	2	4	14,14,15	0.54	0	17,19,21	0.57	0
4	BMA	C	3	4	11,11,12	0.56	0	15,15,17	1.01	1 (6%)
4	MAN	C	4	4	11,11,12	0.74	0	15,15,17	1.16	2 (13%)
4	MAN	C	5	4	11,11,12	0.82	0	15,15,17	1.15	1 (6%)
5	NAG	I	1	2,5	14,14,15	0.49	0	17,19,21	0.47	0
5	NAG	I	2	5	14,14,15	0.50	0	17,19,21	0.59	0
5	BMA	I	3	5	11,11,12	0.61	0	15,15,17	0.83	0
5	MAN	I	4	5	11,11,12	0.80	0	15,15,17	0.86	1 (6%)

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	4,2	-	0/6/23/26	0/1/1/1
4	NAG	C	2	4	-	0/6/23/26	0/1/1/1
4	BMA	C	3	4	-	0/2/19/22	0/1/1/1
4	MAN	C	4	4	-	0/2/19/22	0/1/1/1
4	MAN	C	5	4	-	2/2/19/22	0/1/1/1
5	NAG	I	1	2,5	-	1/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1
5	MAN	I	4	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	5	MAN	C1-O5-C5	3.50	116.88	112.19
4	C	4	MAN	C1-O5-C5	3.18	116.45	112.19
4	C	3	BMA	C1-O5-C5	2.92	116.10	112.19
4	C	4	MAN	O2-C2-C3	-2.76	104.43	110.15
5	I	4	MAN	C1-O5-C5	2.13	115.05	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

