



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:22 PM UTC

PDB ID : 8IDO / pdb_00008ido
Title : Crystal structure of nanobody VHH-T148 with MERS-CoV RBD
Authors : Wang, X.; Tian, L.
Deposited on : 2023-02-14
Resolution : 2.50 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

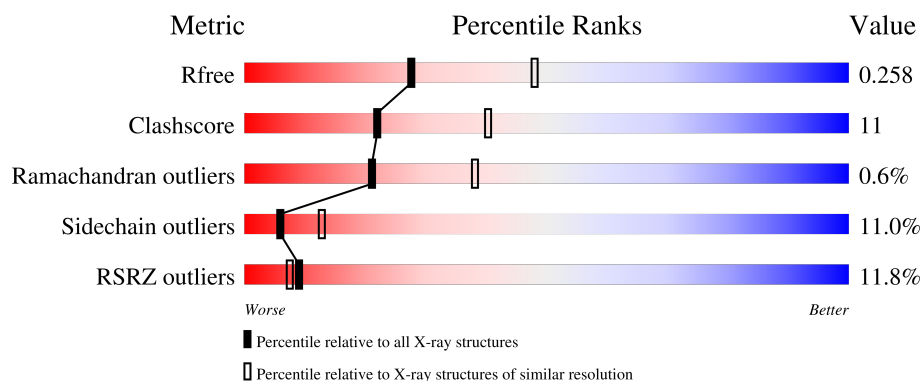
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.



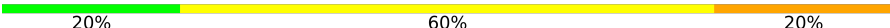
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	229	3% 75% 13% • 9%
1	B	229	7% 61% 18% • 18%
2	C	135	2% 69% 19% 5% • 5%
2	D	135	37% 50% 37% 7% 6%
3	E	5	80% 20%

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Mol	Chain	Length	Quality of chain
3	F	5	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a green segment on the left labeled '20%', a yellow segment in the middle labeled '60%', and an orange segment on the right labeled '20%'. The segments are separated by thin black lines.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5405 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	188	Total	C	N	O	S	0	0	0
			1451	929	228	283	11			
1	A	208	Total	C	N	O	S	0	0	0
			1608	1026	256	315	11			

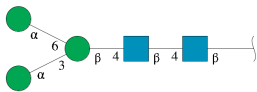
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	590	HIS	-	expression tag	UNP R9UQ53
B	591	HIS	-	expression tag	UNP R9UQ53
B	592	HIS	-	expression tag	UNP R9UQ53
B	593	HIS	-	expression tag	UNP R9UQ53
B	594	HIS	-	expression tag	UNP R9UQ53
B	595	HIS	-	expression tag	UNP R9UQ53
A	590	HIS	-	expression tag	UNP R9UQ53
A	591	HIS	-	expression tag	UNP R9UQ53
A	592	HIS	-	expression tag	UNP R9UQ53
A	593	HIS	-	expression tag	UNP R9UQ53
A	594	HIS	-	expression tag	UNP R9UQ53
A	595	HIS	-	expression tag	UNP R9UQ53

- Molecule 2 is a protein called VHH-T148.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	128	Total	C	N	O	S	0	0	0
			973	609	160	197	7			
2	D	127	Total	C	N	O	S	0	0	0
			964	604	158	195	7			

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



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

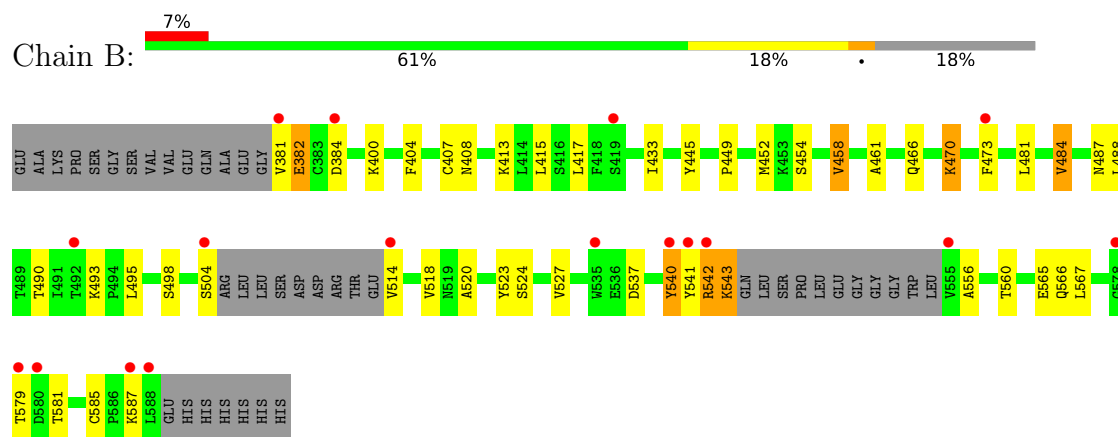
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	84	Total	O	0	0
			84	84		
4	A	143	Total	O	0	0
			143	143		
4	C	37	Total	O	0	0
			37	37		
4	D	23	Total	O	0	0
			23	23		

