



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:07 PM UTC

PDB ID : 7MSQ / pdb_00007msq
Title : Complex between the Fab arm of AB-3467 and the SARS-CoV-2 receptor binding domain (RBD)
Authors : Langley, D.B.; Christ, D.
Deposited on : 2021-05-12
Resolution : 2.29 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

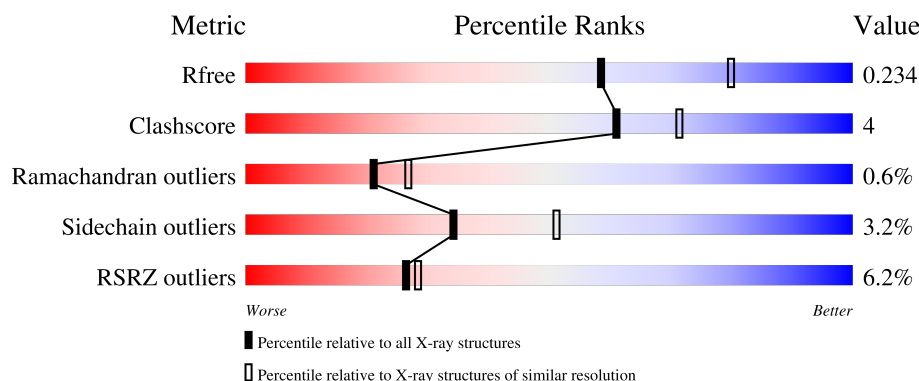
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	204	16% 80% 12% ...
1	B	204	14% 77% 14% 7%
2	D	238	2% 81% 11% 7%
2	H	238	3% 86% 6% 7%
3	E	214	0% 88% 11%

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Mol	Chain	Length	Quality of chain
3	L	214	% 91% 8% .
4	C	5	40% 60%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9962 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	0	0	0
			1541	988	257	288	8			
1	B	189	Total	C	N	O	S	0	0	0
			1492	955	248	281	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	529	GLY	-	expression tag	UNP P0DTC2
A	530	SER	-	expression tag	UNP P0DTC2
A	531	HIS	-	expression tag	UNP P0DTC2
A	532	HIS	-	expression tag	UNP P0DTC2
A	533	HIS	-	expression tag	UNP P0DTC2
A	534	HIS	-	expression tag	UNP P0DTC2
A	535	HIS	-	expression tag	UNP P0DTC2
A	536	HIS	-	expression tag	UNP P0DTC2
B	529	GLY	-	expression tag	UNP P0DTC2
B	530	SER	-	expression tag	UNP P0DTC2
B	531	HIS	-	expression tag	UNP P0DTC2
B	532	HIS	-	expression tag	UNP P0DTC2
B	533	HIS	-	expression tag	UNP P0DTC2
B	534	HIS	-	expression tag	UNP P0DTC2
B	535	HIS	-	expression tag	UNP P0DTC2
B	536	HIS	-	expression tag	UNP P0DTC2

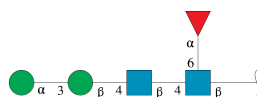
- Molecule 2 is a protein called AB-3467 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	221	Total	C	N	O	S	0	3	0
			1698	1082	279	331	6			
2	H	221	Total	C	N	O	S	0	4	0
			1702	1084	280	332	6			

- Molecule 3 is a protein called AB-3467 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	213	Total	C	N	O	S	0	0	0
			1637	1027	274	332	4			
3	L	214	Total	C	N	O	S	0	0	0
			1640	1027	274	334	5			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

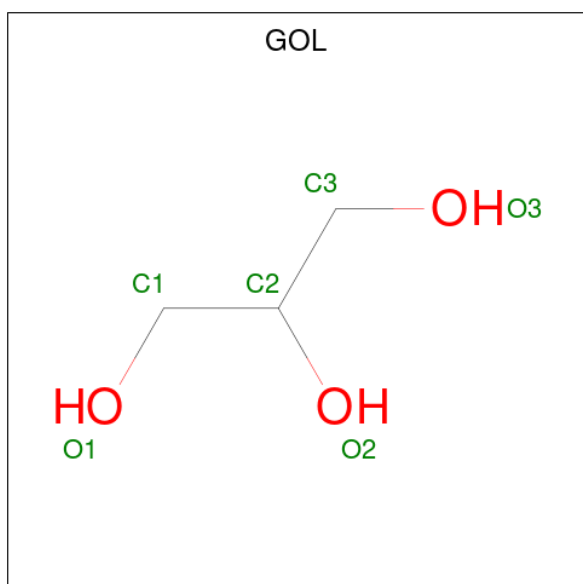
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		
5	B	1	Total	Cl	0	0
			1	1		
5	D	2	Total	Cl	0	0
			2	2		
5	E	2	Total	Cl	0	0
			2	2		
5	H	1	Total	Cl	0	0
			1	1		

