



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:48 PM UTC

PDB ID : 8X0Y / pdb_00008x0y
Title : Crystal structure of JM-1A in complex with SARS-CoV-2 RBD
Authors : Mohapatra, A.; Chen, X.
Deposited on : 2023-11-06
Resolution : 1.94 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

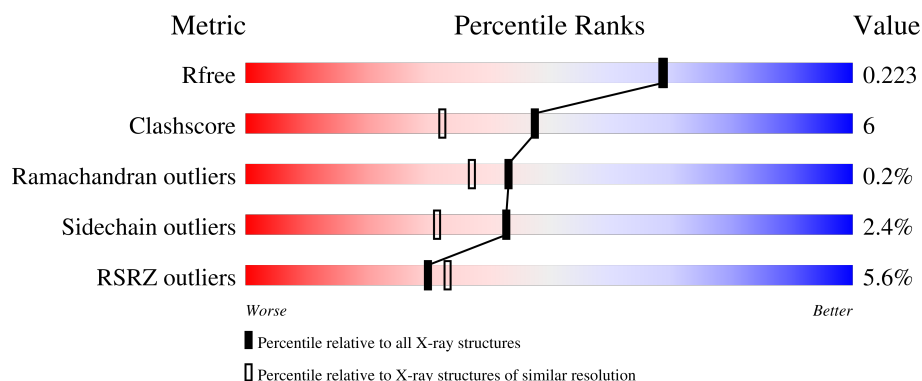
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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.



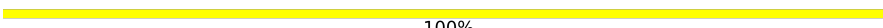
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	196	12% 84% 14%
1	B	196	12% 87% 11%
2	E	219	5% 87% 11%
2	G	219	5% 87% 11%
3	F	212	87% 12%

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Mol	Chain	Length	Quality of chain
3	I	212	 91%8%
4	C	3	 33%67%
4	D	3	 100%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10627 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	B	195	Total	C	N	O	S	0	0	0
			1532	980	255	289	8			
1	A	192	Total	C	N	O	S	0	0	0
			1497	958	250	281	8			

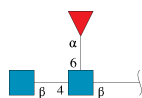
- Molecule 2 is a protein called Heavy chain of JM-1A Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	219	Total	C	N	O	S	0	0	0
			1620	1022	274	317	7			
2	G	217	Total	C	N	O	S	0	0	0
			1608	1016	272	314	6			

- Molecule 3 is a protein called Light chain of JM-1A Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	212	Total	C	N	O	S	0	0	0
			1623	1019	270	330	4			
3	I	212	Total	C	N	O	S	0	0	0
			1623	1019	270	330	4			

- Molecule 4 is an oligosaccharide called 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	3	Total	C	N	O	0	0	0
			38	22	2	14			

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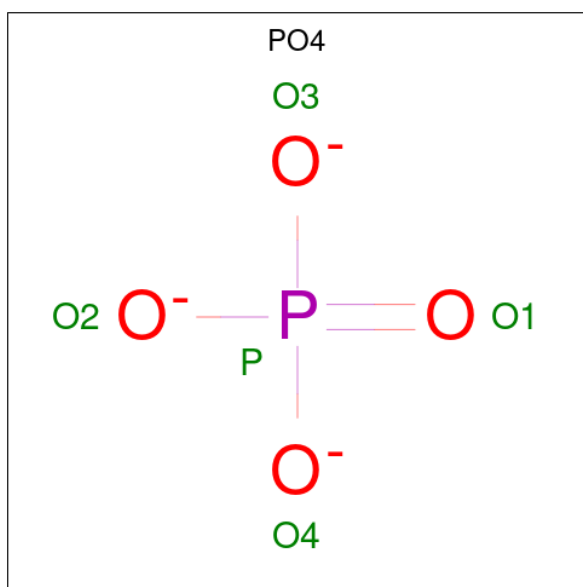
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	3	Total	C	N	O	0	0	0
			38	22	2	14			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total	O	P	5	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	189	Total	O	0	0
			189	189		
7	E	162	Total	O	0	0
			162	162		
7	F	187	Total	O	0	0
			187	187		
7	A	136	Total	O	0	0
			136	136		

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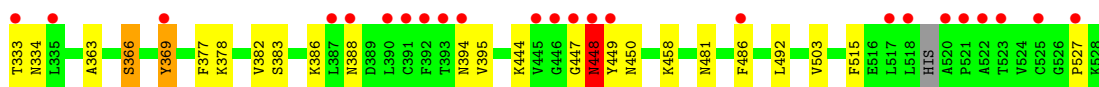
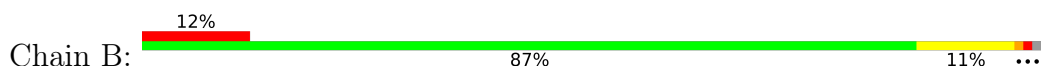
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	191	Total 191	O 191	0	0
7	I	177	Total 177	O 177	0	0

