



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 08:00 PM EDT

PDB ID : 7B0B / pdb_00007b0b
Title : Fab HbnC3t1p1_C6 bound to SARS-CoV-2 RBD
Authors : Borenstein-Katz, A.; Diskin, R.
Deposited on : 2020-11-19
Resolution : 2.98 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

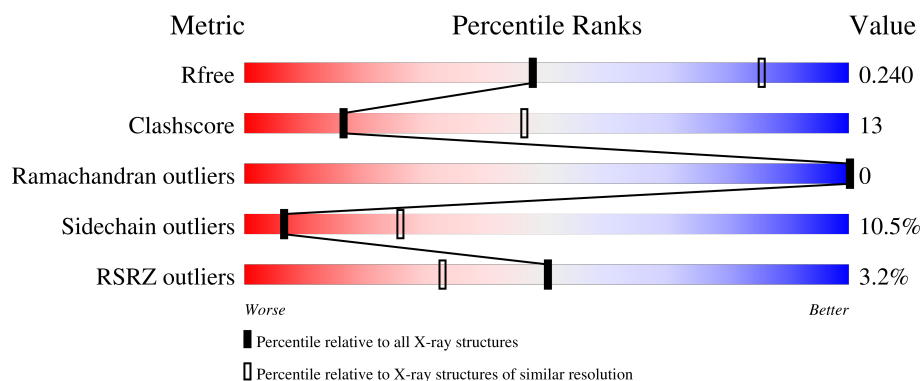
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	L	215	73% 26% •
2	H	230	59% 33% • 5%
3	F	229	7% 57% 26% • 15%
4	A	2	100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4858 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 IGK@ protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	215	Total	C	N	O	S	0	0	0
			1648	1030	279	334	5			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	2	ILE	ASN	conflict	UNP Q6PIL8
L	29	VAL	LEU	conflict	UNP Q6PIL8
L	52	ALA	VAL	conflict	UNP Q6PIL8
L	79	VAL	LEU	conflict	UNP Q6PIL8
L	94	SER	THR	conflict	UNP Q6PIL8
L	?	-	ARG	deletion	UNP Q6PIL8
L	97	TRP	ILE	conflict	UNP Q6PIL8
L	104	LYS	ARG	conflict	UNP Q6PIL8
L	105	VAL	LEU	conflict	UNP Q6PIL8
L	106	GLU	ASP	conflict	UNP Q6PIL8

- Molecule 2 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	0	0	0
			1639	1031	277	321	10			

- Molecule 3 is a protein called Surface glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	195	Total	C	N	O	S	0	0	0
			1543	989	257	289	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	542	HIS	-	expression tag	UNP A0A6M5SXU3
F	543	HIS	-	expression tag	UNP A0A6M5SXU3
F	544	HIS	-	expression tag	UNP A0A6M5SXU3
F	545	HIS	-	expression tag	UNP A0A6M5SXU3
F	546	HIS	-	expression tag	UNP A0A6M5SXU3
F	547	HIS	-	expression tag	UNP A0A6M5SXU3

- 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	A	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

Chain A:

100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.41Å 109.11Å 168.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.36 – 2.98 39.36 – 2.98	Depositor EDS
% Data completeness (in resolution range)	77.2 (39.36-2.98) 77.2 (39.36-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 2.95Å)	Xtriage
Refinement program	PHENIX dev_3965	Depositor
R, R_{free}	0.209 , 0.246 0.210 , 0.240	Depositor DCC
R_{free} test set	2000 reflections (6.15%)	wwPDB-VP
Wilson B-factor (Å ²)	60.7	Xtriage
Anisotropy	0.722	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4858	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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: 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	L	0.26	0/1685	0.53	0/2289
2	H	0.26	0/1677	0.47	0/2284
3	F	0.43	1/1587 (0.1%)	0.88	2/2161 (0.1%)
All	All	0.33	1/4949 (0.0%)	0.65	2/6734 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	355	ARG	CB-CG	-6.43	1.33	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	355	ARG	CG-CD-NE	-12.76	83.93	112.00
3	F	387	LEU	CA-CB-CG	7.36	142.06	116.30

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	L	1648	0	1595	32	0
2	H	1639	0	1606	49	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1543	0	1459	47	1
4	A	28	0	25	2	0
All	All	4858	0	4685	124	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 13.

