

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	6Y0F
Title	:	Structure of human FAPalpha in complex with linagliptin
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Deposited on	:	2020-02-07
Resolution	:	2.92 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 following versions of software and data (see references (1)) 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	:	2.16
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)	:	2.16

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 2.92 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462(2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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	А	722	87%	12%	•
1	В	722	% 8 7%	12%	
1	C	722	07%	1270	
1		720	87% %	13%	•
	D	722	86%	13%	•
2	E	2	100%		



	Chain	I previous	Ouglitan of the in	
IVIOI	Chain	Length	Quality of chain	
	a			
2	G	2	100%	
	тт	2		
2	H	2	50%	50%
	Ŧ			
2	1	2	100%	
	-			
2	J	2	100%	
3	F'	3	67%	33%
	T 7			
4	K	2	50%	50%
	 т			
4	L	2	100%	
4	M	2	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
4	FUC	K	2	-	-	-	Х
4	FUC	L	2	-	-	-	Х

Continued from previous page...



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 24077 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.

Mol	Chain	Residues		A	toms			ZeroOcc	AltConf	Trace
1	Λ	721	Total	С	Ν	Ο	S	0	0	0
	л		5904	3820	964	1098	22	0	0	0
1	В	710	Total	С	Ν	Ο	S	0	0	0
	D	719	5889	3812	961	1094	22	0	0	0
1	C	799	Total	С	Ν	Ο	S	0	0	0
		122	5913	3825	965	1101	22	0	0	U
1	р	720	Total	С	Ν	Ο	S	0	0	0
		(20	5896	3816	962	1096	22			U

• Molecule 1 is a protein called Prolyl endopeptidase FAP.

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace	
9	F	9	Total C N O	0	0	0	
		2	28 16 2 10	0	0	0	
9	C	0	Total C N O	0	0	0	
	G	2	28 16 2 10	0	0	0	
9	Ц	0	Total C N O	0	0	0	
	11	2	28 16 2 10	0	0	0	
9	т	0	Total C N O	0	0	0	
	L	2	28 16 2 10	0	0	0	
0	т	2	Total C N O	0	0	0	
	J	J Z	28 16 2 10	0	0	U	

• Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
3	F	3	Total 39	С 22	N 2	O 15	0	0	0

• Molecule 4 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-bet a-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	Κ	2	Total C N O 24 14 1 9	0	0	0
4	L	2	Total C N O 24 14 1 9	0	0	0
4	М	2	Total C N O 24 14 1 9	0	0	0

• 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
5	Δ	1	Total C N	0	0	Ο
0	Л	T	14 8 1	5	0	0
5	Δ	1	Total C N	Ο	0	0
0	11	I	14 8 1	5	0	0
5	Δ	1	Total C N	Ο	0	0
0	11	I	14 8 1	5	0	0
5	В	1	Total C N	Ο	0	0
0	D	I	$14 \ 8 \ 1$	5	0	0
5	С	1	Total C N	Ο	0	0
0	U	T	$14 \ 8 \ 1$	5	0	0
5	П	1	Total C N	0	0	0
0			$14 \ 8 \ 1$	5		0

• Molecule 6 is 8-[(3R)-3-Aminopiperidin-1-yl]-7-but-2-yn-1-yl-3-methyl-1-[(4-methylqui nazolin-2-yl)methyl]-3,7-dihydro-1H-purine-2,6-d ione (three-letter code: 356) (formula: C₂₅H₂₈N₈O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	Λ	1	Total C N O	0	0
0	л	T	35 25 8 2	0	0
6	В	1	Total C N O	0	0
0	D	L	35 25 8 2	0	0
6	С	1	Total C N O	0	0
0	U	L	35 25 8 2	0	0
6	л	1	Total C N O	0	0
0			35 25 8 2	0	



Chain C:

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.



87%

13%

• Molecule 1: Prolyl endopeptidase FAP



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

Chain E:

100%

NAG1 NAG2

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

Chain G:

100%

NAG1 NAG2

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

Chain H:	50%

50%





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

Chain I:

100%

NAG1 NAG2

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

Chain J:	100	0%
NAG1 NAG2		
• Molecule 3: be etamido-2-deoxy	eta-D-mannopyranose-(1-4 z-beta-D-glucopyranose)-2-acetamido-2-deoxy-beta-D-g
Chain F:	67%	33%
NAG1 NAG2 BNA3		
• Molecule 4: al	pha-L-fucopyranose-(1-6)-	2-acetamido-2-deoxy-beta-D-glu
Chain K:	50%	50%
NAG1 FUC2		
• Molecule 4: al	pha-L-fucopyranose-(1-6)-	2-acetamido-2-deoxy-beta-D-glu
Chain L:	100	0%
NAG1 FUC2		
• Molecule 4: al	pha-L-fucopyranose-(1-6)-	2-acetamido-2-deoxy-beta-D-glu
Chain M:	10	00%
NAG1 FUC2		



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	67.59Å 253.60 Å 115.25 Å	Deperitor
a, b, c, α , β , γ	90.00° 89.76° 90.00°	Depositor
D application $\begin{pmatrix} \hat{\lambda} \end{pmatrix}$	47.93 - 2.92	Depositor
Resolution (A)	47.93 - 2.92	EDS
% Data completeness	98.0 (47.93-2.92)	Depositor
(in resolution range $)$	96.8(47.93-2.92)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) > 1$	$2.01 (at 2.91 \text{\AA})$	Xtriage
Refinement program	BUSTER 2.11.7 (17-DEC-2019)	Depositor
D D.	0.207 , 0.243	Depositor
Π, Π_{free}	0.194 , 0.197	DCC
R_{free} test set	656 reflections $(0.80%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	49.1	Xtriage
Anisotropy	0.624	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , 17.2	EDS
L-test for twinning ²	$< L >=0.44, < L^2>=0.27$	Xtriage
Estimated twinning fraction	0.297 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	24077	wwPDB-VP
Average B, all atoms $(Å^2)$	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: 356, BMA, NAG, FUC

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).

