



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:33 PM UTC

PDB ID : 8YUB / pdb_00008yub
Title : Crystal structure of SARS-CoV-2 ConSp RBD in complex with neutralizing antibody CC25.4 Fab
Authors : Kang, J.M.; Yuan, M.; Han, B.W.; Wilson, I.A.
Deposited on : 2024-03-27
Resolution : 2.49 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

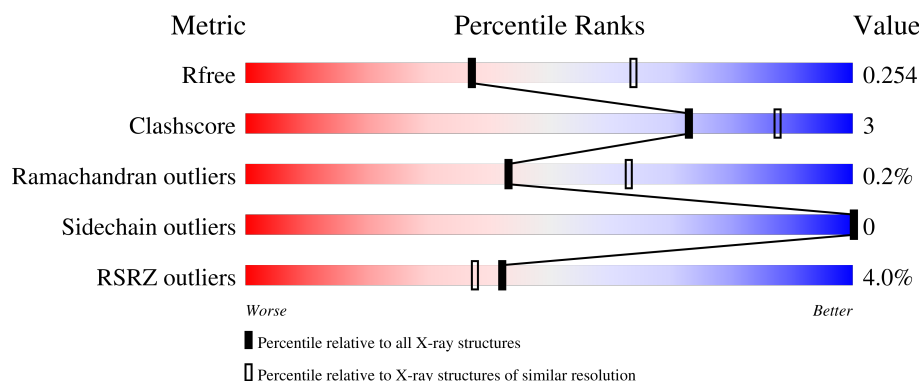
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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.



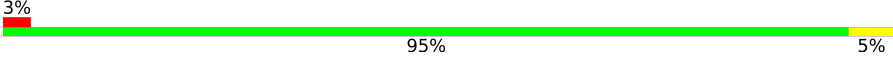
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	228	
1	D	228	
2	B	217	
2	E	217	
3	C	197	

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Mol	Chain	Length	Quality of chain
3	F	197	 3% 95% 5%
4	G	2	 50% 50%
4	H	2	 50% 50%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10211 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 Neutralizing antibody CC25.4 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1758	1107	302	340	9			
1	D	228	Total	C	N	O	S	0	0	0
			1758	1107	302	340	9			

- Molecule 2 is a protein called Neutralizing antibody CC25.4 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1603	996	269	333	5			
2	E	217	Total	C	N	O	S	0	0	0
			1603	996	269	333	5			

- Molecule 3 is a protein called Spike protein S2'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	197	Total	C	N	O	S	0	0	0
			1566	1008	265	285	8			
3	F	197	Total	C	N	O	S	0	0	0
			1566	1008	265	285	8			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	339	HIS	GLY	variant	UNP P0DTC2
C	346	THR	ARG	variant	UNP P0DTC2
C	368	ILE	LEU	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2

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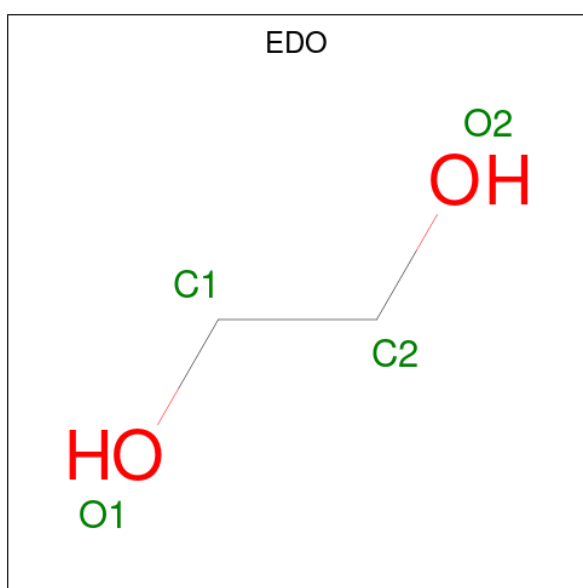
Chain	Residue	Modelled	Actual	Comment	Reference
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	444	THR	LYS	variant	UNP P0DTC2
C	445	PRO	VAL	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	452	ARG	LEU	variant	UNP P0DTC2
C	460	LYS	ASN	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	486	PRO	PHE	variant	UNP P0DTC2
C	490	SER	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
F	339	HIS	GLY	variant	UNP P0DTC2
F	346	THR	ARG	variant	UNP P0DTC2
F	368	ILE	LEU	variant	UNP P0DTC2
F	371	PHE	SER	variant	UNP P0DTC2
F	373	PRO	SER	variant	UNP P0DTC2
F	375	PHE	SER	variant	UNP P0DTC2
F	376	ALA	THR	variant	UNP P0DTC2
F	405	ASN	ASP	variant	UNP P0DTC2
F	408	SER	ARG	variant	UNP P0DTC2
F	417	ASN	LYS	variant	UNP P0DTC2
F	440	LYS	ASN	variant	UNP P0DTC2
F	444	THR	LYS	variant	UNP P0DTC2
F	445	PRO	VAL	variant	UNP P0DTC2
F	446	SER	GLY	variant	UNP P0DTC2
F	452	ARG	LEU	variant	UNP P0DTC2
F	460	LYS	ASN	variant	UNP P0DTC2
F	477	ASN	SER	variant	UNP P0DTC2
F	478	LYS	THR	variant	UNP P0DTC2
F	484	ALA	GLU	variant	UNP P0DTC2
F	486	PRO	PHE	variant	UNP P0DTC2
F	490	SER	PHE	variant	UNP P0DTC2
F	498	ARG	GLN	variant	UNP P0DTC2
F	501	TYR	ASN	variant	UNP P0DTC2
F	505	HIS	TYR	variant	UNP P0DTC2

