



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:34 PM UTC

PDB ID : 7Q0G / pdb_00007q0g
Title : Crystal structure of the receptor binding domain of SARS-CoV-2 beta variant spike glycoprotein in complex with Beta-49 and FI-3A Fabs
Authors : Zhou, D.; Ren, J.; Stuart, D.I.
Deposited on : 2021-10-14
Resolution : 1.82 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:

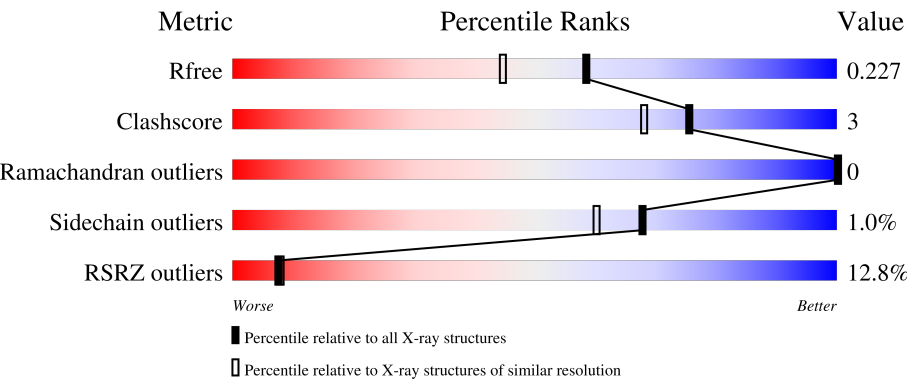
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	E	210	25% 87% 6% 7%
2	H	222	6% 89% 9%
3	L	214	8% 93% 7%
4	B	216	13% 93% 7%
5	A	223	11% 90% 8%

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Mol	Chain	Length	Quality of chain
6	C	5	40% 60%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	TAR	H	404	-	X	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 8581 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	E	196	Total	C	N	O	S	0	0	0
			1549	994	258	289	8			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	319	MET	-	initiating methionine	UNP P0DTC2
E	320	GLY	-	expression tag	UNP P0DTC2
E	321	CYS	-	expression tag	UNP P0DTC2
E	322	VAL	-	expression tag	UNP P0DTC2
E	323	ALA	-	expression tag	UNP P0DTC2
E	324	GLU	-	expression tag	UNP P0DTC2
E	325	THR	-	expression tag	UNP P0DTC2
E	326	GLY	-	expression tag	UNP P0DTC2
E	327	HIS	-	expression tag	UNP P0DTC2
E	328	HIS	-	expression tag	UNP P0DTC2
E	329	HIS	-	expression tag	UNP P0DTC2
E	330	HIS	-	expression tag	UNP P0DTC2
E	331	HIS	-	expression tag	UNP P0DTC2
E	332	HIS	-	expression tag	UNP P0DTC2
E	417	ASN	LYS	variant	UNP P0DTC2
E	484	LYS	GLU	variant	UNP P0DTC2
E	501	TYR	ASN	variant	UNP P0DTC2
E	527	LYS	-	expression tag	UNP P0DTC2
E	528	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called FI-3A Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	0	0	0
			1620	1017	276	319	8			

- Molecule 3 is a protein called FI-3A Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	0	0
			1640	1024	274	337	5			

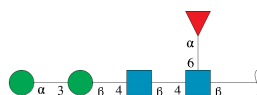
- Molecule 4 is a protein called Beta-49 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	216	Total	C	N	O	S	0	0	0
			1656	1033	283	334	6			

- Molecule 5 is a protein called Beta-49 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	219	Total	C	N	O	S	0	0	0
			1603	1015	264	317	7			

- Molecule 6 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
6	C	5	Total	C	N	O	0	0	0
			60	34	2	24			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	E	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	H	1	Total	C	O	0	0
			6	3	3		
7	H	1	Total	C	O	0	0
			6	3	3		
7	H	1	Total	C	O	0	0
			6	3	3		
7	H	1	Total	C	O	0	0
			6	3	3		
7	L	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		

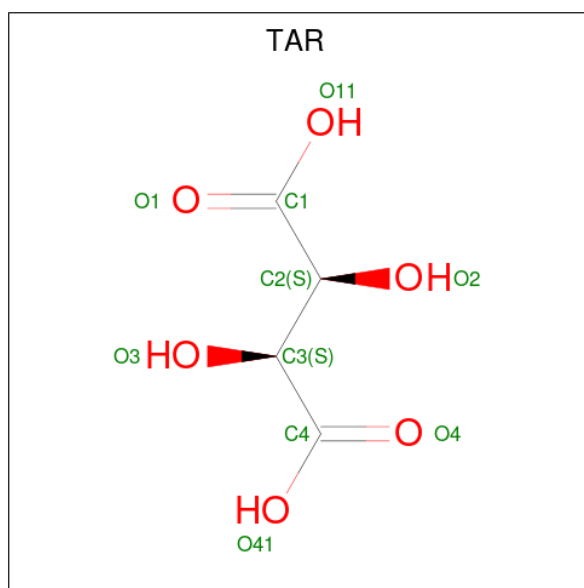
- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	4	Total Cl 4 4	0	0
8	H	1	Total Cl 1 1	0	0
8	L	2	Total Cl 2 2	0	0
8	B	3	Total Cl 3 3	0	0
8	A	4	Total Cl 4 4	0	0

