



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:26 PM UTC

PDB ID : 1QFK / pdb_00001qfk
Title : STRUCTURE OF HUMAN FACTOR VIIA AND ITS IMPLICATIONS FOR
THE TRIGGERING OF BLOOD COAGULATION
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Deposited on : 1999-04-12
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

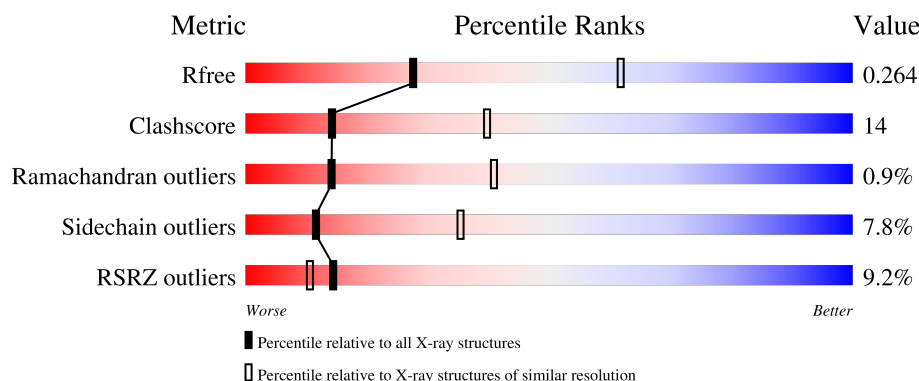
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	104	23% 37% 38% 14% • 8%
2	H	254	3% 54% 35% 10% •
3	A	3	100%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	FUC	L	160	X	-	-	-
6	OZ6	H	1	X	-	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 2928 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.

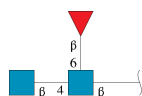
- Molecule 1 is a protein called COAGULATION FACTOR VIIA LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	96	Total	C	N	O	S	0	9	0
			778	465	141	159	13			

- Molecule 2 is a protein called COAGULATION FACTOR VIIA HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	252	Total	C	N	O	S	0	5	0
			1972	1249	351	359	13			

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



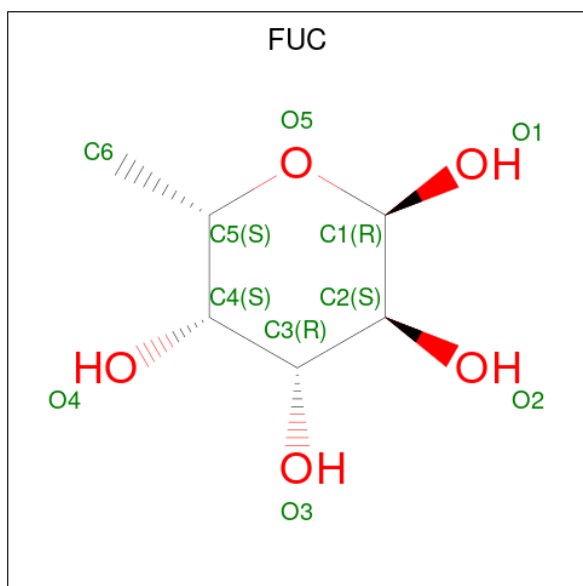
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	A	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 4 is alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆).



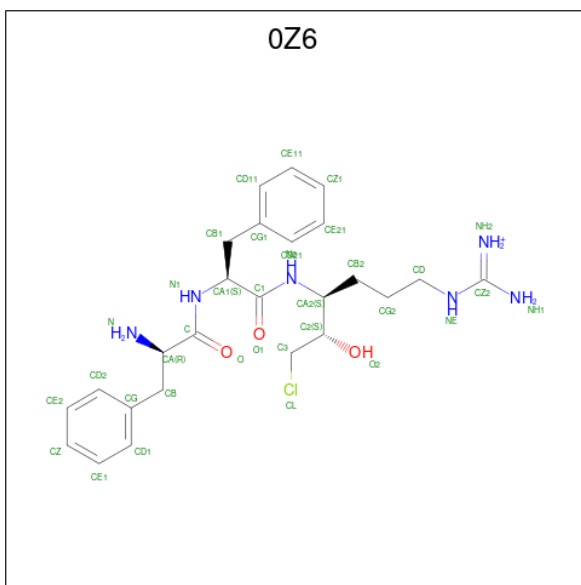
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is alpha-L-fucopyranose (CCD ID: FUC) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is D-phenylalanyl-N-[(2S,3S)-6-{[amino(iminio)methyl]amino}-1-chloro-2-hydroxyhexan-3-yl]-L-phenylalaninamide (CCD ID: 0Z6) (formula: $C_{25}H_{36}ClN_6O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	H	1	Total	C	N	O	0	0
			34	25	6	3		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	1	Total	Ca	0	0
			1	1		

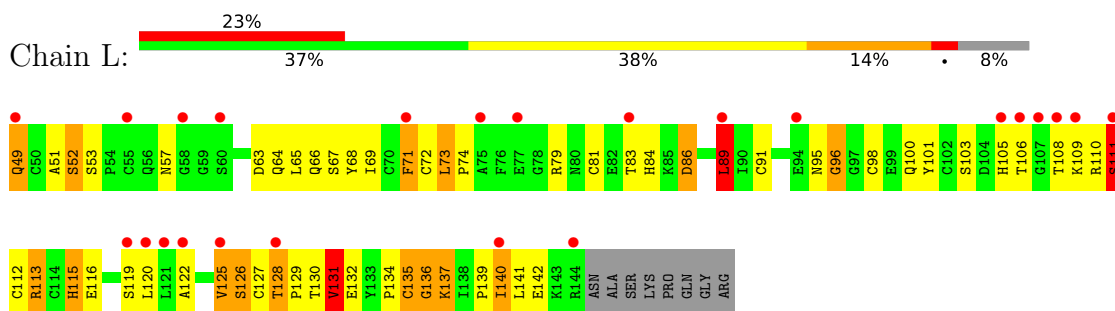
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	L	10	Total O 10 10	0	0
8	H	74	Total O 74 74	0	0