- Molecule 6 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	S	0	0
			3	1	1	1		
6	E	1	Total	C	N	S	0	0
			3	1	1	1		
6	L	1	Total	C	N	S	0	0
			3	1	1	1		
6	L	1	Total	C	N	S	0	0
			3	1	1	1		
6	L	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			6	3	3		

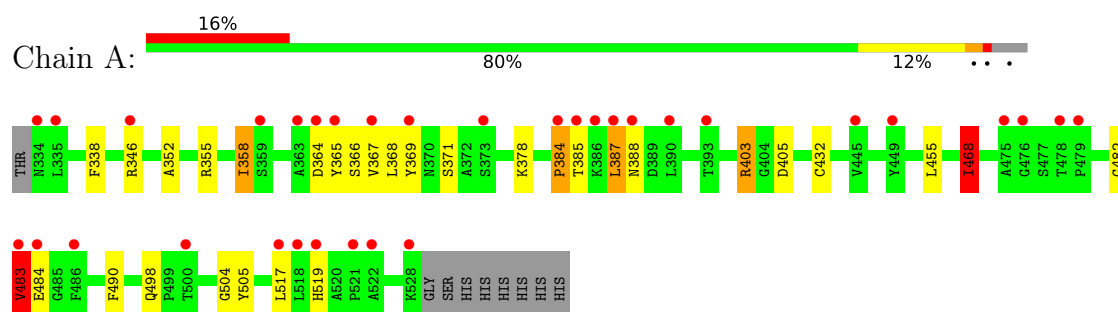
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	10	Total	O	0	0
			10	10		
8	B	18	Total	O	0	0
			18	18		
8	D	32	Total	O	0	0
			32	32		
8	E	35	Total	O	0	0
			35	35		
8	H	38	Total	O	0	0
			38	38		
8	L	31	Total	O	0	0
			31	31		

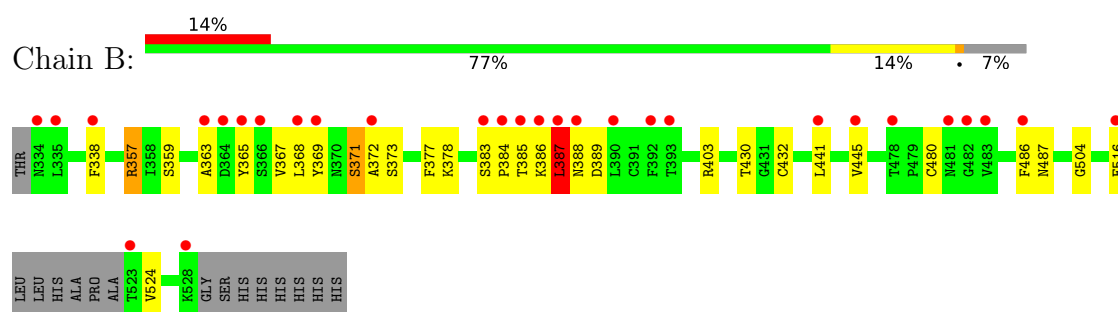
3 Residue-property plots [i](#)

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.