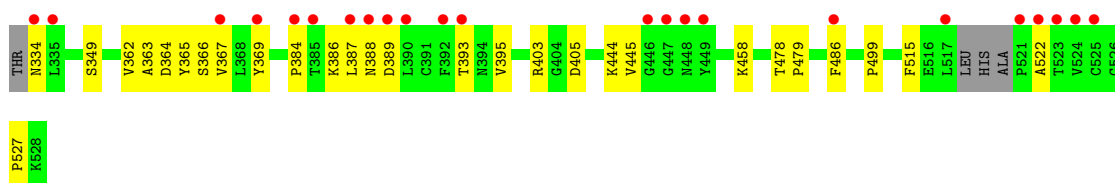
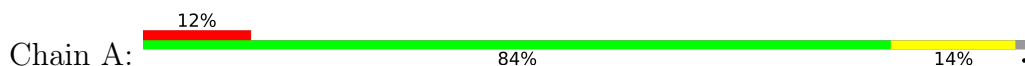
3 Residue-property plots [i](#)

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.

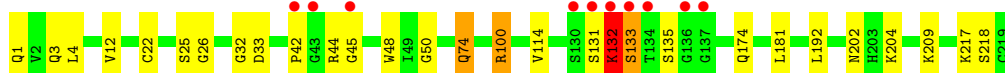
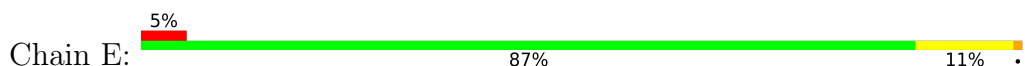
- Molecule 1: Spike protein S1



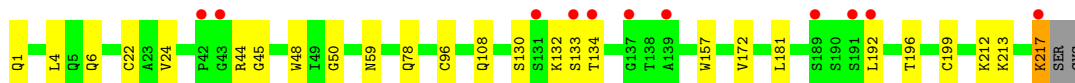
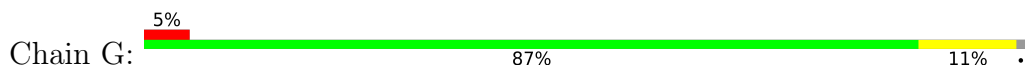
- Molecule 1: Spike protein S1



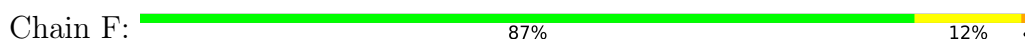
- Molecule 2: Heavy chain of JM-1A Fab



- Molecule 2: Heavy chain of JM-1A Fab



- Molecule 3: Light chain of JM-1A Fab





- Molecule 3: Light chain of JM-1A Fab



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



- Molecule 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 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	148.36Å 107.03Å 87.34Å 90.00° 100.75° 90.00°	Depositor
Resolution (Å)	19.92 – 1.94 19.92 – 1.94	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.92-1.94) 99.8 (19.92-1.94)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 1.94Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.194 , 0.223 0.194 , 0.223	Depositor DCC
R_{free} test set	5271 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.0	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	0.95	EDS
Total number of atoms	10627	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, PO4, NAG, FUC, PCA

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	0.32	0/1538	0.58	0/2093
1	B	0.38	0/1574	0.60	1/2142 (0.0%)
2	E	0.36	0/1655	0.60	0/2262
2	G	0.35	0/1643	0.62	0/2246
3	F	0.36	0/1659	0.59	0/2254
3	I	0.35	0/1659	0.57	0/2254
All	All	0.35	0/9728	0.59	1/13251 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	369	TYR	CA-CB-CG	5.17	123.20	113.90

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	1497	0	1396	20	1
1	B	1532	0	1435	21	0
2	E	1620	0	1594	18	0
2	G	1608	0	1584	17	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1623	0	1578	24	1
3	I	1623	0	1578	16	1
4	C	38	0	34	0	0
4	D	38	0	34	0	0
5	B	1	0	0	1	0
6	F	5	0	0	0	0
7	A	136	0	0	2	1
7	B	189	0	0	5	1
7	E	162	0	0	2	0
7	F	187	0	0	8	2
7	G	191	0	0	3	0
7	I	177	0	0	5	1
All	All	10627	0	9233	106	5

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 6.