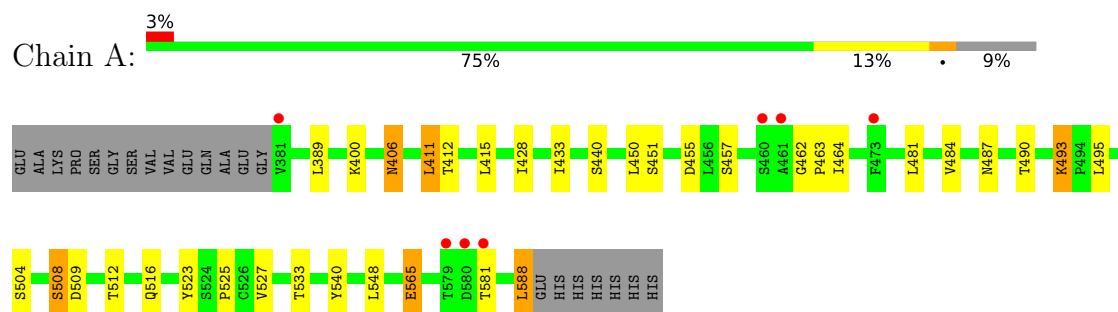
3 Residue-property plots [i](#)

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.

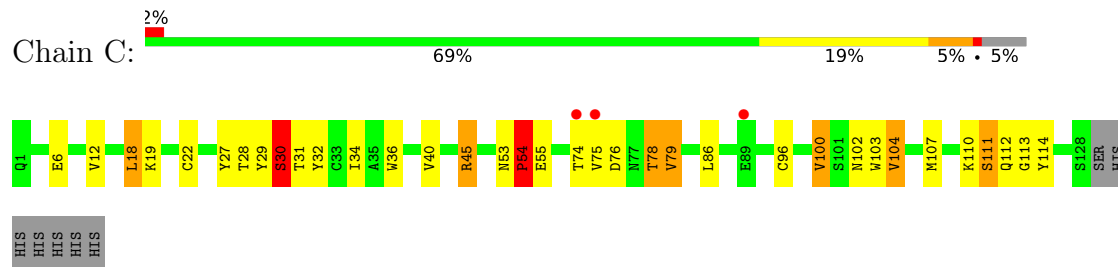
• Molecule 1: Spike protein S1



• Molecule 1: Spike protein S1

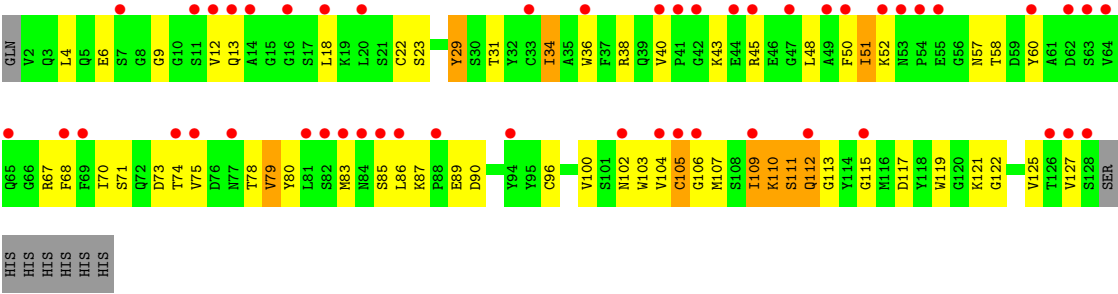


• Molecule 2: VHH-T148

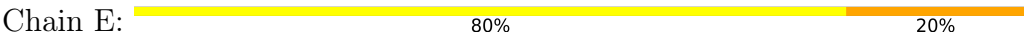


• Molecule 2: VHH-T148





● Molecule 3: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



● Molecule 3: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	175.90Å 47.19Å 124.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.80 – 2.50 16.80 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (16.80-2.50) 97.0 (16.80-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.220 , 0.262 (Not available) , 0.258	Depositor DCC
R_{free} test set	1832 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.448	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5405	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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: MAN, BMA, 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	0.41	0/1647	0.62	0/2249
1	B	0.36	0/1485	0.59	0/2026
2	C	1.12	10/994 (1.0%)	0.94	6/1346 (0.4%)
2	D	0.65	2/985 (0.2%)	0.65	2/1334 (0.1%)
All	All	0.65	12/5111 (0.2%)	0.69	8/6955 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	29	TYR	C-O	-9.33	1.12	1.23
2	C	32	TYR	C-O	-9.12	1.12	1.23
2	C	28	THR	C-O	-7.44	1.13	1.24
2	C	32	TYR	CA-C	-7.42	1.43	1.52
2	C	27	TYR	C-O	-7.15	1.15	1.23
2	C	110	LYS	C-O	-6.53	1.15	1.23
2	C	31	THR	C-O	-6.44	1.15	1.23
2	C	30	SER	CA-CB	-5.93	1.41	1.53
2	C	113	GLY	C-O	-5.76	1.16	1.23
2	D	110	LYS	C-O	-5.32	1.16	1.24
2	C	111	SER	C-O	-5.19	1.16	1.23
2	D	113	GLY	C-O	-5.01	1.16	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	29	TYR	N-CA-C	-16.60	84.36	108.60
2	C	29	TYR	O-C-N	-8.70	114.13	123.26
2	C	29	TYR	CA-C-N	8.49	136.97	121.70
2	C	29	TYR	C-N-CA	8.49	136.97	121.70
2	C	29	TYR	CA-C-O	-6.20	114.81	121.38
2	D	112	GLN	N-CA-C	6.11	119.83	111.39
2	D	111	SER	N-CA-C	5.64	117.07	110.41
2	C	30	SER	CA-CB-OG	-5.55	100.00	111.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	53	ASN	Peptide

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	1608	0	1573	20	0
1	B	1451	0	1419	28	0
2	C	973	0	916	22	0
2	D	964	0	905	42	0
3	E	61	0	52	5	0
3	F	61	0	52	1	0
4	A	143	0	0	6	1
4	B	84	0	0	4	1
4	C	37	0	0	2	0
4	D	23	0	0	4	0
All	All	5405	0	4917	107	1

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 11.

