



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2022 – 06:30 PM JST

PDB ID : 7FC3
Title : structure of NL63 receptor-binding domain complexed with horse ACE2
Authors : Wang, X.Q.; Ge, J.W.; Lan, J.
Deposited on : 2021-07-13
Resolution : 3.19 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 following versions of software and data (see [references](#) ⓘ) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.28.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28.1

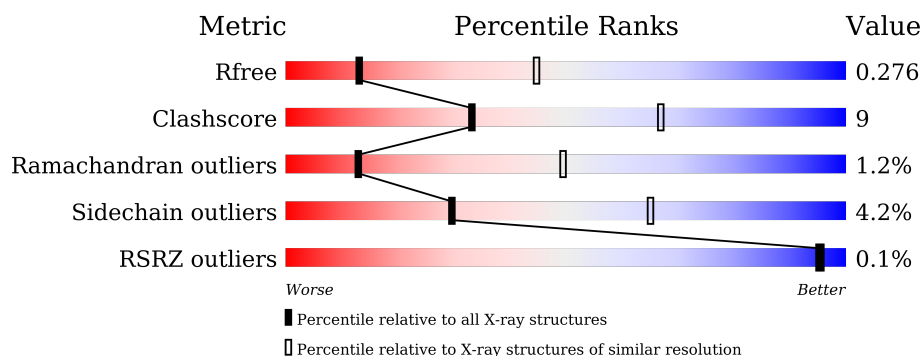
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	131	<div> <div style="width: 69%; background-color: green;"></div> <div style="width: 30%; background-color: yellow;"></div> <div style="width: 1%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> </div> <div>69% 30% .</div>
2	A	595	<div> <div style="width: 76%; background-color: green;"></div> <div style="width: 22%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> <div style="width: 0%; background-color: red;"></div> </div> <div>76% 22% .</div>
3	B	2	<div> <div style="width: 50%; background-color: green;"></div> <div style="width: 50%; background-color: yellow;"></div> </div> <div>50% 50%</div>
4	C	2	<div> <div style="width: 100%; background-color: yellow;"></div> </div> <div>100%</div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FUC	B	2	-	-	-	X
4	NAG	C	1	-	-	-	X
4	NAG	C	2	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5941 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	131	Total	C	N	O	S	0	0	0
			1027	658	171	192	6			

- Molecule 2 is a protein called Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	595	Total	C	N	O	S	0	0	0
			4848	3097	803	919	29			

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	2	Total	C	N	O	0	0	0
			24	14	1	9			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