All (106) 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)
5:B:601:CL:CL	7:B:882:HOH:O	2.10	1.04
2:G:78:GLN:OE1	7:G:301:HOH:O	1.92	0.88
2:G:108:GLN:NE2	7:G:302:HOH:O	2.16	0.77
1:A:366:SER:HA	1:A:369:TYR:CD2	2.19	0.76
1:B:486:PHE:O	7:B:701:HOH:O	2.07	0.73
2:E:32:GLY:O	2:E:100:ARG:HD2	1.90	0.72
3:F:123:GLN:OE1	7:F:402:HOH:O	2.07	0.72
3:F:122:GLU:HA	3:F:125:LYS:HE3	1.75	0.69
1:B:382:VAL:HG23	1:B:386:LYS:HE2	1.76	0.67
2:E:131:SER:C	2:E:133:SER:H	2.06	0.64
1:B:447:GLY:HA3	2:E:26:GLY:HA2	1.80	0.64
1:B:377:PHE:HB3	1:A:384:PRO:HD2	1.80	0.63
1:B:492:LEU:O	2:E:100:ARG:NH2	2.30	0.63
3:F:141:ARG:NH2	7:F:403:HOH:O	2.32	0.62
2:E:42:PRO:O	2:E:44:ARG:NH2	2.25	0.61
3:F:13:VAL:HG23	3:F:78:LEU:HD22	1.81	0.61
2:E:45:GLY:HA2	7:E:424:HOH:O	2.02	0.58
2:E:3:GLN:HB2	2:E:25:SER:OG	2.03	0.58
2:E:74:GLN:HG2	7:E:421:HOH:O	2.02	0.58
2:E:132:LYS:HZ2	2:E:218:SER:HB2	1.69	0.57
3:F:141:ARG:HD2	3:F:162:VAL:HG11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:SER:H	1:B:386:LYS:HD3	1.69	0.56
2:G:59:ASN:OD1	7:G:303:HOH:O	2.18	0.56
1:B:363:ALA:O	1:B:527:PRO:HD3	2.05	0.56
2:G:130:SER:H	2:G:133:SER:HB2	1.72	0.55
1:B:503:VAL:HG23	7:B:845:HOH:O	2.07	0.55
2:E:33:ASP:OD1	2:E:100:ARG:HD3	2.08	0.54
1:A:458:LYS:NZ	7:A:603:HOH:O	2.39	0.54
2:E:4:LEU:HB3	2:E:22:CYS:SG	2.48	0.54
3:I:141:ARG:NH2	7:I:306:HOH:O	2.42	0.53
1:B:366:SER:HA	1:B:369:TYR:CE1	2.44	0.53
1:B:449:TYR:HD1	1:B:450:ASN:H	1.55	0.53
2:G:133:SER:O	3:I:115:PHE:CE2	2.62	0.52
2:G:196:THR:HG23	2:G:213:LYS:HE3	1.92	0.51
1:B:383:SER:HB3	1:B:386:LYS:HD3	1.93	0.51
1:B:481:ASN:HB2	7:B:702:HOH:O	2.09	0.51
2:G:133:SER:O	3:I:115:PHE:CD2	2.63	0.51
1:B:448:ASN:OD1	1:B:448:ASN:N	2.41	0.51
1:A:403:ARG:NH1	1:A:405:ASP:OD2	2.44	0.51
1:A:486:PHE:HE2	3:I:95:PRO:HD3	1.75	0.50
1:B:486:PHE:HE2	3:F:95:PRO:HD3	1.75	0.50
3:I:162:VAL:HG21	7:I:440:HOH:O	2.12	0.50
1:A:369:TYR:HE1	1:A:384:PRO:O	1.95	0.50
1:A:369:TYR:CE1	1:A:384:PRO:O	2.65	0.49
1:A:349:SER:HA	7:A:661:HOH:O	2.13	0.48
1:A:395:VAL:HG22	1:A:515:PHE:HD1	1.78	0.48
1:A:444:LYS:O	1:A:499:PRO:HD3	2.14	0.48
3:F:162:VAL:HG22	3:F:174:LEU:HD12	1.95	0.48
1:B:378:LYS:NZ	7:B:708:HOH:O	2.47	0.48
2:E:174:GLN:HA	3:F:159:GLN:OE1	2.13	0.48
3:I:162:VAL:HG22	3:I:174:LEU:HD12	1.94	0.48
3:F:80:PRO:HA	3:F:105:ILE:CD1	2.43	0.47
3:F:209:ASN:HB3	3:F:212:GLU:HG3	1.96	0.47
1:A:334:ASN:O	1:A:362:VAL:HG12	2.15	0.47
3:F:121:ASP:O	3:F:125:LYS:HG3	2.15	0.47
3:I:167:SER:HB3	7:I:449:HOH:O	2.14	0.47
3:F:209:ASN:CB	3:F:212:GLU:HG3	2.44	0.47
1:A:386:LYS:HE3	1:A:386:LYS:HB3	1.67	0.47
2:G:192:LEU:HD23	2:G:192:LEU:HA	1.79	0.47
3:F:118:PRO:HB3	3:F:208:PHE:CE1	2.50	0.46
2:G:48:TRP:CZ2	2:G:50:GLY:HA2	2.51	0.46
3:F:105:ILE:HD12	7:F:441:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ALA:O	1:A:527:PRO:HD3	2.17	0.45
1:A:364:ASP:O	1:A:367:VAL:HG22	2.17	0.45
2:G:4:LEU:HB3	2:G:22:CYS:SG	2.56	0.45
3:F:23:CYS:HB2	3:F:35:TRP:CH2	2.52	0.45
3:F:210:ARG:NH2	7:F:413:HOH:O	2.50	0.45
1:A:393:THR:HA	1:A:522:ALA:HA	1.98	0.45
2:E:192:LEU:HA	2:E:192:LEU:HD23	1.82	0.45
1:B:486:PHE:CE2	3:F:95:PRO:HD3	2.52	0.44
2:E:131:SER:C	2:E:133:SER:N	2.75	0.44
1:B:447:GLY:O	1:B:448:ASN:C	2.60	0.44
3:I:104:GLU:OE2	7:I:301:HOH:O	2.21	0.44
3:I:107:ARG:HD2	3:I:170:SER:HB2	1.99	0.44
3:F:11:LEU:HD13	3:F:13:VAL:HG13	2.00	0.43
3:F:118:PRO:HB3	3:F:208:PHE:CD1	2.53	0.43
1:B:444:LYS:N	1:B:449:TYR:HE2	2.17	0.43
1:B:369:TYR:OH	1:B:388:ASN:ND2	2.52	0.43
1:B:395:VAL:HG22	1:B:515:PHE:HD1	1.83	0.43
2:E:181:LEU:C	2:E:181:LEU:HD12	2.43	0.43
1:B:444:LYS:HA	1:B:444:LYS:HD3	1.83	0.43
3:F:159:GLN:HG2	7:F:556:HOH:O	2.18	0.43
2:G:217:LYS:NZ	3:I:121:ASP:OD2	2.51	0.43
2:E:12:VAL:O	2:E:114:VAL:HA	2.20	0.42
2:E:202:ASN:OD1	2:E:209:LYS:HG2	2.18	0.42
2:E:48:TRP:CZ2	2:E:50:GLY:HA2	2.55	0.42
2:G:4:LEU:HD22	2:G:24:VAL:HG22	2.01	0.42
3:F:159:GLN:CG	7:F:556:HOH:O	2.68	0.42
2:G:133:SER:O	2:G:134:THR:C	2.62	0.42
2:G:6:GLN:HG2	2:G:96:CYS:SG	2.60	0.41
3:F:27:GLN:HG3	7:F:401:HOH:O	2.20	0.41
3:I:23:CYS:HB2	3:I:35:TRP:CH2	2.56	0.41
3:F:80:PRO:HA	3:F:105:ILE:HD13	2.02	0.41
3:F:24:ARG:NE	7:F:404:HOH:O	2.35	0.41
1:A:387:LEU:C	1:A:389:ASP:H	2.28	0.41
1:A:388:ASN:HB3	1:A:527:PRO:HD2	2.02	0.41
2:G:44:ARG:HB3	2:G:45:GLY:H	1.46	0.41
3:I:45:LYS:NZ	7:I:311:HOH:O	2.53	0.41
3:I:107:ARG:HH11	3:I:107:ARG:HG3	1.86	0.41
2:G:130:SER:O	2:G:133:SER:HB2	2.21	0.41
3:I:19:VAL:HB	3:I:75:ILE:HB	2.03	0.41
1:A:478:THR:HA	1:A:479:PRO:HD3	1.95	0.40
2:G:157:TRP:CH2	2:G:199:CYS:HB3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:89:GLN:HB2	3:I:97:PHE:CD1	2.56	0.40
1:A:365:TYR:CD2	1:A:387:LEU:HB3	2.56	0.40
1:A:486:PHE:CE2	3:I:95:PRO:HD3	2.56	0.40