All (107) 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:C:30:SER:O	2:C:54:PRO:HD2	1.60	1.00
2:D:45:ARG:O	2:D:112:GLN:HB3	1.68	0.93
2:C:34:ILE:HG21	2:C:79:VAL:HG11	1.52	0.92
2:C:30:SER:O	2:C:54:PRO:CD	2.26	0.83
1:A:540:TYR:OH	4:A:601:HOH:O	1.94	0.83
2:D:122:GLY:O	4:D:201:HOH:O	2.02	0.78
2:D:103:TRP:O	4:D:202:HOH:O	2.03	0.77
1:A:487:ASN:ND2	4:A:604:HOH:O	2.20	0.74
1:B:540:TYR:O	1:B:542:ARG:NH2	2.21	0.74
2:D:34:ILE:HG21	2:D:79:VAL:HG11	1.72	0.72
1:B:487:ASN:ND2	4:B:603:HOH:O	2.23	0.72
2:C:45:ARG:O	2:C:112:GLN:HB3	1.92	0.69
2:D:51:ILE:HG13	2:D:58:THR:HG22	1.75	0.68
1:A:588:LEU:O	4:A:602:HOH:O	2.12	0.67
1:B:413:LYS:HA	3:E:1:NAG:H62	1.75	0.67
2:D:9:GLY:HA2	2:D:18:LEU:HD21	1.78	0.66
2:D:107:MET:SD	4:D:203:HOH:O	2.54	0.64
2:D:115:GLY:N	4:D:203:HOH:O	2.21	0.62
2:D:60:TYR:HE2	2:D:70:ILE:H	1.48	0.61
1:B:449:PRO:HG2	1:B:452:MET:HG3	1.82	0.61
2:D:45:ARG:O	2:D:112:GLN:CB	2.47	0.61
2:D:6:GLU:OE2	2:D:96:CYS:N	2.32	0.59
1:A:389:LEU:O	1:A:490:THR:HG23	2.02	0.59
2:D:22:CYS:HB3	2:D:79:VAL:HG22	1.84	0.58
2:D:87:LYS:HG3	2:D:89:GLU:HB3	1.85	0.58
1:B:542:ARG:O	4:B:601:HOH:O	2.17	0.58
1:B:413:LYS:HE3	2:D:104:VAL:HG21	1.85	0.57
1:B:543:LYS:NZ	4:B:606:HOH:O	2.29	0.57
1:A:406:ASN:ND2	4:A:612:HOH:O	2.39	0.55
2:D:67:ARG:HD2	2:D:85:SER:HB2	1.88	0.55
2:C:6:GLU:HG3	2:C:96:CYS:HB2	1.91	0.53
2:D:38:ARG:NH1	2:D:90:ASP:HA	2.24	0.53
2:C:45:ARG:NH2	4:C:205:HOH:O	2.42	0.52
1:A:565:GLU:OE1	4:A:603:HOH:O	2.19	0.52
2:D:23:SER:HA	2:D:78:THR:HG22	1.92	0.51
2:D:36:TRP:HE1	2:D:79:VAL:HG23	1.75	0.51
2:C:55:GLU:H	2:C:55:GLU:CD	2.17	0.51
2:D:38:ARG:HG2	2:D:48:LEU:HD21	1.92	0.51
1:B:384:ASP:OD2	4:B:602:HOH:O	2.19	0.51
2:D:68:PHE:CE1	2:D:83:MET:HB3	2.46	0.50
1:B:524:SER:O	1:B:527:VAL:HG22	2.12	0.50
2:D:86:LEU:HB3	2:D:127:VAL:HG21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:50:PHE:HB2	2:D:105:CYS:SG	2.52	0.50
1:B:537:ASP:HB2	1:B:560:THR:OG1	2.13	0.49
2:C:76:ASP:HB3	2:C:78:THR:OG1	2.12	0.49
1:B:484:VAL:HG13	1:B:567:LEU:O	2.13	0.48
2:D:34:ILE:HB	2:D:51:ILE:HG22	1.95	0.48
2:D:29:TYR:CD1	2:D:29:TYR:N	2.81	0.48
1:B:523:TYR:HB3	1:B:527:VAL:HG11	1.96	0.48
2:D:52:LYS:HE3	2:D:102:ASN:HB2	1.94	0.48
1:B:400:LYS:HD3	1:B:445:TYR:OH	2.14	0.47
1:A:516:GLN:HB3	1:A:525:PRO:HG2	1.96	0.47
2:C:30:SER:O	2:C:54:PRO:HD3	2.13	0.47
