

Full wwPDB X-ray Structure Validation Report (i)

Apr 20, 2024 – 01:21 pm BST

PDB ID	:	6F7Q
Title	:	Human Butyrylcholinesterase complexed with N-Propargyliperidines
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Deposited on	:	2017-12-11
Resolution	:	2.60 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.60 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.



Motric	Whole archive	Similar resolution
IVIETIC	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R _{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	529	83%	16%	•					
1	В	529	74%	25%	•					
2	С	2	50% 50%	6	_					
3	D	3	33% 67%							
3	Е	3	100%							



Mol	Chain	Length	Quality of chain					
3	Н	3	33%	67%				
4	F	2	50%	50%				
5	G	3	33%	67%				

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
10	SO4	А	620	-	-	Х	-
3	NAG	D	2	-	-	-	Х
3	FUL	D	3	-	-	-	Х
3	NAG	Е	2	-	-	-	Х
3	NAG	Н	2	-	-	-	Х
3	FUL	Н	3	-	-	-	Х
9	NAG	В	605	-	-	Х	-



2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 8943 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 Cholinesterase.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
1	А	527	Total 4171	C 2690	N 696	O 770	S 15	0	3	0
1	В	527	Total 4189	C 2701	N 704	O 769	S 15	0	2	0

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



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

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



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

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



cetamido-2-deoxy-beta-D-glucopyranose.

$$\beta$$
 4 β

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

• Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[al pha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



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

• Molecule 6 is 2-[[(3 {R})-1-(2,3-dihydro-1 {H}-inden-2-yl)piperidin-3-yl]methyl-(8-oxidany lquinolin-2-yl)carbonyl-amino]ethyl-dimethyl-azanium (three-letter code: CWQ) (formula: $C_{29}H_{37}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	А	1	Total 35	C 29	N 4	O 2	0	0



Mol	Chain	Residues	A	Aton	ns		ZeroOcc	AltConf
6	Λ	1	Total	С	Ν	Ο	0	0
0	A		35	29	4	2	0	
6	В	1	Total	С	Ν	Ο	0	0
0	0 Б	T	35	29	4	2		
6	В	1	Total	С	Ν	0	0	0
U	В		35	29	4	2	U	0

• Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
7	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

• Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
8	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
8	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
8	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0

• Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	А	1	Total C N O 14 8 1 5	0	0
9	А	1	Total C N O 14 8 1 5	0	0
9	В	1	Total C N O 14 8 1 5	0	0
9	В	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{N} & \text{O} \\ 14 & 8 & 1 & 5 \end{array}$	0	0

• Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
10	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
10	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
10	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
10	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	В	1	Total Cl 1 1	0	0



• Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	А	87	Total O 87 87	0	0
12	В	36	Total O 36 36	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: Cholinesterase

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

Chain C:

50%

50%



NAG1 FUL2

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

Chain D. 💳	220/	
Unam D.	33%	67%

NAG1 NAG2 FUL3

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

Chain E	100%
Cham E.	10070

NAG1 NAG2 FUL3

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

Chain H:	33%	67%	
NAG1 NAG2 FUL3			
• Molecule	4: 2-acetamido-2-de	eoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-de	oxv-beta-

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

Chain E.		
Unain F:	50%	50%

NAG1 NAG2

 • Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)] 2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:	33%	67%
NAG1 NAG2 FUC3		



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants	152.14Å 152.14Å 141.91Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	49.11 - 2.60	Depositor
Resolution (A)	49.11 - 2.60	EDS
% Data completeness	94.1 (49.11-2.60)	Depositor
(in resolution range)	94.1 (49.11-2.60)	EDS
R _{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.27 (at 2.61 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
D D.	0.192 , 0.248	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.192 , 0.247	DCC
R_{free} test set	2435 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	63.3	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34 , 49.5	EDS
L-test for $twinning^2$	$ L > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8943	wwPDB-VP
Average B, all atoms $(Å^2)$	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.52% 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: GOL, SO4, CL, FUC, FUL, NAG, EDO, CWQ

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		Bond lengths		Bond angles	
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.34	0/4297	0.52	0/5841
1	В	0.43	0/4311	0.58	0/5859
All	All	0.39	0/8608	0.55	0/11700

There are no bond length outliers.

There are no bond angle outliers.

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	4171	0	4034	61	0
1	В	4189	0	4060	103	0
2	С	24	0	22	0	0
3	D	38	0	34	1	0
3	Е	38	0	34	0	0
3	Н	38	0	34	3	0
4	F	28	0	25	3	0
5	G	38	0	34	1	0
6	А	70	0	0	0	0
6	В	70	0	0	1	0
7	А	18	0	24	4	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	А	12	0	18	2	0
8	В	4	0	6	2	0
9	А	28	0	26	0	0
9	В	28	0	26	13	0
10	А	15	0	0	3	0
10	В	10	0	0	1	0
11	В	1	0	0	0	0
12	А	87	0	0	4	0
12	В	36	0	0	1	0
All	All	8943	0	8377	166	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 10.