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	2	Total	C	N	O	0	0	0
			24	14	1	9			
4	H	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			3	2	1		
5	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	75	Total	O	0	0
			75	75		
6	B	42	Total	O	0	0
			42	42		
6	C	50	Total	O	0	0
			50	50		

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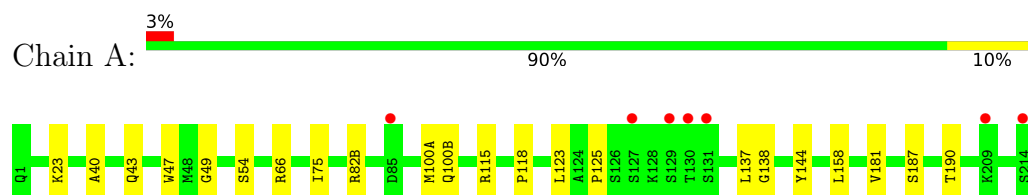
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	51	Total 51	O 51	0	0
6	E	21	Total 21	O 21	0	0
6	F	63	Total 63	O 63	0	0

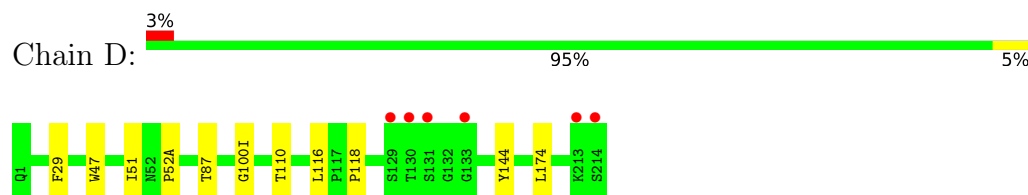
3 Residue-property plots [i](#)

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.

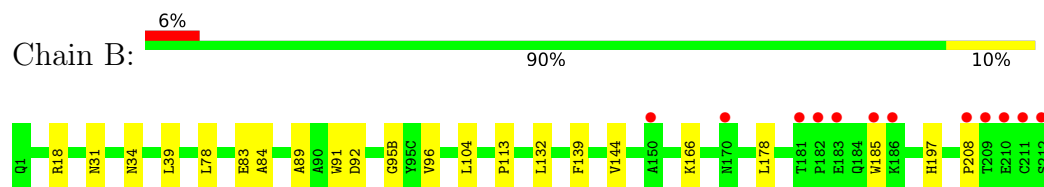
- Molecule 1: Neutralizing antibody CC25.4 heavy chain



