Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2023 – 05:54 PM EDT

PDB ID	:	1QFK
Title	:	STRUCTURE OF HUMAN FACTOR VIIA AND ITS IMPLICATIONS FOR THE TRIGGERING OF BLOOD COAGULATION
Authors	:	Pike, A.C.W.; Brzozowski, A.M.; Roberts, S.M.; Olsen, O.H.; Persson, E.
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.

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 (i) 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 (i)) were used in the production of this report:

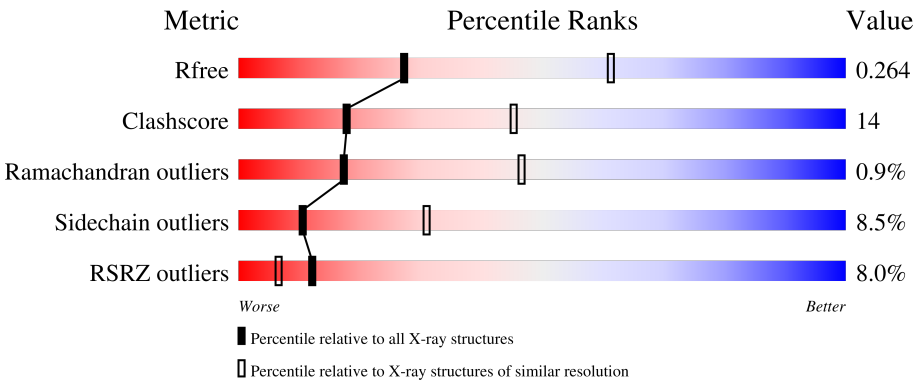
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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%; 42%; 36%; 13%; • ; 8%
2	H	254	2%; 67%; 27%; 5%; ••
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	0Z6	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.

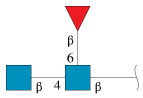
- Molecule 1 is a protein called COAGULATION FACTOR VIIA LIGHT CHAIN.

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

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

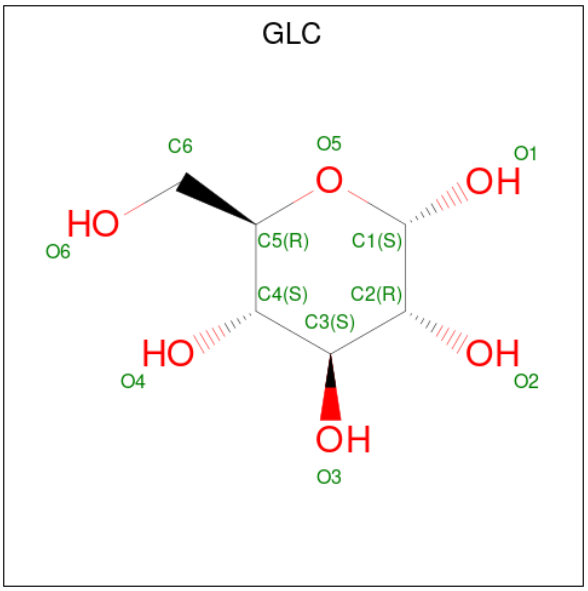
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	252	1972	1249	351	359	13	0	5	0

- 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.



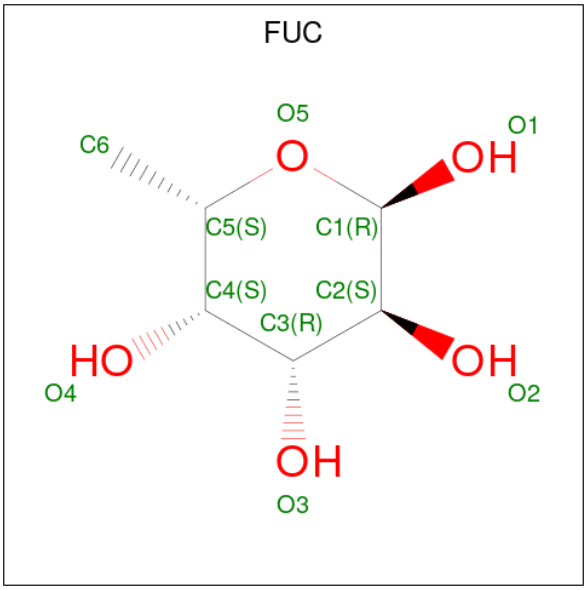
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	A	3	38	22	2	14	0	0	0