Mal	Chain	Bo	nd lengths	Bo	ond angles
10101	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.35	1/6080~(0.0%)	0.54	1/8271~(0.0%)
1	В	0.34	0/6065	0.54	0/8250
1	С	0.35	0/6089	0.54	0/8283
1	D	0.34	0/6072	0.54	0/8260
All	All	0.34	1/24306~(0.0%)	0.54	1/33064~(0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
1	А	679	ASN	CG-ND2	-6.09	1.17	1.32

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	679	ASN	OD1-CG-ND2	-7.44	104.78	121.90

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	А	5904	0	5676	50	0
1	В	5889	0	5663	44	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	С	5913	0	5685	56	0
1	D	5896	0	5672	51	0
2	Е	28	0	25	0	0
2	G	28	0	25	0	0
2	Н	28	0	25	1	0
2	Ι	28	0	25	0	0
2	J	28	0	25	0	0
3	F	39	0	34	0	0
4	Κ	24	0	22	1	0
4	L	24	0	22	0	0
4	М	24	0	22	0	0
5	А	42	0	39	1	0
5	В	14	0	13	1	0
5	С	14	0	13	0	0
5	D	14	0	13	0	0
6	А	35	0	28	2	0
6	В	35	0	28	3	0
6	С	35	0	28	5	0
6	D	35	0	28	4	0
All	All	24077	0	23111	213	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 5.

All (213) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
6:C:806:356:H62	6:C:806:356:H161	1.41	1.03
1:A:679:ASN:OD1	5:A:805:NAG:O5	1.69	0.96
1:A:464:LEU:HD12	1:A:477:HIS:CE1	2.03	0.93
6:D:808:356:H161	6:D:808:356:H62	1.51	0.93
1:D:539:GLN:HG3	1:D:621:TRP:NE1	1.86	0.91
1:B:539:GLN:HG3	1:B:621:TRP:NE1	1.87	0.90
1:D:464:LEU:HD12	1:D:477:HIS:CE1	2.07	0.89
1:A:539:GLN:HG3	1:A:621:TRP:NE1	1.87	0.89
1:C:539:GLN:HG3	1:C:621:TRP:NE1	1.89	0.87
1:C:539:GLN:HG3	1:C:621:TRP:HE1	1.43	0.84
1:D:119:SER:HB3	1:D:127:THR:HG22	1.61	0.83
1:B:539:GLN:HG3	1:B:621:TRP:HE1	1.44	0.82
1:D:539:GLN:HG3	1:D:621:TRP:HE1	1.45	0.81
1:C:464:LEU:HD12	1:C:477:HIS:CE1	2.17	0.78