All (124) 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)
3:F:493:GLN:HE21	3:F:494:SER:H	1.11	0.95
1:L:80:GLU:HG3	1:L:81:PRO:HD2	1.53	0.89
3:F:503:VAL:HA	3:F:506:GLN:HE21	1.46	0.79
2:H:2:MET:HB2	2:H:26:GLY:HA3	1.63	0.77
1:L:84:PHE:CD1	1:L:107:ILE:HG22	2.22	0.75
1:L:84:PHE:CG	1:L:107:ILE:HG22	2.22	0.75
2:H:107:TYR:HD2	2:H:111:ASP:OD2	1.73	0.72
1:L:3:VAL:HG22	1:L:26:SER:HB3	1.74	0.69
1:L:151:VAL:HG13	1:L:156:GLN:HG3	1.74	0.69
2:H:154:ASP:OD1	2:H:181:GLN:NE2	2.29	0.65
3:F:454:ARG:NH2	3:F:469:SER:O	2.30	0.65
2:H:88:SER:O	2:H:91:THR:HG22	1.98	0.64
3:F:493:GLN:HE21	3:F:494:SER:N	1.89	0.64
1:L:124:GLU:OE2	2:H:219:LYS:HE2	1.98	0.63
2:H:6:GLN:H	2:H:115:GLN:HE22	1.46	0.63
3:F:376:THR:HB	3:F:435:ALA:HB3	1.81	0.63
3:F:503:VAL:HA	3:F:506:GLN:NE2	2.12	0.63
3:F:393:THR:HG22	3:F:517:LEU:HA	1.81	0.62
3:F:501:ASN:HD22	3:F:505:TYR:HB3	1.65	0.61
3:F:387:LEU:HA	3:F:390:LEU:HD13	1.81	0.61
3:F:355:ARG:HB2	3:F:398:ASP:OD2	2.01	0.61
2:H:36:TRP:HD1	2:H:70:ILE:HD13	1.67	0.60
2:H:205:ILE:HG22	2:H:220:ARG:HG2	1.82	0.60
2:H:107:TYR:CD2	2:H:111:ASP:OD2	2.53	0.60
2:H:111:ASP:OD1	2:H:112:ILE:N	2.35	0.59
1:L:79:VAL:HG23	1:L:83:ASP:HB2	1.84	0.58
2:H:56:GLY:N	2:H:72:ARG:HH21	2.02	0.58
1:L:190:HIS:HB2	1:L:193:TYR:HE2	1.68	0.58
2:H:36:TRP:CD1	2:H:70:ILE:HD13	2.39	0.57
3:F:359:SER:HA	3:F:524:VAL:HG23	1.86	0.57
1:L:21:LEU:HD12	1:L:74:LEU:HD23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:164:TRP:CZ3	2:H:206:CYS:HB3	2.39	0.57
4:A:1:NAG:H3	4:A:1:NAG:H83	1.88	0.56
1:L:121:PRO:HB2	1:L:126:LEU:HD21	1.89	0.55
1:L:19:ALA:HB3	1:L:76:ILE:HB	1.89	0.55
3:F:503:VAL:CA	3:F:506:GLN:HE21	2.19	0.55
2:H:211:LYS:HG3	2:H:212:PRO:HD3	1.88	0.55
3:F:376:THR:HG23	3:F:378:LYS:HD3	1.88	0.54
1:L:152:ASP:HA	1:L:192:VAL:HG13	1.89	0.54
1:L:150:LYS:HA	1:L:154:ALA:O	2.06	0.54
2:H:107:TYR:HD1	2:H:108:ASP:H	1.56	0.54
2:H:129:PRO:HB3	2:H:155:TYR:HB3	1.88	0.54
1:L:62:ARG:HD2	1:L:83:ASP:OD2	2.08	0.54
3:F:439:ASN:ND2	3:F:506:GLN:OE1	2.30	0.53
2:H:19:LYS:HG3	2:H:82:GLU:HB2	1.91	0.53
2:H:106:CYS:HB2	3:F:475:ALA:O	2.08	0.52
2:H:153:LYS:HA	2:H:187:SER:HB3	1.92	0.52
2:H:118:MET:HE3	2:H:120:THR:HG23	1.92	0.52
3:F:503:VAL:HA	3:F:506:GLN:HG3	1.91	0.52
3:F:417:LYS:NZ	3:F:455:LEU:HD12	2.25	0.51
1:L:116:VAL:HA	1:L:136:LEU:O	2.09	0.51
2:H:6:GLN:H	2:H:115:GLN:NE2	2.08	0.51
3:F:350:VAL:HG22	3:F:401:VAL:O	2.11	0.51
2:H:53:VAL:O	2:H:74:MET:HE2	2.11	0.51
3:F:468:ILE:HG12	3:F:468:ILE:O	2.10	0.51
3:F:404:GLY:O	3:F:407:VAL:HG22	2.11	0.50
3:F:417:LYS:HZ2	3:F:455:LEU:HD12	1.76	0.50
2:H:158:GLU:OE2	2:H:178:ALA:HB3	2.10	0.50
3:F:472:ILE:HD12	3:F:482:GLY:HA2	1.92	0.50
3:F:401:VAL:HG21	3:F:451:TYR:CD2	2.46	0.49
3:F:421:TYR:HE2	3:F:457:ARG:H	1.61	0.49
2:H:13:LYS:O	2:H:16:THR:OG1	2.30	0.48