- Molecule 4 is alpha-D-glucopyranose (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



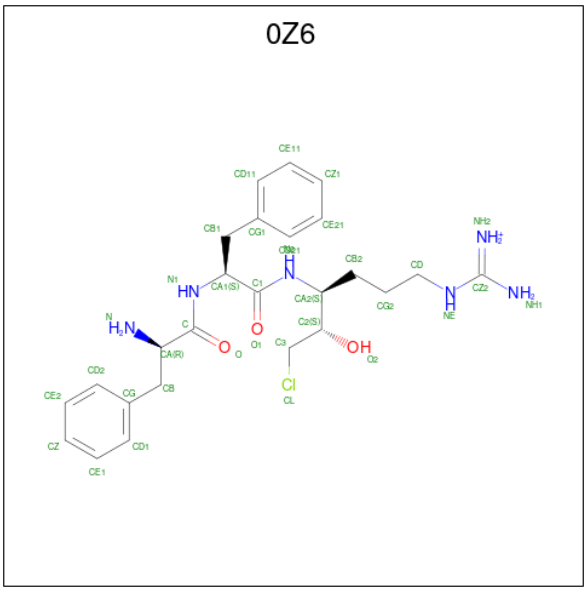
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	L	1	11	6	5	0	0

- Molecule 5 is alpha-L-fucopyranose (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



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

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



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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is water.

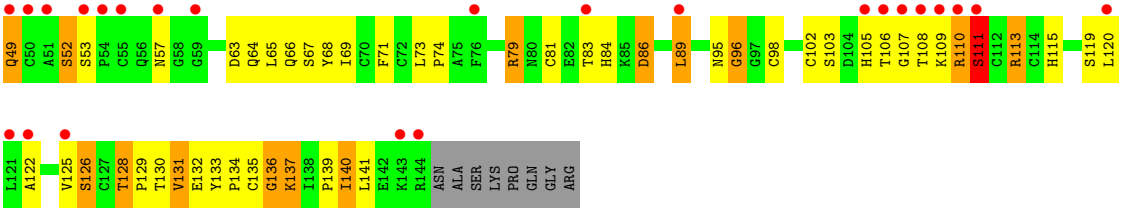
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	L	10	10	10	0	0
			Total	O		
8	H	74	74	74	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

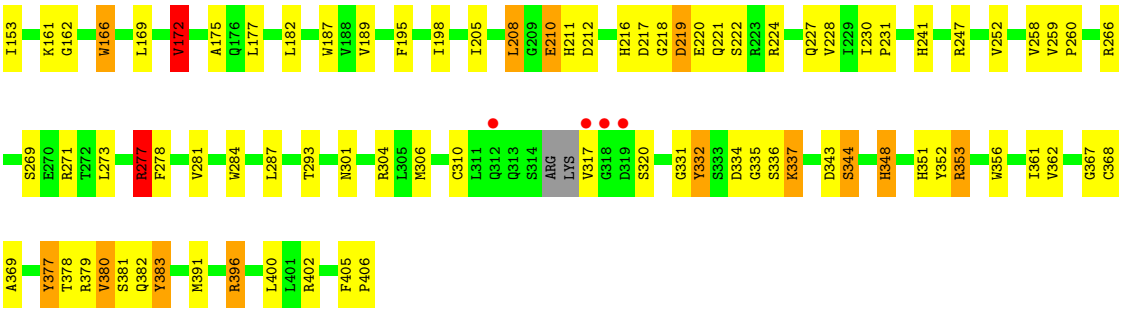
• Molecule 1: COAGULATION FACTOR VIIA LIGHT CHAIN

Chain L: 23% 42% 36% 13% • 8%



• Molecule 2: COAGULATION FACTOR VIIA HEAVY CHAIN

Chain H: 2% 67% 27% 5% ••



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

Chain A: 100%

4 Data and refinement statistics (i)

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 34.17 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.4 (35.00-2.80) 95.5 (34.17-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [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 , 49.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, GLC, 0Z6, NAG, CA, FUL

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	0.62	0/797	1.58	12/1076 (1.1%)
2	H	0.76	1/2043 (0.0%)	1.87	49/2780 (1.8%)
All	All	0.73	1/2840 (0.0%)	1.79	61/3856 (1.6%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	344	SER	CB-OG	7.13	1.51	1.42