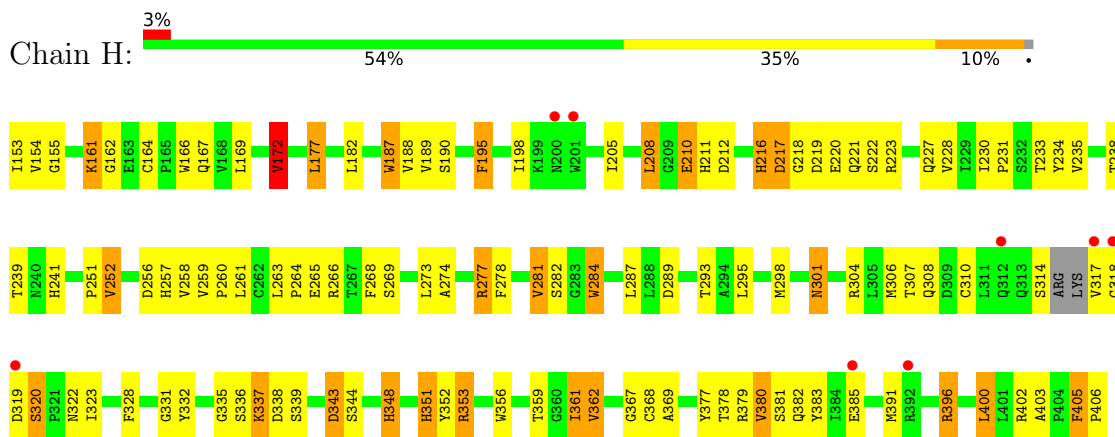
3 Residue-property plots

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: COAGULATION FACTOR VIIA LIGHT CHAIN



• Molecule 2: COAGULATION FACTOR VIIA HEAVY CHAIN



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	115.30Å 115.30Å 98.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.80 35.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.4 (35.00-2.80) 95.6 (35.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.215 , 0.267 0.213 , 0.264	Depositor DCC
R_{free} test set	818 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	59.4	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2928	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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: CA, NAG, GLC, FUC, FUL, OZ6

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	0.70	0/797	1.93	24/1076 (2.2%)
2	H	0.97	0/2043	2.28	104/2780 (3.7%)
All	All	0.90	0/2840	2.19	128/3856 (3.3%)

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
1	L	0	1

There are no bond length outliers.