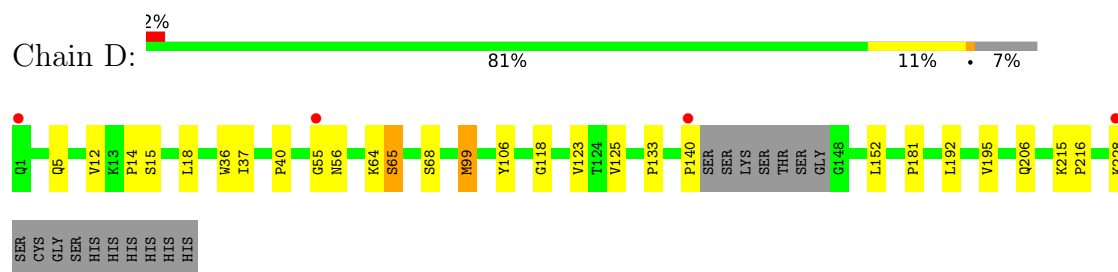
• Molecule 1: Spike protein S1



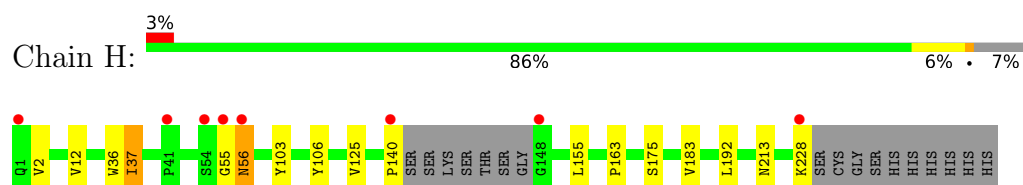
• Molecule 1: Spike protein S1



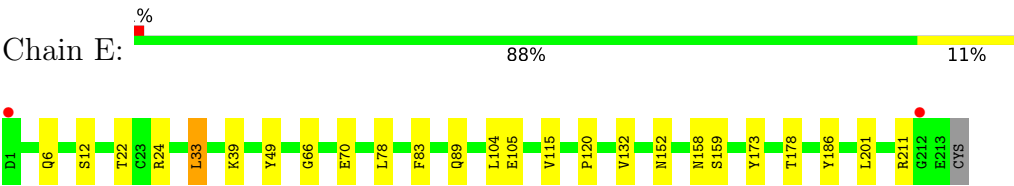
• Molecule 2: AB-3467 Fab Heavy Chain



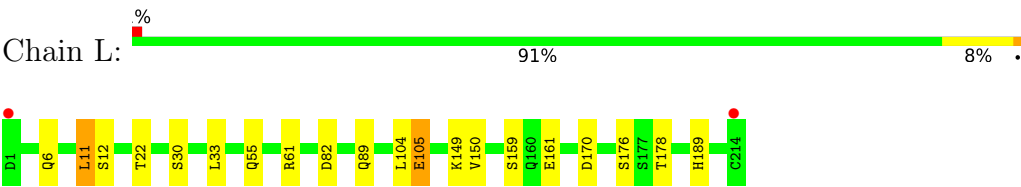
• Molecule 2: AB-3467 Fab Heavy Chain



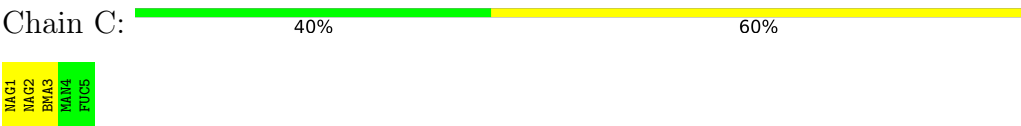
● Molecule 3: AB-3467 Fab Light Chain



● Molecule 3: AB-3467 Fab Light Chain



● Molecule 4: alpha-D-mannopyranose-(1-3)-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	109.76Å 115.49Å 240.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.00 – 2.29 48.00 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.00-2.29) 99.8 (48.00-2.29)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.194 , 0.245 (Not available) , 0.234	Depositor DCC
R_{free} test set	3368 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 28.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.023 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9962	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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: SCN, NAG, FUC, BMA, CL, GOL, MAN

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	1.13	1/1585 (0.1%)	1.39	6/2158 (0.3%)
1	B	1.07	1/1533 (0.1%)	1.35	2/2084 (0.1%)
2	D	1.10	4/1744 (0.2%)	1.33	1/2382 (0.0%)
2	H	1.08	1/1748 (0.1%)	1.32	0/2388
3	E	1.13	2/1673 (0.1%)	1.32	1/2273 (0.0%)
3	L	1.09	0/1676	1.29	3/2277 (0.1%)
All	All	1.10	9/9959 (0.1%)	1.33	13/13562 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	430	THR	C-O	6.98	1.32	1.24
2	D	181	PRO	C-O	-5.95	1.16	1.23
3	E	115	VAL	C-O	-5.86	1.17	1.24
1	A	355	ARG	C-O	-5.75	1.17	1.24
2	D	99	MET	C-O	5.61	1.30	1.23
3	E	201	LEU	C-O	5.54	1.30	1.23
2	D	133	PRO	C-O	-5.36	1.17	1.23
2	D	118	GLY	C-O	5.22	1.29	1.23
2	H	183	VAL	C-O	5.19	1.29	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	468	ILE	N-CA-CB	-7.97	102.00	112.36
2	D	40	PRO	N-CA-CB	6.72	106.95	103.19
1	A	384	PRO	CA-C-N	5.66	128.13	120.44
1	A	384	PRO	C-N-CA	5.66	128.13	120.44
3	L	105	GLU	CB-CG-CD	5.53	122.00	112.60
3	L	170	ASP	CB-CA-C	5.27	118.40	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	468	ILE	CB-CA-C	5.18	116.63	110.93
3	E	66	GLY	CA-C-O	-5.14	118.75	122.45
3	L	30	SER	CB-CA-C	-5.12	110.26	117.23
1	A	403	ARG	CA-C-N	5.07	125.70	120.03
1	A	403	ARG	C-N-CA	5.07	125.70	120.03
1	B	368	LEU	CA-C-N	5.01	127.40	120.29
1	B	368	LEU	C-N-CA	5.01	127.40	120.29