All (5) 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)
7:F:577:HOH:O	7:A:736:HOH:O[4_446]	2.05	0.15
1:A:334:ASN:OD1	2:G:196:THR:OG1[4_445]	2.11	0.09
7:B:799:HOH:O	7:B:800:HOH:O[2_555]	2.13	0.07
3:F:187:LYS:NZ	3:I:155:SER:O[2_546]	2.17	0.03
7:F:544:HOH:O	7:I:411:HOH:O[2_556]	2.19	0.01

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	188/196 (96%)	178 (95%)	10 (5%)	0	100	100
1	B	191/196 (97%)	179 (94%)	11 (6%)	1 (0%)	24	15
2	E	217/219 (99%)	212 (98%)	3 (1%)	2 (1%)	14	6
2	G	215/219 (98%)	207 (96%)	8 (4%)	0	100	100
3	F	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
3	I	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
All	All	1231/1254 (98%)	1184 (96%)	44 (4%)	3 (0%)	43	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	133	SER

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Mol	Chain	Res	Type
1	B	448	ASN
2	E	132	LYS

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	160/169 (95%)	159 (99%)	1 (1%)	78	78
1	B	165/169 (98%)	159 (96%)	6 (4%)	31	17
2	E	185/185 (100%)	179 (97%)	6 (3%)	34	20
2	G	183/185 (99%)	178 (97%)	5 (3%)	39	26
3	F	185/185 (100%)	179 (97%)	6 (3%)	34	20
3	I	185/185 (100%)	183 (99%)	2 (1%)	65	60
All	All	1063/1078 (99%)	1037 (98%)	26 (2%)	43	31

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	333	THR
1	B	334	ASN
1	B	366	SER
1	B	394	ASN
1	B	448	ASN
1	B	458	LYS
2	E	74	GLN
2	E	100	ARG
2	E	132	LYS
2	E	135	SER
2	E	204	LYS
2	E	217	LYS
3	F	141	ARG
3	F	142	GLU
3	F	153	LEU
3	F	159	GLN

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Mol	Chain	Res	Type
3	F	180	LEU
3	F	189	LYS
1	A	445	VAL
2	G	132	LYS
2	G	172	VAL
2	G	181	LEU
2	G	212	LYS
2	G	217	LYS
3	I	141	ARG
3	I	189	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	394	ASN
1	B	450	ASN
2	E	40	GLN
2	E	78	GLN
3	F	38	GLN
1	A	481	ASN
1	A	498	GLN
1	A	501	ASN
2	G	74	GLN
2	G	78	GLN
2	G	167	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
2	PCA	E	1	2	7,8,9	1.86	1 (14%)	9,10,12	2.47	4 (44%)
2	PCA	G	1	2	7,8,9	1.85	1 (14%)	9,10,12	2.17	3 (33%)