- Molecule 9 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	E	1	Total K 1 1	0	0
9	H	5	Total K 5 5	0	0
9	L	5	Total K 5 5	0	0
9	B	2	Total K 2 2	0	0
9	A	1	Total K 1 1	0	0

- Molecule 10 is D(-)-TARTARIC ACID (CCD ID: TAR) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	H	1	Total C O 10 4 6	0	0
10	A	1	Total C O 10 4 6	0	0
10	A	1	Total C O 10 4 6	0	0

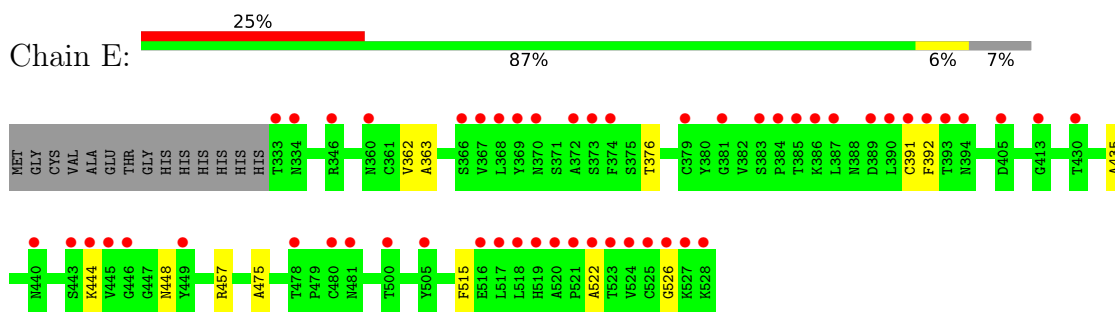
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	E	47	Total O 47 47	0	0
11	H	90	Total O 90 90	0	0
11	L	67	Total O 67 67	0	0
11	B	43	Total O 43 43	0	0
11	A	70	Total O 70 70	0	0

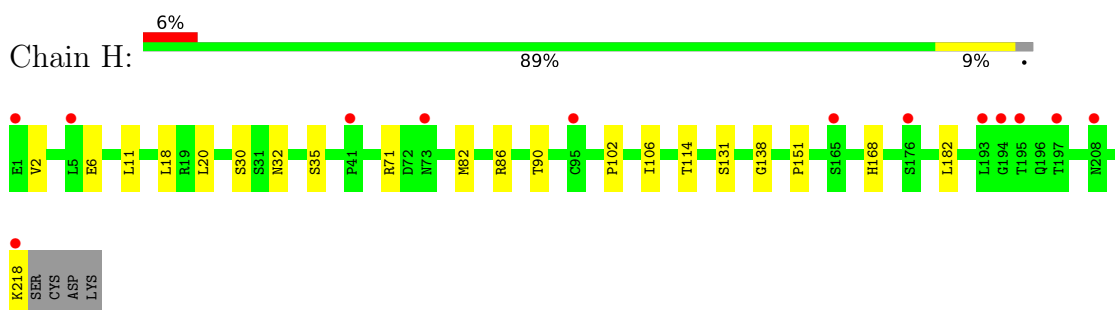
3 Residue-property plots [i](#)

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.

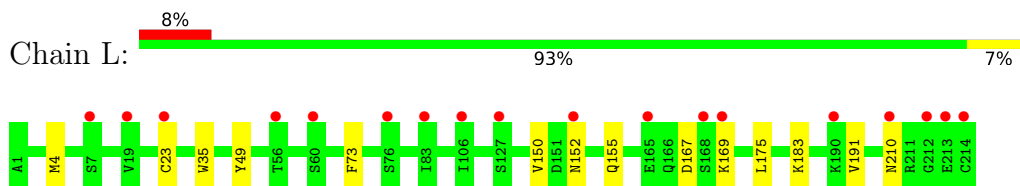
- Molecule 1: Spike protein S1



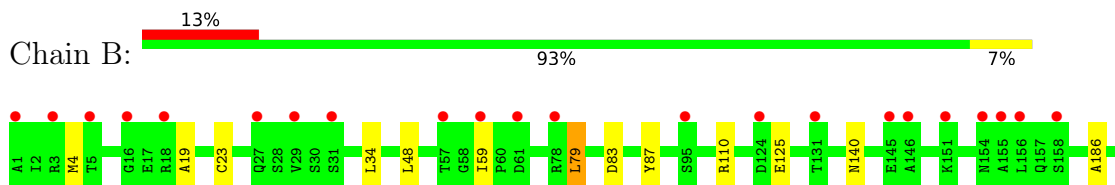
- Molecule 2: FI-3A Fab heavy chain

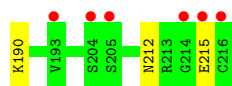


- Molecule 3: FI-3A Fab light chain

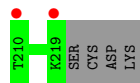
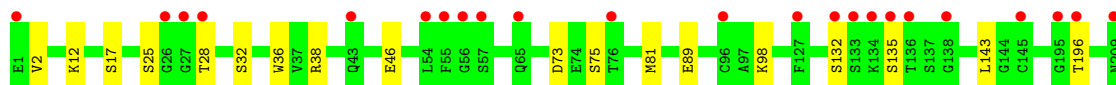
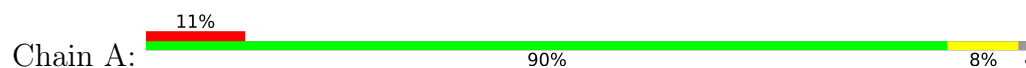