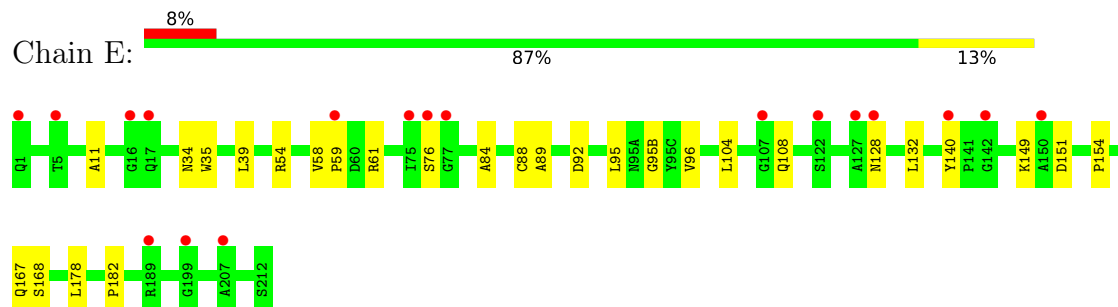
- Molecule 1: Neutralizing antibody CC25.4 heavy chain



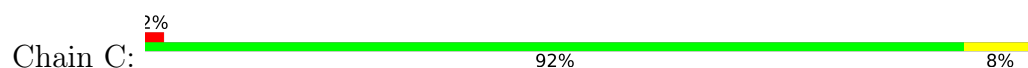
- Molecule 2: Neutralizing antibody CC25.4 light chain



- Molecule 2: Neutralizing antibody CC25.4 light chain

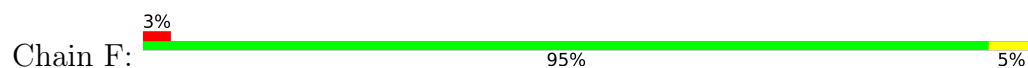


- Molecule 3: Spike protein S2'





- Molecule 3: Spike protein S2'



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.35Å 124.90Å 85.74Å 90.00° 104.37° 90.00°	Depositor
Resolution (Å)	41.20 – 2.49 41.20 – 2.49	Depositor EDS
% Data completeness (in resolution range)	78.8 (41.20-2.49) 78.8 (41.20-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.205 , 0.255 0.206 , 0.254	Depositor DCC
R_{free} test set	2280 reflections (3.92%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 25.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10211	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: FUC, EDO, NAG

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	0.09	0/1804	0.27	0/2458
1	D	0.09	0/1804	0.27	0/2458
2	B	0.10	0/1641	0.28	0/2243
2	E	0.09	0/1641	0.28	0/2243
3	C	0.09	0/1615	0.25	0/2200
3	F	0.09	0/1615	0.24	0/2200
All	All	0.09	0/10120	0.27	0/13802