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	396	ARG	CD-NE-CZ	13.26	142.97	124.40
1	L	100	GLN	CA-C-O	-11.46	113.24	119.77
2	H	268	PHE	CA-CB-CG	10.52	124.32	113.80
1	L	140	ILE	CA-C-O	-9.75	110.01	120.64
2	H	338	ASP	CA-CB-CG	9.74	122.34	112.60
2	H	172	VAL	N-CA-CB	9.59	124.37	112.10
2	H	295	LEU	N-CA-C	-9.41	102.31	113.88
2	H	304	ARG	CD-NE-CZ	8.82	136.75	124.40
2	H	281	VAL	CA-C-O	-8.79	111.09	121.28
2	H	348	HIS	N-CA-C	-8.63	90.34	107.69
2	H	380	VAL	O-C-N	-8.40	113.54	121.94
2	H	298	MET	CA-C-O	-8.27	111.52	121.28
2	H	221	GLN	CG-CD-NE2	8.24	128.76	116.40
2	H	187	TRP	N-CA-C	8.22	121.81	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	155	GLY	CA-C-N	-8.18	115.15	122.43
2	H	155	GLY	C-N-CA	-8.18	115.15	122.43
2	H	239	THR	N-CA-C	7.92	122.76	113.18
2	H	322	ASN	CA-CB-CG	-7.88	104.72	112.60
1	L	131	VAL	N-CA-CB	7.83	124.02	112.35
2	H	217	ASP	CA-CB-CG	7.62	120.22	112.60
2	H	238	THR	CA-C-O	-7.56	112.61	121.16
2	H	322	ASN	OD1-CG-ND2	7.45	130.04	122.60
2	H	261	LEU	CA-C-O	-7.43	112.44	121.36
2	H	266	ARG	NE-CZ-NH2	7.24	125.71	119.20
2	H	400	LEU	CA-C-O	-7.21	112.83	120.40
2	H	402	ARG	CD-NE-CZ	7.13	134.38	124.40
2	H	405	PHE	CA-C-O	7.13	126.21	119.72
2	H	337	LYS	N-CA-C	7.12	120.78	108.76
2	H	252	VAL	N-CA-CB	6.94	119.98	112.07
2	H	218	GLY	CA-C-O	-6.92	111.25	119.00
2	H	154	VAL	O-C-N	6.88	130.69	123.26
2	H	323	ILE	CA-C-O	-6.86	112.64	120.95
2	H	289	ASP	CA-C-O	-6.84	113.82	121.00
1	L	140	ILE	N-CA-CB	6.83	121.26	110.54
2	H	216	HIS	CA-C-O	-6.83	112.82	120.54
2	H	252	VAL	N-CA-C	-6.80	100.08	109.46
1	L	115	HIS	CA-C-O	-6.80	113.66	121.47
2	H	190	SER	CA-C-O	-6.67	113.80	120.80
2	H	339	SER	N-CA-C	-6.57	101.06	110.59
2	H	289	ASP	CA-C-N	-6.57	112.81	122.86
2	H	289	ASP	C-N-CA	-6.57	112.81	122.86
1	L	137	LYS	CA-CB-CG	6.53	127.16	114.10
1	L	137	LYS	N-CA-C	-6.50	98.01	109.06
2	H	167	GLN	CA-C-O	-6.46	114.09	121.19
1	L	135	CYS	N-CA-CB	6.43	119.42	109.97
2	H	353	ARG	CD-NE-CZ	6.36	133.30	124.40
1	L	91	CYS	N-CA-C	6.30	120.23	112.54
2	H	403	ALA	CA-C-O	6.26	126.62	120.23
2	H	337	LYS	N-CA-CB	-6.25	99.98	110.80
2	H	362	VAL	CA-C-O	-6.25	113.29	120.98
2	H	227	GLN	N-CA-CB	-6.24	100.47	111.39
1	L	127	CYS	CA-C-O	-6.19	113.88	121.06
2	H	379	ARG	CD-NE-CZ	6.17	133.03	124.40
2	H	281	VAL	N-CA-C	-6.16	98.82	108.86
2	H	320	SER	N-CA-C	-6.16	102.11	110.36
2	H	318	GLY	N-CA-C	-6.14	104.65	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	235	VAL	CB-CA-C	-6.11	103.99	110.16
2	H	339	SER	CA-C-O	-6.07	114.79	121.89
2	H	319	ASP	CA-CB-CG	-6.02	106.58	112.60
1	L	72	CYS	N-CA-C	5.99	119.85	110.32
2	H	361	ILE	CA-C-O	-5.98	113.98	120.67
2	H	257	HIS	CA-CB-CG	-5.96	107.84	113.80
2	H	405	PHE	CA-CB-CG	-5.95	107.85	113.80
2	H	234	TYR	CA-C-N	5.94	128.01	122.85
2	H	234	TYR	C-N-CA	5.94	128.01	122.85
2	H	164	CYS	CA-C-N	5.91	126.02	119.87
2	H	164	CYS	C-N-CA	5.91	126.02	119.87
2	H	195	PHE	CA-CB-CG	-5.88	107.92	113.80
2	H	348	HIS	CA-CB-CG	5.84	119.64	113.80
2	H	322	ASN	O-C-N	-5.84	116.57	123.22
1	L	101	TYR	N-CA-C	5.81	119.02	110.59
2	H	210	GLU	CG-CD-OE1	-5.80	105.05	118.40
2	H	265[A]	GLU	CB-CA-C	5.79	118.93	109.90
2	H	265[B]	GLU	CB-CA-C	5.79	118.93	109.90
2	H	219	ASP	N-CA-CB	5.76	119.11	110.53
2	H	310	CYS	N-CA-C	5.71	118.28	111.71
1	L	89	LEU	CA-C-N	5.71	128.38	122.27
1	L	89	LEU	C-N-CA	5.71	128.38	122.27
2	H	212	ASP	CA-C-O	-5.68	114.23	120.70
2	H	343	ASP	CA-CB-CG	5.60	118.20	112.60
2	H	264	PRO	N-CA-C	5.58	120.26	111.38
2	H	304	ARG	NH1-CZ-NH2	-5.55	112.08	119.30
1	L	51	ALA	CA-C-O	-5.55	114.98	120.70
2	H	351	HIS	CA-C-O	-5.54	114.66	120.80
2	H	268	PHE	N-CA-C	-5.51	105.36	111.36
2	H	263	LEU	CA-C-N	5.49	125.40	119.85
2	H	263	LEU	C-N-CA	5.49	125.40	119.85
2	H	307	THR	O-C-N	-5.47	115.97	122.20
2	H	251	PRO	N-CA-CB	5.44	108.51	103.39
2	H	252	VAL	O-C-N	5.44	127.18	122.12
1	L	136	GLY	N-CA-C	5.43	126.06	113.18
2	H	221	GLN	CA-CB-CG	5.43	124.95	114.10
2	H	352	TYR	N-CA-CB	5.43	119.55	110.59
1	L	112	CYS	CB-CA-C	-5.39	103.58	111.77
1	L	113	ARG	CA-CB-CG	5.38	124.87	114.10
2	H	306	MET	N-CA-C	-5.38	102.31	110.28
2	H	177	LEU	CA-C-O	-5.35	113.55	119.81
1	L	125	VAL	CB-CA-C	-5.32	102.56	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	306	MET	CA-CB-CG	5.31	124.72	114.10
2	H	187	TRP	CA-C-O	5.30	125.97	120.30
2	H	281	VAL	O-C-N	5.30	128.67	123.00
2	H	301	ASN	CB-CA-C	5.28	119.39	110.79
2	H	314	SER	CA-C-O	5.27	129.76	120.80
2	H	233	THR	O-C-N	5.25	129.30	122.42
2	H	256	ASP	CA-CB-CG	5.24	117.84	112.60
2	H	289	ASP	N-CA-CB	5.22	117.53	109.91
2	H	223	ARG	CA-C-O	-5.18	114.17	120.54
2	H	238	THR	N-CA-CB	5.17	119.12	110.85
2	H	301	ASN	N-CA-CB	-5.17	101.89	110.47
2	H	328	PHE	CA-CB-CG	5.15	118.95	113.80
2	H	274	ALA	CA-C-O	-5.14	113.05	119.38
2	H	308	GLN	OE1-CD-NE2	-5.14	117.46	122.60
2	H	385	GLU	N-CA-CB	5.13	117.58	109.94
2	H	210	GLU	OE1-CD-OE2	5.12	135.19	122.90
1	L	142	GLU	CA-C-O	5.12	125.83	119.79
2	H	282	SER	CA-C-O	-5.11	115.76	121.23
2	H	284	TRP	N-CA-C	-5.10	106.37	112.59
1	L	73	LEU	CA-C-N	5.10	126.21	119.84
1	L	73	LEU	C-N-CA	5.10	126.21	119.84
2	H	359	THR	CA-C-N	-5.09	112.86	121.47
2	H	359	THR	C-N-CA	-5.09	112.86	121.47
1	L	71	PHE	CB-CA-C	5.09	118.92	110.78
2	H	382	GLN	CG-CD-OE1	-5.09	110.62	120.80
2	H	172	VAL	N-CA-C	-5.08	98.70	107.24
2	H	348	HIS	CA-C-O	-5.07	114.19	120.57
1	L	130	THR	N-CA-CB	5.05	119.88	111.49
2	H	161	LYS	CA-C-O	-5.05	116.14	120.88
2	H	195	PHE	N-CA-CB	-5.04	103.21	110.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	111[B]	SER	Mainchain