- Molecule 4: Beta-49 Fab light chain

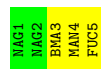




- Molecule 5: Beta-49 Fab heavy chain



- Molecule 6: 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	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.29Å 106.54Å 215.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	107.81 – 1.82 107.81 – 1.82	Depositor EDS
% Data completeness (in resolution range)	51.2 (107.81-1.82) 51.2 (107.81-1.82)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 1.82Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.192 , 0.224 0.201 , 0.227	Depositor DCC
R_{free} test set	4710 reflections (2.57%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8581	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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: GOL, CL, FUC, K, BMA, NAG, MAN, TAR

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	E	0.32	0/1593	0.49	0/2169
2	H	0.37	0/1657	0.58	0/2255
3	L	0.37	0/1674	0.59	0/2275
4	B	0.32	0/1693	0.53	0/2298
5	A	0.35	0/1640	0.54	0/2237
All	All	0.34	0/8257	0.55	0/11234

There are no bond length outliers.

There are no bond angle outliers.

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	E	1549	0	1459	8	0
2	H	1620	0	1598	15	0
3	L	1640	0	1584	8	0
4	B	1656	0	1604	9	0
5	A	1603	0	1583	9	0
6	C	60	0	52	0	0
7	A	6	0	8	0	0
7	B	18	0	24	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	24	0	32	1	0
7	H	24	0	32	4	0
7	L	6	0	7	1	0
8	A	4	0	0	0	0
8	B	3	0	0	0	0
8	E	4	0	0	0	0
8	H	1	0	0	0	0
8	L	2	0	0	0	0
9	A	1	0	0	0	0
9	B	2	0	0	0	0
9	E	1	0	0	0	0
9	H	5	0	0	0	0
9	L	5	0	0	0	0
10	A	20	0	8	2	0
10	H	10	0	4	0	0
11	A	70	0	0	2	0
11	B	43	0	0	0	0
11	E	47	0	0	0	0
11	H	90	0	0	0	0
11	L	67	0	0	1	0
All	All	8581	0	7995	49	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 (49) 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:86:ARG:HH22	7:H:402:GOL:H2	1.49	0.78
4:B:110:ARG:NH2	7:B:401:GOL:O1	2.24	0.70
5:A:89:GLU:OE2	11:A:401:HOH:O	2.10	0.69
1:E:391:CYS:HB3	1:E:522:ALA:HB1	1.78	0.66
4:B:4:MET:HE3	4:B:23:CYS:SG	2.39	0.63
4:B:19:ALA:HB2	4:B:79:LEU:HD21	1.80	0.63
5:A:38:ARG:NH1	5:A:46:GLU:OE1	2.33	0.61
4:B:140:ASN:HD22	7:B:401:GOL:H31	1.65	0.60
10:A:302:TAR:O4	10:A:302:TAR:O2	2.19	0.59
4:B:212:ASN:HB2	4:B:215:GLU:HG3	1.88	0.55
2:H:168:HIS:CE1	7:L:301:GOL:H11	2.42	0.54
1:E:444:LYS:HG3	1:E:448:ASN:HB2	1.90	0.54
2:H:138:GLY:O	7:H:403:GOL:O2	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:457:ARG:HH22	7:E:703:GOL:H2	1.72	0.53
4:B:212:ASN:HB2	4:B:215:GLU:CG	2.39	0.53
3:L:191:VAL:HG22	3:L:210:ASN:OD1	2.09	0.53
2:H:30:SER:HA	2:H:71:ARG:HD2	1.92	0.51
3:L:4:MET:HE3	3:L:23:CYS:SG	2.51	0.49
5:A:38:ARG:NE	11:A:407:HOH:O	2.45	0.49
3:L:150:VAL:CG2	3:L:155:GLN:HG3	2.42	0.49
2:H:11:LEU:HB2	2:H:151:PRO:HG3	1.95	0.49
2:H:2:VAL:HG12	2:H:106:ILE:HD13	1.95	0.48
2:H:35:SER:OG	7:H:401:GOL:O1	2.31	0.48
1:E:376:THR:HB	1:E:435:ALA:HB3	1.94	0.48
2:H:86:ARG:NH2	7:H:402:GOL:H2	2.25	0.48
5:A:132:SER:CB	5:A:135:SER:HB3	2.44	0.48
2:H:18:LEU:HB3	2:H:82:MET:HE3	1.95	0.47
2:H:182:LEU:C	2:H:182:LEU:HD12	2.40	0.47
5:A:12:LYS:HE2	5:A:17:SER:O	2.15	0.47
2:H:90:THR:HG23	2:H:114:THR:HA	1.97	0.46
2:H:102:PRO:HG3	3:L:49:TYR:CZ	2.51	0.46
5:A:2:VAL:HA	5:A:25:SER:O	2.16	0.46
2:H:131:SER:OG	2:H:218:LYS:HE3	2.16	0.45
5:A:73:ASP:OD1	5:A:75:SER:OG	2.34	0.45
1:E:392:PHE:CD1	1:E:515:PHE:HB3	2.52	0.45
3:L:35:TRP:CE2	3:L:73:PHE:HB2	2.52	0.45
1:E:475:ALA:HB1	2:H:32:ASN:HD21	1.82	0.45
1:E:391:CYS:CB	1:E:522:ALA:HB1	2.44	0.44
1:E:363:ALA:O	1:E:526:GLY:HA2	2.18	0.43
4:B:83:ASP:O	4:B:87:TYR:OH	2.24	0.43
4:B:48:LEU:HD23	4:B:59:ILE:HD12	2.00	0.42
2:H:20:LEU:HG	2:H:82:MET:HE2	2.02	0.42
4:B:186:ALA:O	4:B:190:LYS:HG3	2.20	0.41
5:A:36:TRP:CE2	5:A:81:MET:HB2	2.56	0.41
10:A:302:TAR:O11	10:A:302:TAR:O3	2.35	0.41
5:A:28:THR:OG1	5:A:98:LYS:NZ	2.39	0.41
3:L:167:ASP:OD2	3:L:169:LYS:HB3	2.20	0.41
3:L:175:LEU:C	3:L:175:LEU:HD23	2.46	0.41
3:L:183:LYS:NZ	11:L:414:HOH:O	2.55	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	E	194/210 (92%)	189 (97%)	5 (3%)	0	100	100
2	H	216/222 (97%)	213 (99%)	3 (1%)	0	100	100
3	L	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
4	B	214/216 (99%)	208 (97%)	6 (3%)	0	100	100
5	A	217/223 (97%)	214 (99%)	3 (1%)	0	100	100
All	All	1053/1085 (97%)	1031 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	E	167/180 (93%)	166 (99%)	1 (1%)	78	74
2	H	183/187 (98%)	182 (100%)	1 (0%)	81	77
3	L	187/188 (100%)	186 (100%)	1 (0%)	81	77
4	B	186/186 (100%)	183 (98%)	3 (2%)	55	44
5	A	180/187 (96%)	177 (98%)	3 (2%)	53	41
All	All	903/928 (97%)	894 (99%)	9 (1%)	68	60