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
2	PCA	E	1	2	-	0/0/11/13	0/1/1/1
2	PCA	G	1	2	-	0/0/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	PCA	CD-N	4.64	1.46	1.34
2	G	1	PCA	CD-N	4.48	1.45	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	PCA	OE-CD-CG	-5.30	117.26	126.72
2	G	1	PCA	OE-CD-CG	-4.60	118.50	126.72
2	E	1	PCA	CG-CD-N	2.83	115.32	108.39
2	E	1	PCA	CA-N-CD	-2.70	104.32	113.58
2	E	1	PCA	CB-CG-CD	-2.45	100.62	104.41
2	G	1	PCA	CA-N-CD	-2.34	105.58	113.58
2	G	1	PCA	CG-CD-N	2.12	113.56	108.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

6 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	0.40	0	17,19,21	0.74	0
4	NAG	C	2	4	14,14,15	0.27	0	17,19,21	0.69	1 (5%)
4	FUC	C	3	4	10,10,11	1.03	0	14,14,16	1.04	1 (7%)
4	NAG	D	1	4,1	14,14,15	0.70	0	17,19,21	0.95	1 (5%)
4	NAG	D	2	4	14,14,15	0.77	1 (7%)	17,19,21	0.57	0
4	FUC	D	3	4	10,10,11	1.01	0	14,14,16	1.06	1 (7%)

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	-	3/6/23/26	0/1/1/1
4	FUC	C	3	4	-	-	0/1/1/1
4	NAG	D	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	3/6/23/26	0/1/1/1
4	FUC	D	3	4	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2	NAG	O5-C1	2.75	1.48	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3	FUC	C1-C2-C3	2.90	113.87	109.64
4	D	1	NAG	O4-C4-C3	-2.63	104.18	110.38
4	D	3	FUC	O5-C5-C4	2.61	114.25	109.55
4	C	2	NAG	C1-O5-C5	2.09	114.99	112.19

There are no chirality outliers.

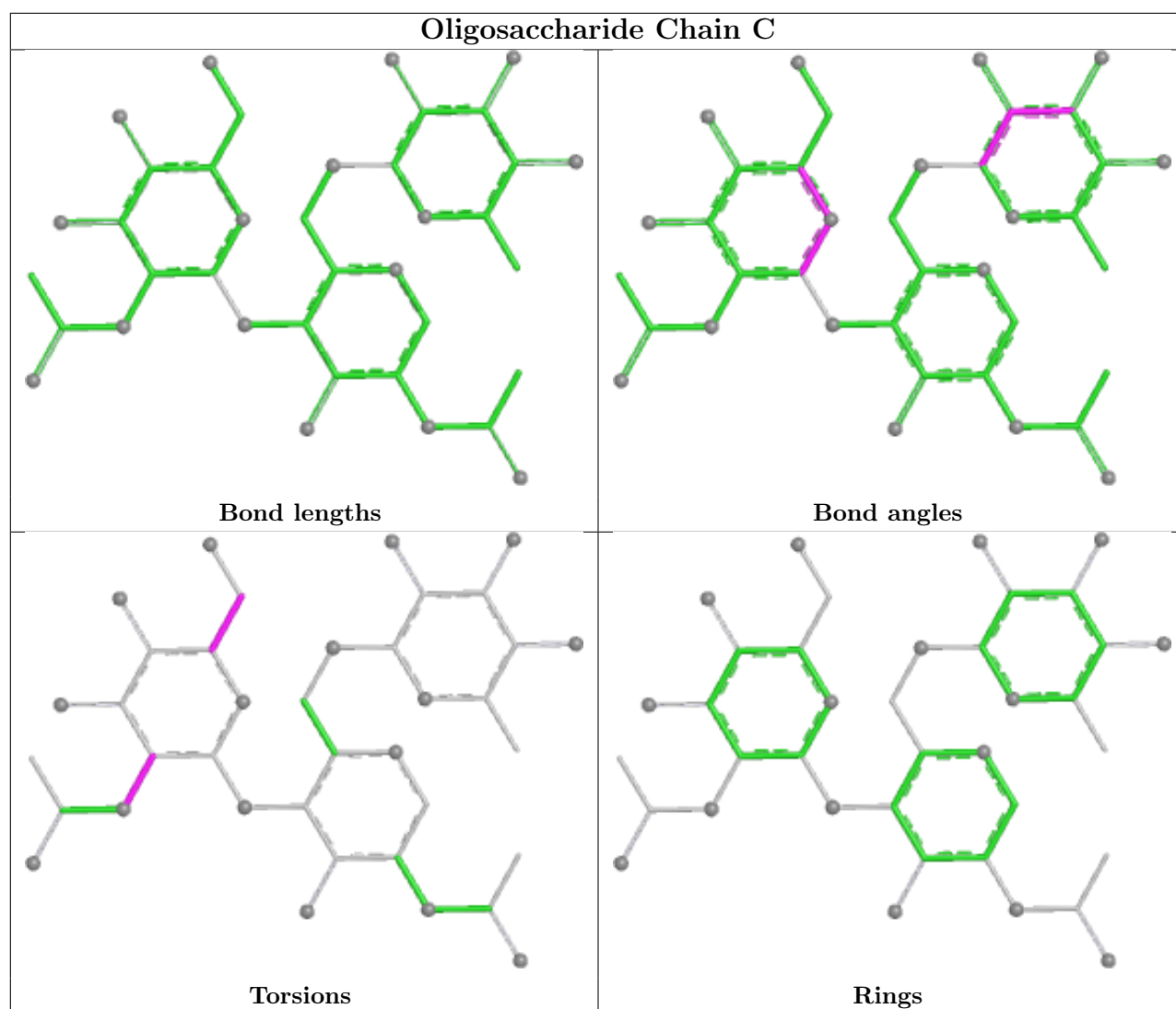
All (8) torsion outliers are listed below:

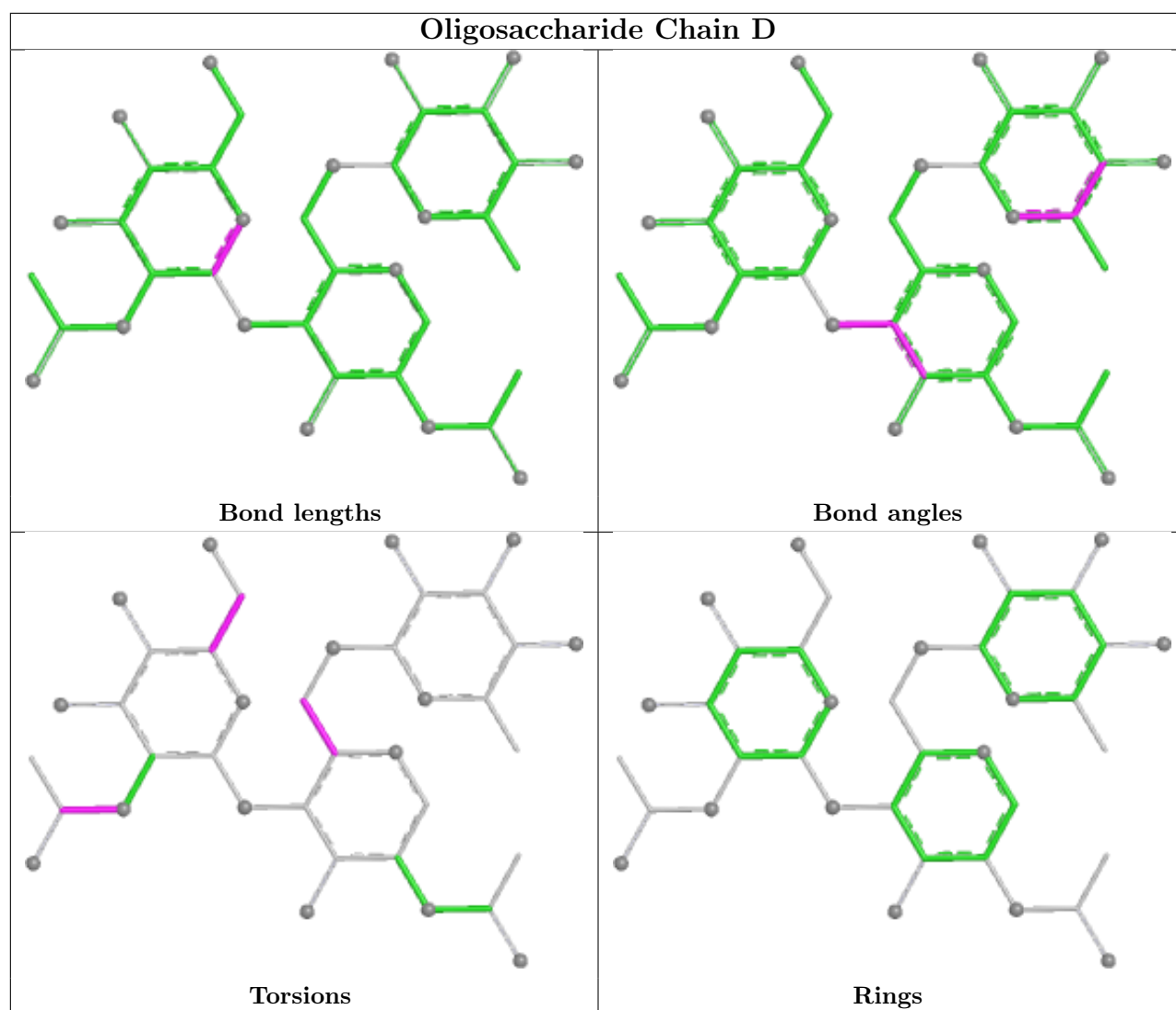
Mol	Chain	Res	Type	Atoms
4	C	2	NAG	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	C	2	NAG	C4-C5-C6-O6
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	D	2	NAG	O5-C5-C6-O6
4	C	2	NAG	C1-C2-N2-C7