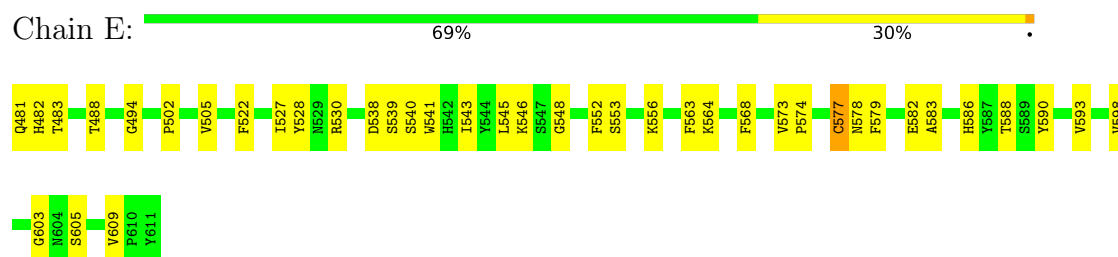


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	14	8	1	5	0	0

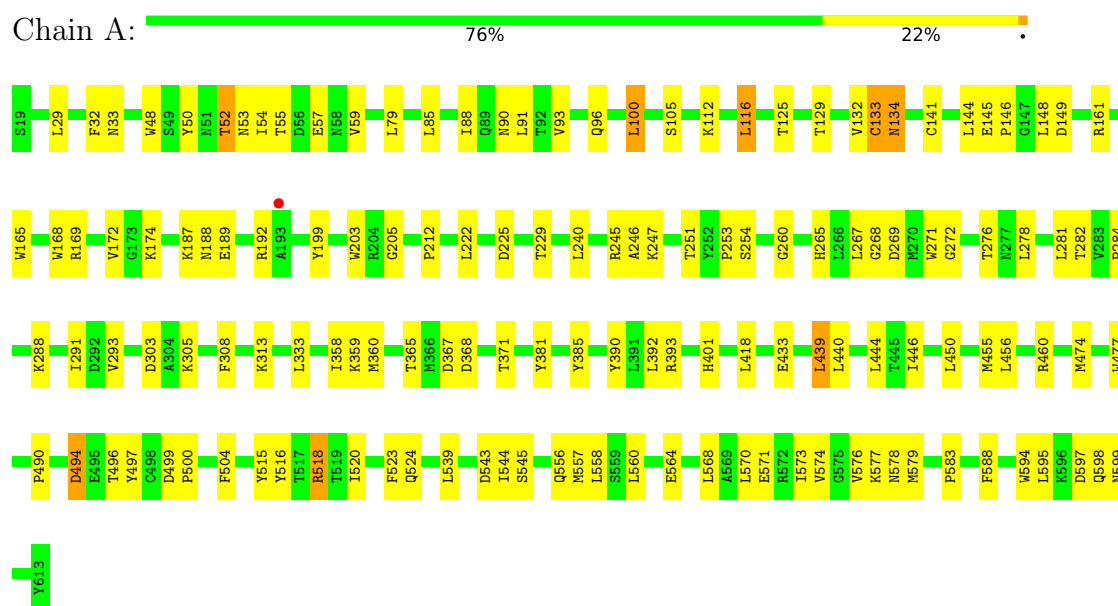
3 Residue-property plots

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: Angiotensin-converting enzyme



- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	112.91Å 112.91Å 328.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.23 – 3.19 34.23 – 3.19	Depositor EDS
% Data completeness (in resolution range)	98.9 (34.23-3.19) 98.9 (34.23-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.74 (at 3.18Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.232 , 0.283 0.243 , 0.276	Depositor DCC
R_{free} test set	1082 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	64.1	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 22.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5941	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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, 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	E	0.61	0/1060	0.82	0/1445
2	A	0.62	0/4984	0.84	1/6768 (0.0%)
All	All	0.62	0/6044	0.83	1/8213 (0.0%)

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	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	149	ASP	CB-CA-C	5.23	120.86	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	132	VAL	Peptide

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	1027	0	968	24	0
2	A	4848	0	4635	76	1
3	B	24	0	22	0	0
4	C	28	0	25	0	0
5	A	14	0	13	0	0
All	All	5941	0	5663	100	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 9.