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	362	VAL
2	H	6	GLU
3	L	152	ASN
4	B	34	LEU
4	B	79	LEU
4	B	125	GLU
5	A	32	SER
5	A	143	LEU
5	A	196	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	498	GLN
3	L	137	ASN
4	B	191	HIS
4	B	212	ASN

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	$\# Z > 2$
6	NAG	C	1	6,1	14,14,15	0.39	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	C	2	6	14,14,15	0.44	0	17,19,21	0.57	0
6	BMA	C	3	6	11,11,12	1.04	1 (9%)	15,15,17	0.71	0
6	MAN	C	4	6	11,11,12	1.23	1 (9%)	15,15,17	1.04	0
6	FUC	C	5	6	10,10,11	1.10	1 (10%)	14,14,16	0.76	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	C	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	C	2	6	-	0/6/23/26	0/1/1/1
6	BMA	C	3	6	-	2/2/19/22	0/1/1/1
6	MAN	C	4	6	-	0/2/19/22	0/1/1/1
6	FUC	C	5	6	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	3	BMA	C4-C5	2.56	1.58	1.53
6	C	4	MAN	O5-C5	2.12	1.47	1.43
6	C	5	FUC	C2-C3	2.10	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

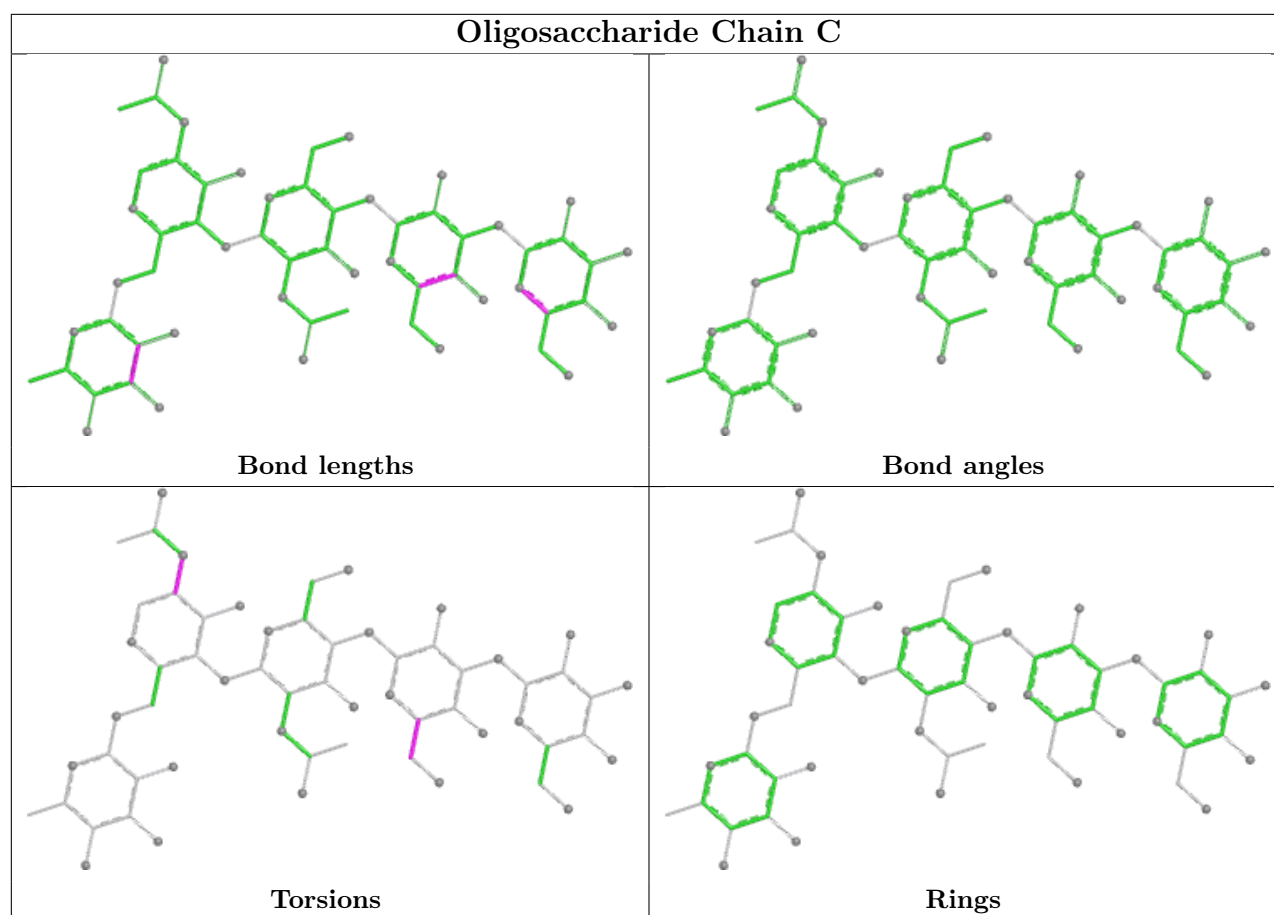
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	3	BMA	O5-C5-C6-O6
6	C	3	BMA	C4-C5-C6-O6
6	C	1	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 44 ligands modelled in this entry, 28 are monoatomic - leaving 16 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	$\# Z > 2$
7	GOL	H	403	-	5,5,5	1.27	0	5,5,5	0.72	0
10	TAR	A	301	-	9,9,9	0.55	0	12,12,12	0.85	0
7	GOL	B	403	-	5,5,5	1.06	0	5,5,5	0.99	0
7	GOL	A	303	-	5,5,5	0.89	0	5,5,5	1.09	0
7	GOL	E	701	-	5,5,5	1.05	0	5,5,5	0.97	0
7	GOL	H	401	-	5,5,5	1.28	0	5,5,5	0.78	0
7	GOL	B	402	-	5,5,5	1.61	2 (40%)	5,5,5	1.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	B	401	-	5,5,5	0.92	0	5,5,5	1.38	1 (20%)