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	A	1758	0	1704	14	0
1	D	1758	0	1704	8	0
2	B	1603	0	1546	13	0
2	E	1603	0	1546	18	0
3	C	1566	0	1494	9	0
3	F	1566	0	1494	6	0
4	G	24	0	22	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	24	0	22	0	0
5	B	3	0	3	0	0
5	E	4	0	6	0	0
6	A	75	0	0	1	0
6	B	42	0	0	1	0
6	C	50	0	0	0	0
6	D	51	0	0	0	0
6	E	21	0	0	0	0
6	F	63	0	0	0	0
All	All	10211	0	9541	63	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 (63) 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:D:118:PRO:HB3	1:D:144:TYR:HB3	1.72	0.71
1:A:66:ARG:HG2	1:A:82(B):ARG:HH21	1.61	0.66
2:B:39:LEU:HD23	2:B:84:ALA:HB2	1.84	0.60
1:A:115:ARG:NH2	6:A:303:HOH:O	2.38	0.57
1:A:125:PRO:HD3	1:A:137:LEU:HD23	1.86	0.56
3:C:440:LYS:HG3	3:C:441:LEU:HG	1.87	0.56
3:C:345:THR:OG1	4:G:2:FUC:O2	2.24	0.56
2:E:39:LEU:HD23	2:E:84:ALA:HB2	1.87	0.55
2:E:167:GLN:HG2	2:E:168:SER:H	1.72	0.55
1:A:158:LEU:HD21	1:A:181:VAL:HG21	1.89	0.55
3:C:379:CYS:SG	3:C:384:PRO:HG3	2.48	0.54
2:B:132:LEU:HD12	2:B:178:LEU:HD23	1.89	0.53
1:D:87:THR:HG23	1:D:110:THR:HA	1.88	0.53
1:A:23:LYS:NZ	1:A:75:ILE:O	2.41	0.53
1:A:118:PRO:HB3	1:A:144:TYR:HB3	1.89	0.53
2:B:78:LEU:HD11	2:B:104:LEU:HD21	1.91	0.52
3:C:377:PHE:CZ	3:C:384:PRO:HG2	2.45	0.51
2:E:132:LEU:HD12	2:E:178:LEU:HD23	1.92	0.51
2:E:59:PRO:HB2	2:E:61:ARG:HG2	1.92	0.51
2:E:54:ARG:NH1	2:E:58:VAL:O	2.44	0.51
2:E:149:LYS:HD3	2:E:154:PRO:HA	1.94	0.50
1:A:123:LEU:HB2	1:A:138:GLY:HA3	1.94	0.49
1:D:100(I):GLY:HA2	2:E:34:ASN:HD22	1.77	0.49
3:C:412:PRO:HG3	3:C:429:PHE:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:TRP:CG	2:E:96:VAL:HB	2.48	0.48
2:B:185:TRP:CZ3	2:B:208:PRO:HG3	2.50	0.47
3:C:380:TYR:O	3:C:430:THR:HA	2.16	0.45
2:B:83:GLU:OE2	2:B:166:LYS:NZ	2.48	0.45
3:C:383:SER:HB2	3:C:386:LYS:HD3	1.99	0.45
2:B:34:ASN:OD1	2:B:89:ALA:HB3	2.17	0.45
2:E:132:LEU:HB2	2:E:178:LEU:HB3	1.98	0.44
1:D:100(I):GLY:HA2	2:E:34:ASN:ND2	2.31	0.44
2:E:61:ARG:HB2	2:E:76:SER:O	2.17	0.44
1:A:187:SER:HA	1:A:190:THR:HG22	1.99	0.44
1:A:100(A):MET:HE1	3:F:464:PHE:CD2	2.54	0.43
3:F:350:VAL:HG21	3:F:402:ILE:HG22	2.00	0.43
3:F:517:LEU:HD23	3:F:517:LEU:HA	1.90	0.43
1:A:40:ALA:HB3	1:A:43:GLN:HB2	2.00	0.43
2:B:144:VAL:HG12	2:B:197:HIS:HB2	2.02	0.42
2:E:92:ASP:O	2:E:95(B):GLY:HA2	2.18	0.42
1:A:54:SER:OG	1:A:100(B):GLN:OE1	2.34	0.42
1:A:66:ARG:HG2	1:A:82(B):ARG:NH2	2.30	0.42
2:B:92:ASP:O	2:B:95(B):GLY:HA2	2.19	0.42
2:B:31:ASN:ND2	2:B:91:TRP:O	2.45	0.42
2:E:95:LEU:HD13	2:E:95:LEU:HA	1.90	0.42
1:A:47:TRP:CG	2:B:96:VAL:HB	2.54	0.42
2:E:11:ALA:O	2:E:104:LEU:HA	2.20	0.42
1:A:47:TRP:CH2	1:A:49:GLY:HA2	2.55	0.42
1:D:29:PHE:CE2	1:D:52(A):PRO:HB3	2.55	0.42
2:B:132:LEU:HB2	2:B:178:LEU:HB3	2.02	0.41
2:E:34:ASN:OD1	2:E:89:ALA:HB3	2.20	0.41
2:B:113:PRO:HA	2:B:139:PHE:HB3	2.02	0.41
2:B:18:ARG:NH1	6:B:403:HOH:O	2.39	0.41
3:C:350:VAL:HG22	3:C:422:ASN:HB3	2.03	0.41
2:E:108:GLN:HB3	2:E:140:TYR:CE2	2.55	0.41
2:E:128:ASN:HA	2:E:182:PRO:HG2	2.03	0.41
3:F:350:VAL:O	3:F:353:TRP:HD1	2.03	0.41
3:F:396:TYR:HB2	3:F:514:SER:HB2	2.01	0.41
1:D:51:ILE:O	1:D:52(A):PRO:HD3	2.21	0.41
3:C:516:GLU:HG2	3:C:518:LEU:HG	2.03	0.40
1:D:116:LEU:HD12	1:D:174:LEU:HD21	2.04	0.40
3:F:439:ASN:O	3:F:443:SER:OG	2.31	0.40
2:E:35:TRP:CZ3	2:E:88:CYS:HB3	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	A	226/228 (99%)	222 (98%)	4 (2%)	0	100	100
1	D	226/228 (99%)	220 (97%)	6 (3%)	0	100	100
2	B	215/217 (99%)	206 (96%)	9 (4%)	0	100	100
2	E	215/217 (99%)	206 (96%)	8 (4%)	1 (0%)	24	43
3	C	195/197 (99%)	186 (95%)	9 (5%)	0	100	100
3	F	195/197 (99%)	186 (95%)	8 (4%)	1 (0%)	24	43
All	All	1272/1284 (99%)	1226 (96%)	44 (4%)	2 (0%)	43	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	151	ASP
3	F	372	ALA