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	L	778	0	699	37	0
2	H	1972	0	1935	45	0
3	A	38	0	33	0	0
4	L	11	0	10	1	0
5	L	10	0	10	0	0
6	H	34	0	31	0	0
7	H	1	0	0	0	0
8	H	74	0	0	1	0
8	L	10	0	0	1	0
All	All	2928	0	2718	79	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (79) 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:L:129:PRO:HB3	1:L:134:PRO:HG3	1.59	0.83
1:L:89:LEU:HD11	1:L:110[B]:ARG:HH11	1.48	0.78
2:H:195:PHE:HA	2:H:198:ILE:HD12	1.71	0.71
1:L:108[B]:THR:OG1	1:L:109[B]:LYS:N	2.25	0.69
1:L:105[B]:HIS:NE2	1:L:111[B]:SER:HB3	2.08	0.68
1:L:89:LEU:O	1:L:110[B]:ARG:HG2	1.96	0.66
2:H:189:VAL:CG1	2:H:361:ILE:HD11	2.29	0.62
1:L:105[B]:HIS:CD2	1:L:110[B]:ARG:HA	2.36	0.60
1:L:105[B]:HIS:HD2	1:L:110[B]:ARG:HA	1.68	0.59
2:H:210:GLU:OE1	2:H:211:HIS:N	2.30	0.59
1:L:89:LEU:HD11	1:L:110[B]:ARG:NH1	2.17	0.58
2:H:335:GLY:HA2	2:H:369:ALA:O	2.04	0.57
2:H:380:VAL:O	2:H:381:SER:C	2.44	0.57
1:L:98:CYS:O	2:H:353:ARG:NH1	2.39	0.56
1:L:120:LEU:HD12	1:L:126:SER:O	2.06	0.55
1:L:89:LEU:O	1:L:110[A]:ARG:HG2	2.06	0.55
1:L:89:LEU:CD1	1:L:110[B]:ARG:HH11	2.19	0.53
1:L:137:LYS:O	1:L:139:PRO:HD3	2.08	0.53
2:H:228:VAL:HB	2:H:400:LEU:HD12	1.91	0.53
1:L:68:TYR:O	1:L:79:ARG:NH2	2.42	0.53
1:L:49:GLN:HB3	4:L:153:GLC:O6	2.08	0.53
2:H:405:PHE:CG	2:H:406:PRO:HA	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:136:GLY:HA2	2:H:166:TRP:CZ3	2.44	0.53
2:H:182:LEU:HD22	2:H:208:LEU:HD22	1.90	0.53
2:H:343:ASP:O	2:H:344:SER:C	2.48	0.53
1:L:69:ILE:HG21	1:L:71:PHE:CZ	2.45	0.52
2:H:241:HIS:HA	2:H:383:TYR:OH	2.09	0.52
1:L:67:SER:OG	1:L:68:TYR:N	2.41	0.52
2:H:351:HIS:HB2	2:H:356:TRP:CH2	2.46	0.51
2:H:208:LEU:HD13	2:H:252:VAL:HG11	1.93	0.51
2:H:216:HIS:HA	2:H:220:GLU:OE2	2.12	0.50
2:H:230:ILE:HB	2:H:231:PRO:HD2	1.93	0.50
2:H:278:PHE:HB3	2:H:301:ASN:ND2	2.27	0.49
1:L:84:HIS:CD2	1:L:86:ASP:H	2.30	0.48
2:H:161:LYS:NZ	2:H:217:ASP:OD2	2.34	0.48
2:H:344:SER:HA	2:H:362:VAL:HG12	1.95	0.48
1:L:125:VAL:HG23	1:L:126:SER:N	2.29	0.48
2:H:269:SER:HA	2:H:273:LEU:HB2	1.95	0.48
2:H:153:ILE:O	2:H:287:LEU:HA	2.13	0.47
2:H:336:SER:OG	2:H:337:LYS:HG3	2.14	0.47
2:H:351:HIS:HB2	2:H:356:TRP:CZ3	2.48	0.47
2:H:278:PHE:HB3	2:H:301:ASN:HD21	1.79	0.47
2:H:277[A]:ARG:HG2	2:H:277[A]:ARG:HH11	1.80	0.47
1:L:95:ASN:O	1:L:96:GLY:C	2.57	0.47
2:H:189:VAL:HG11	2:H:361:ILE:HD11	1.97	0.47
1:L:49:GLN:NE2	1:L:63:ASP:OD1	2.48	0.47
2:H:284:TRP:O	2:H:293:THR:HB	2.14	0.47
1:L:49:GLN:HE22	1:L:63:ASP:HB3	1.80	0.46
1:L:98:CYS:HB3	8:L:163:HOH:O	2.15	0.46
2:H:344:SER:HA	2:H:362:VAL:CG1	2.46	0.46
1:L:52:SER:O	1:L:53:SER:C	2.59	0.45
1:L:115:HIS:CD2	1:L:135:CYS:SG	3.09	0.45
1:L:128:THR:HG23	1:L:129:PRO:HD2	2.00	0.44
2:H:361:ILE:HB	2:H:378:THR:HB	1.99	0.44
2:H:187:TRP:CE2	2:H:391:MET:HG2	2.52	0.44
1:L:68:TYR:N	1:L:68:TYR:CD1	2.85	0.44
1:L:73:LEU:HB3	1:L:74:PRO:HD2	2.00	0.43
1:L:64:GLN:O	1:L:65:LEU:HB2	2.18	0.43
2:H:332:TYR:CD2	2:H:337:LYS:HB2	2.53	0.43
2:H:368:CYS:O	2:H:369:ALA:HB3	2.19	0.43
1:L:139:PRO:O	1:L:140:ILE:C	2.60	0.42
2:H:169:LEU:HB2	2:H:284:TRP:CZ3	2.54	0.42
2:H:172:VAL:HG23	2:H:177:LEU:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:89:LEU:C	1:L:89:LEU:HD12	2.45	0.42
1:L:105[B]:HIS:HB2	1:L:109[B]:LYS:O	2.19	0.42
2:H:189:VAL:HG12	2:H:361:ILE:HD11	2.00	0.42
2:H:331:GLY:HA3	8:H:526:HOH:O	2.19	0.42
2:H:259:VAL:HG13	2:H:260:PRO:HD2	2.02	0.42
1:L:140:ILE:HD13	2:H:162:GLY:HA3	2.02	0.41
2:H:281:VAL:HG12	2:H:348:HIS:HA	2.02	0.41
2:H:182:LEU:HD22	2:H:208:LEU:CD2	2.50	0.41
2:H:362:VAL:HG22	2:H:377:TYR:HE1	1.86	0.41
2:H:153:ILE:HD13	2:H:343:ASP:OD2	2.21	0.40
1:L:115:HIS:O	1:L:116:GLU:C	2.64	0.40
2:H:258:VAL:O	2:H:258:VAL:HG12	2.21	0.40
1:L:57:ASN:ND2	1:L:81:CYS:O	2.51	0.40
1:L:131:VAL:HG23	1:L:132:GLU:N	2.36	0.40

There are no symmetry-related clashes.