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:539:GLN:HG3	1:A:621:TRP:HE1	1.46	0.78
6:C:806:356:H62	6:C:806:356:C16	2.16	0.74
1:C:415:PHE:HE2	1:C:445:LYS:HZ3	1.35	0.74
1:D:432:TYR:HB3	1:D:433:PRO:HD3	1.70	0.74
1:A:188:ARG:HH21	1:A:191:LYS:HZ1	1.37	0.72
1:A:432:TYR:HB3	1:A:433:PRO:HD3	1.71	0.72
1:C:432:TYR:HB3	1:C:433:PRO:HD3	1.70	0.71
6:C:806:356:C6	6:C:806:356:H161	2.19	0.71
1:A:80:ASN:HB3	1:A:83:THR:HG22	1.71	0.70
1:C:119:SER:HB3	1:C:127:THR:HG22	1.73	0.70
1:D:227:ASN:HB3	1:D:261:VAL:HG22	1.73	0.70
1:C:206:LEU:HB3	1:C:208:THR:HG22	1.74	0.70
1:B:432:TYR:HB3	1:B:433:PRO:HD3	1.74	0.70
1:C:227:ASN:HB3	1:C:261:VAL:HG22	1.73	0.69
6:D:808:356:C16	6:D:808:356:H62	2.22	0.69
1:D:321:CYS:SG	1:D:332:CYS:HB2	2.32	0.69
1:C:321:CYS:SG	1:C:332:CYS:HB2	2.34	0.68
1:A:119:SER:HB3	1:A:127:THR:HG22	1.75	0.68
1:D:421:ARG:HD2	1:D:449:GLN:HB3	1.78	0.66
1:A:169:ASN:HD21	1:A:187:GLY:H	1.44	0.65
1:C:169:ASN:HD21	1:C:187:GLY:H	1.44	0.65
1:A:267:ILE:HD12	1:A:277:PRO:HG3	1.80	0.64
1:C:76:ILE:HB	1:C:90:LEU:HB3	1.80	0.62
1:D:409:PHE:HZ	1:D:426:ARG:NH1	1.99	0.61
1:D:324:ARG:HD2	1:D:331:ASP:HB2	1.82	0.60
1:B:169:ASN:HD21	1:B:187:GLY:H	1.47	0.60
1:C:69:HIS:HB3	1:C:79:TYR:HE2	1.68	0.59
1:D:653:TRP:HB3	1:D:661:THR:HG21	1.85	0.59
1:B:413:ASN:HD21	1:B:579:PHE:HB3	1.69	0.58
1:C:206:LEU:HB3	1:C:208:THR:CG2	2.32	0.58
1:A:413:ASN:HD21	1:A:579:PHE:HB3	1.67	0.58
1:C:413:ASN:HD21	1:C:579:PHE:HB3	1.68	0.58
6:B:809:356:H62	6:B:809:356:H161	1.86	0.57
1:B:132:ILE:HD13	1:B:176:PRO:HB3	1.87	0.56
1:D:418:TYR:HB2	1:D:421:ARG:HG3	1.88	0.56
1:D:413:ASN:HD21	1:D:579:PHE:HB3	1.71	0.56
1:B:73:ASP:HB3	5:B:804:NAG:H2	1.88	0.56
1:A:310:LYS:HD3	1:A:315:VAL:HG13	1.87	0.56
1:A:161:LYS:NZ	1:A:269:THR:HG22	2.22	0.55
1:D:132:ILE:HD13	1:D:176:PRO:HB3	1.88	0.55
6:D:808:356:C6	6:D:808:356:H161	2.30	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:B:347:ALA:O	1:B:663:ARG:NH2	2.39	0.55
1:B:506:GLU:HG2	1:B:523:ILE:HG12	1.89	0.55
1:D:169:ASN:HD21	1:D:187:GLY:H	1.55	0.55
1:C:132:ILE:HD13	1:C:176:PRO:HB3	1.88	0.54
1:A:188:ARG:NH2	1:A:191:LYS:HZ1	2.04	0.54
1:C:498:LEU:HD22	1:C:503:LEU:HD11	1.89	0.54
1:B:498:LEU:HD22	1:B:503:LEU:HD11	1.90	0.53
1:C:574:GLY:O	1:C:577:THR:HB	2.08	0.53
1:A:648:ALA:HA	1:A:698:HIS:ND1	2.24	0.53
1:B:648:ALA:HA	1:B:698:HIS:ND1	2.23	0.53
1:C:415:PHE:HE2	1:C:445:LYS:NZ	2.05	0.52
1:C:506:GLU:HG2	1:C:523:ILE:HG12	1.90	0.52
1:C:648:ALA:HA	1:C:698:HIS:ND1	2.23	0.52
1:D:742:ASN:H	1:D:742:ASN:HD22	1.55	0.52
1:A:440:THR:HB	1:A:451:TYR:CE1	2.44	0.52
1:B:55:LYS:H	1:B:491:ASN:HD21	1.58	0.52
1:D:648:ALA:HA	1:D:698:HIS:ND1	2.25	0.52
1:A:324:ARG:CZ	1:A:327:TRP:HD1	2.21	0.52
1:C:267:ILE:HD12	1:C:277:PRO:HG3	1.91	0.52
1:C:254:LYS:NZ	1:C:706:HIS:ND1	2.57	0.52
1:B:129:THR:HG23	1:B:148:ARG:HG2	1.92	0.52
1:C:55:LYS:H	1:C:491:ASN:HD21	1.58	0.52
1:B:324:ARG:NH1	1:B:327:TRP:CE3	2.78	0.52
6:B:809:356:H161	6:B:809:356:C6	2.40	0.51
1:D:293:PHE:HZ	1:D:296:LEU:HB2	1.76	0.51
1:A:498:LEU:HD22	1:A:503:LEU:HD11	1.91	0.51
1:D:506:GLU:HG2	1:D:523:ILE:HG12	1.92	0.51
1:C:624:SER:HG	1:C:734:HIS:CE1	2.28	0.51
1:D:216:PRO:HD3	1:D:298:TRP:HB3	1.93	0.50
1:C:697:ILE:HG12	1:C:727:MET:HB3	1.93	0.50
1:C:624:SER:OG	1:C:734:HIS:CE1	2.64	0.50
1:B:464:LEU:HD12	1:B:477:HIS:CE1	2.46	0.50
1:D:498:LEU:HD22	1:D:503:LEU:HD11	1.93	0.50
1:A:172:LEU:HD21	1:A:269:THR:HG23	1.94	0.50
1:A:55:LYS:H	1:A:491:ASN:HD21	1.60	0.50
1:A:324:ARG:CZ	1:A:327:TRP:CD1	2.95	0.50
1:B:123:ARG:HD2	1:B:124:TYR:CE2	2.47	0.50
1:D:55:LYS:H	1:D:491:ASN:HD21	1.59	0.49
1:A:216:PRO:HD3	1:A:298:TRP:HB3	1.94	0.49
1:B:216:PRO:HD3	1:B:298:TRP:HB3	1.94	0.49
1:C:129:THR:HG23	1:C:148:ARG:HG2	1.94	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:218:GLY:O	1:B:269:THR:OG1	2.30	0.49
1:B:254:LYS:NZ	1:B:706:HIS:ND1	2.59	0.49
1:D:129:THR:HG23	1:D:148:ARG:HG2	1.94	0.49
1:B:697:ILE:HG12	1:B:727:MET:HB3	1.95	0.49
1:C:216:PRO:HD3	1:C:298:TRP:HB3	1.95	0.49
1:C:733:ASN:ND2	1:C:735:GLY:H	2.11	0.49
1:B:172:LEU:HB2	1:B:183:ILE:HD11	1.95	0.48
1:A:254:LYS:HE3	1:A:655:TYR:HA	1.94	0.48
1:C:43:THR:HB	1:C:45:LYS:HD2	1.93	0.48
1:A:697:ILE:HG12	1:A:727:MET:HB3	1.95	0.48
1:B:127:THR:HB	1:B:149:PRO:HB2	1.95	0.48
1:C:521:LYS:HB2	1:C:549:VAL:HG13	1.96	0.48
1:D:697:ILE:HG12	1:D:727:MET:HB3	1.96	0.48
1:B:107:PRO:HG2	1:B:156:SER:O	2.14	0.48
1:A:624:SER:OG	1:A:734:HIS:CE1	2.67	0.47
6:B:809:356:H62	6:B:809:356:C16	2.43	0.47
1:C:733:ASN:HD22	1:C:735:GLY:H	1.61	0.47
6:C:806:356:C20	6:C:806:356:O19	2.62	0.47
1:A:107:PRO:HG2	1:A:156:SER:O	2.14	0.47
1:D:204:GLU:OE1	1:D:660:TYR:HB2	2.14	0.47
1:B:323:PHE:HZ	1:B:328:GLN:HG3	1.79	0.47
1:C:742:ASN:H	1:C:742:ASN:HD22	1.63	0.47
1:B:318:LEU:HD11	1:B:355:PRO:HG3	1.97	0.47
1:C:44:LEU:H	1:C:45:LYS:HZ2	1.63	0.47
1:C:621:TRP:HB2	1:C:645:ILE:HB	1.96	0.47
1:D:123:ARG:HD2	1:D:124:TYR:CE2	2.50	0.47
1:C:254:LYS:HE3	1:C:655:TYR:HA	1.97	0.46
1:A:521:LYS:HB2	1:A:549:VAL:HG13	1.97	0.46
1:A:742:ASN:HD22	1:A:742:ASN:H	1.64	0.46
1:C:107:PRO:HG2	1:C:156:SER:O	2.15	0.46
1:D:418:TYR:CB	1:D:421:ARG:HG3	2.45	0.46
1:B:281:PRO:HD2	1:B:332:CYS:SG	2.56	0.46
1:A:123:ARG:HD2	1:A:124:TYR:CE2	2.49	0.46
1:D:107:PRO:HG2	1:D:156:SER:O	2.15	0.46
1:D:690:ARG:NH2	1:D:720:ALA:O	2.49	0.46
1:B:69:HIS:HB3	1:B:79:TYR:HE2	1.81	0.46
1:C:172:LEU:HB2	1:C:183:ILE:HD11	1.97	0.46
1:D:318:LEU:HD11	1:D:355:PRO:HG3	1.98	0.46
1:A:501:ILE:HG22	1:A:503:LEU:HG	1.98	0.46
1:B:690:ARG:NH2	1:B:720:ALA:O	2.49	0.46
1:D:408:LEU:HB3	1:D:427:ILE:HG22	1.98	0.46