All (166) 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	distance (Å)	overlap (Å)
1:B:57:ASN:HD21	9:B:605:NAG:C1	1.30	1.44
1:B:57:ASN:HD21	9:B:605:NAG:C2	1.45	1.29
1:B:57:ASN:CG	9:B:605:NAG:C1	2.35	0.94
1:B:346:THR:HG23	1:B:349:GLU:H	1.36	0.90
1:B:234:THR:HG22	10:B:615:SO4:O4	1.71	0.89
1:B:14:ARG:NH1	9:B:605:NAG:C1	2.37	0.86
1:B:457:THR:HG22	1:B:459:ALA:H	1.44	0.83
1:B:57:ASN:ND2	9:B:605:NAG:C2	2.30	0.78
1:B:14:ARG:HH11	9:B:605:NAG:C1	1.97	0.76
1:B:57:ASN:HD22	9:B:605:NAG:H83	1.51	0.74
1:B:57:ASN:OD1	9:B:605:NAG:C1	2.36	0.72
1:B:470:ARG:HH11	8:B:604:EDO:H21	1.54	0.71
1:A:499:LYS:HG2	1:A:512:THR:HG22	1.71	0.71
1:B:57:ASN:ND2	9:B:605:NAG:H83	2.09	0.68
1:B:250:THR:O	1:B:267:LYS:NZ	2.27	0.67
1:B:159:ASN:HD21	1:B:258:THR:HG22	1.60	0.67
1:A:63:ASN:N	10:A:620:SO4:O4	2.24	0.65
1:A:87:ASP:OD2	12:A:701:HOH:O	2.14	0.65
1:B:361:VAL:O	1:B:366:LYS:NZ	2.30	0.64
1:A:250:THR:O	1:A:267:LYS:NZ	2.23	0.64
1:B:308:GLU:OE2	1:B:408:LYS:HE2	1.96	0.64
1:B:319:VAL:O	1:B:418:PHE:HA	1.98	0.63
1:A:218:THR:HA	7:A:605:GOL:H31	1.80	0.62
1:A:509:ARG:NH2	12:A:706:HOH:O	2.32	0.62



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:57:ASN:ND2	9:B:605:NAG:N2	2.43	0.62	
1:B:5:ILE:HD12	1:B:55:ILE:HD11	1.82	0.62	
1:B:256:ASN:HB3	1:B:259:GLU:HB2	1.82	0.60	
1:A:383:GLU:OE1	1:A:383:GLU:N	2.27	0.60	
1:A:277:ALA:N	12:A:704:HOH:O	2.30	0.60	
1:B:479:ASN:OD1	1:B:481:ASN:ND2	2.35	0.59	
1:B:213:SER:HA	1:B:216:LEU:HD12	1.84	0.59	
1:B:109:VAL:HB	1:B:192:VAL:HG22	1.85	0.59	
1:A:9:LYS:HD2	1:A:180:LYS:HB3	1.84	0.58	
1:B:197:GLU:HB3	12:B:729:HOH:O	2.03	0.58	
1:B:190:LYS:NZ	4:F:2:NAG:HN2	2.01	0.57	
1:B:457:THR:HG22	1:B:459:ALA:N	2.18	0.57	
1:B:76:PHE:CE2	1:B:339:LYS:HE2	2.40	0.57	
1:B:515:ARG:HH21	1:B:515:ARG:HG2	1.69	0.57	
1:B:522:TRP:O	1:B:527:PRO:HD3	2.06	0.56	
1:B:111:ILE:HA	1:B:142:VAL:O	2.06	0.56	
1:A:361:VAL:O	1:A:366:LYS:NZ	2.40	0.55	
1:A:156:LEU:HD11	1:A:261:ILE:HD11	1.88	0.55	
1:B:76:PHE:CZ	1:B:339:LYS:HE2	2.42	0.55	
1:B:35[A]:GLN:HG3	1:B:48:SER:O	2.07	0.54	
1:B:386:ARG:NH1	1:B:433:TRP:HB2	2.22	0.54	
1:B:312:PHE:O	1:B:314:LYS:HE3	2.07	0.54	
1:B:337:PHE:HA	1:B:343:SER:OG	2.08	0.54	
1:A:319:VAL:O	1:A:418:PHE:HA	2.08	0.53	
1:B:28:PHE:HB3	1:B:31:ILE:HD11	1.89	0.53	
1:B:346:THR:HG22	1:B:349:GLU:OE1	2.08	0.53	
1:B:254:ARG:HB2	1:B:260:ILE:HB	1.90	0.53	
1:A:166:MET:H	1:A:166:MET:HE2	1.73	0.53	
1:B:190:LYS:HZ3	4:F:2:NAG:HN2	1.55	0.53	
1:A:69:ILE:HD13	1:A:84:PRO:HD2	1.90	0.52	
1:A:135:ARG:HH12	7:A:603:GOL:H2	1.75	0.52	
1:B:57:ASN:ND2	9:B:605:NAG:C7	2.72	0.52	
1:A:62:ALA:HB1	10:A:620:SO4:O4	2.10	0.51	
1:A:470:ARG:HH11	8:A:608:EDO:H22	1.76	0.51	
1:B:386:ARG:HD3	1:B:433:TRP:CE3	2.47	0.50	
1:B:156:LEU:HD12	1:B:261:ILE:HD11	1.93	0.50	
1:B:474:PHE:HB2	1:B:480:PRO:HB3	1.92	0.50	
1:A:227:PHE:CD1	1:A:303:PRO:HB2	2.46	0.50	
1:B:197:GLU:OE1	1:B:198:SER:HB2	2.12	0.50	
1:B:245:ASN:ND2	3:H:1:NAG:H62	2.27	0.50	
1:A:135:ARG:NH1	7:A:603:GOL:H2	2.27	0.50	