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	396	ARG	CD-NE-CZ	13.83	142.97	123.60
2	H	266	ARG	NE-CZ-NH2	10.83	125.71	120.30
2	H	379	ARG	NE-CZ-NH2	-10.48	115.06	120.30
2	H	212	ASP	CB-CG-OD2	-10.25	109.07	118.30
2	H	396	ARG	NE-CZ-NH2	-10.02	115.29	120.30
2	H	210	GLU	OE1-CD-OE2	9.91	135.19	123.30
2	H	247[A]	ARG	NE-CZ-NH2	-9.76	115.42	120.30
2	H	247[B]	ARG	NE-CZ-NH2	-9.76	115.42	120.30
2	H	304	ARG	CD-NE-CZ	9.39	136.75	123.60
2	H	377	TYR	CB-CG-CD1	-8.79	115.73	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	379	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	L	113	ARG	NE-CZ-NH2	-8.31	116.14	120.30
2	H	304	ARG	NE-CZ-NH1	8.09	124.34	120.30
2	H	352	TYR	CB-CG-CD1	7.89	125.73	121.00
2	H	402	ARG	CD-NE-CZ	7.70	134.38	123.60
2	H	348	HIS	N-CA-C	-7.65	90.34	111.00
2	H	383	TYR	CB-CG-CD1	7.42	125.45	121.00
2	H	332	TYR	CB-CG-CD1	-7.31	116.61	121.00
2	H	352	TYR	CB-CG-CD2	-7.15	116.71	121.00
2	H	353	ARG	CD-NE-CZ	6.93	133.30	123.60
1	L	107[A]	GLY	N-CA-C	6.78	130.06	113.10
1	L	107[B]	GLY	N-CA-C	6.78	130.06	113.10
2	H	379	ARG	CD-NE-CZ	6.74	133.03	123.60
2	H	306	MET	CA-CB-CG	6.72	124.72	113.30
2	H	277[A]	ARG	CG-CD-NE	6.68	125.82	111.80
2	H	277[B]	ARG	CG-CD-NE	6.68	125.82	111.80
2	H	304	ARG	NH1-CZ-NH2	-6.65	112.08	119.40
2	H	210	GLU	CG-CD-OE1	-6.63	105.05	118.30
2	H	224	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	L	102	CYS	CA-CB-SG	6.56	125.81	114.00
2	H	304	ARG	NE-CZ-NH2	6.54	123.57	120.30
1	L	113	ARG	NE-CZ-NH1	6.53	123.56	120.30
2	H	219	ASP	CB-CG-OD1	-6.45	112.50	118.30
2	H	353	ARG	NE-CZ-NH2	6.27	123.43	120.30
1	L	137	LYS	CA-CB-CG	6.25	127.16	113.40
2	H	224	ARG	NE-CZ-NH2	-6.24	117.18	120.30
2	H	277[A]	ARG	CD-NE-CZ	6.16	132.22	123.60
2	H	277[B]	ARG	CD-NE-CZ	6.16	132.22	123.60
1	L	140	ILE	CA-C-N	6.13	130.68	117.20
2	H	247[A]	ARG	CD-NE-CZ	6.10	132.14	123.60
2	H	247[B]	ARG	CD-NE-CZ	6.10	132.14	123.60
2	H	377	TYR	CB-CG-CD2	5.93	124.56	121.00
2	H	337	LYS	N-CA-CB	-5.90	99.98	110.60
2	H	172	VAL	N-CA-CB	5.85	124.37	111.50
2	H	380	VAL	O-C-N	-5.73	113.54	122.70
1	L	131	VAL	N-CA-CB	5.69	124.02	111.50
2	H	227	GLN	N-CA-CB	-5.62	100.47	110.60
2	H	334	ASP	CA-C-N	5.56	127.33	116.20
2	H	382	GLN	CG-CD-OE1	-5.49	110.62	121.60
2	H	396	ARG	NE-CZ-NH1	5.47	123.04	120.30
2	H	310	CYS	CA-CB-SG	-5.27	104.52	114.00
2	H	221	GLN	CA-CB-CG	5.25	124.95	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	113	ARG	CA-CB-CG	5.21	124.87	113.40
2	H	218	GLY	CA-C-O	-5.20	111.25	120.60
1	L	136	GLY	N-CA-C	5.18	126.06	113.10
1	L	133	TYR	CB-CG-CD2	5.06	124.04	121.00
2	H	271	ARG	CD-NE-CZ	5.05	130.67	123.60
1	L	130	THR	N-CA-CB	5.04	119.88	110.30
2	H	175	ALA	CB-CA-C	-5.04	102.54	110.10
2	H	221	GLN	CG-CD-NE2	5.03	128.76	116.70
2	H	353	ARG	NH1-CZ-NH2	-5.01	113.89	119.40