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	1541	0	1454	15	0
1	B	1492	0	1395	19	0
2	D	1698	0	1645	13	0
2	H	1702	0	1644	12	0
3	E	1637	0	1590	12	0
3	L	1640	0	1584	11	0
4	C	60	0	52	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
5	H	1	0	0	0	0
6	B	3	0	0	0	0
6	E	3	0	0	0	0
6	L	9	0	0	0	0
7	D	6	0	8	0	0
8	A	10	0	0	0	0
8	B	18	0	0	0	0
8	D	32	0	0	0	0
8	E	35	0	0	0	0
8	H	38	0	0	2	0
8	L	31	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9962	0	9372	80	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 (80) 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:213[A]:ASN:OD1	8:H:401:HOH:O	1.85	0.94
1:B:365:TYR:HB3	1:B:387:LEU:HD13	1.60	0.82
2:H:36:TRP:C	2:H:37:ILE:HD12	2.21	0.66
1:B:371:SER:O	1:B:373:SER:N	2.29	0.65
2:H:192:LEU:C	2:H:192:LEU:HD12	2.22	0.65
1:B:371:SER:C	1:B:373:SER:H	2.04	0.65
3:L:11:LEU:CD2	3:L:104:LEU:HD13	2.27	0.63
3:L:11:LEU:HD22	3:L:104:LEU:HD13	1.82	0.62
1:B:403:ARG:HG2	1:B:504:GLY:O	2.00	0.61
2:D:36:TRP:C	2:D:37:ILE:HD12	2.25	0.61
1:B:384:PRO:HA	1:B:387:LEU:HD12	1.83	0.61
1:A:352:ALA:HA	1:A:468:ILE:HD11	1.82	0.60
3:E:39:LYS:HE2	3:E:83:PHE:O	2.04	0.56
2:D:55[B]:GLY:HA2	2:D:106:TYR:CD1	2.40	0.56
1:A:484:GLU:OE2	1:A:490:PHE:HB2	2.06	0.55
1:A:364:ASP:OD1	1:A:388:ASN:ND2	2.41	0.54
1:B:383:SER:O	1:B:387:LEU:HG	2.08	0.54
3:L:12:SER:HA	3:L:105:GLU:O	2.08	0.53
2:D:192:LEU:C	2:D:192:LEU:HD12	2.34	0.53
3:L:55:GLN:OE1	3:L:55:GLN:HA	2.10	0.52
2:D:37:ILE:HD12	2:D:37:ILE:N	2.24	0.52
2:H:55[B]:GLY:HA2	2:H:106:TYR:CE1	2.45	0.51
1:A:384:PRO:HA	1:A:387:LEU:HD22	1.91	0.51
2:H:37:ILE:HD12	2:H:37:ILE:N	2.26	0.51
1:B:365:TYR:HB2	1:B:387:LEU:HB3	1.93	0.51
3:E:78:LEU:HD11	3:E:104:LEU:HD21	1.92	0.50
2:H:55[B]:GLY:HA2	2:H:106:TYR:CD1	2.47	0.49
3:E:39:LYS:CE	3:E:83:PHE:O	2.60	0.49
3:E:33:LEU:HD22	3:E:89:GLN:O	2.12	0.49
1:B:357:ARG:HH11	1:B:357:ARG:HG2	1.78	0.48
1:A:369:TYR:CD1	1:A:384:PRO:HB2	2.49	0.48
1:B:369:TYR:HA	1:B:377:PHE:CE2	2.48	0.48
1:B:384:PRO:O	1:B:387:LEU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:61:ARG:NH1	3:L:82:ASP:OD1	2.47	0.48
3:L:33:LEU:HD22	3:L:89:GLN:O	2.15	0.47
1:B:388:ASN:HB2	1:B:389:ASP:OD1	2.14	0.47
3:E:105:GLU:OE2	3:E:173:TYR:OH	2.18	0.47
1:B:359:SER:HA	1:B:524:VAL:HG22	1.97	0.47
1:B:357:ARG:HG2	1:B:357:ARG:NH1	2.30	0.46
2:D:14:PRO:O	2:D:15:SER:HB2	2.14	0.46
2:D:206:GLN:HA	2:D:206:GLN:OE1	2.14	0.46
1:A:378:LYS:HB2	2:H:103:TYR:CD1	2.51	0.46
1:B:357:ARG:HH11	1:B:357:ARG:CG	2.29	0.46
2:H:55[B]:GLY:CA	2:H:106:TYR:CD1	2.99	0.46
2:H:12:VAL:O	2:H:125:VAL:HA	2.16	0.46
2:D:18:LEU:HD12	2:D:123:VAL:HG11	1.98	0.45
2:D:64:LYS:O	2:D:65:SER:CB	2.64	0.45
3:E:6:GLN:HA	3:E:22:THR:O	2.17	0.45
3:E:12:SER:HA	3:E:105:GLU:O	2.16	0.45
2:H:155:LEU:HD11	8:H:436:HOH:O	2.16	0.45
1:A:378:LYS:O	1:A:432:CYS:HA	2.16	0.45
1:B:486:PHE:CE2	1:B:487:ASN:ND2	2.85	0.45
2:D:99:MET:HE1	3:E:49:TYR:CZ	2.51	0.45
2:D:55[B]:GLY:CA	2:D:106:TYR:CD1	3.00	0.45
1:B:386:LYS:C	1:B:387:LEU:O	2.60	0.44
2:D:12:VAL:O	2:D:125:VAL:HA	2.17	0.44
2:D:64:LYS:O	2:D:65:SER:OG	2.34	0.44
1:B:371:SER:C	1:B:373:SER:N	2.74	0.44
3:E:24:ARG:HD3	3:E:70:GLU:OE1	2.18	0.43
3:L:150:VAL:CG1	3:L:189:HIS:CG	3.01	0.43
2:D:215:LYS:HB3	2:D:216:PRO:HD3	2.01	0.43
2:H:192:LEU:C	2:H:192:LEU:CD1	2.91	0.43
1:A:338:PHE:CE1	1:A:358:ILE:HD12	2.54	0.43
1:A:403:ARG:HD2	1:A:505:TYR:HA	2.01	0.43
3:L:159:SER:HA	3:L:178:THR:O	2.19	0.42
2:H:55[B]:GLY:O	2:H:56[B]:ASN:CB	2.67	0.42
1:B:378:LYS:O	1:B:432:CYS:HA	2.20	0.42
1:A:482:GLY:O	1:A:483:VAL:HG22	2.20	0.42
3:E:186:TYR:CE2	3:E:211:ARG:HD2	2.55	0.42
1:A:468:ILE:HD13	1:A:468:ILE:HA	1.83	0.41
1:A:482:GLY:C	1:A:483:VAL:HG13	2.45	0.41
1:A:405:ASP:HB2	1:A:504:GLY:O	2.20	0.41
3:L:161:GLU:HA	3:L:176:SER:O	2.20	0.41
1:A:365:TYR:O	1:A:368:LEU:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:PHE:HE2	1:B:363:ALA:HB1	1.85	0.41
1:A:366:SER:OG	1:A:385:THR:O	2.39	0.41
3:E:120:PRO:HD3	3:E:132:VAL:HG22	2.03	0.41
3:L:6:GLN:HA	3:L:22:THR:O	2.21	0.41
3:L:11:LEU:HD23	3:L:11:LEU:C	2.45	0.40
3:E:159:SER:HA	3:E:178:THR:O	2.20	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	193/204 (95%)	174 (90%)	17 (9%)	2 (1%)	12	15
1	B	185/204 (91%)	174 (94%)	9 (5%)	2 (1%)	11	13
2	D	220/238 (92%)	210 (96%)	7 (3%)	3 (1%)	9	9
2	H	221/238 (93%)	213 (96%)	5 (2%)	3 (1%)	9	9
3	E	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
3	L	212/214 (99%)	202 (95%)	10 (5%)	0	100	100
All	All	1242/1312 (95%)	1177 (95%)	55 (4%)	10 (1%)	21	20