1:L:151:VAL:CG1	1:L:156:GLN:HG3	2.43	0.48
1:L:109:ARG:HG2	1:L:172:SER:HB2	1.96	0.47
2:H:136:PRO:HG2	2:H:199:LEU:HD21	1.95	0.47
3:F:355:ARG:CB	3:F:398:ASP:OD2	2.63	0.47
1:L:107:ILE:HD11	1:L:172:SER:OG	2.14	0.46
3:F:408:ARG:NH1	3:F:409:GLN:HE21	2.14	0.46
2:H:135:ALA:HB1	2:H:223:PRO:HA	1.98	0.46
3:F:518:LEU:C	3:F:520:ALA:H	2.23	0.46
2:H:178:ALA:HA	2:H:188:LEU:HB3	1.98	0.46
3:F:440:ASN:OD1	3:F:441:LEU:HD22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:83:LEU:HD12	2:H:83:LEU:HA	1.71	0.45
2:H:210:HIS:CD2	2:H:212:PRO:HD2	2.51	0.45
2:H:211:LYS:CG	2:H:212:PRO:HD3	2.46	0.45
3:F:358:ILE:HG13	3:F:395:VAL:CG2	2.45	0.45
1:L:119:PHE:CD1	2:H:134:LEU:HB3	2.51	0.45
3:F:493:GLN:NE2	3:F:493:GLN:HA	2.32	0.45
2:H:55:SER:C	2:H:72:ARG:HH21	2.25	0.45
2:H:72:ARG:NH1	2:H:74:MET:HE3	2.31	0.45
1:L:187:TYR:CE1	1:L:193:TYR:HE1	2.35	0.44
1:L:187:TYR:CD1	1:L:193:TYR:HE1	2.34	0.44
3:F:416:GLY:O	3:F:420:ASP:OD2	2.36	0.44
2:H:63:LYS:HE2	2:H:63:LYS:HB3	1.91	0.44
2:H:91:THR:HB	2:H:121:VAL:H	1.82	0.44
2:H:136:PRO:HD2	2:H:223:PRO:HB3	2.00	0.43
2:H:6:GLN:HA	2:H:21:SER:O	2.18	0.43
2:H:127:LYS:HE3	2:H:154:ASP:O	2.17	0.43
3:F:340:GLU:O	3:F:344:ALA:HB2	2.18	0.43
2:H:40:ALA:HB3	2:H:43:GLN:HB2	1.99	0.43
1:L:210:PHE:C	1:L:210:PHE:CD1	2.96	0.43
1:L:107:ILE:HD13	1:L:107:ILE:HG21	1.82	0.43
1:L:190:HIS:HB2	1:L:193:TYR:CE2	2.51	0.43
3:F:359:SER:HA	3:F:524:VAL:CG2	2.49	0.43
1:L:49:ILE:HD12	1:L:74:LEU:HD12	1.99	0.43
3:F:371:SER:C	3:F:373:SER:H	2.27	0.43
3:F:454:ARG:HD3	3:F:457:ARG:HB2	2.01	0.43
3:F:369:TYR:HD2	3:F:384:PRO:HB2	1.83	0.43
3:F:379:CYS:HB2	3:F:384:PRO:HD3	1.99	0.43
2:H:136:PRO:HG3	2:H:148:LEU:HB3	2.00	0.42
3:F:358:ILE:CG1	3:F:395:VAL:HG23	2.49	0.42
1:L:122:SER:OG	2:H:132:PHE:HB3	2.19	0.42
1:L:171:ASP:OD2	1:L:173:THR:OG1	2.32	0.42
1:L:109:ARG:NH1	1:L:171:ASP:O	2.53	0.42
3:F:378:LYS:HB2	3:F:378:LYS:HE2	1.68	0.42
3:F:383:SER:HB3	3:F:386:LYS:HB2	2.02	0.42
1:L:32:SER:HB3	3:F:478:THR:HG21	2.02	0.41
1:L:35:ALA:HA	1:L:49:ILE:O	2.20	0.41
1:L:57:THR:HG23	2:H:107:TYR:OH	2.20	0.41
2:H:17:SER:HA	2:H:83:LEU:O	2.20	0.41
2:H:206:CYS:O	2:H:218:ASP:HA	2.20	0.41
3:F:393:THR:O	3:F:523:THR:OG1	2.35	0.41
2:H:72:ARG:O	2:H:72:ARG:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:335:LEU:HD12	3:F:362:VAL:HG13	2.02	0.41
3:F:462:LYS:N	3:F:465:GLU:OE1	2.41	0.41
4:A:1:NAG:O3	4:A:2:NAG:N2	2.53	0.41
2:H:7:SER:OG	2:H:21:SER:N	2.44	0.41
3:F:350:VAL:HG21	3:F:402:ILE:HG22	2.03	0.41
2:H:161:THR:O	2:H:208:VAL:HA	2.21	0.40
1:L:55:ARG:HD3	1:L:59:ILE:O	2.21	0.40
3:F:388:ASN:O	3:F:526:GLY:HA3	2.21	0.40
2:H:4:LEU:HD22	2:H:112:ILE:HG22	2.03	0.40
2:H:6:GLN:NE2	2:H:96:CYS:H	2.20	0.40
3:F:493:GLN:NE2	3:F:494:SER:H	1.94	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:H:220:ARG:NH1	3:F:369:TYR:O[2_454]	2.19	0.01