All (100) 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:E:481:GLN:HG3	1:E:482:HIS:H	1.47	0.78
1:E:540:SER:HB3	1:E:586:HIS:HB2	1.66	0.77
2:A:365:THR:HG22	2:A:367:ASP:H	1.50	0.77
1:E:488:THR:HG22	1:E:527:ILE:HB	1.69	0.75
2:A:245:ARG:NH1	2:A:260:GLY:O	2.20	0.74
2:A:293:VAL:HG11	2:A:418:LEU:HD12	1.75	0.69
1:E:546:LYS:HD2	1:E:582:GLU:OE1	1.94	0.67
2:A:253:PRO:O	2:A:254:SER:OG	2.13	0.67
2:A:474:MET:HE1	2:A:499:ASP:HB2	1.78	0.66
2:A:269:ASP:HB2	2:A:272:GLY:H	1.59	0.65
1:E:538:ASP:O	1:E:539:SER:OG	2.13	0.65
2:A:564:GLU:OE1	2:A:568:LEU:HD22	1.97	0.64
1:E:505:VAL:HG11	1:E:593:VAL:HB	1.80	0.63
1:E:582:GLU:OE2	1:E:590:TYR:HB3	2.00	0.61
2:A:556:GLN:O	2:A:560:LEU:HD13	2.01	0.60
2:A:267:LEU:HA	2:A:278:LEU:HD11	1.82	0.60
1:E:548:GLY:HA3	1:E:578:ASN:O	2.01	0.60
2:A:446:ILE:HD13	2:A:523:PHE:HZ	1.66	0.59
2:A:245:ARG:HG2	2:A:246:ALA:N	2.17	0.59
2:A:308:PHE:CD2	2:A:333:LEU:HD13	2.38	0.58
2:A:494:ASP:HB2	2:A:496:THR:HG22	1.85	0.58
1:E:564:LYS:HB2	1:E:603:GLY:HA3	1.87	0.56
2:A:390:TYR:HA	2:A:393:ARG:NE	2.21	0.56
2:A:284:PRO:HB3	2:A:594:TRP:CH2	2.40	0.56
2:A:144:LEU:HA	2:A:148:LEU:HB2	1.89	0.55
2:A:571:GLU:OE2	2:A:577:LYS:HE3	2.07	0.55
1:E:543:ILE:HG12	1:E:583:ALA:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:269:ASP:HB3	2:A:271:TRP:HE3	1.72	0.54
2:A:578:ASN:OD1	2:A:579:MET:N	2.41	0.54
1:E:528:TYR:CE1	1:E:543:ILE:HB	2.43	0.53
2:A:269:ASP:HB3	2:A:271:TRP:CE3	2.43	0.53
2:A:247:LYS:HD3	2:A:282:THR:HA	1.90	0.52
1:E:528:TYR:HE1	1:E:543:ILE:HD12	1.73	0.52
2:A:543:ASP:O	2:A:545:SER:N	2.44	0.51
2:A:225:ASP:O	2:A:229:THR:HG22	2.10	0.51
2:A:515:TYR:HA	2:A:518:ARG:HG2	1.92	0.51
2:A:50:TYR:CE1	2:A:59:VAL:HG22	2.45	0.51
1:E:552:PHE:CZ	1:E:563:PHE:HE2	2.29	0.51
1:E:577:CYS:HB3	1:E:598:VAL:HB	1.93	0.51
2:A:269:ASP:HB2	2:A:272:GLY:N	2.26	0.48
1:E:530:ARG:CZ	1:E:539:SER:HA	2.42	0.48
2:A:240:LEU:HD21	2:A:444:LEU:HD12	1.95	0.47
2:A:229:THR:HG23	2:A:516:TYR:OH	2.15	0.47
2:A:390:TYR:HA	2:A:393:ARG:HE	1.79	0.47
2:A:32:PHE:CE2	2:A:100:LEU:HD21	2.50	0.47
2:A:165:TRP:O	2:A:169:ARG:HG2	2.15	0.47
2:A:543:ASP:C	2:A:545:SER:H	2.18	0.47
2:A:576:VAL:HG12	2:A:577:LYS:N	2.30	0.47
2:A:251:THR:OG1	2:A:281:LEU:HD12	2.15	0.46
2:A:288:LYS:NZ	2:A:433:GLU:HB2	2.30	0.46
2:A:456:LEU:HD23	2:A:460:ARG:HD2	1.96	0.46
2:A:96:GLN:HG2	2:A:392:LEU:HD13	1.97	0.46
2:A:133:CYS:HA	2:A:141:CYS:HA	1.96	0.46
2:A:524:GLN:HA	2:A:583:PRO:HG2	1.97	0.46
1:E:543:ILE:HG12	1:E:583:ALA:CB	2.45	0.46
2:A:597:ASP:O	2:A:599:ASN:N	2.49	0.46
2:A:539:LEU:H	2:A:539:LEU:HD23	1.82	0.45
1:E:545:LEU:HD12	1:E:579:PHE:HB3	1.98	0.45
2:A:288:LYS:HZ2	2:A:433:GLU:HB2	1.82	0.45
2:A:359:LYS:HE3	2:A:359:LYS:HB3	1.65	0.45
2:A:368:ASP:HA	2:A:371:THR:HB	1.98	0.45
1:E:568:PHE:CD1	1:E:598:VAL:HG22	2.52	0.45
2:A:358:ILE:HG21	2:A:360:MET:HE3	2.00	0.44
2:A:203:TRP:O	2:A:205:GLY:N	2.51	0.44
2:A:313:LYS:HA	2:A:313:LYS:HD2	1.73	0.44
2:A:450:LEU:HD23	2:A:450:LEU:HA	1.74	0.44
1:E:502:PRO:HD3	1:E:541:TRP:CZ3	2.53	0.43
2:A:161:ARG:HH22	2:A:268:GLY:H	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:597:ASP:C	2:A:599:ASN:H	2.21	0.43
2:A:145:GLU:HA	2:A:146:PRO:HA	1.70	0.43
2:A:570:LEU:HD22	2:A:574:VAL:HG21	2.00	0.43
2:A:571:GLU:HG3	2:A:577:LYS:HB3	2.01	0.43
2:A:303:ASP:OD2	2:A:305:LYS:HB3	2.18	0.43
2:A:265:HIS:CE1	2:A:490:PRO:HB3	2.54	0.43
2:A:112:LYS:NZ	2:A:189:GLU:OE2	2.48	0.42
2:A:439:LEU:HD23	2:A:588:PHE:HA	2.01	0.42
2:A:477:TRP:CE3	2:A:500:PRO:HG3	2.54	0.42
1:E:481:GLN:HG3	1:E:482:HIS:N	2.23	0.42
2:A:188:ASN:HB3	2:A:192:ARG:NH1	2.34	0.42
2:A:543:ASP:C	2:A:545:SER:N	2.72	0.42
2:A:48:TRP:O	2:A:52:THR:HB	2.19	0.42
1:E:564:LYS:HD2	1:E:605:SER:OG	2.20	0.42
2:A:199:TYR:CE2	2:A:203:TRP:CZ2	3.07	0.42
2:A:418:LEU:HD13	2:A:418:LEU:HA	1.89	0.42
2:A:33:ASN:HD21	2:A:96:GLN:HE22	1.67	0.42
2:A:174:LYS:HE2	2:A:497:TYR:CE1	2.54	0.41
2:A:573:ILE:HD13	2:A:573:ILE:HG21	1.80	0.41
2:A:90:ASN:HB3	2:A:93:VAL:HG22	2.02	0.41
2:A:291:ILE:HD13	2:A:291:ILE:HA	1.86	0.41
2:A:520:ILE:HG21	2:A:579:MET:HB3	2.03	0.41
2:A:557:MET:HE3	2:A:558:LEU:HD12	2.03	0.41
2:A:543:ASP:OD1	2:A:545:SER:HB2	2.20	0.41
2:A:125:THR:O	2:A:129:THR:HG23	2.21	0.41
2:A:116:LEU:HD21	2:A:187:LYS:HD2	2.02	0.41
2:A:187:LYS:HE2	2:A:199:TYR:CE1	2.56	0.41
2:A:293:VAL:HG11	2:A:418:LEU:CD1	2.49	0.41
1:E:553:SER:O	1:E:556:LYS:N	2.55	0.40
2:A:168:TRP:O	2:A:172:VAL:HG22	2.20	0.40
1:E:483:THR:HG23	1:E:522:PHE:HB2	2.04	0.40
1:E:502:PRO:HD3	1:E:541:TRP:CH2	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)
2:A:134:ASN:OD1	2:A:134:ASN:OD1[12_545]	1.53	0.67