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	372	ALA
1	A	519	HIS
1	B	387	LEU
2	D	65	SER
1	A	483	VAL
2	H	56[A]	ASN

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Mol	Chain	Res	Type
2	H	56[B]	ASN
2	D	56[A]	ASN
2	D	56[B]	ASN
2	H	2	VAL

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	167/176 (95%)	157 (94%)	10 (6%)	17	25
1	B	161/176 (92%)	152 (94%)	9 (6%)	19	28
2	D	190/207 (92%)	184 (97%)	6 (3%)	34	51
2	H	190/207 (92%)	185 (97%)	5 (3%)	40	59
3	E	186/187 (100%)	183 (98%)	3 (2%)	55	73
3	L	186/187 (100%)	184 (99%)	2 (1%)	65	81
All	All	1080/1140 (95%)	1045 (97%)	35 (3%)	34	51

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	346	ARG
1	A	358	ILE
1	A	367	VAL
1	A	371	SER
1	A	387	LEU
1	A	455	LEU
1	A	468	ILE
1	A	483	VAL
1	A	498	GLN
1	A	517	LEU
1	B	357	ARG
1	B	367	VAL
1	B	371	SER
1	B	385	THR

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Mol	Chain	Res	Type
1	B	387	LEU
1	B	441	LEU
1	B	445	VAL
1	B	480	CYS
1	B	516	GLU
2	D	5	GLN
2	D	68	SER
2	D	140	PRO
2	D	152	LEU
2	D	195	VAL
2	D	228	LYS
3	E	33	LEU
3	E	152	ASN
3	E	158	ASN
2	H	37	ILE
2	H	140	PRO
2	H	163	PRO
2	H	175	SER
2	H	228	LYS
3	L	11	LEU
3	L	149	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	354	ASN
1	A	448	ASN
1	A	450	ASN
1	B	343	ASN
1	B	487	ASN
3	E	92	ASN
2	H	77	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