Interatomic Class				
Atom-1	Atom-2	distance $(Å)$	overlap(Å)	
1:C:206:LEU:CB	1:C:208:THR:HG22	2 45	0.45	
1:C:318:LEU:HD11	1:C:355:PRO:HG3	1.98	0.45	
$1 \cdot A \cdot 310 \cdot LYS \cdot HD3$	1·A·315·VAL·CG1	2 46	0.45	
$1 \cdot C \cdot 132 \cdot ILE \cdot HG21$	1.C.176.PRO.HB3	1 99	0.45	
1:C:573:ASP:HB3	1:C:577:THR:HG21	1.98	0.45	
$1 \cdot A \cdot 129 \cdot THB \cdot HG22$	1·A·148·ABG·HG2	1.99	0.45	
1:A:733:ASN:ND2	1:A:735:GLY:H	2.15	0.45	
$1 \cdot \text{R} \cdot 401 \cdot \text{PHE} \cdot \text{HE} 2$	1·B·411·SEB·HB3	1.80	0.45	
1:B:424:ILE:HD13	1:B:453:ALA:HB2	1.98	0.45	
1:D:733:ASN:ND2	1:D:735:GLY:H	2.15	0.45	
1:D:521:LYS:HB2	1:D:549:VAL:HG13	1 99	0.45	
1:B:254:LYS:HE3	1:B:655:TYB:HA	1.99	0.45	
$1 \cdot D \cdot 263 \cdot ABG \cdot HH 21$	1.D.265.PHE.HZ	1.65	0.45	
1:D:733:ASN:HD22	1:D:735:GLY:H	1.65	0.45	
1:B:521:LYS:HB2	1:B:549:VAL:HG13	1.99	0.45	
1:C:123:ARG:HD2	1:C:124:TYB:CE2	2.52	0.45	
1:A:690:ARG:NH2	1:A:720:ALA:O	2.02	0.45	
1:B:733:ASN:ND2	1:B:735:GLY:H	2.13	0.45	
1:A:318:LEU:HD11	1:A:355:PRO:HG3	1.99	0.44	
1:B:293:PHE:HZ	1:B:296:LEU:HB2	1.82	0.44	
1:A:132:ILE:HG21	1:A:176:PRO:HB3	1.98	0.44	
2:H:2:NAG:H3	2:H:2:NAG:O7	2.16	0.44	
6:D:808:356:C20	6:D:808:356:O19	2.64	0.44	
1:C:690:ARG:NH2	1:C:720:ALA:O	2.51	0.44	
1:A:558:ILE:HB	1:A:569:ILE:HG21	2.00	0.44	
1:A:77:VAL:HG22	1:A:86:SER:HB2	1.99	0.44	
1:B:157:PRO:HD3	1:B:214:TRP:HB3	2.00	0.44	
1:D:254:LYS:HE3	1:D:655:TYR:HA	1.98	0.44	
1:A:313:GLN:HG3	1:A:663:ARG:HA	2.00	0.44	
1:B:211:ALA:HB1	1:B:224:ALA:HB3	1.99	0.44	
1:C:76:ILE:HD13	1:C:90:LEU:HD23	1.99	0.44	
1:D:105:LEU:HD21	1:D:109:ARG:HG2	1.99	0.44	
1:A:324:ARG:NE	1:A:327:TRP:HD1	2.16	0.43	
1:D:132:ILE:HG21	1:D:176:PRO:HB3	1.99	0.43	
1:A:281:PRO:HD2	1:A:332:CYS:SG	2.58	0.43	
1:D:157:PRO:HD3	1:D:214:TRP:HB3	2.00	0.43	
6:A:806:356:H161	6:A:806:356:C6	2.48	0.43	
1:B:733:ASN:HD22	1:B:735:GLY:H	1.65	0.43	
1:A:624:SER:HG	1:A:734:HIS:CE1	2.32	0.43	
1:C:243:GLN:HG2	1:D:254:LYS:HD3	2.01	0.43	
1:A:254:LYS:NZ	1:A:706:HIS:ND1	2.67	0.43	