1:A:455:ASP:HB3	1:A:464:ILE:HB	1.97	0.47
1:A:490:THR:CG2	2:C:107:MET:HG2	2.45	0.47
1:B:466:GLN:O	1:B:518:VAL:HG12	2.15	0.47
1:B:541:TYR:O	1:B:556:ALA:N	2.43	0.47
2:C:22:CYS:HB3	2:C:79:VAL:HG13	1.97	0.46
2:D:83:MET:HE3	2:D:86:LEU:HD21	1.98	0.46
1:B:490:THR:O	1:B:490:THR:OG1	2.31	0.46
1:A:433:ILE:HD12	1:A:433:ILE:HA	1.82	0.45
2:D:87:LYS:HG2	2:D:90:ASP:OD2	2.17	0.45
2:D:73:ASP:HB2	2:D:80:TYR:HE1	1.82	0.45
1:A:523:TYR:HB3	1:A:527:VAL:HG11	1.99	0.45
1:A:508:SER:HB3	4:A:706:HOH:O	2.17	0.44
2:D:106:GLY:O	2:D:110:LYS:HG3	2.17	0.44
1:B:408:ASN:HA	1:B:585:CYS:O	2.17	0.44
1:A:490:THR:HG22	2:C:107:MET:HG2	1.98	0.44
1:B:587:LYS:NZ	3:E:1:NAG:O7	2.51	0.44
2:C:74:THR:HG23	2:C:75:VAL:HG13	1.99	0.44
2:D:4:LEU:HD22	2:D:22:CYS:SG	2.58	0.44
1:B:493:LYS:NZ	1:B:565:GLU:O	2.49	0.44
1:A:493:LYS:NZ	1:A:565:GLU:O	2.50	0.44
2:D:103:TRP:CD1	2:D:103:TRP:H	2.34	0.43
2:D:119:TRP:H	3:E:4:MAN:HO4	1.64	0.43
2:C:19:LYS:NZ	4:C:202:HOH:O	2.18	0.43
2:D:117:ASP:HB3	3:E:2:NAG:H61	2.00	0.43
2:D:73:ASP:HB2	2:D:80:TYR:CE1	2.54	0.43
1:B:413:LYS:HB2	3:E:1:NAG:O5	2.19	0.43
2:C:86:LEU:HA	2:C:86:LEU:HD23	1.86	0.43
1:B:541:TYR:HD1	1:B:556:ALA:O	2.02	0.43
2:D:38:ARG:HH12	2:D:90:ASP:HA	1.83	0.42
1:B:404:PHE:HB3	1:B:407:CYS:SG	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:103:TRP:CZ3	2:C:104:VAL:HG23	2.55	0.42
2:C:45:ARG:O	2:C:112:GLN:CB	2.65	0.42
1:B:458:VAL:HG13	1:B:461:ALA:HB3	2.01	0.42
1:B:487:ASN:O	2:D:111:SER:HB2	2.19	0.42
2:C:18:LEU:HD22	2:C:19:LYS:N	2.35	0.42
2:C:111:SER:O	2:C:112:GLN:HG2	2.20	0.42
1:B:382:GLU:HA	1:B:408:ASN:O	2.20	0.41
2:D:52:LYS:HD3	2:D:57:ASN:HD21	1.83	0.41
1:A:509:ASP:OD2	1:A:512:THR:OG1	2.23	0.41
1:B:417:LEU:O	1:B:488:LEU:HD12	2.20	0.41
1:A:400:LYS:HB2	1:A:400:LYS:HE3	1.61	0.41
1:B:470:LYS:HG2	1:B:520:ALA:HA	2.02	0.41
1:B:540:TYR:HB3	1:B:542:ARG:CZ	2.50	0.41
2:D:12:VAL:HG22	2:D:18:LEU:HD13	2.03	0.41
1:A:428:ILE:HD13	1:A:433:ILE:HD13	2.03	0.41
2:C:100:VAL:HG11	3:F:1:NAG:H2	2.02	0.41
2:D:109:ILE:HA	2:D:109:ILE:HD13	1.72	0.41
1:A:411:LEU:HD22	1:A:415:LEU:HG	2.03	0.41
2:D:107:MET:HE3	2:D:107:MET:HB3	1.93	0.41
1:A:462:GLY:HA2	1:A:463:PRO:HD2	1.97	0.40
2:C:22:CYS:HB2	2:C:36:TRP:CZ2	2.56	0.40
2:D:83:MET:HE1	2:D:125:VAL:HG11	2.04	0.40
2:D:43:LYS:HB3	2:D:43:LYS:HE2	1.74	0.40
1:A:487:ASN:HB3	2:C:114:TYR:CD1	2.57	0.40