5 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	0.87	1 (7%)	17,19,21	1.10	1 (5%)
4	NAG	C	2	4	14,14,15	0.65	0	17,19,21	1.30	1 (5%)
4	BMA	C	3	4	11,11,12	0.60	0	15,15,17	1.52	2 (13%)
4	MAN	C	4	4	11,11,12	0.42	0	15,15,17	1.02	0
4	FUC	C	5	4	10,10,11	0.52	0	14,14,16	0.89	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	-	0/6/23/26	0/1/1/1
4	NAG	C	2	4	-	1/6/23/26	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	FUC	C	5	4	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1	NAG	O5-C1	-2.03	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3	BMA	C1-O5-C5	3.93	117.45	112.19
4	C	3	BMA	O2-C2-C1	-3.14	102.04	109.22
4	C	2	NAG	O7-C7-N2	2.38	126.18	121.98
4	C	1	NAG	O7-C7-C8	-2.29	117.98	122.05

There are no chirality outliers.

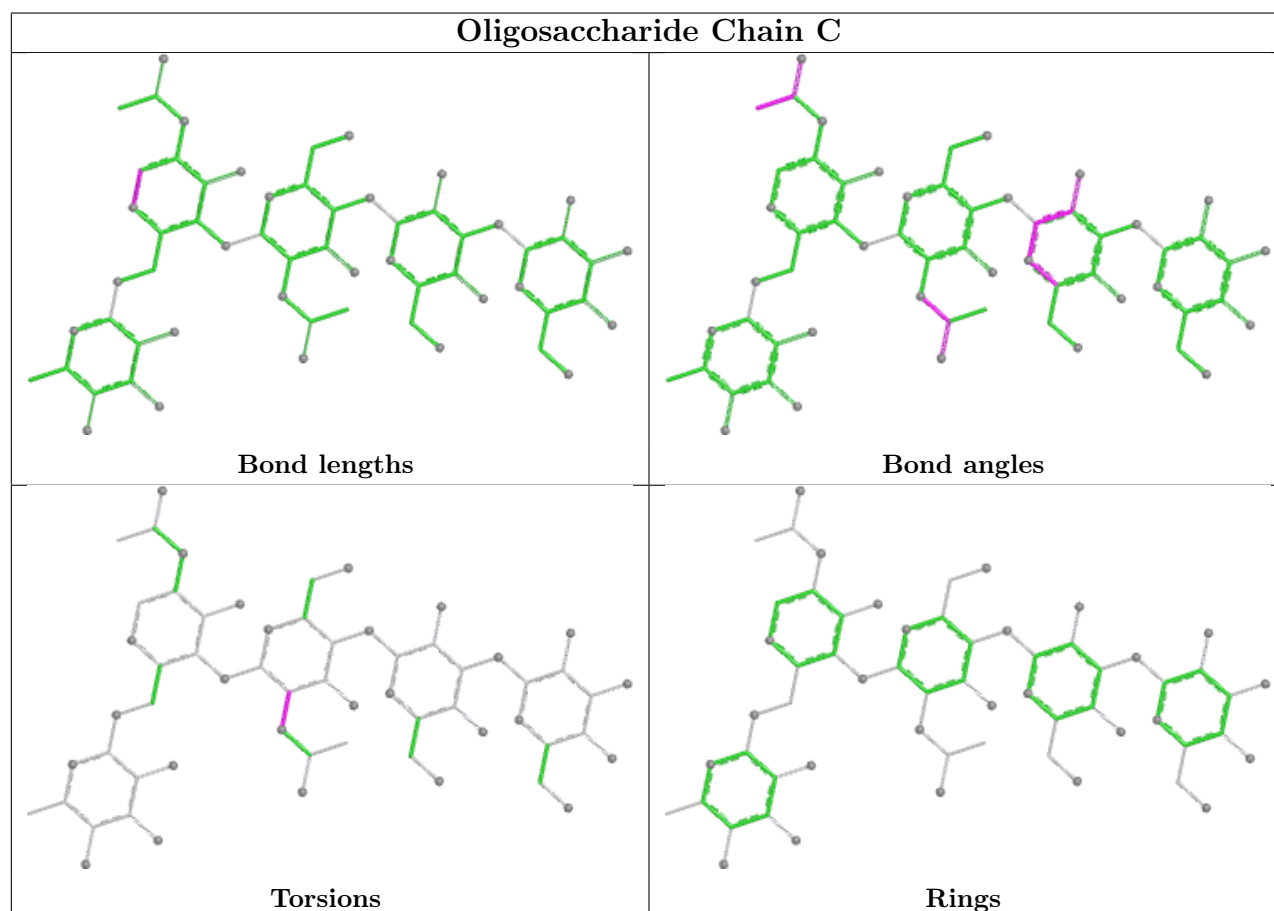
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2	NAG	C1-C2-N2-C7

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 [i](#)

Of 13 ligands modelled in this entry, 7 are monoatomic - leaving 6 for Mogul analysis.