10	TAR	A	302	-	9,9,9	1.57	2 (22%)	12,12,12	1.26	2 (16%)
7	GOL	E	703	-	5,5,5	1.04	0	5,5,5	1.03	0
7	GOL	H	405	-	5,5,5	1.06	0	5,5,5	0.99	0
7	GOL	L	301	9	5,5,5	1.43	0	5,5,5	0.72	0
7	GOL	E	704	-	5,5,5	1.39	1 (20%)	5,5,5	1.17	0
7	GOL	E	702	-	5,5,5	1.11	0	5,5,5	1.12	1 (20%)
10	TAR	H	404	-	9,9,9	1.98	4 (44%)	12,12,12	1.98	4 (33%)
7	GOL	H	402	-	5,5,5	1.16	0	5,5,5	0.98	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
7	GOL	H	403	-	-	4/4/4/4	-
10	TAR	A	301	-	-	4/12/12/12	-
7	GOL	B	403	-	-	4/4/4/4	-
7	GOL	A	303	-	-	1/4/4/4	-
7	GOL	E	701	-	-	1/4/4/4	-
7	GOL	H	401	-	-	1/4/4/4	-
7	GOL	B	402	-	-	1/4/4/4	-
7	GOL	B	401	-	-	0/4/4/4	-
10	TAR	A	302	-	-	8/12/12/12	-
7	GOL	E	703	-	-	2/4/4/4	-
7	GOL	H	405	-	-	3/4/4/4	-
7	GOL	L	301	9	-	2/4/4/4	-
7	GOL	E	704	-	-	2/4/4/4	-
7	GOL	E	702	-	-	0/4/4/4	-
10	TAR	H	404	-	-	7/12/12/12	-
7	GOL	H	402	-	-	2/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	302	TAR	O4-C4	3.36	1.32	1.22
10	H	404	TAR	O1-C1	3.34	1.32	1.22
10	H	404	TAR	O4-C4	2.96	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	402	GOL	C3-C2	2.76	1.62	1.51
10	H	404	TAR	O41-C4	-2.72	1.22	1.30
10	A	302	TAR	O41-C4	-2.71	1.22	1.30
10	H	404	TAR	O11-C1	-2.55	1.22	1.30
7	E	704	GOL	C3-C2	2.41	1.60	1.51
7	B	402	GOL	C1-C2	2.20	1.60	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	H	404	TAR	O41-C4-C3	3.39	122.72	113.31
10	H	404	TAR	O4-C4-C3	-3.35	112.70	121.62
10	H	404	TAR	O11-C1-C2	3.28	122.41	113.31
10	H	404	TAR	O1-C1-C2	-3.10	113.37	121.62
10	A	302	TAR	O41-C4-C3	3.04	121.77	113.31
10	A	302	TAR	O4-C4-C3	-2.85	114.03	121.62
7	B	401	GOL	C3-C2-C1	-2.44	102.86	111.80
7	E	702	GOL	C3-C2-C1	-2.01	104.42	111.80