Atom-1	Atom-2	Interatomic	Clash
	Atom-2	distance (Å)	overlap (Å)
1:A:733:ASN:HD22	1:A:735:GLY:H	1.65	0.43
1:D:292:TYR:CE2	1:D:311:ARG:HA	2.54	0.43
1:A:105:LEU:HD21	1:A:109:ARG:HG2	2.01	0.42
1:B:590:ARG:HA	1:B:665:MET:HA	2.01	0.42
6:A:806:356:H161	6:A:806:356:H62	2.01	0.42
1:B:132:ILE:HG21	1:B:176:PRO:HB3	2.01	0.42
1:B:193:PHE:HB2	1:B:226:PHE:HB2	2.00	0.42
1:C:37:ASN:HA	1:C:500:ASN:ND2	2.35	0.42
1:A:286:ILE:HD13	1:A:310:LYS:HG3	2.01	0.42
1:D:324:ARG:HG2	1:D:329:THR:O	2.20	0.42
1:B:558:ILE:HB	1:B:569:ILE:HG21	2.00	0.42
1:C:592:LEU:HG	1:C:665:MET:HG2	2.02	0.42
1:B:502:GLN:HG2	1:B:502:GLN:H	1.72	0.41
1:D:47:ILE:HD13	1:D:560:TYR:HB2	2.02	0.41
1:D:175:ARG:HG2	1:D:178:ASP:CG	2.40	0.41
1:D:267:ILE:HD12	1:D:277:PRO:HG3	2.03	0.41
1:B:105:LEU:HD21	1:B:109:ARG:HG2	2.02	0.41
1:C:319:SER:OG	1:C:332:CYS:SG	2.71	0.41
1:B:197:PRO:HA	1:B:226:PHE:CE2	2.56	0.41
1:C:254:LYS:HD3	1:D:243:GLN:HG2	2.03	0.41
1:A:197:PRO:HA	1:A:226:PHE:CE2	2.56	0.41
1:A:157:PRO:HD3	1:A:214:TRP:HB3	2.03	0.41
1:C:624:SER:OG	6:C:806:356:H231	2.21	0.41
1:D:197:PRO:HA	1:D:226:PHE:CE2	2.56	0.41
1:D:562:ALA:HB2	1:D:569:ILE:HD13	2.03	0.41
1:D:358:SER:HB2	1:D:360:ASP:OD1	2.21	0.41
1:A:47:ILE:HD13	1:A:560:TYR:HB2	2.03	0.41
1:C:558:ILE:HB	1:C:569:ILE:HG21	2.03	0.40
1:D:212:LEU:HD13	1:D:221:LEU:HD11	2.02	0.40
1:C:170:ILE:HG22	1:C:183:ILE:HD13	2.02	0.40
1:A:76:ILE:HD13	1:A:90:LEU:HD23	2.03	0.40
1:C:157:PRO:HD3	1:C:214:TRP:HB3	2.02	0.40
1:C:47:ILE:HD13	1:C:560:TYR:HB2	2.04	0.40
1:D:73:ASP:HB2	4:K:1:NAG:H2	2.04	0.40
1:C:523:ILE:HB	1:C:569:ILE:HB	2.03	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	Perce	ntiles
1	А	719/722~(100%)	681~(95%)	36~(5%)	2(0%)	41	70
1	В	717/722~(99%)	679~(95%)	35~(5%)	3 (0%)	34	65
1	С	720/722~(100%)	678~(94%)	41 (6%)	1 (0%)	51	81
1	D	718/722~(99%)	676~(94%)	41 (6%)	1 (0%)	51	81
All	All	2874/2888~(100%)	2714 (94%)	153 (5%)	7 (0%)	47	77

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	84	GLY
1	А	414	GLU
1	В	313	GLN
1	В	414	GLU
1	С	414	GLU
1	D	414	GLU
1	А	313	GLN

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	Percer	ntiles
1	А	636/637~(100%)	621~(98%)	15~(2%)	49	78
1	В	634/637~(100%)	618~(98%)	16 (2%)	47	77
1	С	637/637~(100%)	617~(97%)	20 (3%)	40	72



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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	635/637~(100%)	623~(98%)	12 (2%)	57 83
All	All	2542/2548~(100%)	2479 (98%)	63(2%)	47 77