All (1) 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)
4:B:670:HOH:O	4:A:692:HOH:O[3_957]	2.13	0.07

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	99/229 (43%)	95 (96%)	4 (4%)	0	100	100
2	C	86/135 (64%)	80 (93%)	4 (5%)	2 (2%)	5	8
2	D	125/135 (93%)	114 (91%)	11 (9%)	0	100	100
All	All	310/499 (62%)	289 (93%)	19 (6%)	2 (1%)	21	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	30	SER
2	C	54	PRO

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	190/207 (92%)	172 (90%)	18 (10%)	8	17
1	B	173/207 (84%)	153 (88%)	20 (12%)	5	11
2	C	105/112 (94%)	94 (90%)	11 (10%)	6	14
2	D	104/112 (93%)	90 (86%)	14 (14%)	4	8
All	All	572/638 (90%)	509 (89%)	63 (11%)	6	13

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	381	VAL
1	B	382	GLU
1	B	415	LEU
1	B	433	ILE
1	B	454	SER
1	B	458	VAL
1	B	470	LYS
1	B	473	PHE

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Mol	Chain	Res	Type
1	B	481	LEU
1	B	484	VAL
1	B	495	LEU
1	B	498	SER
1	B	504	SER
1	B	514	VAL
1	B	540	TYR
1	B	542	ARG
1	B	543	LYS
1	B	566	GLN
1	B	579	THR
1	B	581	THR
1	A	406	ASN
1	A	411	LEU
1	A	412	THR
1	A	440	SER
1	A	450	LEU
1	A	451	SER
1	A	457	SER
1	A	481	LEU
1	A	484	VAL
1	A	493	LYS
1	A	495	LEU
1	A	504	SER
1	A	508	SER
1	A	533	THR
1	A	548	LEU
1	A	565	GLU
1	A	581	THR
1	A	588	LEU
2	C	12	VAL
2	C	18	LEU
2	C	30	SER
2	C	40	VAL
2	C	45	ARG
2	C	54	PRO
2	C	78	THR
2	C	79	VAL
2	C	100	VAL
2	C	102	ASN
2	C	104	VAL
2	D	13	GLN

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Mol	Chain	Res	Type
2	D	29	TYR
2	D	31	THR
2	D	34	ILE
2	D	40	VAL
2	D	51	ILE
2	D	71	SER
2	D	74	THR
2	D	75	VAL
2	D	79	VAL
2	D	100	VAL
2	D	105	CYS
2	D	109	ILE
2	D	121	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	576	GLN
1	A	427	GLN
1	A	475	ASN
1	A	576	GLN
2	C	77	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

10 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	$\# Z > 2$
3	NAG	E	1	3,1	14,14,15	0.40	0	17,19,21	0.48	0
3	NAG	E	2	3	14,14,15	0.19	0	17,19,21	0.47	0
3	BMA	E	3	3	11,11,12	1.13	2 (18%)	15,15,17	1.01	0
3	MAN	E	4	3	11,11,12	1.29	2 (18%)	15,15,17	1.09	1 (6%)
3	MAN	E	5	3	11,11,12	1.12	1 (9%)	15,15,17	0.87	0
3	NAG	F	1	3,1	14,14,15	0.72	1 (7%)	17,19,21	0.56	0
3	NAG	F	2	3	14,14,15	0.31	0	17,19,21	0.58	0
3	BMA	F	3	3	11,11,12	0.55	0	15,15,17	0.91	1 (6%)
3	MAN	F	4	3	11,11,12	0.75	0	15,15,17	1.32	2 (13%)
3	MAN	F	5	3	11,11,12	1.24	1 (9%)	15,15,17	1.25	2 (13%)

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	5	MAN	C4-C5	2.72	1.58	1.53
3	F	1	NAG	C1-C2	2.41	1.55	1.52
3	E	3	BMA	C2-C3	2.40	1.56	1.52
3	E	4	MAN	C4-C5	2.25	1.57	1.53
3	E	3	BMA	C1-C2	2.19	1.57	1.52
3	E	5	MAN	C2-C3	2.19	1.55	1.52
3	E	4	MAN	O5-C5	2.02	1.47	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	4	MAN	C1-O5-C5	3.75	117.21	112.19
3	F	5	MAN	C1-O5-C5	3.01	116.22	112.19
3	E	4	MAN	C1-O5-C5	2.90	116.08	112.19
3	F	3	BMA	C1-O5-C5	2.48	115.50	112.19
3	F	4	MAN	O2-C2-C3	-2.06	105.89	110.15
3	F	5	MAN	C3-C4-C5	2.05	113.95	110.23

There are no chirality outliers.

All (3) torsion outliers are listed below:

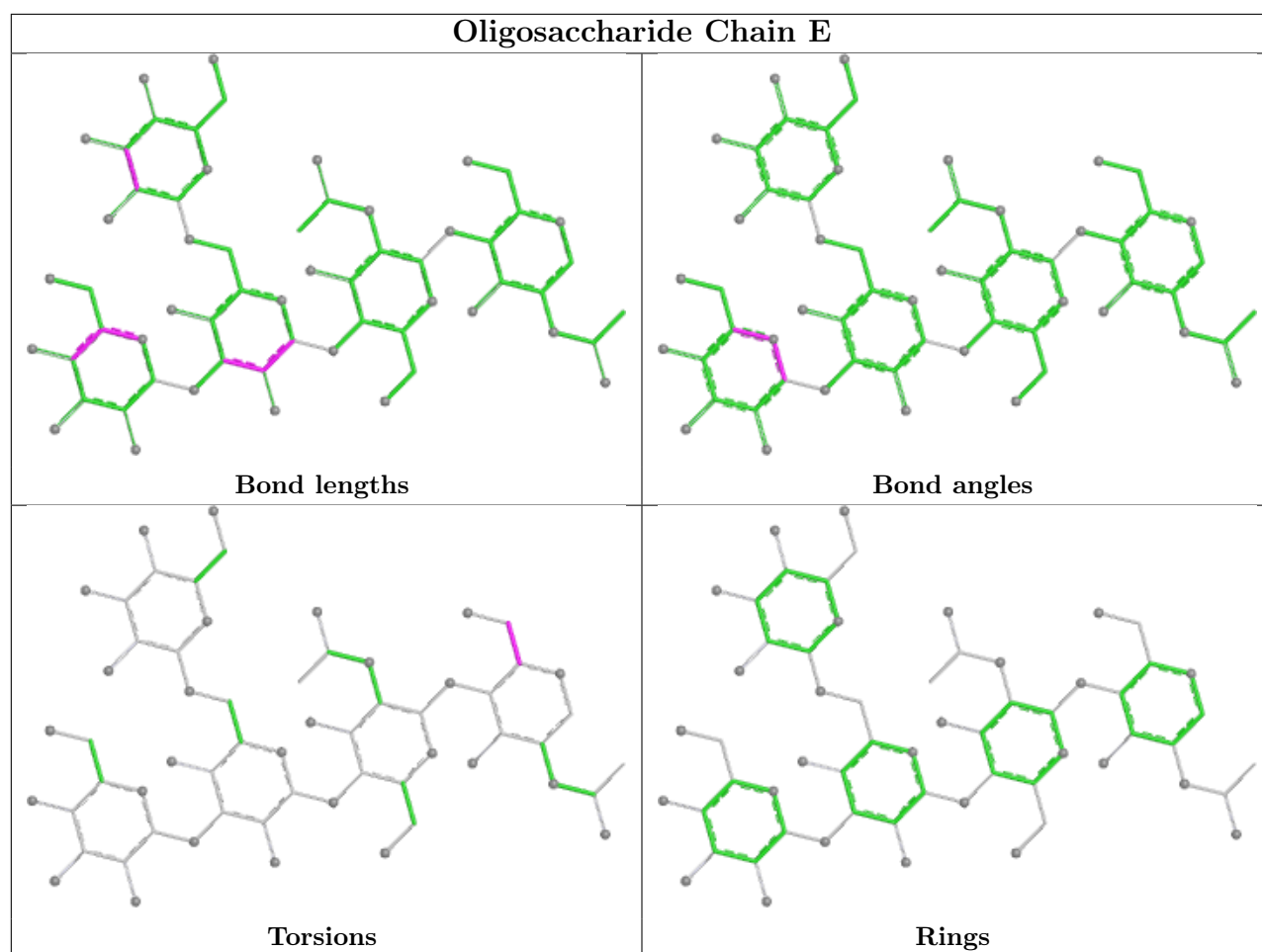
Mol	Chain	Res	Type	Atoms
3	F	5	MAN	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6

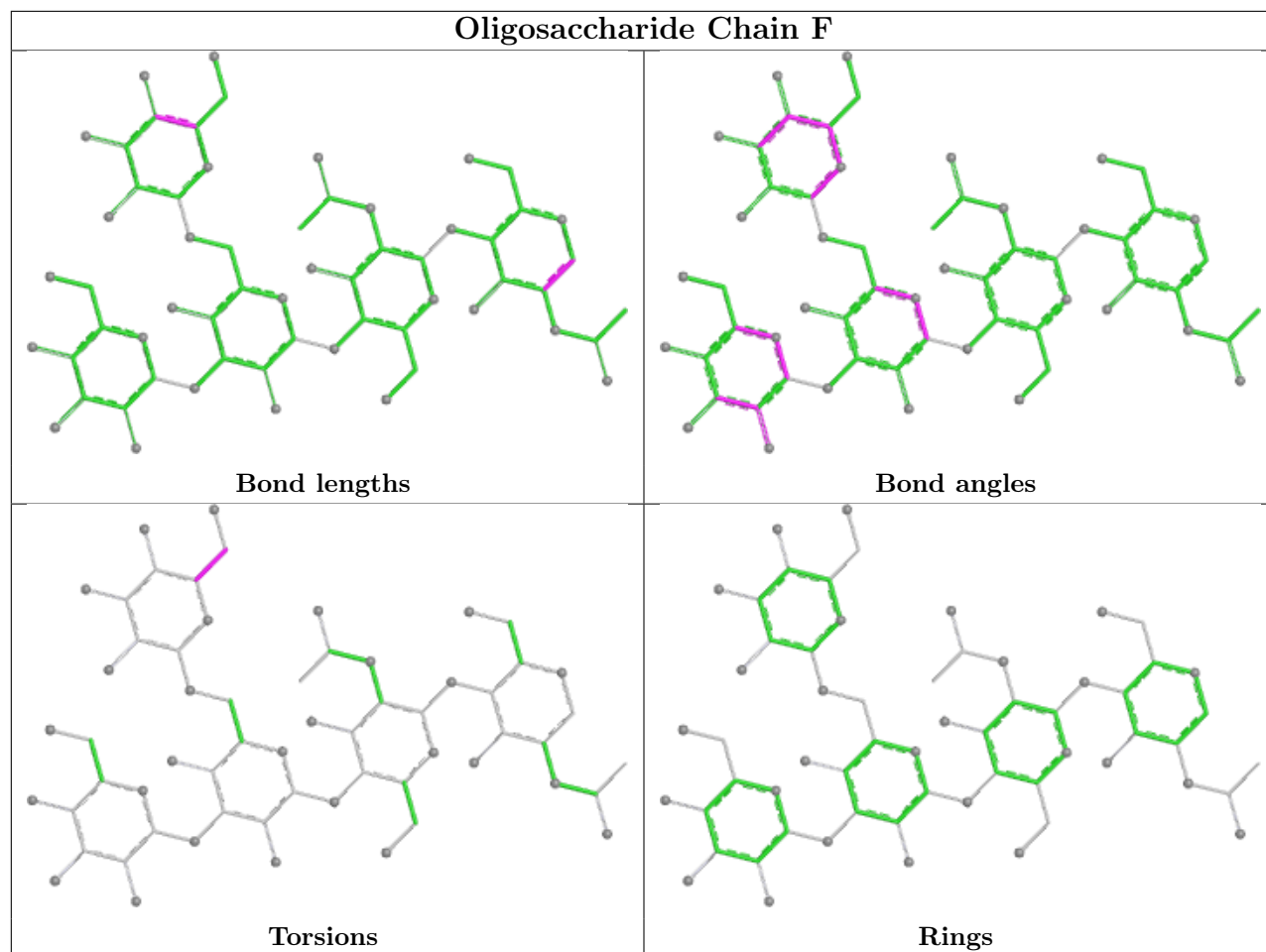
There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	4	MAN	1	0
3	E	2	NAG	1	0
3	F	1	NAG	1	0
3	E	1	NAG	3	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](#)