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:63:ASN:ND2	10:A:620:SO4:O1	2.45	0.49
1:B:227:PHE:CD1	1:B:303:PRO:HB2	2.47	0.49
1:B:500:TYR:CZ	1:B:511:MET:HB2	2.48	0.49
1:B:338:SER:HB3	5:G:1:NAG:H62	1.95	0.49
1:A:206:LEU:HD22	1:A:299:LEU:HD11	1.94	0.49
1:B:219:ARG:NH2	1:B:475:ALA:O	2.46	0.49
1:A:374:THR:HA	1:A:376:TRP:CZ3	2.47	0.49
1:B:200:GLY:O	1:B:204:VAL:HG23	2.13	0.49
1:B:76:PHE:CD2	1:B:339:LYS:HE2	2.48	0.48
1:A:314:LYS:NZ	12:A:710:HOH:O	2.40	0.48
1:B:42:ARG:HD2	1:B:151:LEU:HD22	1.93	0.48
1:B:39:GLY:O	1:B:265:ARG:HD3	2.13	0.47
1:B:365:GLY:O	1:B:369:ILE:HG13	2.13	0.47
1:A:218:THR:OG1	7:A:605:GOL:H2	2.13	0.47
1:A:494:LYS:HE2	1:A:497:GLU:HG3	1.95	0.47
1:B:99:ILE:HG21	1:B:185:PHE:HB3	1.96	0.47
1:A:109:VAL:HB	1:A:192:VAL:HG22	1.96	0.46
1:A:156:LEU:CD1	1:A:261:ILE:HD11	2.45	0.46
1:A:494:LYS:HE2	1:A:494:LYS:HB2	1.75	0.46
1:B:57:ASN:ND2	9:B:605:NAG:C8	2.76	0.46
1:A:453:ARG:H	1:A:453:ARG:HD2	1.81	0.46
1:B:209:LEU:HD23	1:B:312:PHE:HB3	1.96	0.46
1:B:35[B]:GLN:HG2	1:B:49:LEU:HD12	1.97	0.46
1:A:321:VAL:HG11	1:A:399:ILE:HA	1.97	0.46
1:A:411:GLU:HG3	1:A:495:SER:OG	2.16	0.46
1:B:52:TRP:HD1	1:B:54:ASP:H	1.63	0.46
1:B:301:ASP:OD1	1:B:302:MET:N	2.44	0.45
1:B:76:PHE:CE1	1:B:339:LYS:HE2	2.52	0.45
1:B:245:ASN:HD21	3:H:1:NAG:H62	1.81	0.45
1:A:12:LYS:HB2	1:A:55:ILE:HG12	1.97	0.45
1:A:347:ARG:HB2	1:A:385:TYR:CZ	2.52	0.45
1:B:284:THR:HG22	1:B:356:ILE:O	2.16	0.45
1:B:342:ASN:OD1	1:B:344:ILE:HG12	2.16	0.45
1:A:195:PHE:CB	1:A:221:ILE:HB	2.47	0.45
1:A:42:ARG:HH22	1:A:269:PRO:HD3	1.82	0.44
1:A:526:PHE:O	1:A:529:VAL:HG22	2.17	0.44
1:A:172:GLN:NE2	1:A:213:SER:OG	2.41	0.44
1:A:470:ARG:HE	8:A:608:EDO:H22	1.83	0.44
1:B:117:GLY:O	1:B:119:GLN:HG2	2.18	0.44
1:B:424:ARG:NH1	1:B:432:GLU:HA	2.33	0.44
3:H:1:NAG:H62	3:H:3:FUL:H2	1.76	0.44