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

Mol	Chain	Res	Type
1	А	127	THR
1	А	142	ARG
1	А	246	ARG
1	А	313	GLN
1	А	382	ASP
1	А	385	GLU
1	А	402	ARG
1	А	405	GLN
1	А	432	TYR
1	А	476	LEU
1	А	541	TYR
1	А	621	TRP
1	А	624	SER
1	А	730	SER
1	А	757	SER
1	В	45	LYS
1	В	73	ASP
1	В	83	THR
1	В	142	ARG
1	В	200	VAL
1	В	208	THR
1	В	225	GLU
1	В	246	ARG
1	В	328	GLN
1	В	382	ASP
1	В	402	ARG
1	В	432	TYR
1	В	541	TYR
1	В	621	TRP
1	В	665	MET
1	В	730	SER
1	С	36	GLU
1	С	37	ASN
1	С	45	LYS
1	С	127	THR
1	С	225	GLU



	U	-	10
Mol	Chain	Res	Type
1	С	246	ARG
1	С	324	ARG
1	С	328	GLN
1	С	350	PHE
1	С	382	ASP
1	С	402	ARG
1	С	405	GLN
1	С	412	SER
1	С	432	TYR
1	С	541	TYR
1	С	621	TRP
1	С	624	SER
1	С	730	SER
1	С	741	THR
1	С	754	GLN
1	D	127	THR
1	D	200	VAL
1	D	208	THR
1	D	246	ARG
1	D	311	ARG
1	D	382	ASP
1	D	432	TYR
1	D	512	GLU
1	D	541	TYR
1	D	621	TRP
1	D	624	SER
1	D	730	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	144	ASN
1	А	169	ASN
1	А	413	ASN
1	А	477	HIS
1	А	491	ASN
1	А	733	ASN
1	А	742	ASN
1	А	754	GLN
1	В	144	ASN
1	В	169	ASN
1	В	413	ASN



Mol	Chain	Res	Type
1	В	477	HIS
1	В	483	GLN
1	В	491	ASN
1	В	691	ASN
1	В	704	ASN
1	В	733	ASN
1	В	742	ASN
1	В	754	GLN
1	С	144	ASN
1	С	169	ASN
1	С	413	ASN
1	С	477	HIS
1	С	491	ASN
1	С	500	ASN
1	С	733	ASN
1	С	742	ASN
1	D	169	ASN
1	D	413	ASN
1	D	477	HIS
1	D	483	GLN
1	D	491	ASN
1	D	691	ASN
1	D	733	ASN
1	D	742	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

19 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



Mal	Tune	Chain	Dog	Link	Bo	ond leng	ths	В	ond ang	les
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	Е	1	1,2	14, 14, 15	0.26	0	$17,\!19,\!21$	0.58	0
2	NAG	Е	2	2	14, 14, 15	0.29	0	$17,\!19,\!21$	0.57	0
3	NAG	F	1	1,3	14, 14, 15	0.26	0	$17,\!19,\!21$	0.57	0
3	NAG	F	2	3	14,14,15	0.35	0	$17,\!19,\!21$	1.38	3(17%)
3	BMA	F	3	3	11,11,12	0.26	0	$15,\!15,\!17$	0.48	0
2	NAG	G	1	1,2	14,14,15	0.26	0	17,19,21	0.58	0
2	NAG	G	2	2	$14,\!14,\!15$	0.27	0	$17,\!19,\!21$	0.73	0
2	NAG	Н	1	1,2	14, 14, 15	0.37	0	$17,\!19,\!21$	0.77	1(5%)
2	NAG	Н	2	2	14,14,15	0.39	0	$17,\!19,\!21$	1.03	1(5%)
2	NAG	Ι	1	1,2	14,14,15	0.27	0	17,19,21	0.62	0
2	NAG	Ι	2	2	14, 14, 15	0.29	0	$17,\!19,\!21$	0.63	0
2	NAG	J	1	1,2	$14,\!14,\!15$	0.28	0	$17,\!19,\!21$	0.58	0
2	NAG	J	2	2	$14,\!14,\!15$	0.29	0	$17,\!19,\!21$	0.51	0
4	NAG	К	1	1,4	14,14,15	0.33	0	$17,\!19,\!21$	1.42	3 (17%)
4	FUC	K	2	4	10, 10, 11	0.32	0	14, 14, 16	0.61	0
4	NAG	L	1	1,4	14,14,15	0.30	0	17,19,21	0.72	0
4	FUC	L	2	4	10, 10, 11	0.53	0	$14,\!14,\!16$	0.80	0
4	NAG	М	1	1,4	14,14,15	0.38	0	17,19,21	1.38	2 (11%)
4	FUC	М	2	4	10, 10, 11	0.35	0	$14,\!14,\!16$	1.00	1 (7%)

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).

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
2	NAG	Е	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Е	2	2	-	1/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	3/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	Н	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	Н	2	2	-	4/6/23/26	0/1/1/1
2	NAG	Ι	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Ι	2	2	-	0/6/23/26	0/1/1/1



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	1/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	4/6/23/26	0/1/1/1
4	FUC	K	2	4	-	-	0/1/1/1
4	NAG	L	1	1,4	-	0/6/23/26	0/1/1/1
4	FUC	L	2	4	-	_	0/1/1/1
4	NAG	М	1	1,4	-	1/6/23/26	0/1/1/1
4	FUC	М	2	4	-	_	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
4	М	1	NAG	O5-C1-C2	4.23	117.96	111.29
3	F	2	NAG	O5-C1-C2	-3.82	105.26	111.29
4	Κ	1	NAG	C1-C2-N2	3.49	116.44	110.49
4	Κ	1	NAG	O5-C1-C2	-3.15	106.32	111.29
3	F	2	NAG	C1-C2-N2	3.04	115.69	110.49
4	М	1	NAG	C1-C2-N2	-2.97	105.41	110.49
2	Η	2	NAG	O5-C1-C2	2.95	115.95	111.29
4	Κ	1	NAG	C2-N2-C7	2.40	126.32	122.90
3	F	2	NAG	C2-N2-C7	2.14	125.96	122.90
4	М	2	FUC	O2-C2-C1	2.13	113.52	109.15
2	Н	1	NAG	O5-C1-C2	-2.05	108.06	111.29