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	L	103/104 (99%)	83 (81%)	17 (16%)	3 (3%)	3	13
2	H	253/254 (100%)	239 (94%)	14 (6%)	0	100	100
All	All	356/358 (99%)	322 (90%)	31 (9%)	3 (1%)	14	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	96	GLY
1	L	122	ALA
1	L	86	ASP

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	89/90 (99%)	72 (81%)	17 (19%)	1	5
2	H	217/216 (100%)	207 (95%)	10 (5%)	24	58
All	All	306/306 (100%)	279 (91%)	27 (9%)	11	29

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

Mol	Chain	Res	Type
1	L	49	GLN
1	L	52	SER
1	L	66	GLN
1	L	83	THR
1	L	89	LEU
1	L	103[A]	SER
1	L	103[B]	SER
1	L	106[A]	THR
1	L	106[B]	THR
1	L	111[A]	SER
1	L	111[B]	SER
1	L	113	ARG
1	L	119	SER
1	L	126	SER
1	L	128	THR
1	L	131	VAL
1	L	141	LEU
2	H	172	VAL
2	H	188	VAL
2	H	205	ILE
2	H	208	LEU
2	H	222	SER
2	H	277[A]	ARG
2	H	277[B]	ARG
2	H	317	VAL
2	H	320	SER
2	H	396	ARG

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	49	GLN
1	L	80	ASN
1	L	84	HIS
2	H	203	ASN
2	H	286	GLN
2	H	301	ASN
2	H	312	GLN

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 ⓘ

3 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	A	1	2,3	14,14,15	1.36	1 (7%)	17,19,21	1.90	6 (35%)
3	NAG	A	2	3	14,14,15	1.29	2 (14%)	17,19,21	1.71	6 (35%)
3	FUL	A	3	3	10,10,11	0.73	0	14,14,16	2.73	5 (35%)

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	A	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	A	2	3	-	1/6/23/26	0/1/1/1
3	FUL	A	3	3	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	NAG	O7-C7	-4.08	1.14	1.23
3	A	2	NAG	O7-C7	-2.83	1.16	1.23
3	A	2	NAG	C2-N2	2.02	1.49	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3	FUL	O2-C2-C1	7.16	125.61	109.22
3	A	3	FUL	O3-C3-C4	-3.62	101.84	110.38
3	A	3	FUL	O3-C3-C2	-3.45	103.02	110.05
3	A	1	NAG	C3-C4-C5	3.32	116.26	110.23
3	A	1	NAG	O4-C4-C5	3.24	117.31	109.32
3	A	3	FUL	O5-C1-C2	-3.10	103.38	110.79
3	A	1	NAG	O6-C6-C5	3.06	121.76	111.33
3	A	2	NAG	C2-N2-C7	-3.00	118.89	122.90
3	A	2	NAG	O5-C1-C2	-2.97	106.69	111.29
3	A	2	NAG	C4-C3-C2	2.62	114.86	111.02
3	A	1	NAG	O3-C3-C2	-2.55	104.11	109.40
3	A	1	NAG	O4-C4-C3	2.54	116.35	110.38
3	A	3	FUL	C1-C2-C3	2.41	113.15	109.64
3	A	2	NAG	O4-C4-C5	-2.10	104.16	109.32
3	A	1	NAG	C1-O5-C5	-2.05	109.44	112.19
3	A	2	NAG	C1-O5-C5	-2.02	109.48	112.19
3	A	2	NAG	O3-C3-C2	2.01	113.57	109.40

There are no chirality outliers.