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	196/196 (100%)	196 (100%)	0	100	100
1	D	196/196 (100%)	196 (100%)	0	100	100
2	B	182/182 (100%)	182 (100%)	0	100	100
2	E	182/182 (100%)	182 (100%)	0	100	100
3	C	170/170 (100%)	170 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	170/170 (100%)	170 (100%)	0	100	100
All	All	1096/1096 (100%)	1096 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	198	ASN
2	B	1	GLN
2	B	53	GLN
2	B	108	GLN
3	C	481	ASN
3	C	505	HIS
1	D	52	ASN
1	D	163	HIS
2	E	53	GLN
3	F	450	ASN
3	F	505	HIS

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 ⓘ

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	G	1	3,4	14,14,15	0.40	0	17,19,21	0.86	1 (5%)
4	FUC	G	2	4	10,10,11	1.42	2 (20%)	14,14,16	1.22	1 (7%)
4	NAG	H	1	3,4	14,14,15	0.66	1 (7%)	17,19,21	0.56	0
4	FUC	H	2	4	10,10,11	0.77	0	14,14,16	0.88	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	G	1	3,4	-	2/6/23/26	0/1/1/1
4	FUC	G	2	4	-	-	0/1/1/1
4	NAG	H	1	3,4	-	3/6/23/26	0/1/1/1
4	FUC	H	2	4	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	2	FUC	C2-C3	2.68	1.56	1.52
4	G	2	FUC	C1-C2	2.25	1.57	1.52
4	H	1	NAG	C1-C2	2.25	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	NAG	C1-O5-C5	2.80	115.94	112.19
4	G	2	FUC	O5-C5-C4	2.60	114.24	109.55

There are no chirality outliers.

All (5) torsion outliers are listed below:

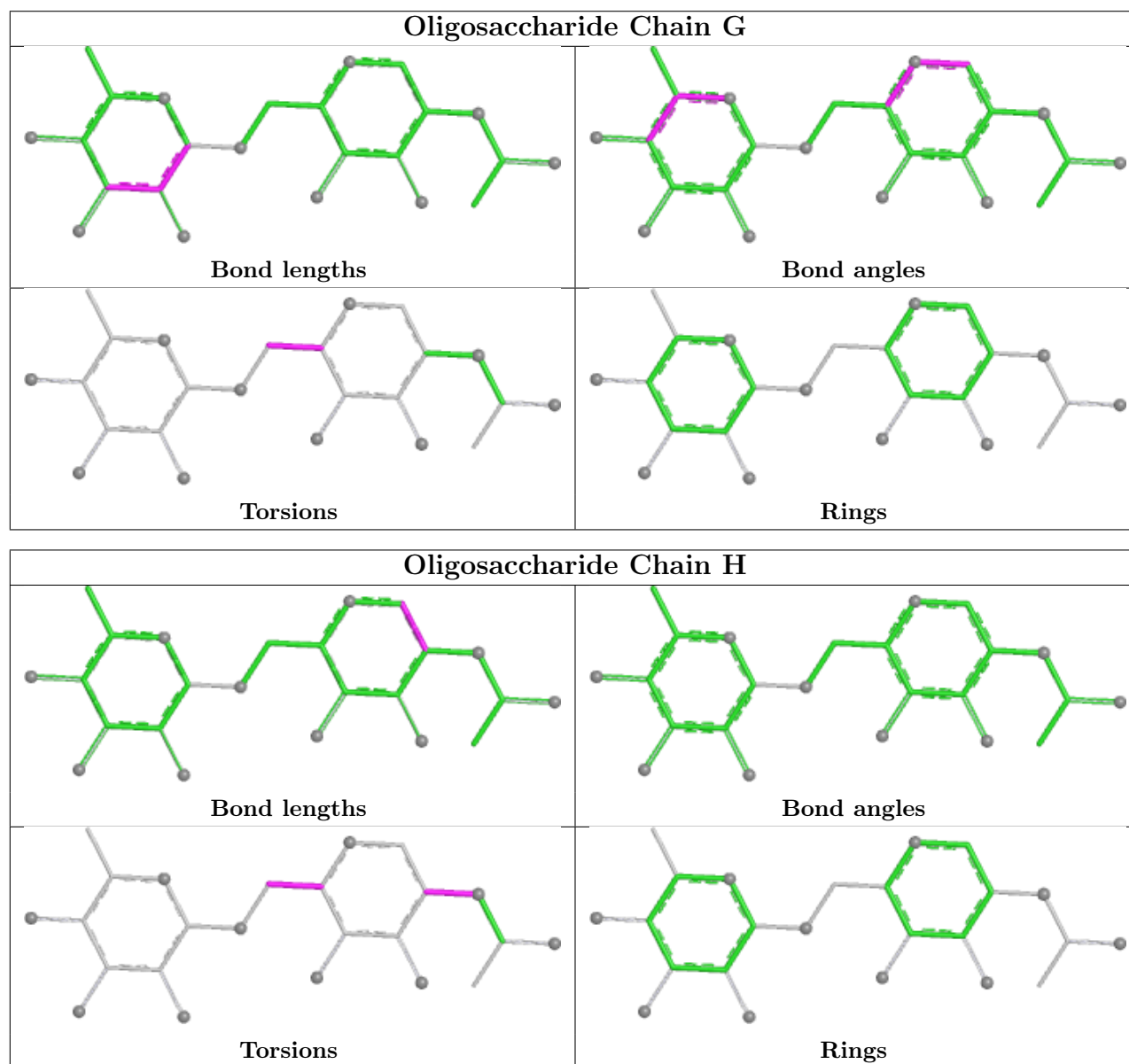
Mol	Chain	Res	Type	Atoms
4	H	1	NAG	O5-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	H	1	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	2	FUC	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 [i](#)

2 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	$\# Z > 2$
5	EDO	E	301	-	3,3,3	0.42	0	2,2,2	0.42	0
5	EDO	B	301	-	2,2,3	0.48	0	1,1,2	0.37	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	E	301	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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	228/228 (100%)	0.15	7 (3%) 51 47	23, 36, 59, 108	0
1	D	228/228 (100%)	0.25	6 (2%) 57 52	25, 38, 52, 69	0
2	B	217/217 (100%)	0.35	12 (5%) 30 27	23, 41, 74, 92	0
2	E	217/217 (100%)	0.76	18 (8%) 17 15	30, 50, 70, 77	0
3	C	197/197 (100%)	0.15	4 (2%) 65 61	25, 37, 64, 74	0
3	F	197/197 (100%)	0.01	5 (2%) 58 54	24, 35, 54, 74	0
All	All	1284/1284 (100%)	0.28	52 (4%) 42 38	23, 39, 66, 108	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	212	SER	4.8
1	D	129	SER	4.1
3	F	372	ALA	3.7
1	D	214	SER	3.6
2	B	209	THR	3.4
2	B	208	PRO	3.3
2	B	181	THR	3.3
3	F	449	TYR	3.2
1	A	131	SER	3.2
2	B	211	CYS	3.2
2	B	182	PRO	3.1
2	B	185	TRP	3.0
1	D	213	LYS	2.9
2	E	140	TYR	2.8
1	D	131	SER	2.8
3	C	333	THR	2.8
2	E	16	GLY	2.7
2	B	186	LYS	2.7
2	E	127	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	E	75	ILE	2.6
1	A	214	SER	2.6
2	E	77	GLY	2.6
2	E	207	ALA	2.6
3	C	481	ASN	2.5
3	C	483	VAL	2.5
1	D	130	THR	2.5
2	E	17	GLN	2.5
2	B	170	ASN	2.5
2	E	199	GLY	2.5
2	B	210	GLU	2.4
2	E	128	ASN	2.4
2	B	150	ALA	2.4
3	C	381	GLY	2.4
1	A	129	SER	2.3
2	E	1	GLN	2.3
2	E	76	SER	2.3
1	A	209	LYS	2.3
2	E	150	ALA	2.2
3	F	447	GLY	2.2
2	E	142	GLY	2.2
1	A	127	SER	2.2
2	E	122	SER	2.2
1	A	85	ASP	2.2
2	E	189	ARG	2.1
2	B	183	GLU	2.1
2	E	107	GLY	2.0
2	E	5	THR	2.0
2	E	59	PRO	2.0
3	F	371	PHE	2.0
1	D	133	GLY	2.0
1	A	130	THR	2.0
3	F	333	THR	2.0