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Н	2	NAG	C8-C7-N2-C2
2	Н	2	NAG	O7-C7-N2-C2
2	Н	1	NAG	O5-C5-C6-O6
2	Н	1	NAG	C4-C5-C6-O6
4	Κ	1	NAG	C4-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
4	Κ	1	NAG	O5-C5-C6-O6
2	Н	2	NAG	O5-C5-C6-O6
2	Е	2	NAG	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
4	М	1	NAG	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6



Mol	Chain	\mathbf{Res}	Type	Atoms
2	Н	2	NAG	C3-C2-N2-C7
4	K	1	NAG	C1-C2-N2-C7
3	F	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C3-C2-N2-C7
4	K	1	NAG	C3-C2-N2-C7
3	F	2	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

M	ol	Chain	Res	Type	Clashes	Symm-Clashes
2		Н	2	NAG	1	0
4		K	1	NAG	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 oligosaccharide.































5.6 Ligand geometry (i)

10 ligands 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).



Mal	Turne	Chain	Dec	Tink	Bo	ond leng	$_{\rm ths}$	Bond angles		
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
6	356	А	806	-	32,39,39	1.01	3 (9%)	$35,\!57,\!57$	1.71	5 (14%)
5	NAG	В	804	1	14,14,15	0.29	0	17,19,21	0.71	1 (5%)
6	356	С	806	-	32,39,39	1.02	2 (6%)	$35,\!57,\!57$	1.88	6 (17%)
6	356	В	809	-	32,39,39	1.07	2 (6%)	35,57,57	1.85	4 (11%)
5	NAG	А	803	1	14,14,15	0.32	0	17,19,21	0.74	1(5%)
5	NAG	D	801	1	14,14,15	0.25	0	17,19,21	0.66	0
6	356	D	808	-	$32,\!39,\!39$	1.10	2(6%)	$35,\!57,\!57$	1.78	4 (11%)
5	NAG	С	805	1	14,14,15	0.29	0	17,19,21	0.77	1 (5%)
5	NAG	А	805	1	14,14,15	0.32	0	17,19,21	1.38	3 (17%)
5	NAG	А	804	1	14,14,15	0.27	0	17,19,21	0.92	1 (5%)

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	356	А	806	-	-	3/6/22/22	0/5/5/5
5	NAG	В	804	1	-	0/6/23/26	0/1/1/1
6	356	С	806	-	-	4/6/22/22	0/5/5/5
6	356	В	809	-	-	2/6/22/22	0/5/5/5
5	NAG	А	803	1	-	2/6/23/26	0/1/1/1
5	NAG	D	801	1	-	0/6/23/26	0/1/1/1
6	356	D	808	-	-	4/6/22/22	0/5/5/5
5	NAG	С	805	1	-	0/6/23/26	0/1/1/1
5	NAG	А	805	1	-	1/6/23/26	0/1/1/1
5	NAG	А	804	1	-	0/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
6	В	809	356	C3-N7	3.90	1.37	1.33
6	С	806	356	C3-N7	3.79	1.37	1.33
6	D	808	356	C3-N7	3.78	1.37	1.33
6	А	806	356	C3-N7	3.69	1.36	1.33
6	D	808	356	C4-N9	2.77	1.42	1.38
6	В	809	356	C4-N9	2.68	1.42	1.38
6	А	806	356	C4-N9	2.46	1.41	1.38
6	С	806	356	C4-N9	2.39	1.41	1.38



Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
6	А	806	356	C1-C3	-2.08	1.36	1.39

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
6	D	808	356	C1-C4-N9	-7.28	112.82	120.30
6	С	806	356	C1-C4-N9	-7.24	112.86	120.30
6	А	806	356	C1-C4-N9	-7.23	112.87	120.30
6	В	809	356	C1-C4-N9	-7.19	112.91	120.30
6	В	809	356	C12-C6-N2	5.17	119.39	112.10
6	D	808	356	C12-C6-N2	4.64	118.64	112.10
6	С	806	356	C12-C6-N2	4.30	118.16	112.10
6	В	809	356	C4-C1-C3	4.10	122.59	119.96
6	С	806	356	C4-C1-C3	4.03	122.55	119.96
6	А	806	356	C4-C1-C3	3.98	122.51	119.96
5	А	805	NAG	C1-C2-N2	3.77	116.92	110.49
6	D	808	356	C4-C1-C3	3.48	122.19	119.96
5	А	804	NAG	C1-O5-C5	2.95	116.19	112.19
5	С	805	NAG	C1-O5-C5	2.71	115.86	112.19
5	А	805	NAG	O5-C1-C2	-2.60	107.19	111.29
5	А	805	NAG	C2-N2-C7	2.54	126.51	122.90
6	С	806	356	C26-C21-C16	-2.53	107.41	110.65
6	С	806	356	C14-N8-C3	2.48	121.77	118.25
6	С	806	356	C16-N11-C5	-2.48	116.72	122.03
5	В	804	NAG	O5-C1-C2	-2.34	107.60	111.29
6	В	809	356	C14-N8-C3	2.32	121.53	118.25
6	А	806	356	C14-N8-C3	2.30	121.51	118.25
5	А	803	NAG	C1-C2-N2	-2.29	106.57	110.49
6	А	806	356	C17-N11-C5	-2.29	117.13	122.03
6	D	808	356	C14-N8-C3	2.10	121.23	118.25
6	A	806	356	C12-C6-N2	2.06	115.00	112.10