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	E	703	GOL	C1-C2-C3-O3
7	E	703	GOL	O2-C2-C3-O3
7	E	704	GOL	C1-C2-C3-O3
7	H	403	GOL	C1-C2-C3-O3
7	L	301	GOL	O1-C1-C2-O2
7	L	301	GOL	O1-C1-C2-C3
7	B	403	GOL	O1-C1-C2-C3
10	H	404	TAR	O1-C1-C2-O2
10	H	404	TAR	O3-C3-C4-O4
10	H	404	TAR	O3-C3-C4-O41
10	A	302	TAR	O3-C3-C4-O4
10	A	302	TAR	O3-C3-C4-O41
10	A	302	TAR	O2-C2-C3-O3
10	A	302	TAR	C1-C2-C3-C4
10	A	302	TAR	C1-C2-C3-O3
10	A	302	TAR	O2-C2-C3-C4
10	H	404	TAR	O11-C1-C2-O2
7	B	403	GOL	O2-C2-C3-O3
10	H	404	TAR	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
10	H	404	TAR	O2-C2-C3-O3
7	H	401	GOL	C1-C2-C3-O3
7	H	402	GOL	O1-C1-C2-C3
7	H	403	GOL	O1-C1-C2-C3
7	H	405	GOL	O1-C1-C2-C3
7	B	403	GOL	C1-C2-C3-O3
10	A	302	TAR	C2-C3-C4-O4
10	A	302	TAR	C2-C3-C4-O41
7	H	403	GOL	O2-C2-C3-O3
7	E	704	GOL	O2-C2-C3-O3
10	A	301	TAR	C1-C2-C3-C4
10	A	301	TAR	O2-C2-C3-C4
7	H	405	GOL	O2-C2-C3-O3
7	B	402	GOL	O2-C2-C3-O3
10	A	301	TAR	C1-C2-C3-O3
7	E	701	GOL	O2-C2-C3-O3
7	B	403	GOL	O1-C1-C2-O2
7	H	405	GOL	O1-C1-C2-O2
7	A	303	GOL	O1-C1-C2-C3
7	H	403	GOL	O1-C1-C2-O2
7	H	402	GOL	O1-C1-C2-O2
10	H	404	TAR	O2-C2-C3-C4
10	A	301	TAR	O2-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	403	GOL	1	0
7	H	401	GOL	1	0
7	B	401	GOL	2	0
10	A	302	TAR	2	0
7	E	703	GOL	1	0
7	L	301	GOL	1	0
7	H	402	GOL	2	0

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	E	196/210 (93%)	1.58	52 (26%) 1 1	31, 46, 97, 142	0
2	H	218/222 (98%)	0.81	13 (5%) 27 31	27, 37, 59, 90	0
3	L	214/214 (100%)	0.94	18 (8%) 17 19	29, 43, 60, 99	0
4	B	216/216 (100%)	1.16	28 (12%) 7 8	32, 48, 77, 120	0
5	A	219/223 (98%)	1.07	25 (11%) 10 11	31, 42, 68, 103	0
All	All	1063/1085 (97%)	1.10	136 (12%) 7 8	27, 43, 74, 142	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	528	LYS	10.2
3	L	214	CYS	9.9
1	E	522	ALA	9.5
1	E	517	LEU	9.3
5	A	135	SER	7.8
1	E	520	ALA	7.6
1	E	333	THR	7.3
1	E	518	LEU	7.3
1	E	523	THR	7.2
1	E	524	VAL	6.9
1	E	526	GLY	6.7
1	E	521	PRO	6.7
1	E	519	HIS	6.6
4	B	216	CYS	6.6
1	E	527	LYS	6.4
5	A	136	THR	5.6
2	H	218	LYS	5.5
5	A	1	GLU	5.3
1	E	525	CYS	5.0
5	A	133	SER	5.0