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:4:ILE:H	1:A:4:ILE:HD12	1.83	0.44
1:A:500:TYR:CZ	1:A:511:MET:HB2	2.52	0.44
1:B:500:TYR:CE1	1:B:514:LEU:HB2	2.52	0.44
1:B:49:LEU:HD12	1:B:49:LEU:HA	1.66	0.44
1:B:195:PHE:CB	1:B:221:ILE:HB	2.47	0.44
1:A:227:PHE:CE1	1:A:303:PRO:HB2	2.52	0.44
1:A:465:ARG:HA	1:A:465:ARG:HD2	1.87	0.44
1:B:205:SER:O	1:B:208:LEU:HB2	2.17	0.43
1:A:430:TRP:HB3	1:A:431:PRO:HD2	2.01	0.43
1:B:515:ARG:HH21	1:B:515:ARG:CG	2.31	0.43
1:B:335:PRO:HD3	1:B:356:ILE:CD1	2.48	0.43
1:A:39:GLY:O	1:A:265:ARG:HD2	2.18	0.43
1:A:182:ILE:HD12	1:A:182:ILE:HA	1.81	0.43
1:A:474:PHE:HB2	1:A:480:PRO:HB3	2.00	0.43
1:B:508:THR:HG21	8:B:604:EDO:H11	2.00	0.43
1:B:24:THR:O	1:B:101:ALA:HB3	2.19	0.43
1:B:13:VAL:HG12	1:B:28:PHE:HD2	1.83	0.43
1:B:14:ARG:HH12	9:B:605:NAG:C1	2.24	0.43
1:B:388:ALA:O	1:B:392:VAL:HG23	2.17	0.43
1:B:411:GLU:HG3	1:B:495:SER:OG	2.19	0.43
1:B:133:LEU:HD23	1:B:468:VAL:HG13	2.00	0.42
1:B:154:LEU:HD23	1:B:162:ALA:HB1	2.00	0.42
1:B:227:PHE:CE1	1:B:303:PRO:HB2	2.54	0.42
1:B:256:ASN:O	1:B:260:ILE:HG22	2.19	0.42
1:B:526:PHE:O	1:B:529:VAL:HB	2.19	0.42
1:A:195:PHE:HB3	1:A:221:ILE:HB	2.00	0.42
1:A:14:ARG:HD2	1:A:57:ASN:OD1	2.20	0.42
1:A:337:PHE:HE1	1:A:386:ARG:HG2	1.85	0.42
1:A:407:LYS:HE3	1:A:407:LYS:HB2	1.53	0.42
1:B:197:GLU:O	1:B:200:GLY:N	2.52	0.42
1:A:320:GLY:HA3	1:A:419:TYR:CE2	2.55	0.42
1:B:361:VAL:CG1	1:B:366:LYS:HG3	2.50	0.42
1:B:420:TYR:OH	1:B:515:ARG:NH1	2.52	0.41
1:B:195:PHE:HB2	1:B:221:ILE:HB	2.02	0.41
1:A:386:ARG:HD3	1:A:433:TRP:CE3	2.55	0.41
1:B:19:THR:HA	1:B:23:GLY:O	2.20	0.41
1:B:321:VAL:HG11	1:B:399:ILE:HA	2.02	0.41
1:B:407:LYS:HE3	1:B:407:LYS:HB2	1.43	0.41
1:B:457:THR:HB	1:B:460:GLU:HG3	2.01	0.41
1:A:173:LEU:HD12	1:A:173:LEU:HA	1.86	0.41
1:B:227:PHE:CD1	1:B:227:PHE:C	2.94	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	$distance ({ m \AA})$	overlap (Å)
1:A:374:THR:HG22	1:A:376:TRP:CH2	2.56	0.41
1:B:106:ASN:HB2	4:F:1:NAG:H83	2.01	0.41
1:B:169:PHE:CZ	1:B:298:PHE:HB2	2.56	0.41
1:B:242:ARG:O	1:B:279:VAL:HG11	2.21	0.41
1:B:372:HIS:HB3	6:B:601:CWQ:CAQ	2.50	0.41
3:D:1:NAG:H62	3:D:3:FUL:H2	1.76	0.41
1:A:427:LYS:HE2	1:A:427:LYS:HB3	1.88	0.41
1:A:479:ASN:OD1	1:A:481:ASN:ND2	2.54	0.41
1:A:492:VAL:HG12	1:A:494:LYS:HG3	2.03	0.41
1:A:395:ASP:CG	1:A:515[A]:ARG:HE	2.25	0.40
1:B:197:GLU:HA	1:B:223:GLN:O	2.21	0.40
1:B:430:TRP:HB3	1:B:431:PRO:HD2	2.03	0.40
1:A:166:MET:H	1:A:166:MET:CE	2.34	0.40
1:B:102:PRO:O	1:B:138:ARG:NH2	2.54	0.40
1:B:299:LEU:HD23	1:B:299:LEU:HA	1.78	0.40
1:B:35[A]:GLN:HB2	1:B:47:GLN:HB2	2.02	0.40
1:A:457:THR:OG1	1:A:460:GLU:HG3	2.21	0.40
1:B:428:LEU:HD21	1:B:437:MET:SD	2.62	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	528/529~(100%)	500~(95%)	27~(5%)	1 (0%)	47	71
1	В	527/529~(100%)	489 (93%)	34~(6%)	4 (1%)	19	39
All	All	1055/1058~(100%)	989 (94%)	61 (6%)	5 (0%)	29	52

All (5) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	В	55	ILE
1	А	281	PRO
1	В	48	SER
1	В	281	PRO
1	В	253	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	446/454~(98%)	437~(98%)	9~(2%)	55	78	
1	В	448/454 (99%)	435 (97%)	13 (3%)	42	68	
All	All	894/908~(98%)	872 (98%)	22~(2%)	47	73	

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	166	MET
1	А	195	PHE
1	А	255	GLU
1	А	338	SER
1	А	363	GLU
1	А	471	TRP
1	А	495	SER
1	А	507	SER
1	А	524	SER
1	В	48	SER
1	В	50	THR
1	В	96	ASN
1	В	119	GLN
1	В	198	SER
1	В	246	LEU
1	В	286	LEU
1	В	287	SER
1	В	338	SER
1	В	424	ARG



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Mol	Chain	Res	Type
1	В	466	SER
1	В	471	TRP
1	В	524	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type	
1	В	57	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)

16 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).

Mal	Turne	Chain	Dec	Tink	Bond lengths		Bond angles			
	Type	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	С	1	2,1	14,14,15	0.25	0	17,19,21	0.47	0
2	FUL	C	2	2	10,10,11	1.71	2 (20%)	14,14,16	0.77	0
3	NAG	D	1	1,3	14,14,15	0.43	0	17,19,21	1.44	1 (5%)
3	NAG	D	2	3	14,14,15	0.61	0	17,19,21	0.93	2 (11%)
3	FUL	D	3	3	10,10,11	1.03	1 (10%)	14,14,16	1.43	3 (21%)
3	NAG	Е	1	1,3	14,14,15	0.60	0	17,19,21	1.35	2 (11%)
3	NAG	Е	2	3	14,14,15	0.63	0	17,19,21	1.26	2 (11%)
3	FUL	Е	3	3	10,10,11	1.23	1 (10%)	14,14,16	1.83	6 (42%)