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

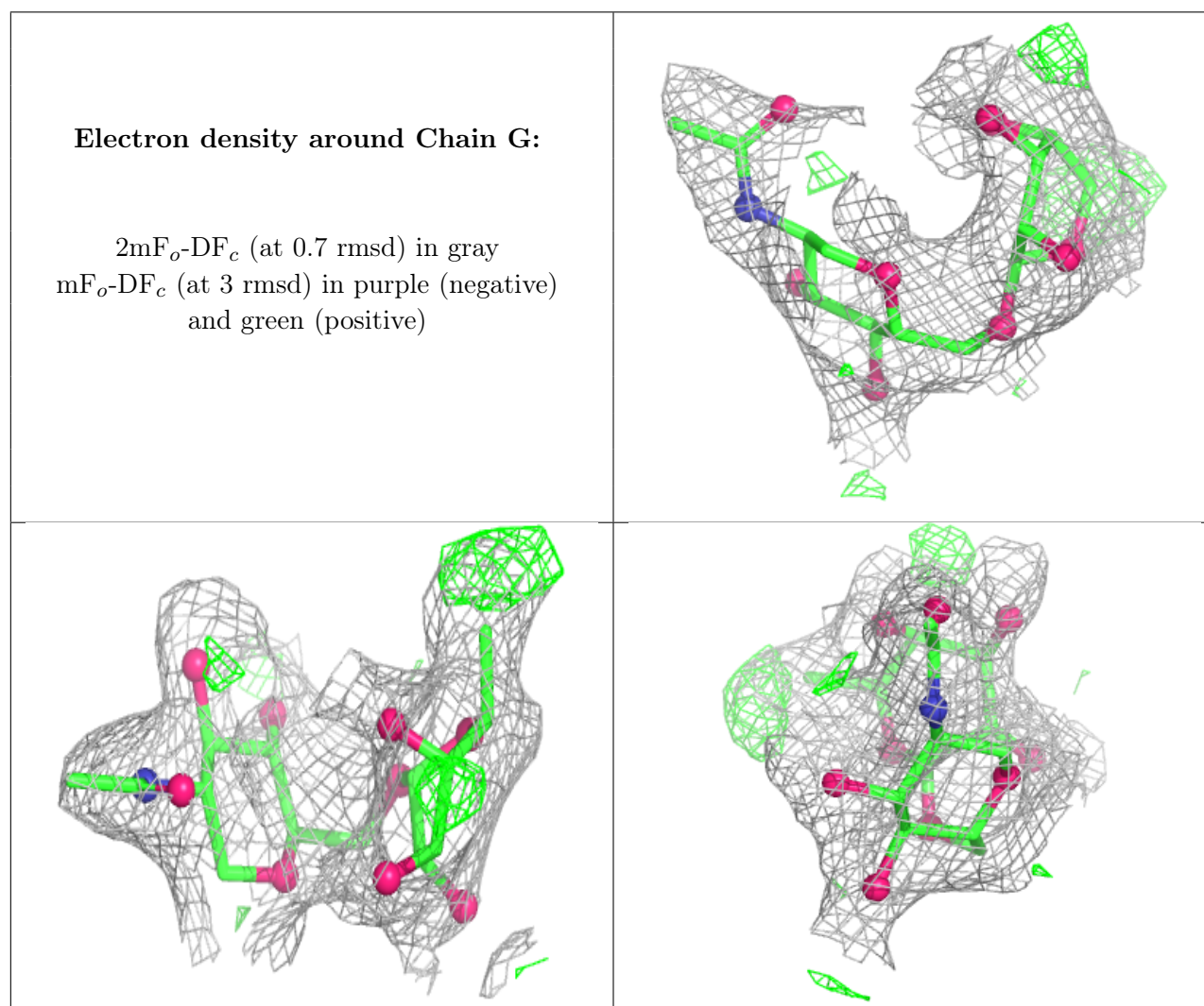
There are no non-standard protein/DNA/RNA residues in this entry.