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 (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	778	0	699	34	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	76	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 (76) 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
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
2:H:380:VAL:O	2:H:381:SER:C	2.44	0.54
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
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
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:343:ASP:O	2:H:344:SER:C	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:277[A]:ARG:HG2	2:H:277[A]:ARG:HH11	1.80	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: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:95:ASN:O	1:L:96:GLY:C	2.57	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
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
1:L:52:SER:O	1:L:53:SER:C	2.59	0.40
2:H:153:ILE:HD13	2:H:343:ASP:OD2	2.21	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%)	4 15
2	H	253/254 (100%)	239 (94%)	14 (6%)	0	100 100
All	All	356/358 (99%)	322 (90%)	31 (9%)	3 (1%)	17 49

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 (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	L	89/90 (99%)	70 (79%)	19 (21%)	1 3
2	H	217/216 (100%)	206 (95%)	11 (5%)	24 55
All	All	306/306 (100%)	276 (90%)	30 (10%)	10 24

All (30) 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	79	ARG
1	L	83	THR
1	L	89	LEU
1	L	103[A]	SER
1	L	103[B]	SER
1	L	106[A]	THR

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Mol	Chain	Res	Type
1	L	106[B]	THR
1	L	110[A]	ARG
1	L	110[B]	ARG
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	141	LEU
2	H	166	TRP
2	H	172	VAL
2	H	205	ILE
2	H	208	LEU
2	H	219	ASP
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 (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)

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	3,2	14,14,15	1.33	1 (7%)	17,19,21	1.90	6 (35%)
3	NAG	A	2	3	14,14,15	1.29	1 (7%)	17,19,21	1.68	4 (23%)
3	FUL	A	3	3	10,10,11	0.71	0	14,14,16	3.11	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	3,2	-	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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	NAG	O7-C7	-4.03	1.14	1.23
3	A	2	NAG	O7-C7	-2.80	1.16	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	3	FUL	O2-C2-C1	8.04	125.61	109.15
3	A	3	FUL	O5-C1-C2	-4.79	103.38	110.77
3	A	3	FUL	O3-C3-C4	-3.68	101.84	110.35
3	A	3	FUL	O3-C3-C2	-3.64	103.02	109.99
3	A	1	NAG	C3-C4-C5	3.37	116.26	110.24
3	A	1	NAG	O4-C4-C5	3.23	117.31	109.30
3	A	1	NAG	O6-C6-C5	3.05	121.76	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2	NAG	O5-C1-C2	-2.91	106.69	111.29
3	A	3	FUL	C1-C2-C3	2.84	113.15	109.67
3	A	2	NAG	C2-N2-C7	-2.82	118.89	122.90
3	A	2	NAG	C4-C3-C2	2.62	114.86	111.02
3	A	1	NAG	O4-C4-C3	2.60	116.35	110.35
3	A	1	NAG	O3-C3-C2	-2.59	104.11	109.47
3	A	2	NAG	O4-C4-C5	-2.07	104.16	109.30
3	A	1	NAG	C1-O5-C5	-2.03	109.44	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