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	L	213/215 (99%)	201 (94%)	12 (6%)	0	100	100
2	H	214/230 (93%)	208 (97%)	6 (3%)	0	100	100
3	F	193/229 (84%)	181 (94%)	12 (6%)	0	100	100
All	All	620/674 (92%)	590 (95%)	30 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	186/186 (100%)	163 (88%)	23 (12%)	4	19
2	H	187/198 (94%)	158 (84%)	29 (16%)	2	12
3	F	168/202 (83%)	163 (97%)	5 (3%)	36	67
All	All	541/586 (92%)	484 (90%)	57 (10%)	6	26

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	5	THR
1	L	7	SER
1	L	10	THR
1	L	12	SER
1	L	14	SER
1	L	28	SER
1	L	31	SER
1	L	54	SER
1	L	74	LEU
1	L	75	THR
1	L	86	VAL
1	L	115	SER
1	L	116	VAL
1	L	122	SER
1	L	128	SER
1	L	133	VAL
1	L	134	VAL
1	L	160	SER
1	L	169	SER
1	L	172	SER
1	L	197	VAL
1	L	203	SER
1	L	207	THR
2	H	4	LEU
2	H	7	SER
2	H	11	VAL

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Mol	Chain	Res	Type
2	H	22	CYS
2	H	25	SER
2	H	31	SER
2	H	67	ARG
2	H	75	SER
2	H	89	GLU
2	H	91	THR
2	H	93	VAL
2	H	96	CYS
2	H	100	HIS
2	H	104	THR
2	H	120	THR
2	H	125	SER
2	H	137	SER
2	H	138	SER
2	H	150	CYS
2	H	151	LEU
2	H	153	LYS
2	H	180	LEU
2	H	181	GLN
2	H	187	SER
2	H	190	SER
2	H	196	SER
2	H	197	SER
2	H	201	THR
2	H	207	ASN
3	F	350	VAL
3	F	367	VAL
3	F	421	TYR
3	F	443	SER
3	F	477	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	101	GLN
1	L	148	GLN
3	F	409	GLN
3	F	414	GLN
3	F	474	GLN
3	F	493	GLN
3	F	501	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

2 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	A	1	4,3	14,14,15	0.37	0	17,19,21	1.51	2 (11%)
4	NAG	A	2	4	14,14,15	1.02	2 (14%)	17,19,21	0.58	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	A	1	4,3	-	6/6/23/26	0/1/1/1
4	NAG	A	2	4	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2	NAG	C1-C2	2.90	1.56	1.52
4	A	2	NAG	O5-C1	2.37	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	NAG	C2-N2-C7	4.51	128.94	122.90
4	A	1	NAG	C1-C2-N2	2.65	114.61	110.43

There are no chirality outliers.