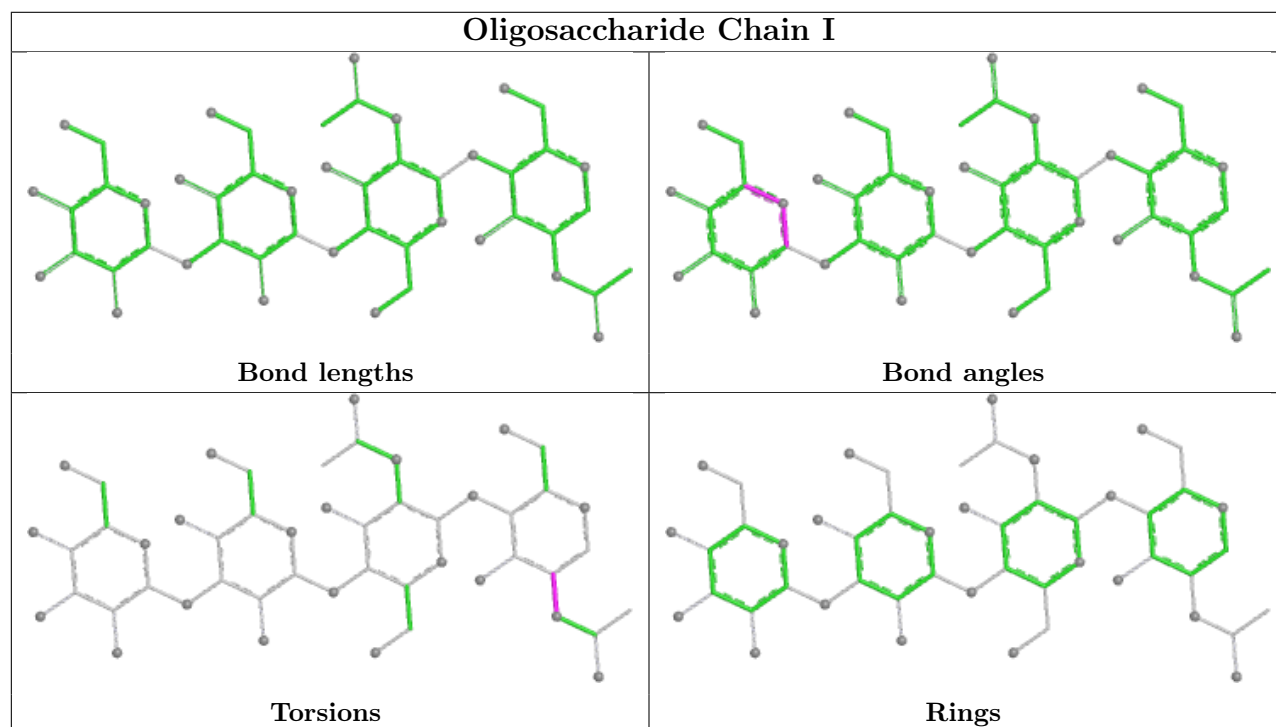
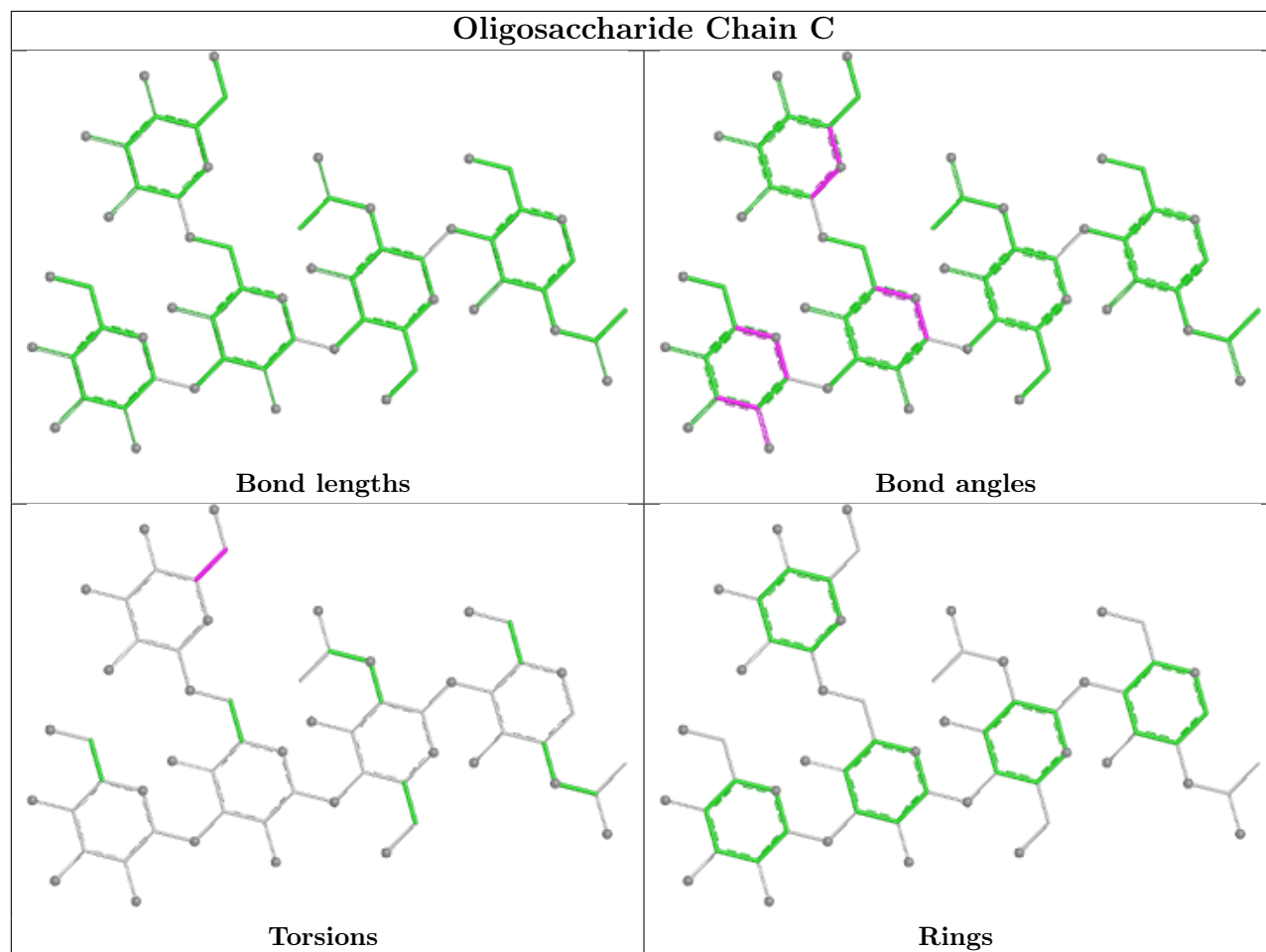
Mol	Chain	Res	Type	Atoms
4	C	5	MAN	O5-C5-C6-O6
4	C	5	MAN	C4-C5-C6-O6
5	I	1	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	1	NAG	2	0
5	I	3	BMA	0	1
4	C	4	MAN	1	0