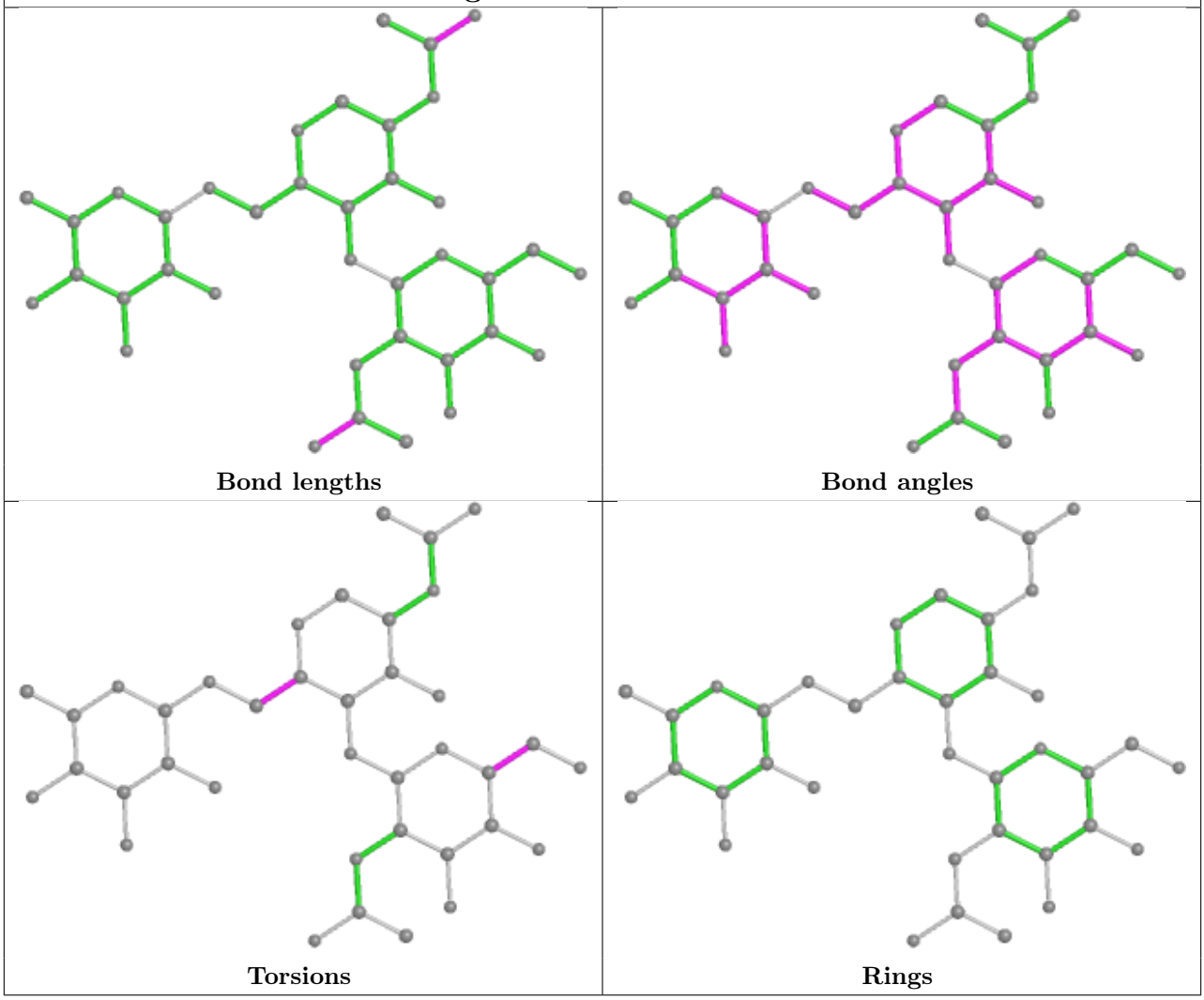
Mol	Chain	Res	Type	Atoms
3	A	1	NAG	O5-C5-C6-O6
3	A	1	NAG	C4-C5-C6-O6
3	A	2	NAG	O5-C5-C6-O6

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.

Oligosaccharide Chain A



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	$\#\|Z\| > 2$
4	GLC	L	153	1	11,11,12	0.63	0	15,15,17	1.50	3 (20%)
6	0Z6	H	1	2	34,35,36	1.18	2 (5%)	41,45,46	1.87	8 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	FUC	L	160	1	10,10,11	0.86	1 (10%)	14,14,16	2.38	4 (28%)