All (7) torsion outliers are listed below:

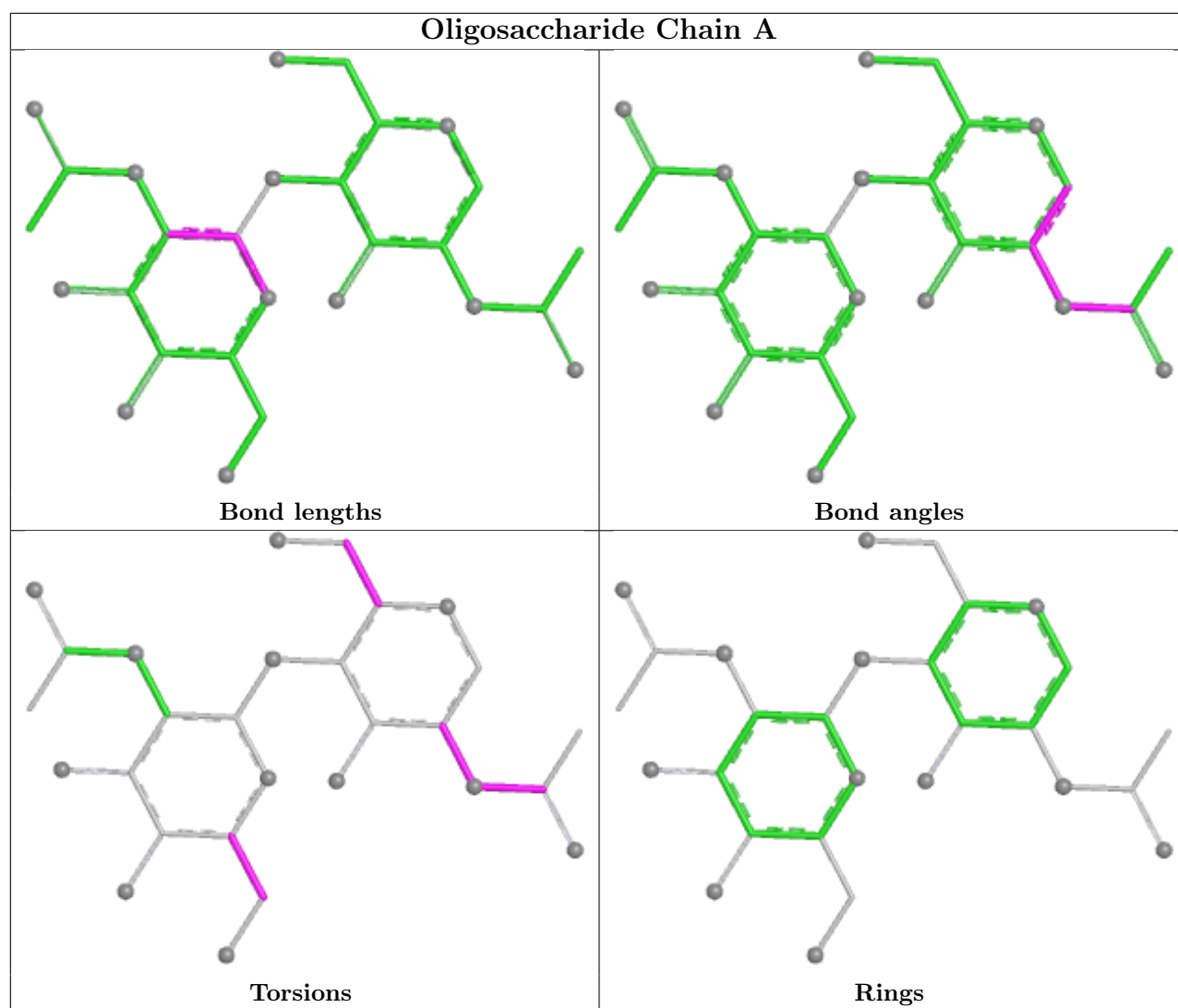
Mol	Chain	Res	Type	Atoms
4	A	1	NAG	C8-C7-N2-C2
4	A	1	NAG	O7-C7-N2-C2
4	A	1	NAG	C4-C5-C6-O6
4	A	2	NAG	O5-C5-C6-O6
4	A	1	NAG	O5-C5-C6-O6
4	A	1	NAG	C1-C2-N2-C7
4	A	1	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2	NAG	1	0
4	A	1	NAG	2	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	L	215/215 (100%)	-0.28	2 (0%) 81 65	30, 52, 75, 105	0
2	H	218/230 (94%)	-0.14	1 (0%) 87 75	33, 51, 82, 103	0
3	F	195/229 (85%)	0.35	17 (8%) 16 10	40, 71, 116, 149	0
All	All	628/674 (93%)	-0.04	20 (3%) 50 33	30, 56, 98, 149	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	385	THR	4.3
1	L	153	ASN	4.0
2	H	224	LYS	3.8
3	F	522	ALA	3.3
1	L	215	CYS	3.2
3	F	520	ALA	3.1
3	F	387	LEU	3.1
3	F	517	LEU	2.9
3	F	521	PRO	2.8
3	F	518	LEU	2.8
3	F	444	LYS	2.8
3	F	519	HIS	2.7
3	F	384	PRO	2.7
3	F	527	PRO	2.7
3	F	354	ASN	2.4
3	F	372	ALA	2.3
3	F	381	GLY	2.3
3	F	386	LYS	2.1
3	F	371	SER	2.1
3	F	382	VAL	2.0