Mal	Turne	Chain	Dec	Dog Link		ond leng	$_{\rm ths}$	В	ond ang	les
INIOI	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	F	1	1,4	14,14,15	1.42	1 (7%)	17,19,21	1.46	2 (11%)
4	NAG	F	2	4	14,14,15	0.53	0	17,19,21	0.48	0
5	NAG	G	1	1,5	14,14,15	0.54	0	17,19,21	0.72	0
5	NAG	G	2	5	14,14,15	0.62	0	17,19,21	0.67	0
5	FUC	G	3	5	10,10,11	1.25	2 (20%)	14,14,16	1.14	1 (7%)
3	NAG	Н	1	1,3	14,14,15	0.42	0	17,19,21	1.44	1 (5%)
3	NAG	Н	2	3	14,14,15	0.61	0	17,19,21	0.93	2 (11%)
3	FUL	Н	3	3	10,10,11	1.03	1 (10%)	14,14,16	1.42	3 (21%)

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	С	1	2,1	-	2/6/23/26	0/1/1/1
2	FUL	С	2	2	-	-	0/1/1/1
3	NAG	D	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	D	2	3	-	4/6/23/26	0/1/1/1
3	FUL	D	3	3	-	-	0/1/1/1
3	NAG	Е	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Е	2	3	-	3/6/23/26	0/1/1/1
3	FUL	Е	3	3	-	-	0/1/1/1
4	NAG	F	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	F	2	4	-	4/6/23/26	0/1/1/1
5	NAG	G	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	FUC	G	3	5	-	-	0/1/1/1
3	NAG	Н	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	Н	2	3	-	4/6/23/26	0/1/1/1
3	FUL	Н	3	3	-	-	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1	NAG	O5-C1	-5.08	1.35	1.43
2	С	2	FUL	O5-C1	4.12	1.50	1.43
3	D	3	FUL	C1-C2	2.69	1.58	1.52
3	Н	3	FUL	C1-C2	2.69	1.58	1.52



f = f = f = f = f = f = f = f = f = f =									
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)		
5	G	3	FUC	C4-C5	2.63	1.58	1.52		
3	Е	3	FUL	C2-C3	2.56	1.56	1.52		
2	С	2	FUL	C2-C3	-2.45	1.48	1.52		
5	G	3	FUC	C4-C3	2.20	1.57	1.52		

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	D	1	NAG	C1-O5-C5	5.35	119.44	112.19
3	Н	1	NAG	C1-O5-C5	5.33	119.42	112.19
3	Е	1	NAG	O4-C4-C3	-3.90	101.33	110.35
4	F	1	NAG	C3-C4-C5	3.82	117.06	110.24
4	F	1	NAG	C4-C3-C2	3.73	116.48	111.02
3	Е	3	FUL	C1-C2-C3	3.37	113.81	109.67
3	D	3	FUL	O5-C1-C2	3.24	115.77	110.77
3	Н	3	FUL	O5-C1-C2	3.22	115.73	110.77
3	Е	1	NAG	C4-C3-C2	2.91	115.28	111.02
3	Е	3	FUL	O5-C5-C4	2.87	114.67	109.52
3	D	3	FUL	C1-O5-C5	2.85	119.24	112.78
3	Н	3	FUL	C1-O5-C5	2.85	119.23	112.78
5	G	3	FUC	O5-C5-C4	2.63	114.24	109.52
3	Е	2	NAG	O5-C1-C2	-2.60	107.18	111.29
3	Е	3	FUL	C1-O5-C5	2.52	118.50	112.78
3	Е	3	FUL	C3-C4-C5	2.47	113.63	109.77
3	Е	3	FUL	O5-C1-C2	2.25	114.24	110.77
3	D	2	NAG	C4-C3-C2	2.24	114.29	111.02
3	Н	2	NAG	C4-C3-C2	2.23	114.28	111.02
3	Е	2	NAG	C1-C2-N2	2.13	114.13	110.49
3	Е	3	FUL	C2-C3-C4	2.10	114.54	110.89
3	Н	3	FUL	C1-C2-C3	2.10	112.25	109.67
3	D	3	FUL	C1-C2-C3	2.09	112.24	109.67
3	D	2	NAG	C1-O5-C5	2.05	114.97	112.19
3	Н	2	NAG	C1-O5-C5	2.03	114.94	112.19

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2



Mol	Chain	Res	Type	Atoms
3	Е	1	NAG	C8-C7-N2-C2
3	Е	1	NAG	O7-C7-N2-C2
3	Н	1	NAG	C8-C7-N2-C2
3	Н	1	NAG	O7-C7-N2-C2
3	Н	2	NAG	C8-C7-N2-C2
3	Н	2	NAG	O7-C7-N2-C2
3	D	1	NAG	C4-C5-C6-O6
3	Н	1	NAG	C4-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
3	Е	2	NAG	C8-C7-N2-C2
2	С	1	NAG	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	Н	1	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
3	Е	2	NAG	O7-C7-N2-C2
4	F	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
2	С	1	NAG	C4-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
4	F	2	NAG	C1-C2-N2-C7
3	Е	2	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	Н	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	Н	2	NAG	C4-C5-C6-O6
4	F	2	NAG	C3-C2-N2-C7

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There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Н	1	NAG	3	0
3	D	3	FUL	1	0
3	D	1	NAG	1	0
4	F	2	NAG	2	0
4	F	1	NAG	1	0
5	G	1	NAG	1	0
3	Н	3	FUL	1	0



Oligosaccharide Chain C Oligosaccharide Chain C Bond lengths Bond lengths Bond angles Torsions Rings

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 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 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).