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	GLC	L	153	1	-	2/2/19/22	0/1/1/1
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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	1	0Z6	O2-C2	-4.83	1.29	1.43
6	H	1	0Z6	C3-C2	3.89	1.63	1.51
5	L	160	FUC	O5-C1	-2.09	1.40	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	1	0Z6	CB2-CA2-C2	8.28	126.89	112.51
5	L	160	FUC	C1-O5-C5	6.35	127.17	112.78
5	L	160	FUC	O5-C5-C4	3.37	115.57	109.52
4	L	153	GLC	O2-C2-C1	3.23	115.77	109.15
6	H	1	0Z6	CB-CA-C	-3.15	101.61	108.97
4	L	153	GLC	C2-C3-C4	-3.02	105.66	110.89
6	H	1	0Z6	C-CA-N	2.75	120.04	109.40
6	H	1	0Z6	O2-C2-C3	2.55	117.31	109.74
4	L	153	GLC	O2-C2-C3	2.48	115.11	110.14
5	L	160	FUC	O3-C3-C4	2.44	115.99	110.35
6	H	1	0Z6	C1-CA1-N1	2.42	117.75	111.16
6	H	1	0Z6	CB2-CA2-N2	-2.40	107.17	110.33
6	H	1	0Z6	CA2-N2-C1	-2.33	118.96	123.07
6	H	1	0Z6	CB1-CG1-CD21	2.31	125.49	120.91
5	L	160	FUC	C6-C5-C4	2.15	117.04	113.07

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	160	FUC	C1
6	H	1	0Z6	C2

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	H	1	0Z6	C3-C2-CA2-N2
6	H	1	0Z6	C3-C2-CA2-CB2
6	H	1	0Z6	C1-CA1-CB1-CG1
4	L	153	GLC	O5-C5-C6-O6
4	L	153	GLC	C4-C5-C6-O6
6	H	1	0Z6	N1-CA1-CB1-CG1
6	H	1	0Z6	CA1-CB1-CG1-CD11
6	H	1	0Z6	CA1-CB1-CG1-CD21

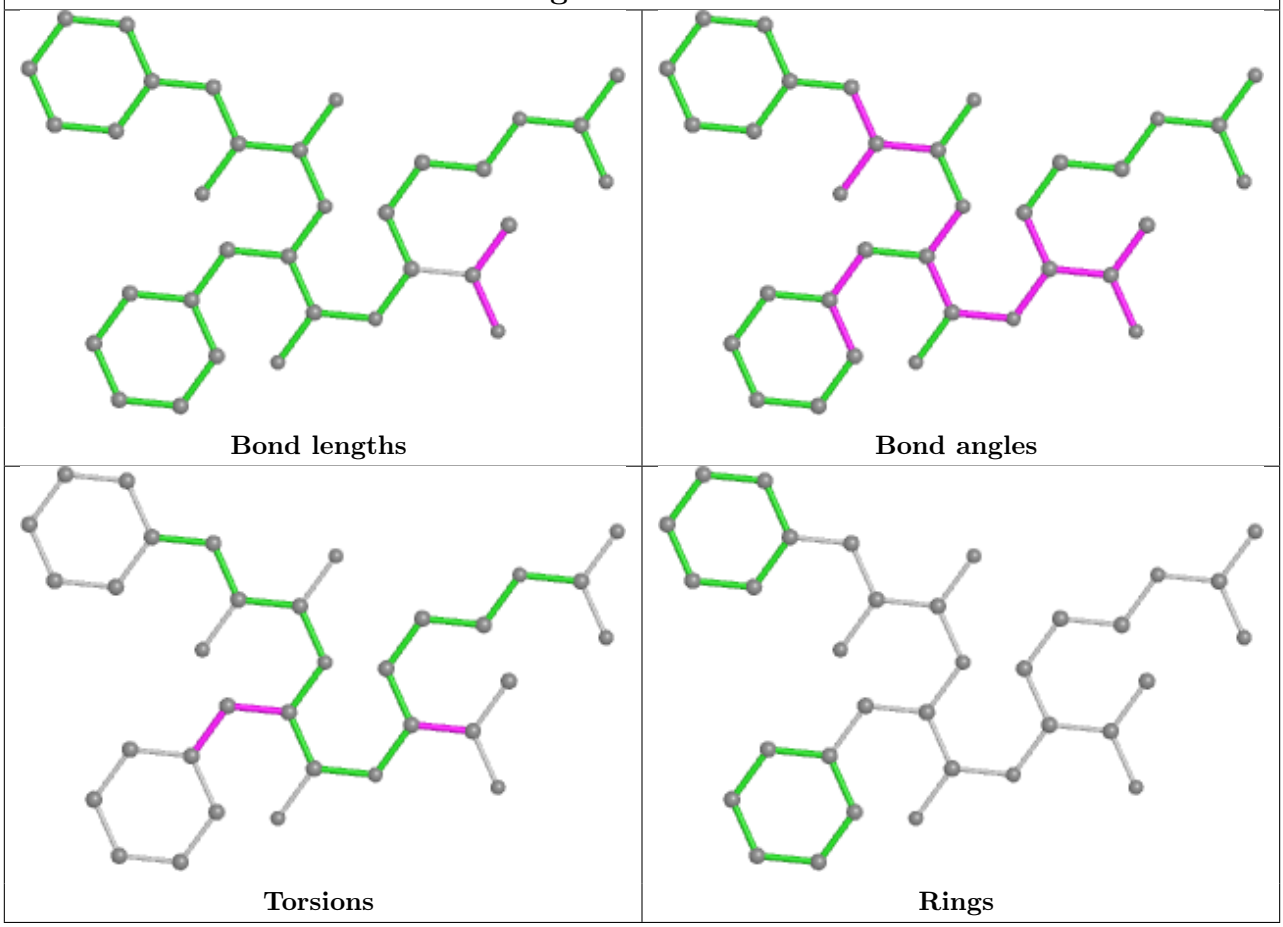
There are no ring outliers.