There are no ligands in this entry.

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	208/229 (90%)	-0.37	7 (3%) 48 43	27, 35, 57, 98	0
1	B	188/229 (82%)	0.35	17 (9%) 15 13	32, 49, 84, 119	0
2	C	128/135 (94%)	0.04	3 (2%) 61 57	34, 47, 75, 101	0
2	D	127/135 (94%)	1.86	50 (39%) 1 0	47, 79, 104, 128	0
All	All	651/728 (89%)	0.35	77 (11%) 9 7	27, 46, 93, 128	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	54	PRO	5.5
2	D	104	VAL	4.8
2	D	105	CYS	4.6
1	B	381	VAL	4.6
1	B	540	TYR	4.3
1	B	514	VAL	4.1
2	C	74	THR	3.9
2	D	13	GLN	3.7
1	B	542	ARG	3.7
2	D	85	SER	3.7
1	B	555	VAL	3.6
1	B	541	TYR	3.6
1	A	461	ALA	3.5
2	D	53	ASN	3.5
2	D	12	VAL	3.4
2	D	86	LEU	3.4
2	D	109	ILE	3.3
2	D	64	VAL	3.2
1	B	535	TRP	3.2
2	D	84	ASN	3.2
2	D	102	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
2	D	60	TYR	3.0
2	D	65	GLN	3.0
1	B	579	THR	3.0
2	D	14	ALA	2.9
2	D	40	VAL	2.9
2	D	112	GLN	2.9
2	D	75	VAL	2.8
1	A	581	THR	2.8
2	D	42	GLY	2.8
1	B	504	SER	2.7
1	B	473	PHE	2.7
1	A	460	SER	2.7
2	D	126	THR	2.7
2	D	45	ARG	2.7
2	D	74	THR	2.6
2	D	106	GLY	2.6
2	D	18	LEU	2.6
1	B	419	SER	2.5
2	D	33	CYS	2.5
1	B	492	THR	2.5
2	D	11	SER	2.5
2	D	63	SER	2.5
1	B	578	GLY	2.5
2	D	47	GLY	2.5
2	D	20	LEU	2.5
1	B	587	LYS	2.4
2	C	89	GLU	2.4
2	D	69	PHE	2.4
2	D	55	GLU	2.4
2	D	62	ASP	2.4
2	D	82	SER	2.3
2	C	75	VAL	2.3
2	D	81	LEU	2.3
2	D	52	LYS	2.3
2	D	127	VAL	2.3
2	D	77	ASN	2.3
2	D	128	SER	2.2
2	D	68	PHE	2.2
1	A	381	VAL	2.2
2	D	44	GLU	2.2
1	A	473	PHE	2.2
2	D	41	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	115	GLY	2.2
2	D	7	SER	2.2
1	A	579	THR	2.1
1	A	580	ASP	2.1
1	B	588	LEU	2.1
1	B	580	ASP	2.1
2	D	50	PHE	2.1
1	B	384	ASP	2.1
2	D	94	TYR	2.1
2	D	49	ALA	2.0
2	D	88	PRO	2.0
2	D	16	GLY	2.0
2	D	36	TRP	2.0
2	D	83	MET	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](#)

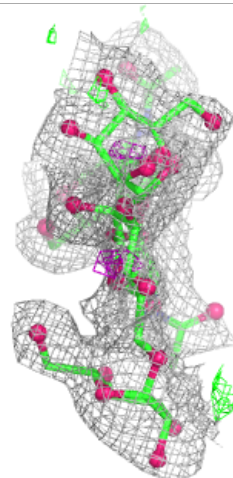
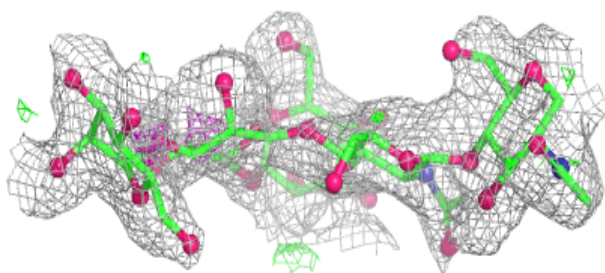
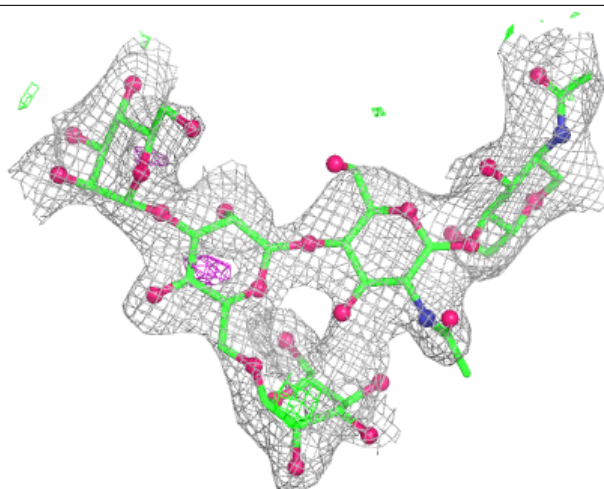
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