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

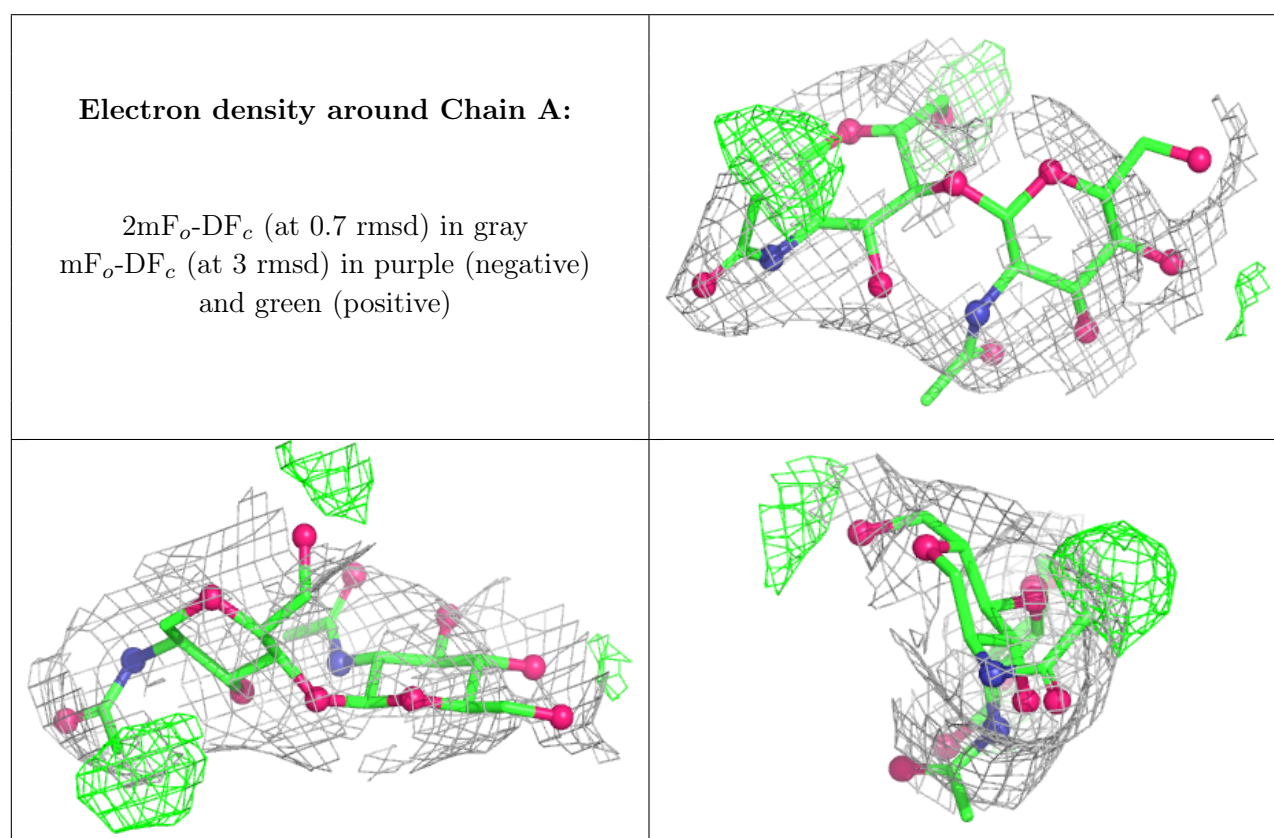
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	1	14/15	-	-	67,102,119,126	0
4	NAG	A	2	14/15	-	-	88,124,142,142	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.