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



5.6 Ligand geometry

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

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	91/101 (90%)	1.08	16 (17%) 4 4	17, 34, 56, 60	0
1	B	91/101 (90%)	0.45	6 (6%) 24 26	15, 24, 43, 56	0
2	H	219/227 (96%)	0.30	9 (4%) 41 44	12, 20, 41, 54	0
2	X	219/227 (96%)	0.15	4 (1%) 67 71	13, 21, 35, 54	0
3	L	215/216 (99%)	0.28	10 (4%) 36 39	14, 23, 39, 70	0
3	Y	215/216 (99%)	0.24	12 (5%) 30 32	13, 22, 38, 48	0
All	All	1050/1088 (96%)	0.33	57 (5%) 31 33	12, 23, 42, 70	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	27(B)	LEU	6.5
2	H	132	SER	5.3
3	L	28	SER	5.2
3	L	27	GLN	5.1
3	L	27(A)	SER	4.5
2	X	133	GLY	4.5
1	B	92	GLY	4.3
3	Y	28	SER	4.3
1	A	92	GLY	4.2
2	X	204	ASN	4.1
2	H	128	SER	3.8
1	B	34	GLY	3.7
3	L	29	SER	3.6
2	H	133	GLY	3.6
1	B	35	ILE	3.5
3	Y	41	GLY	3.5
2	H	98	THR	3.4
2	H	127	SER	3.3
2	H	193	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	40	PHE	3.2
3	L	213	GLU	3.2
3	L	26	SER	3.1
1	A	2	THR	3.1
2	X	129	LYS	3.1
1	A	36	ASP	3.0
3	Y	7	SER	2.9
3	Y	40	PRO	2.9
3	Y	184	ALA	2.8
1	A	30	ILE	2.8
1	B	30	ILE	2.8
1	B	38	LEU	2.7
1	A	45	PHE	2.6
3	Y	27(A)	SER	2.5
1	A	15	THR	2.5
1	A	38	LEU	2.5
3	L	212	GLY	2.5
1	A	18	ILE	2.5
1	A	34	GLY	2.4
3	Y	27(B)	LEU	2.3
1	A	23	ILE	2.3
3	Y	93	ASN	2.3
3	Y	127	SER	2.3
1	A	14	GLU	2.2
1	A	19	PRO	2.2
3	L	24	ARG	2.2
2	H	158	ALA	2.2
1	A	37	GLU	2.2
3	Y	29	SER	2.2
3	Y	212	GLY	2.2
3	L	25	ALA	2.2
2	X	201	LYS	2.2
2	H	156	SER	2.2
1	A	33	LEU	2.1
2	H	100(A)	ASP	2.1
1	A	75	PHE	2.0
1	B	71	THR	2.0
3	Y	27	GLN	2.0

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

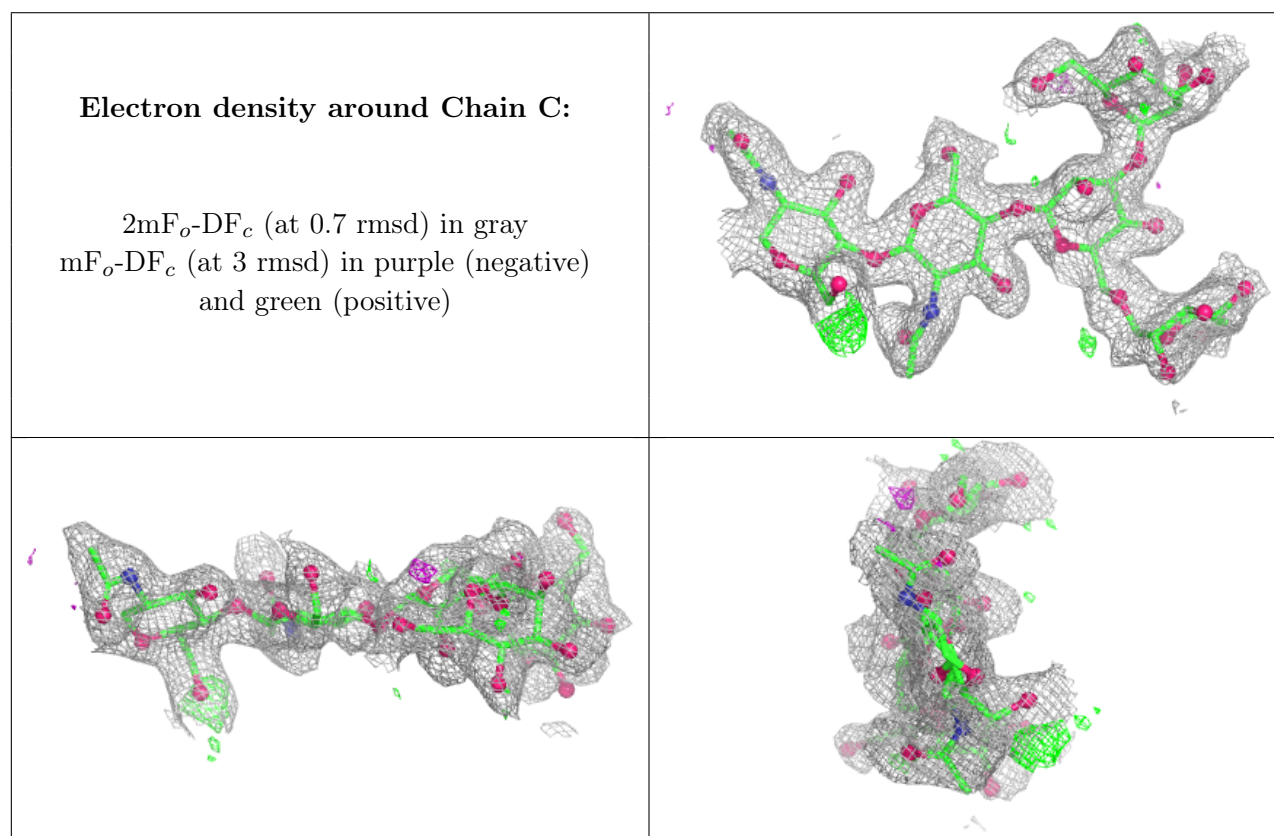
There are no non-standard protein/DNA/RNA residues in this entry.