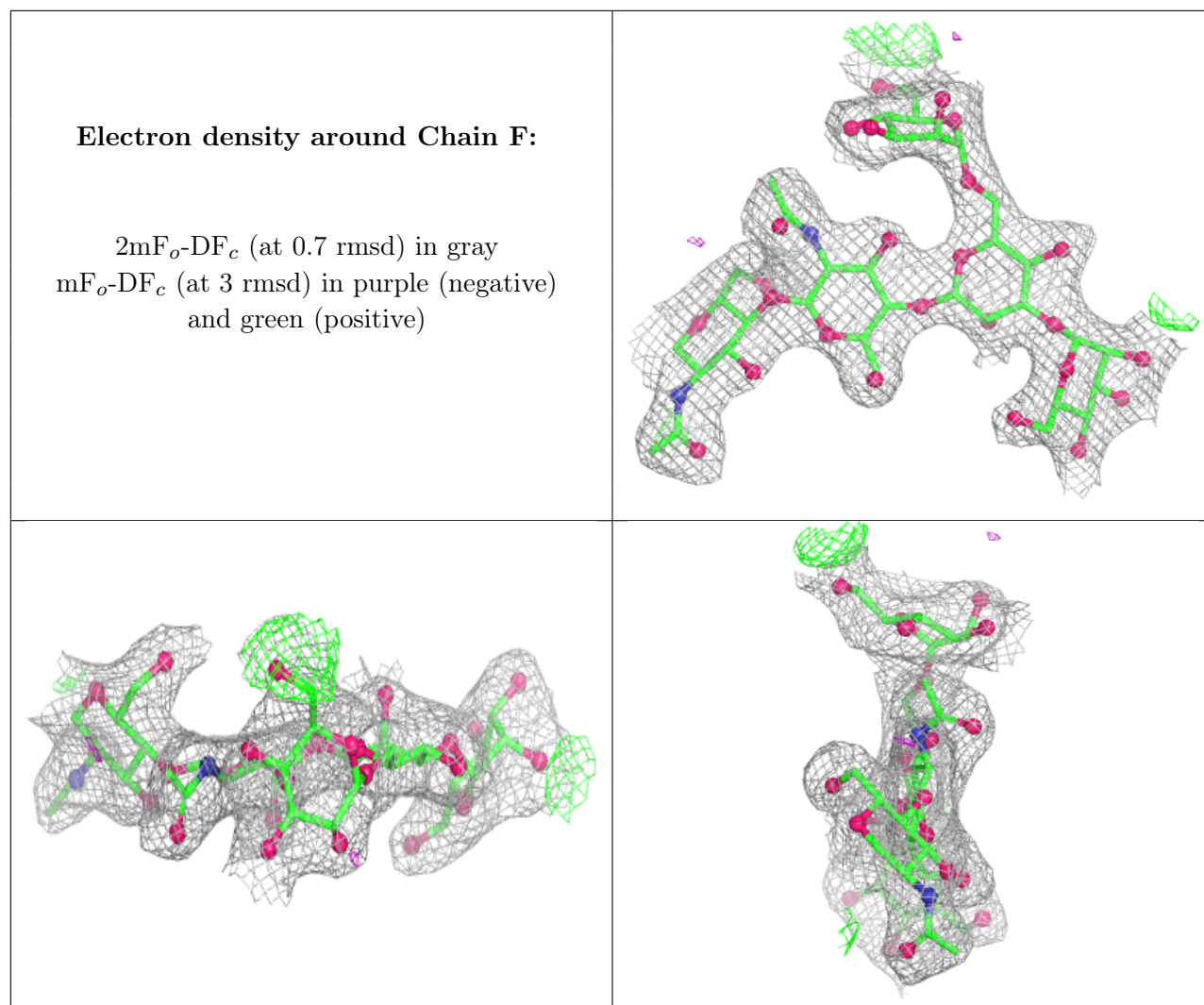
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	E	5	11/12	0.62	0.14	73,89,97,100	0
3	MAN	F	5	11/12	0.67	0.14	66,71,73,77	0
3	BMA	E	3	11/12	0.73	0.15	73,82,91,91	0
3	NAG	E	2	14/15	0.76	0.14	81,96,99,99	0
3	MAN	E	4	11/12	0.76	0.13	66,70,73,73	0
3	NAG	E	1	14/15	0.86	0.11	46,69,78,81	0
3	BMA	F	3	11/12	0.89	0.09	53,56,60,69	0
3	MAN	F	4	11/12	0.92	0.08	49,57,59,64	0
3	NAG	F	2	14/15	0.94	0.08	45,52,55,56	0
3	NAG	F	1	14/15	0.96	0.07	32,34,41,51	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 E:

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





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.