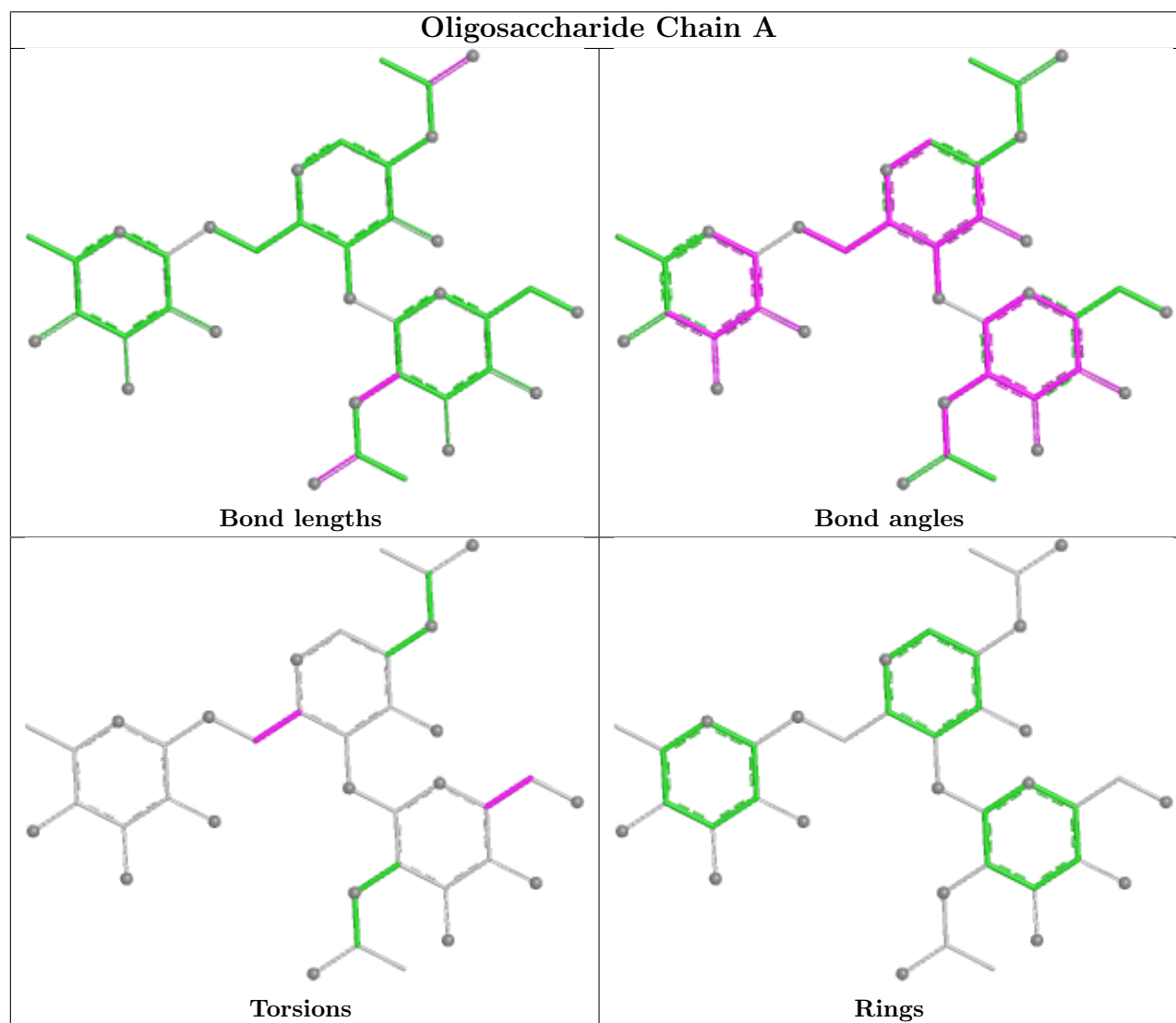
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	NAG	O5-C5-C6-O6
3	A	1	NAG	C4-C5-C6-O6
3	A	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](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	0Z6	H	1	2	34,35,36	1.22	2 (5%)	41,45,46	1.42	7 (17%)
5	FUC	L	160	1	10,10,11	0.83	0	14,14,16	2.28	4 (28%)
4	GLC	L	153	1	11,11,12	0.62	0	15,15,17	1.38	3 (20%)

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
6	0Z6	H	1	2	1/1/7/10	6/35/35/37	0/2/2/2
5	FUC	L	160	1	1/1/4/5	-	0/1/1/1
4	GLC	L	153	1	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	1	0Z6	O2-C2	-4.99	1.29	1.43
6	H	1	0Z6	C3-C2	4.02	1.63	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	160	FUC	C1-O5-C5	6.02	127.17	112.97
5	L	160	FUC	O5-C5-C4	3.34	115.57	109.55
6	H	1	0Z6	CB-CA-C	-3.15	101.61	108.97
4	L	153	GLC	C2-C3-C4	-2.96	105.66	110.86
4	L	153	GLC	O2-C2-C1	2.86	115.77	109.22
6	H	1	0Z6	C-CA-N	2.83	120.04	109.37
6	H	1	0Z6	O2-C2-C3	2.55	117.31	109.68
6	H	1	0Z6	CB1-CG1-CD21	2.46	125.49	120.90
6	H	1	0Z6	CA2-N2-C1	-2.46	118.96	123.25
6	H	1	0Z6	C1-CA1-N1	2.45	117.75	111.11
6	H	1	0Z6	CB2-CA2-N2	-2.41	107.17	110.30
4	L	153	GLC	O2-C2-C3	2.39	115.11	110.15
5	L	160	FUC	O3-C3-C4	2.38	115.99	110.38
5	L	160	FUC	C6-C5-C4	2.17	117.04	113.08

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	160	FUC	C1
6	H	1	OZ6	C2

All (8) torsion outliers are listed below:

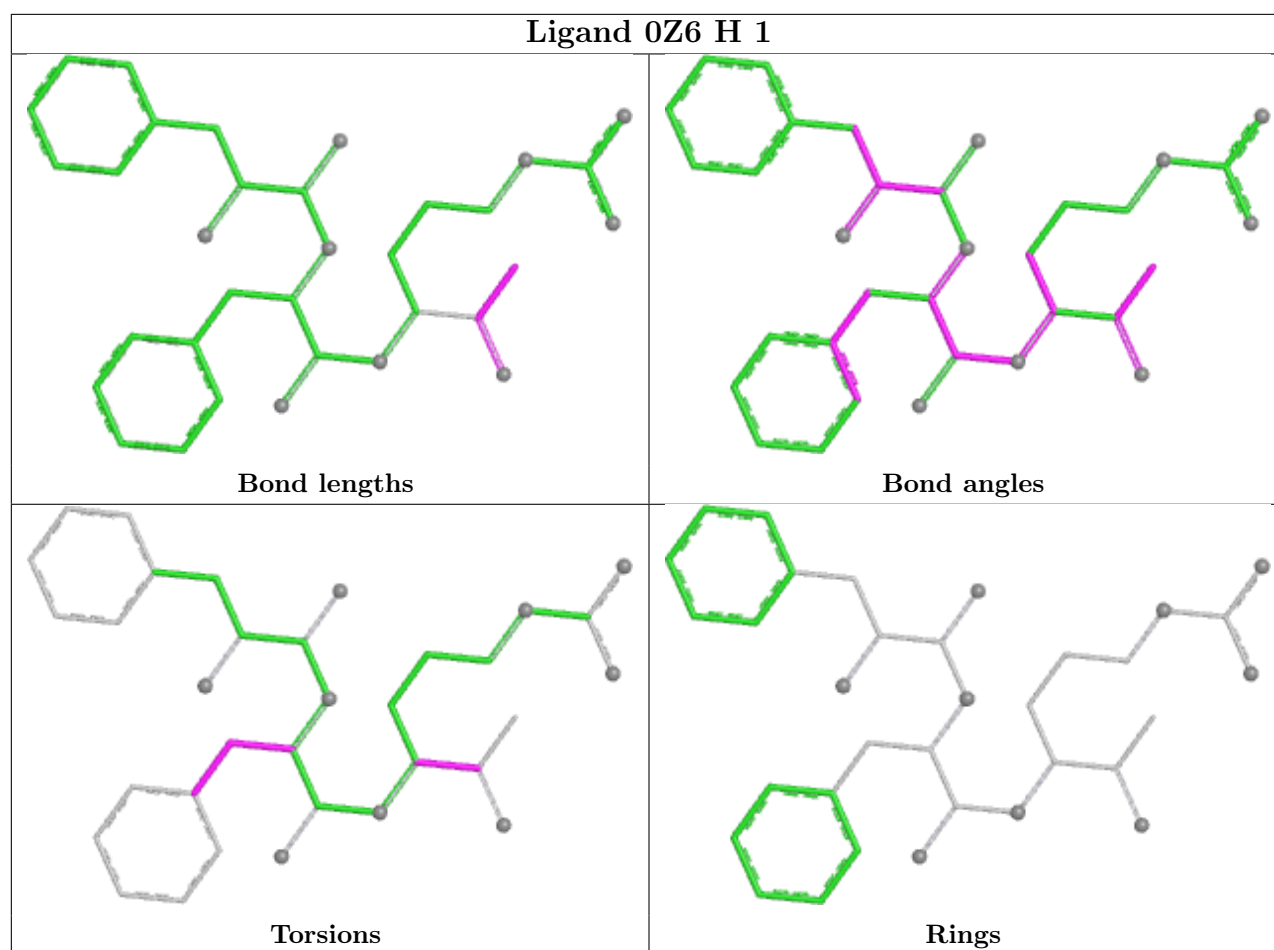
Mol	Chain	Res	Type	Atoms
6	H	1	OZ6	C3-C2-CA2-N2
6	H	1	OZ6	C3-C2-CA2-CB2
6	H	1	OZ6	C1-CA1-CB1-CG1
4	L	153	GLC	O5-C5-C6-O6
4	L	153	GLC	C4-C5-C6-O6
6	H	1	OZ6	N1-CA1-CB1-CG1
6	H	1	OZ6	CA1-CB1-CG1-CD11
6	H	1	OZ6	CA1-CB1-CG1-CD21

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	153	GLC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	96/104 (92%)	1.55	24 (25%) 2 1	39, 76, 95, 98	9 (9%)
2	H	252/254 (99%)	0.06	8 (3%) 50 40	26, 44, 72, 105	5 (1%)
All	All	348/358 (97%)	0.47	32 (9%) 14 10	26, 49, 91, 105	14 (4%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	106[A]	THR	15.1
1	L	108[A]	THR	10.7
1	L	105[A]	HIS	8.8
1	L	109[A]	LYS	7.1
2	H	317	VAL	6.4
1	L	122	ALA	3.4
2	H	318	GLY	3.2
1	L	83	THR	3.2
2	H	200	ASN	3.2
1	L	49	GLN	3.0
1	L	107[A]	GLY	2.9
2	H	392[A]	ARG	2.8
1	L	75	ALA	2.5
1	L	144	ARG	2.5
1	L	58	GLY	2.5
1	L	55	CYS	2.5
2	H	319	ASP	2.5
1	L	125	VAL	2.5
1	L	120	LEU	2.4
1	L	121	LEU	2.4
1	L	71	PHE	2.4
1	L	94	GLU	2.4
2	H	201	TRP	2.4
1	L	77	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	89	LEU	2.3
1	L	111[A]	SER	2.2
2	H	312	GLN	2.2
1	L	140	ILE	2.1
2	H	385	GLU	2.1
1	L	60	SER	2.1
1	L	119	SER	2.1
1	L	128	THR	2.1

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

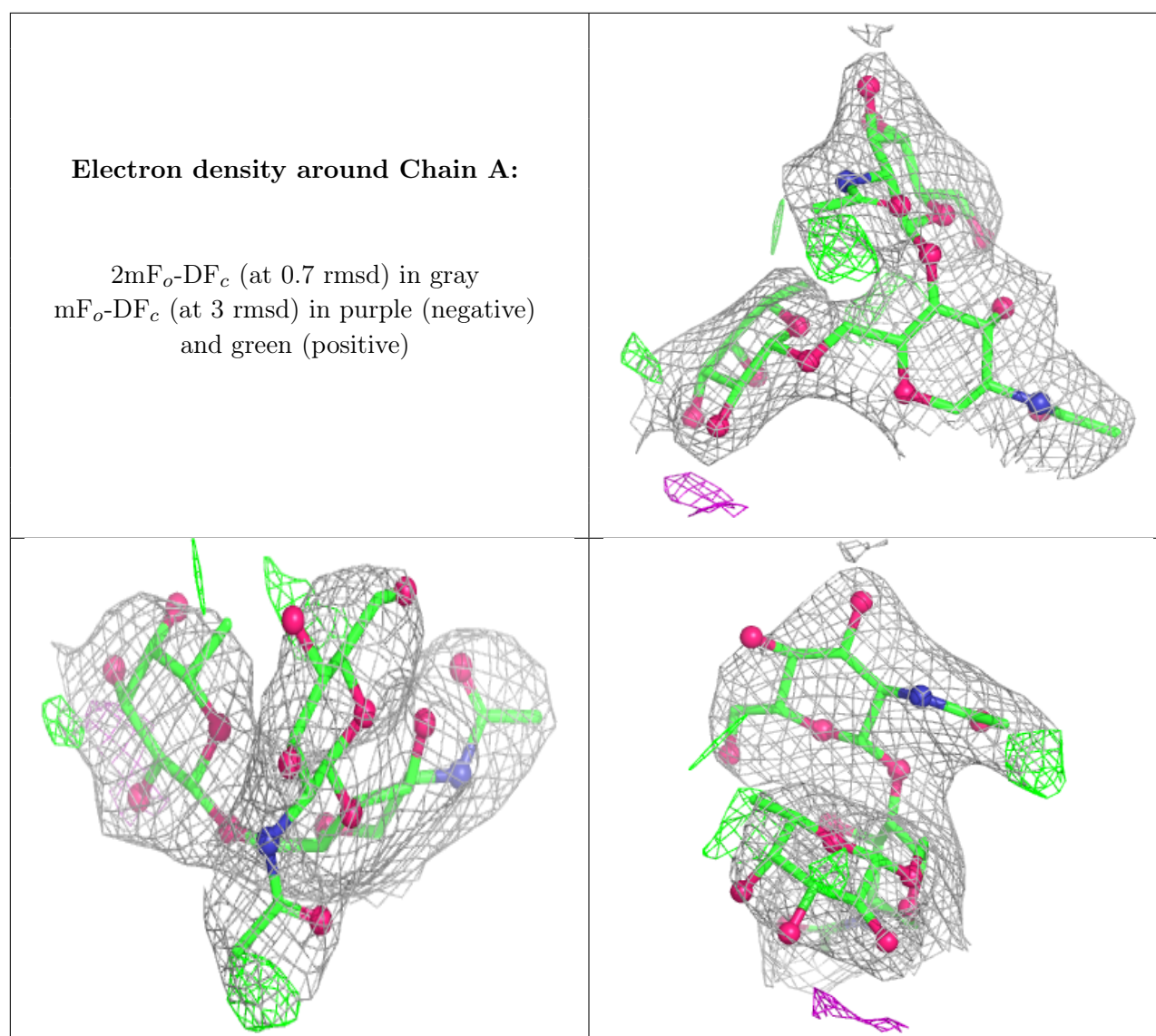
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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
3	NAG	A	1	14/15	-	-	52,54,59,65	0
3	NAG	A	2	14/15	-	-	68,72,74,76	0
3	FUL	A	3	10/11	-	-	57,59,60,62	0