Mal	Turne	Chain	Dec	Tink	Bond lengths			Bond angles		
IVIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
9	NAG	В	611	1	14,14,15	0.82	1 (7%)	17,19,21	0.89	1 (5%)
10	SO4	В	616	-	4,4,4	0.32	0	6,6,6	0.05	0
10	SO4	А	619	-	4,4,4	0.32	0	6,6,6	0.22	0
7	GOL	А	603	-	$5,\!5,\!5$	0.39	0	5,5,5	0.30	0
10	SO4	А	621	-	4,4,4	0.25	0	6,6,6	0.39	0



Mal	Tuno	Chain	Dog	Link	Bond lengths			Bond angles		
	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
10	SO4	В	615	-	4,4,4	0.17	0	$6,\!6,\!6$	0.30	0
6	CWQ	А	602	-	39,39,39	1.98	7 (17%)	50,55,55	1.73	9 (18%)
8	EDO	А	608	-	3,3,3	0.57	0	2,2,2	0.28	0
6	CWQ	В	602	-	39,39,39	2.22	9 (23%)	50,55,55	1.91	14 (28%)
8	EDO	В	604	-	3,3,3	0.57	0	2,2,2	0.16	0
7	GOL	А	604	-	$5,\!5,\!5$	0.40	0	$5,\!5,\!5$	0.66	0
9	NAG	А	615	1	$14,\!14,\!15$	0.50	0	17,19,21	0.55	0
9	NAG	В	605	1	$14,\!14,\!15$	0.39	0	17,19,21	1.14	2 (11%)
6	CWQ	В	601	-	39,39,39	2.18	8 (20%)	50,55,55	1.40	5 (10%)
6	CWQ	А	601	-	39,39,39	2.17	10 (25%)	50,55,55	1.62	8 (16%)
9	NAG	А	611	1	14,14,15	0.65	1 (7%)	17,19,21	0.57	0
8	EDO	А	606	-	3,3,3	0.63	0	2,2,2	0.20	0
10	SO4	А	620	-	4,4,4	0.16	0	6,6,6	0.51	0
8	EDO	А	607	-	3,3,3	0.40	0	2,2,2	0.68	0
7	GOL	А	605	-	5, 5, 5	0.20	0	5, 5, 5	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	А	603	-	-	2/4/4/4	-
8	EDO	А	606	-	-	1/1/1/1	-
8	EDO	В	604	-	-	1/1/1/1	-
7	GOL	А	604	-	-	3/4/4/4	-
6	CWQ	А	602	-	-	4/21/39/39	0/5/5/5
9	NAG	В	611	1	-	0/6/23/26	0/1/1/1
8	EDO	А	608	-	-	1/1/1/1	-
8	EDO	А	607	-	-	1/1/1/1	-
6	CWQ	В	602	-	-	2/21/39/39	0/5/5/5
9	NAG	А	615	1	-	2/6/23/26	0/1/1/1
9	NAG	В	605	1	-	3/6/23/26	0/1/1/1
6	CWQ	В	601	-	-	5/21/39/39	0/5/5/5
6	CWQ	A	601	-	-	4/21/39/39	1/5/5/5
9	NAG	A	611	1	-	3/6/23/26	0/1/1/1
7	GOL	A	605	-	-	4/4/4/4	-

All (36) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
6	В	602	CWQ	CAM-CAN	-6.80	1.39	1.50
6	В	601	CWQ	CAT-CAS	-6.44	1.40	1.50
6	А	601	CWQ	CAM-CAN	-6.43	1.40	1.50
6	В	601	CWQ	CAX-CAW	-6.06	1.40	1.50
6	В	602	CWQ	CAT-CAS	-6.00	1.40	1.50
6	В	602	CWQ	CAX-CAW	-5.92	1.40	1.50
6	В	601	CWQ	CAM-CAN	-5.90	1.41	1.50
6	А	601	CWQ	CAX-CAW	-5.87	1.40	1.50
6	А	602	CWQ	CAM-CAN	-5.66	1.41	1.50
6	А	601	CWQ	CAT-CAS	-5.60	1.41	1.50
6	А	602	CWQ	CAT-CAS	-5.56	1.41	1.50
6	А	602	CWQ	CAX-CAW	-5.22	1.41	1.50
6	В	601	CWQ	CAR-CAS	-3.85	1.33	1.39
6	В	602	CWQ	CAO-CAN	-3.33	1.34	1.39
6	В	601	CWQ	CAM-CAL	-3.33	1.48	1.54
6	А	601	CWQ	CAM-CAL	-3.27	1.48	1.54
6	А	601	CWQ	CAT-CAL	-3.27	1.48	1.54
6	В	601	CWQ	CAO-CAN	-3.24	1.34	1.39
6	В	602	CWQ	CAT-CAL	-3.23	1.49	1.54
6	А	601	CWQ	CAR-CAS	-3.22	1.34	1.39
6	В	602	CWQ	CAR-CAS	-3.21	1.34	1.39
6	А	601	CWQ	CAO-CAN	-3.17	1.34	1.39
6	А	602	CWQ	CAR-CAS	-3.08	1.34	1.39
9	В	611	NAG	O5-C1	2.96	1.48	1.43
6	А	602	CWQ	CAM-CAL	-2.93	1.49	1.54
6	В	601	CWQ	CAT-CAL	-2.81	1.49	1.54
6	А	602	CWQ	CAO-CAN	-2.66	1.35	1.39
6	В	601	CWQ	CAS-CAN	-2.43	1.35	1.39
6	В	602	CWQ	CAM-CAL	-2.34	1.50	1.54
6	А	601	CWQ	CAS-CAN	-2.27	1.35	1.39
6	А	602	CWQ	CBB-CBA	-2.26	1.39	1.42
6	А	601	CWQ	CBE-CBA	-2.24	1.39	1.42
6	А	601	CWQ	CBB-CBA	-2.17	1.39	1.42
6	В	602	CWQ	CBB-CBA	-2.05	1.39	1.42
6	В	602	CWQ	CAS-CAN	-2.03	1.35	1.39
9	А	611	NAG	C1-C2	2.02	1.55	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	В	602	CWQ	CAJ-NAK-CAU	6.58	114.67	108.19
6	А	601	CWQ	CAG-CAF-NAE	5.48	122.48	113.80
6	А	602	CWQ	CAS-CAT-CAL	-4.81	98.25	103.39