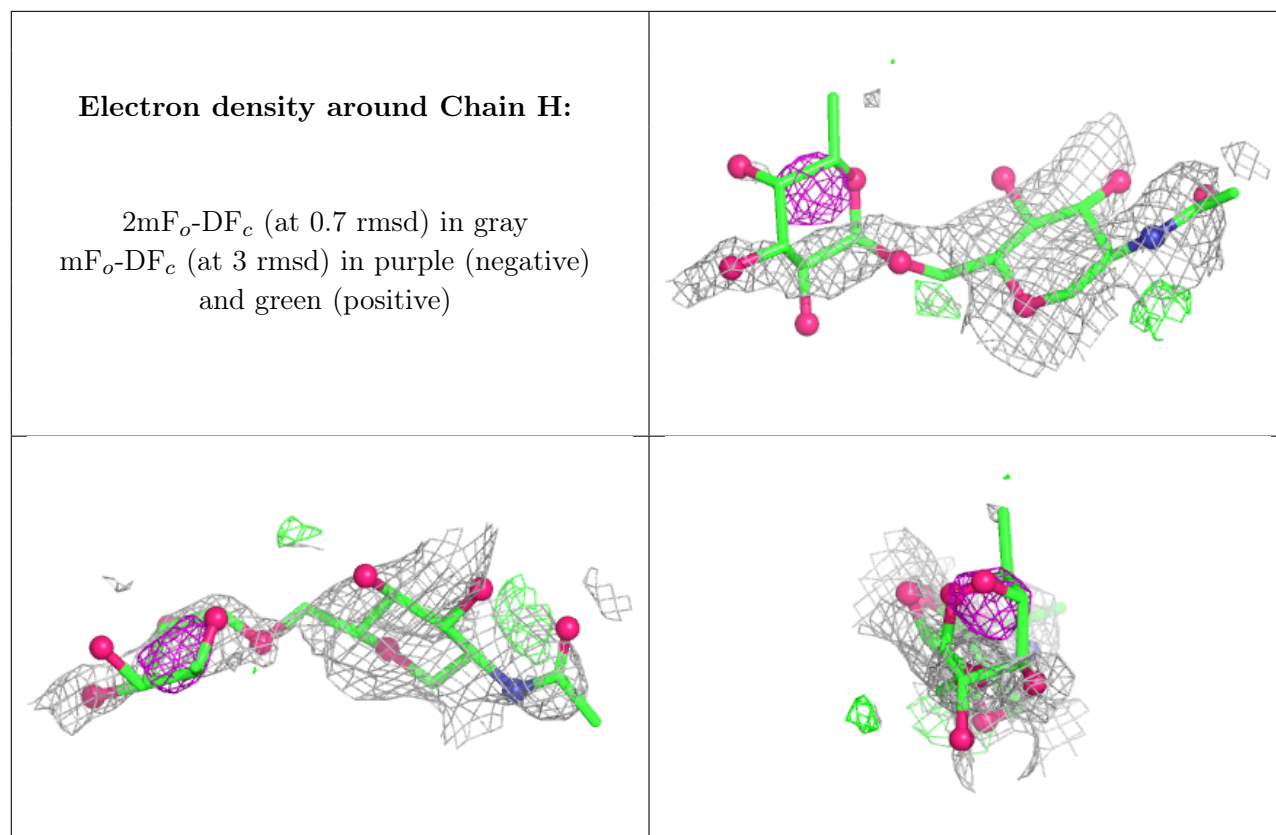
6.3 Carbohydrates [i](#)

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
4	FUC	G	2	10/11	0.33	0.18	62,71,76,77	0
4	NAG	H	1	14/15	0.34	0.19	76,95,109,117	0
4	FUC	H	2	10/11	0.36	0.23	93,114,124,126	0
4	NAG	G	1	14/15	0.71	0.14	54,70,77,77	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
5	EDO	E	301	4/4	0.54	0.27	40,40,41,42	0
5	EDO	B	301	3/4	0.71	0.20	28,28,29,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.