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



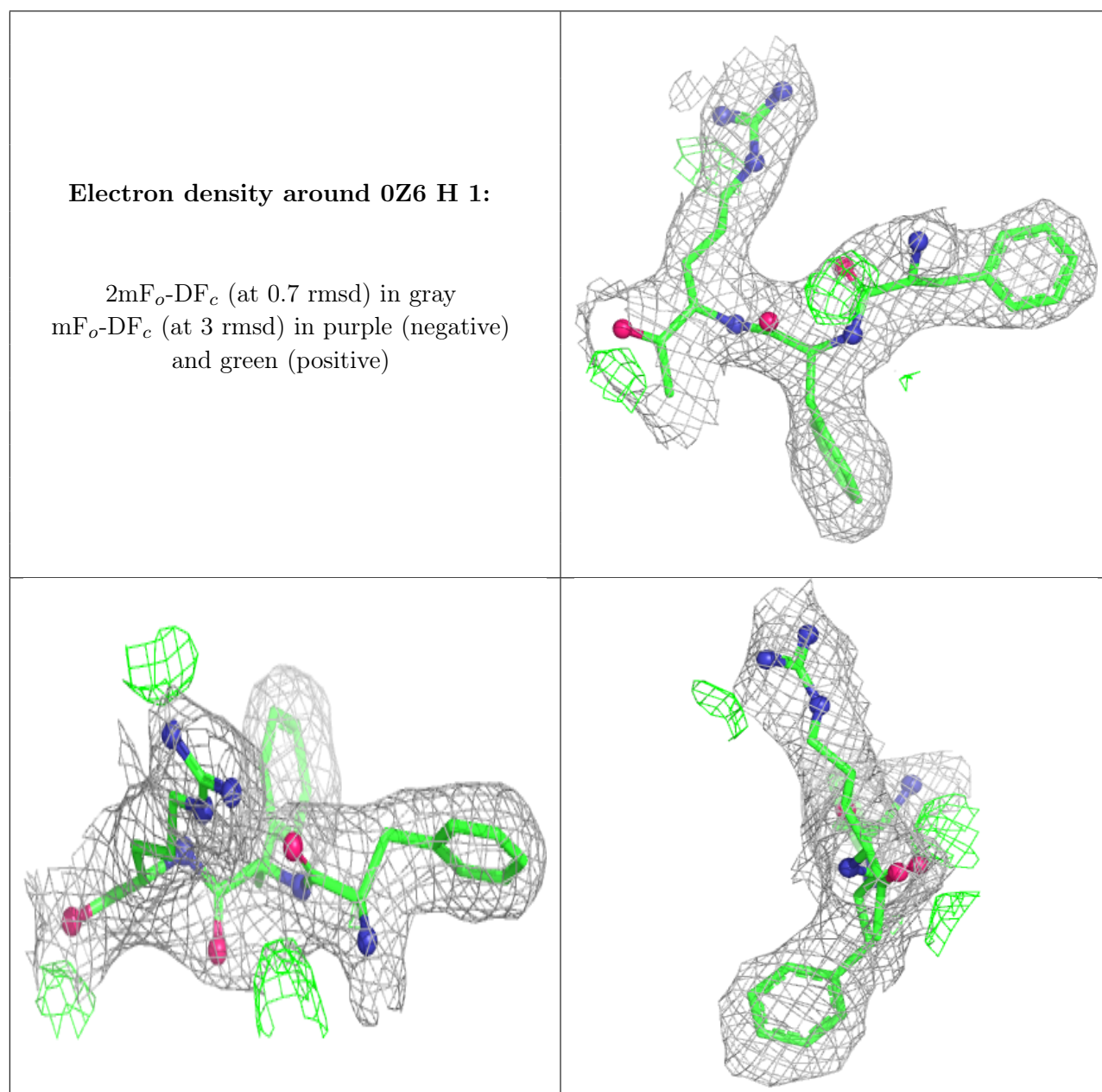
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	FUC	L	160	10/11	0.53	0.22	100,101,102,102	0
4	GLC	L	153	11/12	0.78	0.13	96,97,97,97	0
6	OZ6	H	1	34/35	0.93	0.10	34,40,45,46	0
7	CA	H	500	1/1	0.94	0.07	73,73,73,73	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.