6F''/Q

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	Observed(^o)	Ideal(°)
6	В	601	CWQ	CAG-CAF-NAE	4.73	121.29	113.80
6	А	602	CWQ	CBD-CAX-NAZ	-4.53	117.82	123.42
6	А	602	CWQ	CAN-CAM-CAL	-4.13	98.98	103.39
6	В	602	CWQ	CAG-CAF-NAE	-4.09	107.32	113.80
6	А	601	CWQ	CAJ-NAK-CAU	3.82	111.95	108.19
6	В	602	CWQ	CAS-CAT-CAL	-3.68	99.47	103.39
6	А	601	CWQ	CBD-CAX-NAZ	-3.61	118.95	123.42
6	В	602	CWQ	CBD-CAX-NAZ	-3.54	119.04	123.42
6	А	602	CWQ	CBE-CBA-NAZ	3.43	120.78	117.33
6	А	602	CWQ	CAM-CAN-CAS	-3.23	108.33	110.56
6	В	601	CWQ	CBD-CAX-NAZ	-3.21	119.45	123.42
6	А	602	CWQ	CAG-CAF-NAE	-3.17	108.76	113.80
6	В	602	CWQ	CAN-CAM-CAL	-3.15	100.03	103.39
6	В	602	CWQ	CAM-CAN-CAS	-3.07	108.44	110.56
9	В	611	NAG	C1-O5-C5	2.98	116.22	112.19
6	В	602	CWQ	CAG-CAU-NAK	2.92	116.15	110.45
6	А	602	CWQ	CAX-NAZ-CBA	2.87	123.28	117.24
6	А	601	CWQ	CBE-CBA-NAZ	2.83	120.18	117.33
6	А	601	CWQ	CAD-NAE-CAF	-2.76	113.13	116.41
6	А	601	CWQ	CAM-CAN-CAS	-2.68	108.71	110.56
6	А	601	CWQ	CAX-NAZ-CBA	2.63	122.79	117.24
6	В	602	CWQ	CAI-CAJ-NAK	-2.57	106.95	111.28
9	В	605	NAG	C1-O5-C5	2.54	115.63	112.19
6	В	602	CWQ	CAX-NAZ-CBA	2.53	122.58	117.24
6	А	602	CWQ	CAT-CAS-CAN	-2.53	108.82	110.56
6	В	602	CWQ	CBD-CAX-CAW	2.48	123.79	119.21
6	В	601	CWQ	CAJ-NAK-CAU	2.46	110.61	108.19
6	В	601	CWQ	CBE-CBA-NAZ	2.30	119.64	117.33
6	В	602	CWQ	CAH-CAG-CAU	2.28	111.25	108.68
6	В	602	CWQ	CAU-NAK-CAL	-2.22	106.56	112.69
6	В	601	CWQ	CAX-NAZ-CBA	2.17	121.82	117.24
6	В	602	CWQ	CAT-CAS-CAN	-2.14	109.08	110.56
6	В	602	CWQ	CBG-CBF-CBE	-2.09	117.64	120.28
6	А	602	CWQ	CAD-NAE-CAF	-2.06	113.96	116.41
9	В	605	NAG	O5-C1-C2	-2.05	108.06	111.29
6	А	601	CWQ	CAH-CAI-CAJ	2.02	113.69	110.85

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There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms				
6	А	601	CWQ	NAE-CAF-CAG-CAH				
Continued on next page								



Mol	Chain	Res	Type	Atoms
6	А	601	CWQ	NAE-CAF-CAG-CAU
6	А	602	CWQ	CAM-CAL-NAK-CAJ
6	А	602	CWQ	CAM-CAL-NAK-CAU
6	А	602	CWQ	CAT-CAL-NAK-CAJ
6	А	602	CWQ	CAT-CAL-NAK-CAU
6	В	601	CWQ	NAE-CAF-CAG-CAU
6	В	602	CWQ	CAC-CAD-NAE-CAW
7	А	603	GOL	O1-C1-C2-C3
7	А	605	GOL	O1-C1-C2-C3
7	А	605	GOL	C1-C2-C3-O3
9	А	615	NAG	C4-C5-C6-O6
9	А	611	NAG	C8-C7-N2-C2
9	А	611	NAG	O7-C7-N2-C2
9	В	605	NAG	C8-C7-N2-C2
9	В	605	NAG	O7-C7-N2-C2
9	А	615	NAG	O5-C5-C6-O6
7	А	604	GOL	O1-C1-C2-C3
7	А	603	GOL	O1-C1-C2-O2
7	А	605	GOL	O1-C1-C2-O2
7	А	605	GOL	O2-C2-C3-O3
8	А	606	EDO	O1-C1-C2-O2
9	В	605	NAG	O5-C5-C6-O6
6	В	601	CWQ	NAE-CAF-CAG-CAH
9	А	611	NAG	O5-C5-C6-O6
8	А	607	EDO	O1-C1-C2-O2
8	А	608	EDO	O1-C1-C2-O2
8	В	604	EDO	O1-C1-C2-O2
7	А	604	GOL	O2-C2-C3-O3
6	В	601	CWQ	CAD-CAC-NAB-CAA
6	В	601	CWQ	CAD-CAC-NAB-CAV
6	В	601	CWQ	CAC-CAD-NAE-CAF
6	А	601	CWQ	CAM-CAL-NAK-CAJ
6	В	602	CWQ	CAC-CAD-NAE-CAF
6	А	601	CWQ	CAD-CAC-NAB-CAV
7	А	604	GOL	O1-C1-C2-O2