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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	PO4	F	301	-	4,4,4	0.95	0	6,6,6	0.46	0

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	192/196 (97%)	0.50	23 (11%) 9 10	20, 32, 87, 124	0
1	B	195/196 (99%)	0.37	24 (12%) 8 9	17, 28, 88, 145	0
2	E	218/219 (99%)	0.20	10 (4%) 37 42	17, 30, 71, 113	0
2	G	216/219 (98%)	0.24	11 (5%) 33 38	18, 30, 82, 161	0
3	F	212/212 (100%)	-0.07	1 (0%) 87 91	15, 27, 46, 108	0
3	I	212/212 (100%)	0.03	1 (0%) 87 91	17, 29, 59, 101	0
All	All	1245/1254 (99%)	0.20	70 (5%) 30 33	15, 29, 79, 161	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	133	SER	5.7
1	A	448	ASN	5.7
1	A	449	TYR	4.7
1	B	449	TYR	4.7
2	E	131	SER	4.3
1	B	518	LEU	4.2
1	B	447	GLY	4.1
1	B	448	ASN	4.1
2	G	131	SER	4.0
1	A	385	THR	3.9
1	B	517	LEU	3.9
1	A	522	ALA	3.7
1	A	447	GLY	3.7
1	A	517	LEU	3.6
3	F	212	GLU	3.4
2	E	134	THR	3.4
1	A	392	PHE	3.4
2	E	133	SER	3.3
1	B	333	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	522	ALA	3.1
1	A	369	TYR	3.1
1	B	445	VAL	3.1
1	B	520	ALA	3.1
1	A	521	PRO	3.0
2	G	134	THR	3.0
2	G	42	PRO	2.9
1	B	486	PHE	2.8
2	E	130	SER	2.8
2	G	191	SER	2.8
2	G	43	GLY	2.8
1	B	446	GLY	2.7
2	G	139	ALA	2.7
1	A	446	GLY	2.6
2	G	192	LEU	2.6
2	G	137	GLY	2.6
1	A	367	VAL	2.6
1	B	388	ASN	2.6
1	B	393	THR	2.6
1	B	392	PHE	2.5
2	E	132	LYS	2.5
1	A	335	LEU	2.5
1	A	486	PHE	2.5
2	E	137	GLY	2.5
1	A	523	THR	2.5
1	B	525	CYS	2.4
1	A	525	CYS	2.4
1	B	369	TYR	2.4
1	B	394	ASN	2.4
1	A	389	ASP	2.4
1	A	334	ASN	2.4
1	A	388	ASN	2.4
1	B	387	LEU	2.3
1	A	393	THR	2.3
1	B	521	PRO	2.3
1	A	387	LEU	2.3
1	A	384	PRO	2.3
2	G	217	LYS	2.3
1	A	390	LEU	2.3
1	B	523	THR	2.3
1	A	524	VAL	2.3
1	B	391	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	42	PRO	2.2
2	E	136	GLY	2.2
2	G	189	SER	2.2
1	B	390	LEU	2.2
1	B	527	PRO	2.1
2	E	45	GLY	2.0
1	B	335	LEU	2.0
2	E	43	GLY	2.0
3	I	211	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	PCA	G	1	8/9	0.81	0.13	40,43,54,59	0
2	PCA	E	1	8/9	0.87	0.10	39,42,47,49	0

6.3 Carbohydrates [i](#)

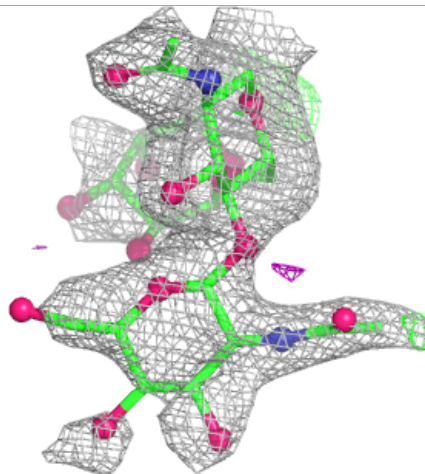
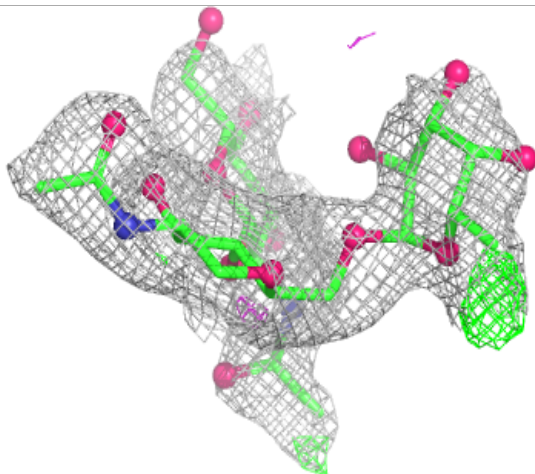
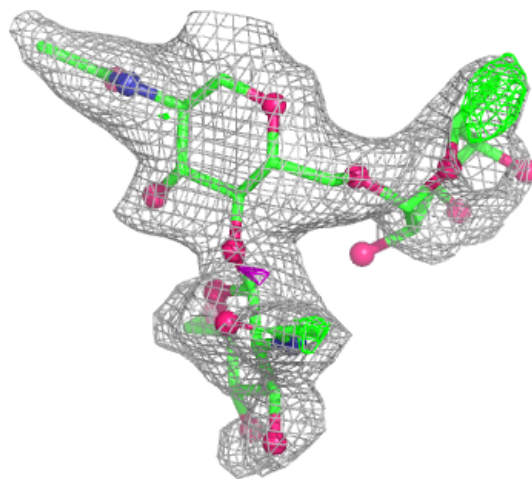
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