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	E	129/131 (98%)	118 (92%)	9 (7%)	2 (2%)	9	43
2	A	593/595 (100%)	550 (93%)	36 (6%)	7 (1%)	13	49
All	All	722/726 (99%)	668 (92%)	45 (6%)	9 (1%)	13	49

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	598	GLN
1	E	494	GLY
2	A	105	SER
2	A	53	ASN
1	E	588	THR
2	A	276	THR
2	A	504	PHE
2	A	544	ILE
2	A	212	PRO

5.3.2 Protein sidechains [i](#)

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	117/117 (100%)	113 (97%)	4 (3%)	37	70
2	A	524/524 (100%)	501 (96%)	23 (4%)	28	64
All	All	641/641 (100%)	614 (96%)	27 (4%)	30	65

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	573	VAL
1	E	574	PRO
1	E	577	CYS
1	E	609	VAL
2	A	29	LEU
2	A	52	THR
2	A	54	ILE
2	A	55	THR
2	A	57	GLU
2	A	79	LEU
2	A	85	LEU
2	A	88	ILE
2	A	91	LEU
2	A	100	LEU
2	A	116	LEU
2	A	133	CYS
2	A	134	ASN
2	A	222	LEU
2	A	381	TYR
2	A	385	TYR
2	A	401	HIS
2	A	439	LEU
2	A	440	LEU
2	A	455	MET
2	A	494	ASP
2	A	518	ARG
2	A	595	LEU