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All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	А	601	CWQ	CAG-CAH-CAI-CAJ-CAU-NAK

8 monomers are involved in 26 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	А	603	GOL	2	0
10	В	615	SO4	1	0
8	А	608	EDO	2	0
8	В	604	EDO	2	0
9	В	605	NAG	13	0
6	В	601	CWQ	1	0
10	А	620	SO4	3	0
7	А	605	GOL	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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	527/529~(99%)	-0.17	17 (3%) 47 40	38, 57, 90, 113	6 (1%)
1	В	527/529~(99%)	-0.17	12 (2%) 60 54	45, 69, 96, 129	7 (1%)
All	All	1054/1058~(99%)	-0.17	29 (2%) 53 46	38, 63, 94, 129	13 (1%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	4	ILE	3.8
1	В	3	ASP	3.8
1	А	254	ARG	3.5
1	В	53	SER	3.5
1	А	54	ASP	3.4
1	А	5	ILE	3.4
1	А	253	SER	3.2
1	А	55	ILE	3.1
1	А	53	SER	3.1
1	А	257	GLU	3.1
1	А	3	ASP	2.9
1	В	258	THR	2.9
1	А	255	GLU	2.9
1	А	258	THR	2.5
1	В	342	ASN	2.4
1	В	345	ILE	2.4
1	А	249	LEU	2.4
1	В	453	ARG	2.3
1	В	255	GLU	2.3
1	В	4	ILE	2.3
1	А	266	ASN	2.3
1	A	52	TRP	2.2
1	A	261	ILE	2.2
1	А	259	GLU	2.2



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Mol	Chain	Res	Type	RSRZ
1	В	5	ILE	2.1
1	В	18	LEU	2.1
1	В	17	ASN	2.1
1	А	161	GLU	2.1
1	В	161	GLU	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	$B-factors(Å^2)$	Q<0.9
3	NAG	D	2	14/15	0.59	0.53	121,134,138,142	0
3	NAG	Е	2	14/15	0.59	0.51	111,127,135,139	0
3	FUL	D	3	10/11	0.69	0.49	92,114,121,129	0
3	NAG	Н	2	14/15	0.72	0.50	116,127,131,134	0
3	FUL	Н	3	10/11	0.72	0.45	98,111,116,122	0
3	FUL	Е	3	10/11	0.73	0.27	105,113,115,115	0
4	NAG	F	2	14/15	0.78	0.22	97,120,133,135	0
5	NAG	G	2	14/15	0.81	0.30	95,105,117,125	0
3	NAG	Н	1	14/15	0.83	0.31	109,123,128,133	0
3	NAG	D	1	14/15	0.85	0.29	107,120,130,135	0
4	NAG	F	1	14/15	0.87	0.11	81,95,106,112	0
5	FUC	G	3	10/11	0.88	0.32	$102,\!111,\!125,\!125$	0
3	NAG	Е	1	14/15	0.89	0.23	86,99,111,122	0
2	FUL	С	2	10/11	0.91	0.29	80,90,93,99	0
2	NAG	C	1	14/15	0.93	0.28	90,96,101,106	0
5	NAG	G	1	14/15	0.94	0.20	84,91,103,109	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	$B-factors(Å^2)$	Q<0.9
7	GOL	А	604	6/6	0.62	0.30	$67,\!78,\!84,\!85$	0
7	GOL	А	603	6/6	0.66	0.33	79,84,89,95	0
9	NAG	В	605	14/15	0.69	0.27	106,116,122,124	0
10	SO4	А	620	5/5	0.70	0.39	85,87,102,106	5
10	SO4	А	621	5/5	0.81	0.29	74,80,89,106	5
10	SO4	В	615	5/5	0.83	0.20	92,94,102,119	5
7	GOL	А	605	6/6	0.84	0.25	61,63,71,75	0
9	NAG	В	611	14/15	0.89	0.14	71,84,100,100	0
9	NAG	А	615	14/15	0.90	0.16	62,86,97,99	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
8	EDO	А	607	4/4	0.90	0.17	$66,\!67,\!68,\!72$	0
9	NAG	А	611	14/15	0.91	0.16	58,70,79,83	0
11	CL	В	603	1/1	0.92	0.17	78,78,78,78	0
6	CWQ	В	602	35/35	0.94	0.20	54,69,89,94	0
6	CWQ	А	602	35/35	0.94	0.24	38,54,63,69	0
8	EDO	А	606	4/4	0.94	0.21	53,74,75,76	0
10	SO4	В	616	5/5	0.95	0.15	62,79,89,100	5
10	SO4	А	619	5/5	0.95	0.19	62,73,84,93	5
6	CWQ	А	601	35/35	0.96	0.14	49,61,73,76	0
8	EDO	А	608	4/4	0.96	0.13	$57,\!61,\!68,\!68$	0
6	CWQ	В	601	35/35	0.97	0.12	50,57,66,72	0
8	EDO	В	604	4/4	0.98	0.11	57,64,68,72	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.