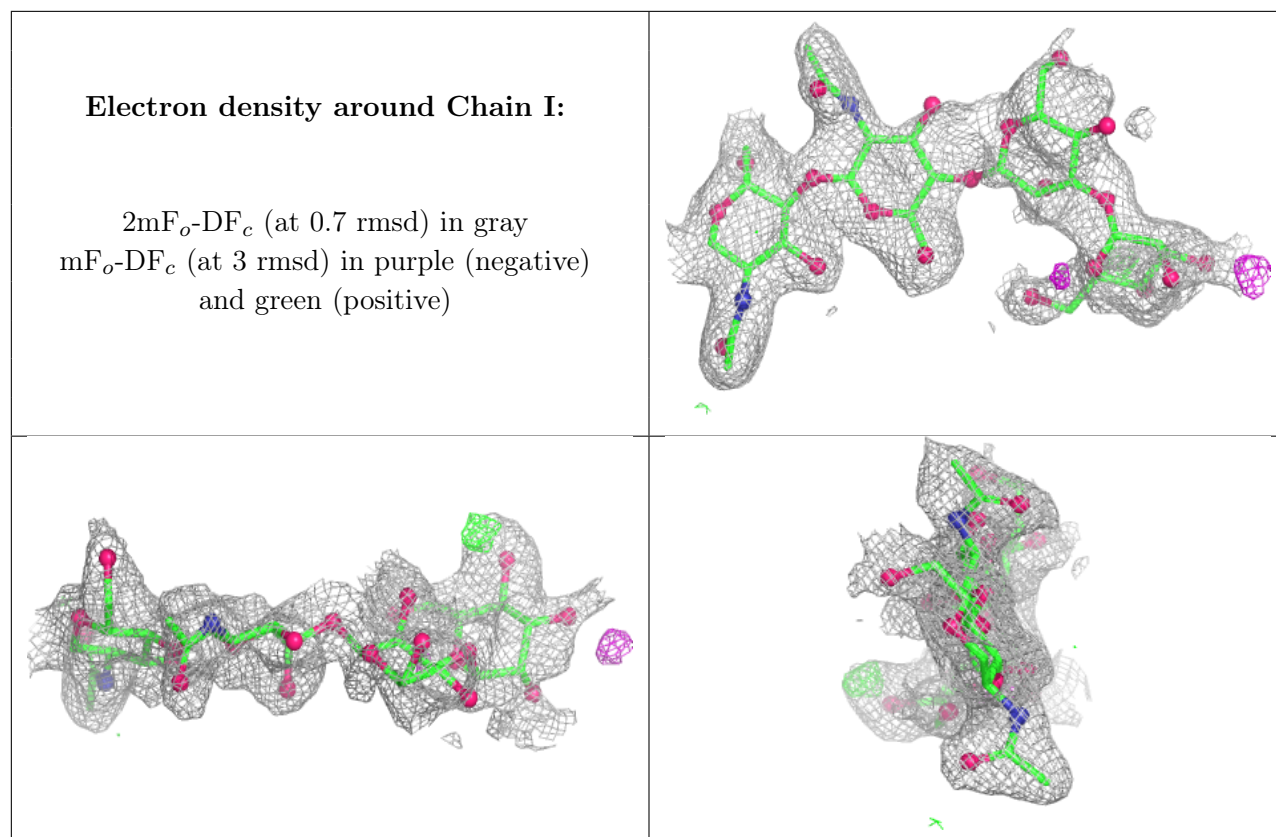
6.3 Carbohydrates ⓘ

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
4	NAG	C	1	14/15	-	-	27,31,33,33	0
4	NAG	C	2	14/15	-	-	27,32,35,37	0
4	BMA	C	3	11/12	-	-	29,36,44,45	0
4	MAN	C	4	11/12	-	-	33,36,39,40	0
4	MAN	C	5	11/12	-	-	54,55,58,61	0
5	NAG	I	1	14/15	-	-	37,40,46,49	0
5	NAG	I	2	14/15	-	-	40,51,56,60	0
5	BMA	I	3	11/12	-	-	47,55,64,65	0
5	MAN	I	4	11/12	-	-	47,55,59,60	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.