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

Mol	Chain	Res	Type
2	A	96	GLN
2	A	134	ASN
2	A	194	ASN
2	A	239	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$
3	NAG	B	1	3,2	14,14,15	0.36	0	17,19,21	0.91	1 (5%)
3	FUC	B	2	3	10,10,11	0.28	0	14,14,16	0.87	0
4	NAG	C	1	2,4	14,14,15	0.35	0	17,19,21	1.17	2 (11%)
4	NAG	C	2	4	14,14,15	0.25	0	17,19,21	1.14	2 (11%)

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1	NAG	C2-N2-C7	3.00	127.17	122.90
4	C	2	NAG	C2-N2-C7	2.80	126.89	122.90
4	C	2	NAG	C1-O5-C5	2.65	115.78	112.19
4	C	1	NAG	C1-O5-C5	2.55	115.64	112.19
3	B	1	NAG	C1-O5-C5	2.43	115.48	112.19

There are no chirality outliers.

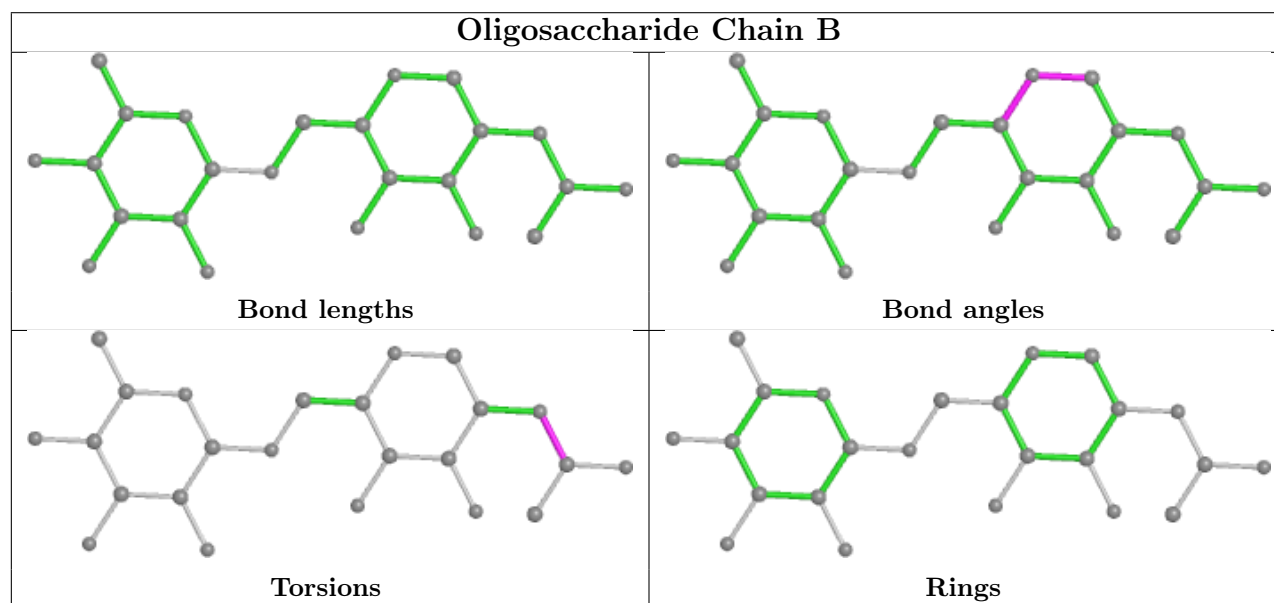
All (9) torsion outliers are listed below:

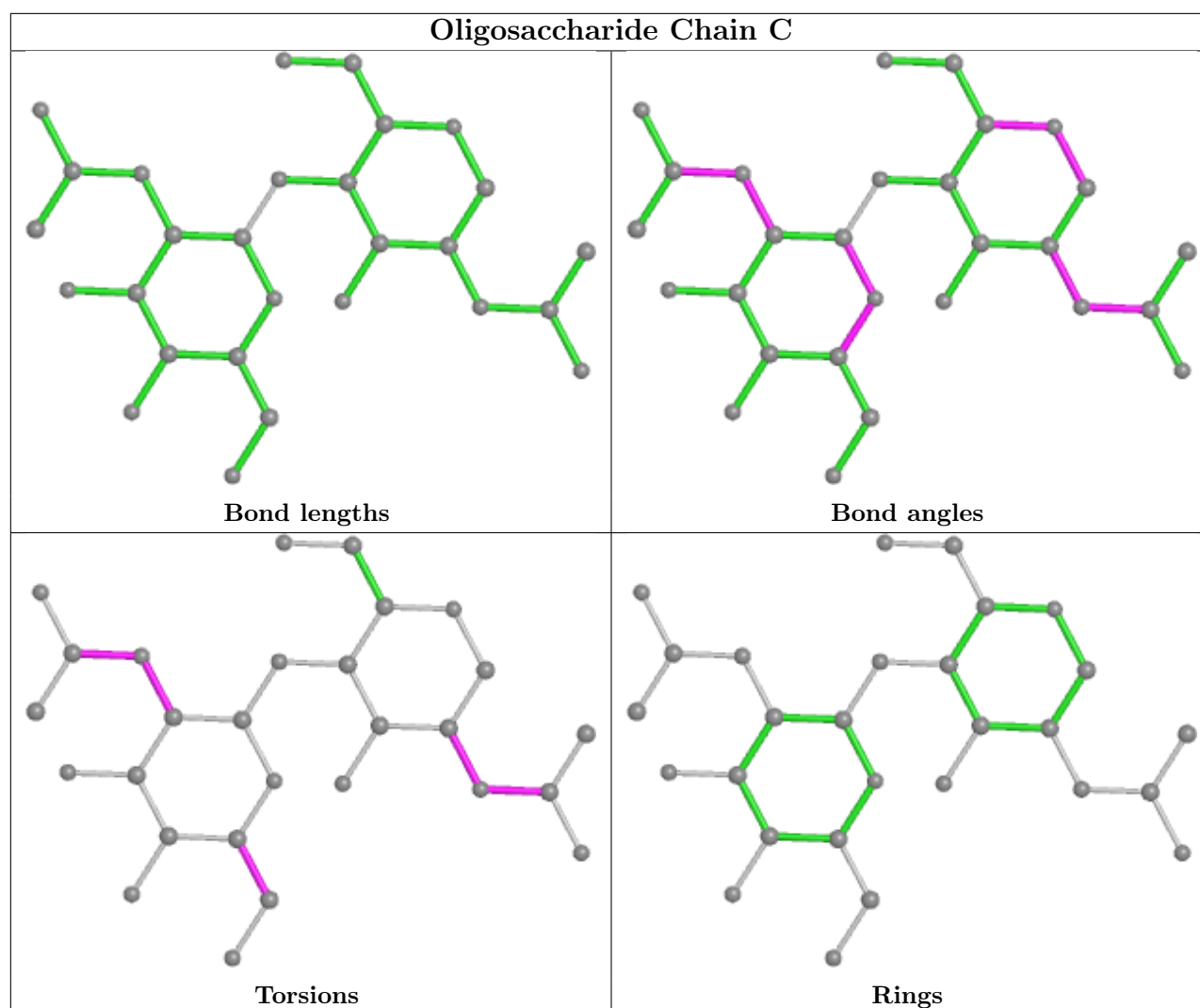
Mol	Chain	Res	Type	Atoms
3	B	1	NAG	C8-C7-N2-C2
3	B	1	NAG	O7-C7-N2-C2
4	C	1	NAG	C8-C7-N2-C2
4	C	1	NAG	O7-C7-N2-C2
4	C	2	NAG	C3-C2-N2-C7
4	C	2	NAG	C8-C7-N2-C2
4	C	2	NAG	O7-C7-N2-C2
4	C	1	NAG	C1-C2-N2-C7
4	C	2	NAG	O5-C5-C6-O6

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](#)

1 ligand is 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	NAG	A	701	2	14,14,15	0.51	0	17,19,21	0.86	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	NAG	A	701	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	701	NAG	C8-C7-N2-C2

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	131/131 (100%)	-0.05	0 100 100	56, 70, 88, 122	0
2	A	595/595 (100%)	-0.26	1 (0%) 95 94	36, 56, 96, 139	0
All	All	726/726 (100%)	-0.22	1 (0%) 95 95	36, 58, 93, 139	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	193	ALA	2.2