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	SCN	L	303	-	1,2,2	0.77	0	0,1,1	-	-
6	SCN	L	302	-	1,2,2	0.90	0	0,1,1	-	-
6	SCN	E	303	-	1,2,2	0.53	0	0,1,1	-	-
6	SCN	B	602	-	1,2,2	0.32	0	0,1,1	-	-
7	GOL	D	303	-	5,5,5	0.22	0	5,5,5	0.58	0
6	SCN	L	301	-	1,2,2	0.73	0	0,1,1	-	-

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
7	GOL	D	303	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	303	GOL	O1-C1-C2-O2
7	D	303	GOL	O1-C1-C2-C3
7	D	303	GOL	C1-C2-C3-O3
7	D	303	GOL	O2-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 ⓘ

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	195/204 (95%)	0.93	33 (16%) 4 5	31, 63, 119, 146	0
1	B	189/204 (92%)	0.71	29 (15%) 5 6	35, 63, 106, 133	0
2	D	221/238 (92%)	0.05	4 (1%) 67 69	23, 46, 71, 101	3 (1%)
2	H	221/238 (92%)	0.08	8 (3%) 46 48	21, 46, 66, 100	4 (1%)
3	E	213/214 (99%)	-0.05	2 (0%) 81 82	31, 46, 68, 96	0
3	L	214/214 (100%)	-0.05	2 (0%) 81 82	36, 48, 66, 124	0
All	All	1253/1312 (95%)	0.26	78 (6%) 26 28	21, 49, 94, 146	7 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	55[A]	GLY	8.4
2	D	55[A]	GLY	6.5
1	A	517	LEU	5.3
1	B	365	TYR	5.0
1	A	385	THR	4.6
1	A	518	LEU	4.3
1	A	387	LEU	4.2
1	B	481	ASN	3.9
1	B	387	LEU	3.9
1	A	486	PHE	3.9
1	B	386	LYS	3.8
1	B	528	LYS	3.8
1	A	445	VAL	3.4
2	H	140	PRO	3.4
1	B	392	PHE	3.4
1	A	334	ASN	3.3
1	B	372	ALA	3.2
1	A	483	VAL	3.2
1	B	335	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	385	THR	3.2
1	B	483	VAL	3.1
2	H	1	GLN	3.1
1	A	476	GLY	3.0
1	A	521	PRO	3.0
1	B	441	LEU	3.0
1	A	478	THR	3.0
1	A	519	HIS	2.9
1	A	335	LEU	2.9
1	A	390	LEU	2.9
1	B	334	ASN	2.9
1	B	486	PHE	2.8
2	D	140	PRO	2.8
1	A	365	TYR	2.8
1	A	528	LYS	2.8
1	B	393	THR	2.8
1	A	449	TYR	2.7
3	L	214	CYS	2.7
2	D	1	GLN	2.7
2	H	56[A]	ASN	2.7
1	A	367	VAL	2.6
1	A	373	SER	2.6
1	A	479	PRO	2.6
1	B	478	THR	2.6
1	A	386	LYS	2.6
3	E	1	ASP	2.6
3	L	1	ASP	2.6
1	B	523	THR	2.6
2	H	148	GLY	2.6
1	B	369	TYR	2.6
2	H	54[A]	SER	2.6
3	E	212	GLY	2.5
1	A	364	ASP	2.5
1	B	388	ASN	2.5
1	B	363	ALA	2.5
1	A	393	THR	2.4
1	A	369	TYR	2.4
1	B	364	ASP	2.4
1	B	366	SER	2.4
1	B	516	GLU	2.4
1	A	363	ALA	2.4
2	H	228	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	384	PRO	2.3
1	B	384	PRO	2.3
1	B	368	LEU	2.3
1	B	338	PHE	2.3
1	A	522	ALA	2.2
2	D	228	LYS	2.2
1	B	445	VAL	2.2
1	A	346	ARG	2.2
1	A	359	SER	2.2
1	A	475	ALA	2.1
1	B	383	SER	2.1
1	A	388	ASN	2.1
2	H	41	PRO	2.1
1	A	500	THR	2.0
1	B	390	LEU	2.0
1	B	482	GLY	2.0
1	A	484	GLU	2.0