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	А	806	356	C18-C12-C6-N2
6	А	806	356	C20-C15-N9-C4
6	С	806	356	C20-C15-N9-C4
6	В	809	356	C20-C15-N9-C4
6	D	808	356	C20-C15-N9-C4
5	А	805	NAG	C1-C2-N2-C7



Mol	Chain	\mathbf{Res}	Type	Atoms
6	А	806	356	N9-C15-C20-N24
6	С	806	356	N9-C15-C20-N24
6	В	809	356	N9-C15-C20-N24
6	D	808	356	N9-C15-C20-N24
5	А	803	NAG	C4-C5-C6-O6
6	С	806	356	N9-C15-C20-N25
6	D	808	356	N9-C15-C20-N25
6	С	806	356	C12-C6-N2-C1
6	D	808	356	C12-C6-N2-C1
5	А	803	NAG	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	А	806	356	2	0
5	В	804	NAG	1	0
6	С	806	356	5	0
6	В	809	356	3	0
6	D	808	356	4	0
5	А	805	NAG	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.











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, 95^{th} 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	А	721/722~(99%)	0.19	11 (1%) 73	73	27, 52, 79, 96	0
1	В	719/722~(99%)	0.16	4 (0%) 89	89	28, 49, 70, 88	0
1	С	722/722~(100%)	0.16	2 (0%) 94	94	29, 51, 76, 92	0
1	D	720/722~(99%)	0.21	4 (0%) 89	89	29, 50, 74, 87	0
All	All	2882/2888 (99%)	0.18	21 (0%) 87	88	27, 50, 75, 96	0

All (21) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	D	432	TYR	5.9
1	В	432	TYR	4.4
1	А	93	ARG	3.8
1	С	432	TYR	3.6
1	А	72	ALA	2.9
1	А	432	TYR	2.8
1	D	79	TYR	2.8
1	D	512	GLU	2.7
1	А	135	LEU	2.5
1	D	518	LEU	2.5
1	А	607	PHE	2.5
1	А	359	TYR	2.5
1	В	306	LEU	2.4
1	С	499	LYS	2.3
1	В	514	ASP	2.3
1	А	44	LEU	2.3
1	А	340	GLU	2.2
1	В	512	GLU	2.1
1	А	170	ILE	2.1
1	А	90	LEU	2.1
1	A	172	LEU	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, 95^{th} 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	$\mathbf{B} extsf{-}\mathbf{B} extsf{-}\mathbf{factors}(\mathbf{A}^2)$	Q < 0.9
4	FUC	L	2	10/11	0.59	0.61	$68,\!68,\!69,\!69$	0
4	FUC	K	2	10/11	0.68	0.44	91,91,91,91	0
4	NAG	K	1	14/15	0.72	0.31	88,88,90,90	0
2	NAG	Е	2	14/15	0.74	0.35	77,78,78,78	0
3	BMA	F	3	11/12	0.75	0.35	$90,\!90,\!90,\!91$	0
2	NAG	Н	2	14/15	0.76	0.29	71,72,72,72	0
3	NAG	F	2	14/15	0.77	0.31	84,86,87,88	0
4	FUC	М	2	10/11	0.81	0.32	$76,\!76,\!77,\!77$	0
2	NAG	G	2	14/15	0.83	0.24	$73,\!74,\!74,\!74$	0
3	NAG	F	1	14/15	0.83	0.30	77,78,80,83	0
4	NAG	М	1	14/15	0.85	0.28	70,72,74,75	0
2	NAG	Ι	2	14/15	0.85	0.38	82,83,84,84	0
4	NAG	L	1	14/15	0.87	0.16	59,61,64,66	0
2	NAG	Ι	1	14/15	0.88	0.22	$77,\!78,\!79,\!81$	0
2	NAG	G	1	14/15	0.88	0.22	$68,\!69,\!70,\!71$	0
2	NAG	Е	1	14/15	0.88	0.22	73,74,75,76	0
2	NAG	J	2	14/15	0.88	0.22	72,72,73,73	0
2	NAG	Н	1	14/15	0.88	0.24	$69,\!69,\!71,\!71$	0
2	NAG	J	1	14/15	0.91	0.15	$67,\!67,\!69,\!70$	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, 95^{th} 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	${f B} ext{-factors}({ m \AA}^2)$	Q<0.9
5	NAG	С	805	14/15	0.81	0.31	$65,\!66,\!66,\!66$	0
5	NAG	А	805	14/15	0.85	0.27	$71,\!72,\!73,\!73$	0
5	NAG	В	804	14/15	0.86	0.21	79,80,80,80	0
5	NAG	А	804	14/15	0.86	0.30	$60,\!60,\!61,\!61$	0
5	NAG	D	801	14/15	0.88	0.20	61,62,62,63	0
5	NAG	А	803	14/15	0.88	0.26	$59,\!60,\!62,\!62$	0
6	356	В	809	35/35	0.94	0.23	44,45,45,46	0
6	356	С	806	35/35	0.95	0.18	$37,\!40,\!41,\!42$	0
6	356	D	808	35/35	0.96	0.20	43,44,45,45	0
6	356	А	806	35/35	0.96	0.19	$45,\!48,\!49,\!49$	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.