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](#)

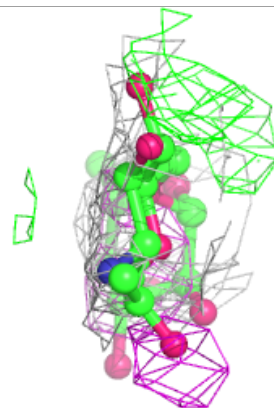
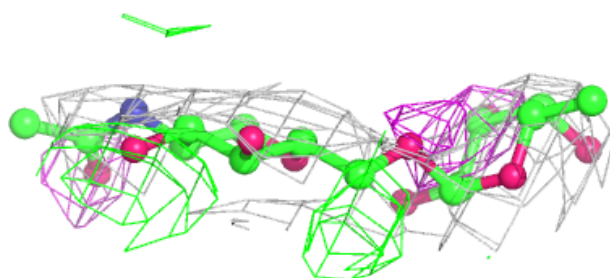
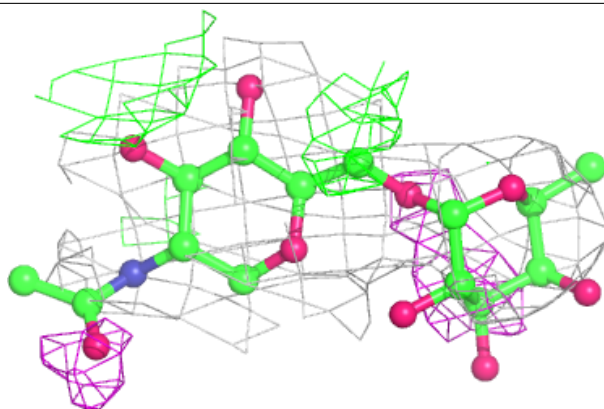
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	C	1	14/15	0.63	0.44	90,90,90,90	0
4	NAG	C	2	14/15	0.64	0.41	90,90,90,90	0
3	NAG	B	1	14/15	0.70	0.38	90,90,90,90	0
3	FUC	B	2	10/11	0.74	0.56	90,90,90,90	0

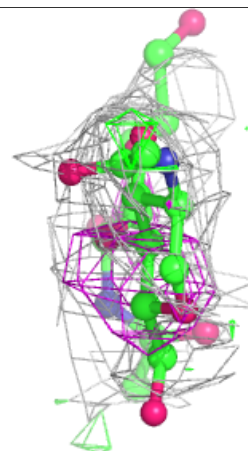
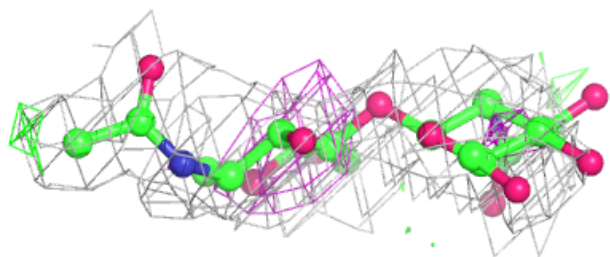
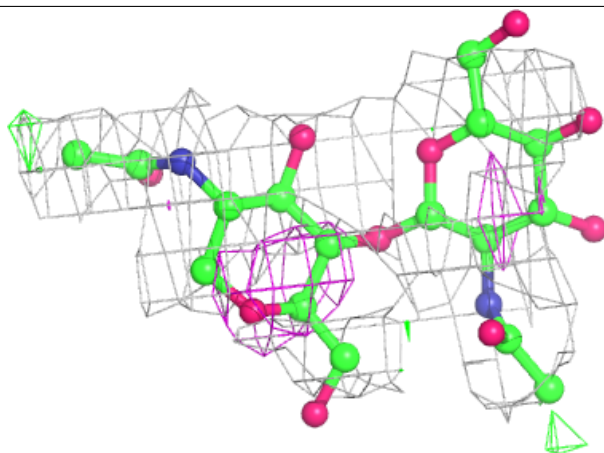
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain B:

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

**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(\AA^2)	Q<0.9
5	NAG	A	701	14/15	0.84	0.26	63,77,84,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.