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Mol	Chain	Res	Type	RSRZ
4	B	156	LEU	4.9
5	A	219	LYS	4.9
3	L	169	LYS	4.4
1	E	480	CYS	4.3
2	H	5	LEU	4.3
5	A	57	SER	4.2
5	A	134	LYS	4.1
1	E	360	ASN	4.1
1	E	372	ALA	4.0
2	H	194	GLY	4.0
3	L	212	GLY	3.9
1	E	369	TYR	3.9
5	A	76	THR	3.9
3	L	23	CYS	3.8
1	E	445	VAL	3.8
1	E	373	SER	3.8
3	L	106	ILE	3.7
1	E	384	PRO	3.7
4	B	1	ALA	3.7
1	E	386	LYS	3.6
4	B	214	GLY	3.5
5	A	26	GLY	3.5
1	E	405	ASP	3.5
5	A	65	GLN	3.4
2	H	1	GLU	3.4
1	E	392	PHE	3.4
1	E	444	LYS	3.3
3	L	56	THR	3.3
5	A	138	GLY	3.3
4	B	3	ARG	3.3
2	H	197	THR	3.2
4	B	131	THR	3.2
1	E	387	LEU	3.2
5	A	28	THR	3.2
4	B	29	VAL	3.1
1	E	393	THR	3.1
3	L	190	LYS	3.1
3	L	127	SER	3.1
1	E	516	GLU	3.1
4	B	154	ASN	3.0
1	E	366	SER	3.0
5	A	209	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
2	H	193	LEU	2.9
1	E	446	GLY	2.9
1	E	390	LEU	2.9
1	E	385	THR	2.8
4	B	95	SER	2.8
5	A	195	GLY	2.8
2	H	195	THR	2.7
1	E	440	ASN	2.7
5	A	56	GLY	2.7
4	B	78	ARG	2.7
4	B	205	SER	2.7
1	E	449	TYR	2.7
3	L	168	SER	2.7
1	E	481	ASN	2.7
4	B	145	GLU	2.6
1	E	391	CYS	2.6
5	A	96	CYS	2.6
5	A	132	SER	2.6
4	B	18	ARG	2.6
5	A	27	GLY	2.6
1	E	430	THR	2.6
3	L	60	SER	2.6
4	B	31	SER	2.5
4	B	5	THR	2.5
1	E	381	GLY	2.5
1	E	368	LEU	2.4
5	A	54	LEU	2.4
1	E	478	THR	2.4
4	B	16	GLY	2.4
2	H	95	CYS	2.4
5	A	196	THR	2.4
1	E	394	ASN	2.4
1	E	346	ARG	2.4
4	B	57	THR	2.4
3	L	213	GLU	2.4
1	E	443	SER	2.4
4	B	151	LYS	2.4
4	B	215	GLU	2.3
3	L	210	ASN	2.3
1	E	367	VAL	2.3
1	E	383	SER	2.3
4	B	158	SER	2.3

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Mol	Chain	Res	Type	RSRZ
4	B	204	SER	2.3
5	A	210	THR	2.3
3	L	165	GLU	2.3
4	B	61	ASP	2.3
5	A	43	GLN	2.3
3	L	19	VAL	2.3
2	H	176	SER	2.2
3	L	76	SER	2.2
2	H	41	PRO	2.2
2	H	165	SER	2.2
3	L	7	SER	2.2
1	E	505	TYR	2.2
5	A	55	PHE	2.2
5	A	145	CYS	2.2
4	B	59	ILE	2.2
1	E	334	ASN	2.1
3	L	83	ILE	2.1
1	E	500	THR	2.1
2	H	208	ASN	2.1
1	E	413	GLY	2.1
2	H	73	ASN	2.1
3	L	152	ASN	2.1
4	B	146	ALA	2.1
4	B	27	GLN	2.0
1	E	379	CYS	2.0
4	B	155	ALA	2.0
1	E	389	ASP	2.0
4	B	124	ASP	2.0
1	E	374	PHE	2.0
5	A	127	PHE	2.0
1	E	370	ASN	2.0
4	B	193	VAL	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.

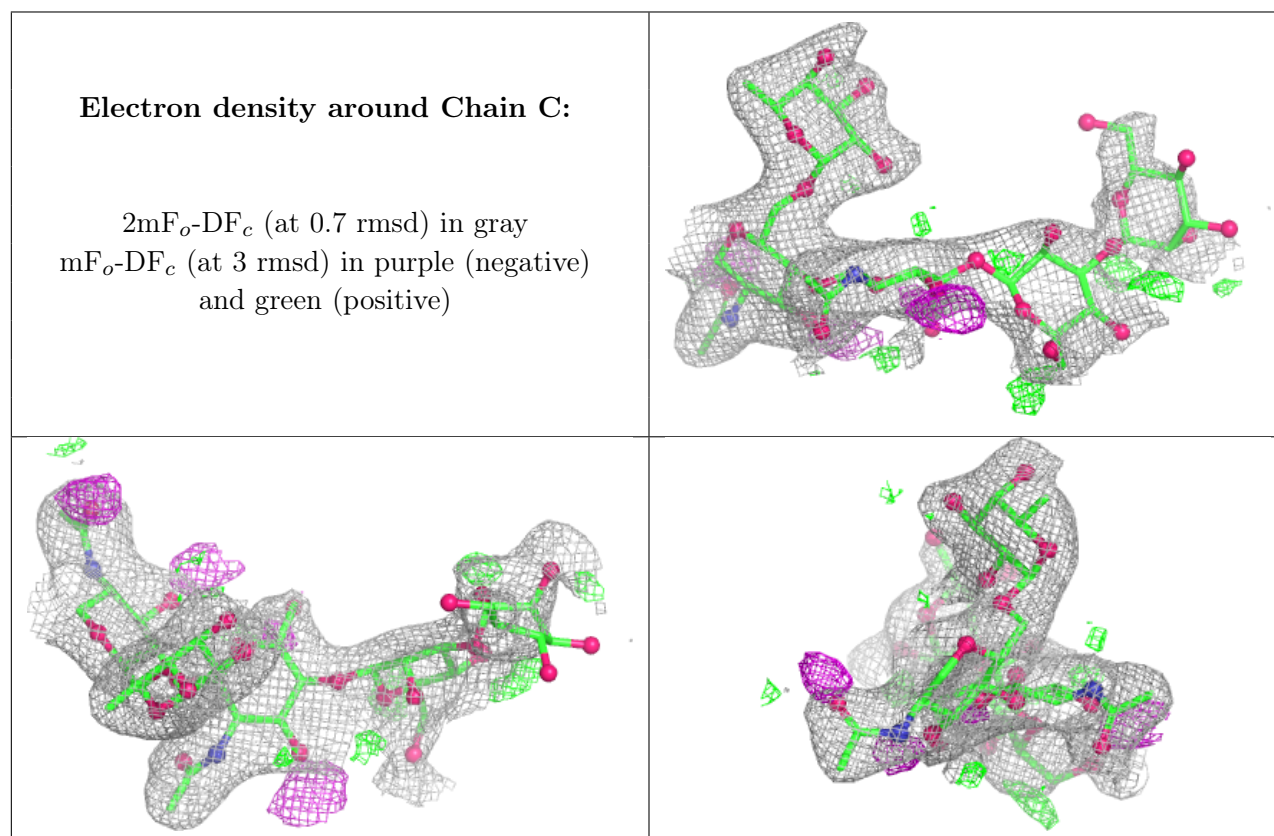
6.3 Carbohydrates [i](#)