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

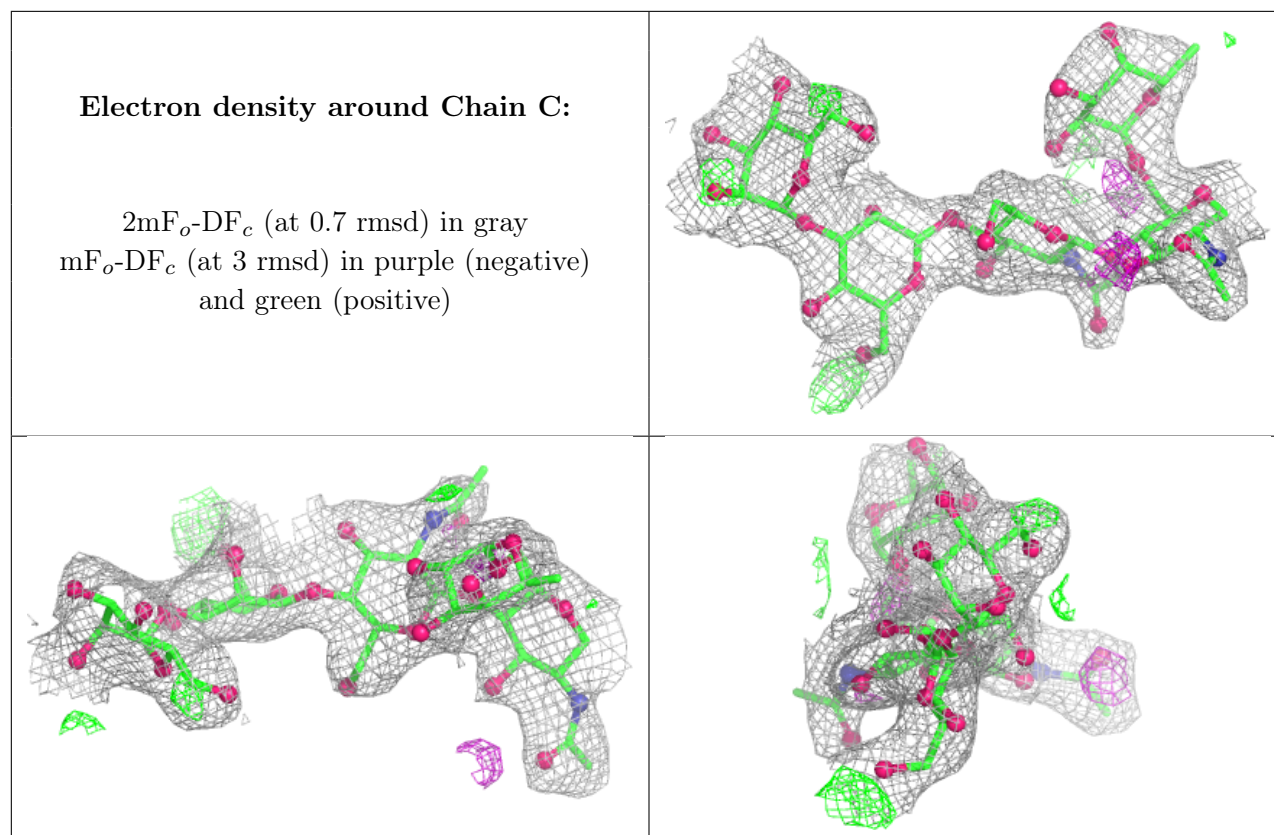
There are no non-standard protein/DNA/RNA residues in this entry.

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	-	-	56,70,82,90	0
4	NAG	C	2	14/15	-	-	70,75,79,81	0
4	BMA	C	3	11/12	-	-	74,76,80,83	0
4	MAN	C	4	11/12	-	-	77,81,85,86	0
4	FUC	C	5	10/11	-	-	112,117,121,121	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($\text{\AA}^2$)	Q<0.9
7	GOL	D	303	6/6	0.72	0.19	44,55,63,67	0
6	SCN	L	301	3/3	0.84	0.13	60,60,69,88	0
5	CL	D	302	1/1	0.86	0.24	89,89,89,89	0
5	CL	A	601	1/1	0.87	0.12	84,84,84,84	0
6	SCN	L	303	3/3	0.89	0.27	46,46,63,75	0
5	CL	E	302	1/1	0.91	0.11	64,64,64,64	0
6	SCN	E	303	3/3	0.92	0.14	47,47,54,60	0
5	CL	B	601	1/1	0.93	0.10	77,77,77,77	0
5	CL	E	301	1/1	0.94	0.12	59,59,59,59	0
6	SCN	L	302	3/3	0.94	0.11	55,55,58,59	0
5	CL	D	301	1/1	0.96	0.07	63,63,63,63	0
6	SCN	B	602	3/3	0.97	0.09	43,43,45,53	0
5	CL	H	301	1/1	0.98	0.06	63,63,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.