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 then 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.

Ligand 0Z6 H 1



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	L	96/104 (92%)	1.10	24 (25%)	0	0	49, 79, 95, 98	0
2	H	252/254 (99%)	-0.13	4 (1%)	72	66	27, 44, 72, 105	0
All	All	348/358 (97%)	0.21	28 (8%)	12	6	27, 50, 93, 105	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	49	GLN	4.6
1	L	106[A]	THR	4.3
1	L	122	ALA	4.2
2	H	318	GLY	4.2
1	L	59	GLY	3.7
1	L	89	LEU	3.5
1	L	110[A]	ARG	3.3
1	L	83	THR	3.0
2	H	319	ASP	2.9
1	L	51	ALA	2.9
1	L	107[A]	GLY	2.9
1	L	111[A]	SER	2.9
1	L	76	PHE	2.9
1	L	105[A]	HIS	2.8
1	L	143	LYS	2.8
1	L	121	LEU	2.8
1	L	125	VAL	2.7
1	L	144	ARG	2.7
1	L	54	PRO	2.6
1	L	55	CYS	2.6
1	L	120	LEU	2.5
2	H	317	VAL	2.5
1	L	50	CYS	2.4
1	L	53	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	312	GLN	2.1
1	L	108[A]	THR	2.1
1	L	109[A]	LYS	2.1
1	L	57	ASN	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)

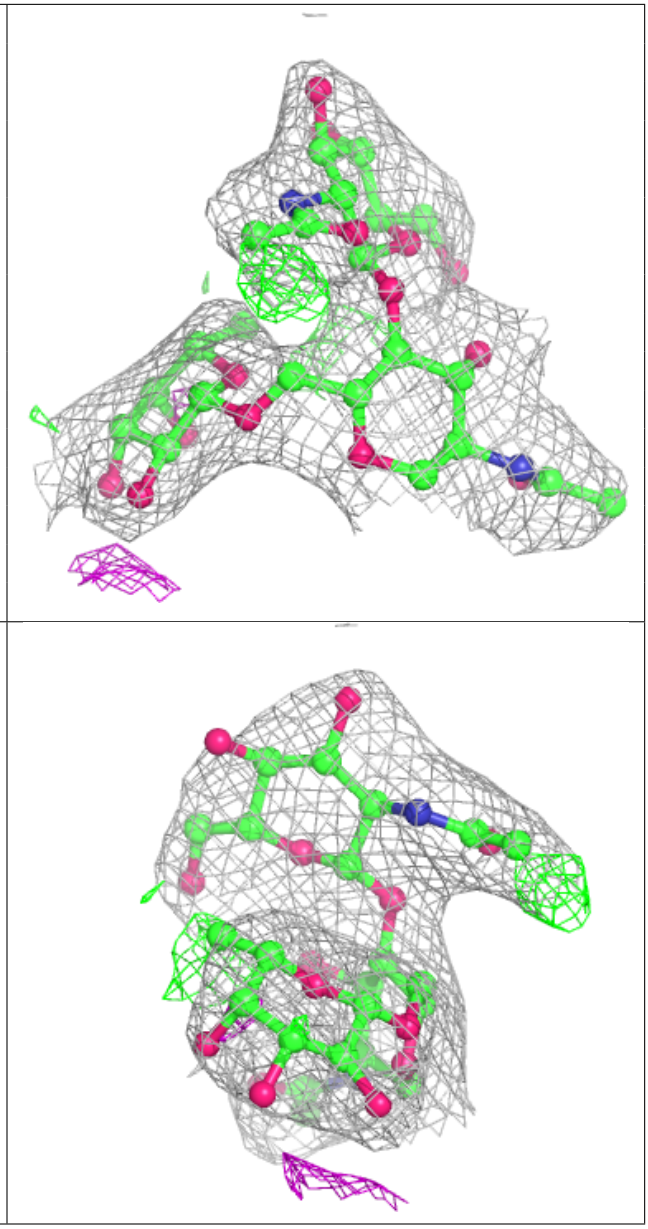
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	NAG	A	2	14/15	0.86	0.33	68,72,74,76	0
3	FUL	A	3	10/11	0.92	0.22	57,59,60,62	0
3	NAG	A	1	14/15	0.93	0.17	52,54,59,65	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 A:

$2mF_o$-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)

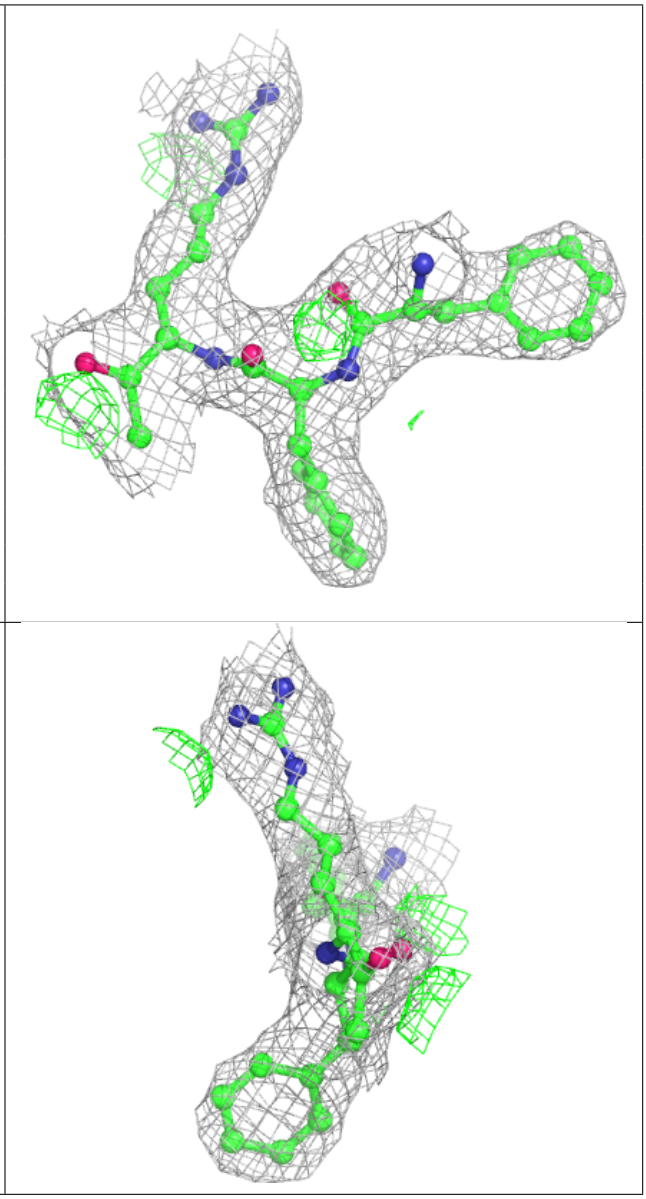
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GLC	L	153	11/12	0.86	0.31	96,97,97,97	0
5	FUC	L	160	10/11	0.87	0.15	100,101,102,102	0
6	0Z6	H	1	34/35	0.92	0.20	34,40,45,46	0
7	CA	H	500	1/1	0.96	0.15	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.

Electron density around 0Z6 H 1:

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



6.5 Other polymers (i)

There are no such residues in this entry.