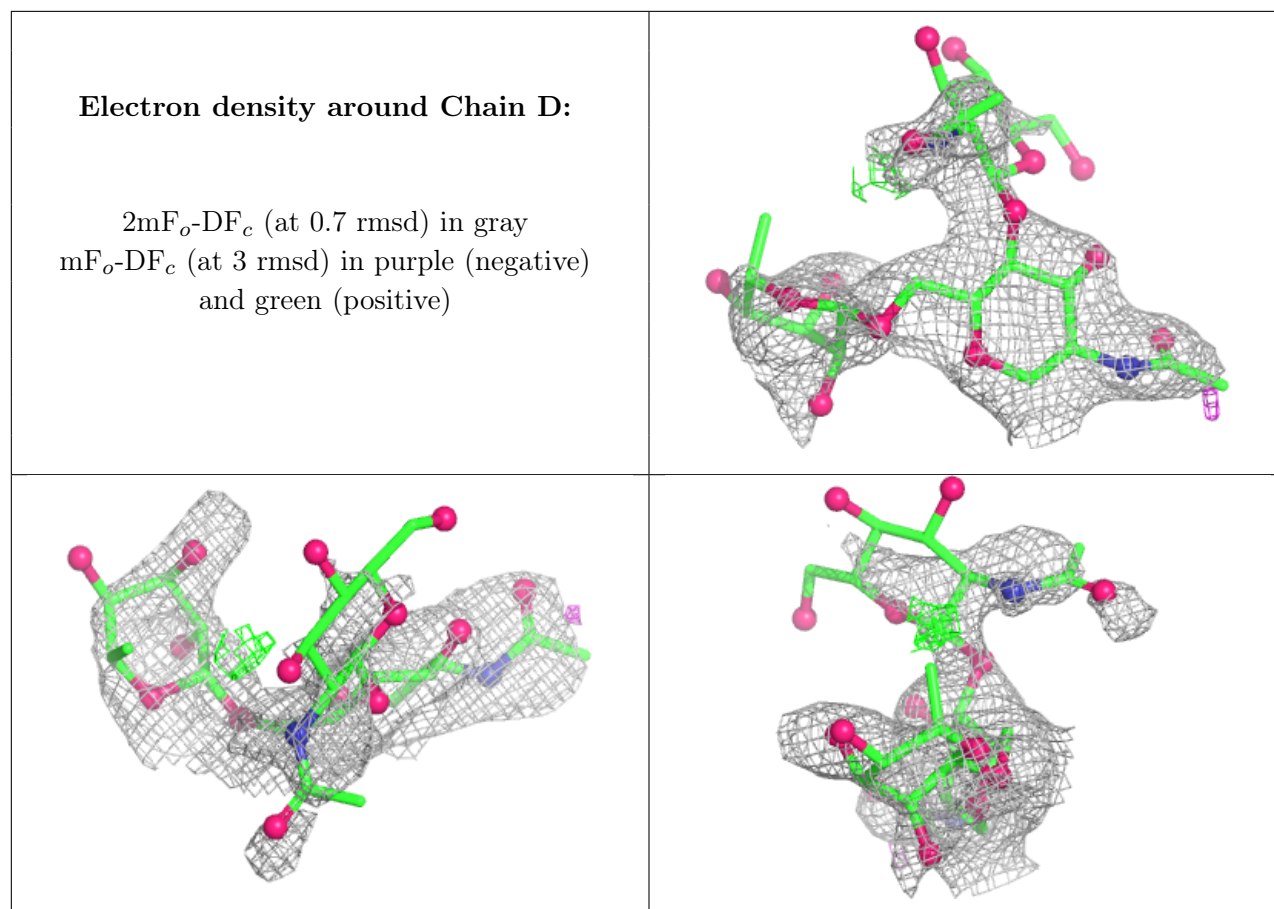
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	C	1	14/15	-	-	40,57,77,78	0
4	NAG	C	2	14/15	-	-	75,84,90,90	0
4	FUC	C	3	10/11	-	-	74,86,89,90	0
4	NAG	D	1	14/15	-	-	58,78,93,97	0
4	NAG	D	2	14/15	-	-	85,102,106,107	0
4	FUC	D	3	10/11	-	-	95,102,110,114	0

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.

Electron density around Chain C:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





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	CL	B	601	1/1	0.88	0.25	56,56,56,56	0
6	PO4	F	301	5/5	-	-	42,42,42,44	5

6.5 Other polymers [i](#)

There are no such residues in this entry.