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
6	NAG	C	1	14/15	-	-	32,40,46,47	0
6	NAG	C	2	14/15	-	-	40,53,73,82	0
6	BMA	C	3	11/12	-	-	82,96,112,113	0
6	MAN	C	4	11/12	-	-	100,117,131,132	0
6	FUC	C	5	10/11	-	-	39,50,59,63	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
7	GOL	H	405	6/6	0.71	0.26	48,49,59,64	0
7	GOL	B	401	6/6	0.72	0.26	52,64,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	K	L	305	1/1	0.73	0.19	81,81,81,81	0
10	TAR	A	302	10/10	0.73	0.19	46,65,77,85	0
7	GOL	E	701	6/6	0.74	0.32	63,66,75,76	0
9	K	A	308	1/1	0.75	0.20	87,87,87,87	0
10	TAR	A	301	10/10	0.76	0.21	36,68,77,92	0
7	GOL	E	704	6/6	0.77	0.23	42,60,67,70	0
8	CL	B	405	1/1	0.77	0.26	60,60,60,60	0
7	GOL	E	703	6/6	0.79	0.21	46,66,72,85	0
7	GOL	L	301	6/6	0.79	0.20	35,48,56,63	0
7	GOL	H	403	6/6	0.80	0.20	45,49,57,71	0
8	CL	A	306	1/1	0.82	0.21	71,71,71,71	0
9	K	H	409	1/1	0.82	0.20	79,79,79,79	0
8	CL	L	303	1/1	0.83	0.15	70,70,70,70	0
7	GOL	A	303	6/6	0.83	0.18	52,58,68,70	0
9	K	L	307	1/1	0.84	0.19	90,90,90,90	0
8	CL	H	406	1/1	0.85	0.19	66,66,66,66	0
9	K	L	308	1/1	0.86	0.18	74,74,74,74	0
8	CL	E	706	1/1	0.86	0.14	61,61,61,61	0
10	TAR	H	404	10/10	0.87	0.12	37,64,71,72	0
7	GOL	B	402	6/6	0.87	0.17	43,55,58,63	0
9	K	L	304	1/1	0.87	0.13	73,73,73,73	0
8	CL	A	305	1/1	0.88	0.14	58,58,58,58	0
8	CL	E	708	1/1	0.88	0.16	66,66,66,66	0
9	K	H	408	1/1	0.88	0.20	69,69,69,69	0
8	CL	L	302	1/1	0.88	0.12	73,73,73,73	0
8	CL	E	707	1/1	0.89	0.20	73,73,73,73	0
7	GOL	B	403	6/6	0.89	0.15	44,56,63,66	0
7	GOL	H	402	6/6	0.89	0.17	39,54,64,84	0
7	GOL	E	702	6/6	0.89	0.18	45,57,68,81	0
9	K	E	709	1/1	0.89	0.17	78,78,78,78	0
9	K	H	407	1/1	0.90	0.20	61,61,61,61	0
9	K	H	410	1/1	0.90	0.23	79,79,79,79	0
9	K	L	306	1/1	0.91	0.24	70,70,70,70	0
9	K	B	408	1/1	0.91	0.14	56,56,56,56	0
8	CL	B	406	1/1	0.93	0.12	64,64,64,64	0
8	CL	B	404	1/1	0.93	0.19	65,65,65,65	0
9	K	B	407	1/1	0.94	0.27	56,56,56,56	0
7	GOL	H	401	6/6	0.94	0.11	34,48,52,52	0
8	CL	A	307	1/1	0.95	0.15	63,63,63,63	0
9	K	H	411	1/1	0.96	0.31	60,60,60,60	0
8	CL	A	304	1/1	0.98	0.20	34,34,34,34	0
8	CL	E	705	1/1	0.99	0.16	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.