

# Full wwPDB X-ray Structure Validation Report (i)

#### Nov 13, 2023 - 03:19 am GMT

:	8QHL
:	Human Angiotensin-1 converting enzyme N-domain in complex with the lac-
	totripeptide VPP
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:	2023-09-08
:	1.90 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
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

# 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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	628	85%	10%	•	
1	В	628	87%	8%	·	•
2	С	3	100%			-
2	D	3	100%			-
3	Е	2	100%			_



Mol	Chain	Length	Quality of chain						
3	F	2	100%						
4	G	4	50%	50%					
5	Н	3	67%	33%					
6	Ι	2	50%	50%					
6	J	2	50%	50%					



#### 8QHL

# 2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 10738 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	Atoms					ZeroOcc	AltConf	Trace
1	В	603	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	1	0
L	1 D 005	4960	3184	850	907	19	0	4	0	
1	Λ	605	Total	С	Ν	Ο	$\mathbf{S}$	0	1	0
	005	4964	3187	850	908	19	0	4	0	

• Molecule 1 is a protein called Angiotensin-converting enzyme.

Chain	Residue	Modelled	Actual	Comment	Reference
В	9	GLN	ASN	engineered mutation	UNP P12821
В	25	GLN	ASN	engineered mutation	UNP P12821
В	82	GLN	ASN	engineered mutation	UNP P12821
В	117	GLN	ASN	engineered mutation	UNP P12821
В	131	GLN	ASN	engineered mutation	UNP P12821
В	289	GLN	ASN	engineered mutation	UNP P12821
В	545	ARG	GLN	engineered mutation	UNP P12821
В	576	LEU	PRO	engineered mutation	UNP P12821
А	9	GLN	ASN	engineered mutation	UNP P12821
А	25	GLN	ASN	engineered mutation	UNP P12821
А	82	GLN	ASN	engineered mutation	UNP P12821
А	117	GLN	ASN	engineered mutation	UNP P12821
А	131	GLN	ASN	engineered mutation	UNP P12821
А	289	GLN	ASN	engineered mutation	UNP P12821
А	545	ARG	GLN	engineered mutation	UNP P12821
А	576	LEU	PRO	engineered mutation	UNP P12821

There are 16 discrepancies between the modelled and reference sequences:

• Molecule 2 is a protein called VAL-PRO-PRO.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	3	Total 22	C 15	N 3	0 4	0	0	0
2	С	3	Total 22	C 15	N 3	0 4	0	0	0



• Molecule 3 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
3	Е	2	Total         C         N         O           28         16         2         10	0	0	0
3	F	2	Total         C         N         O           28         16         2         10	0	0	0

• Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b eta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopy ranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total 49	C 28	N 2	O 19	0	0	0

• Molecule 5 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	Aton	ns	ZeroOcc	AltConf	Trace
5	Н	3	TotalC3922	N O 2 15	0	0	0

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





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

• Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	В	1	Total Zn 1 1	0	0
7	А	1	Total Zn 1 1	0	0

• Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	В	1	Total Cl 1 1	0	0
8	А	1	Total Cl 1 1	0	0

• Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 7  4  3 \end{array}$	0	0
9	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
9	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
9	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
9	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
9	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 7  4  3 \end{array}$	0	0

• Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

• Molecule 11 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	В	1	Total C O	0	0
	L	13  8  5	0	0	
11	Λ	1	Total C O	0	0
	А	L	$13 \ 8 \ 5$	0	0

• Molecule 12 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Ato	$\mathbf{ms}$		ZeroOcc	AltConf
12	В	1	Total 10	C 6	O 4	0	0





Mol	Chain	Residues	A	tor	ns		ZeroOcc	AltConf
13	А	1	Total 11	С 6	N 1	0 4	0	0

 $\bullet\,$  Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	А	1	Total Mg 1 1	0	0

• Molecule 15 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	А	1	Total         C         O           16         10         6	0	0
15	А	1	Total         C         O           16         10         6	0	0

• Molecule 16 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	В	252	Total         O           252         252	0	0
16	D	3	Total O 3 3	0	0
16	А	187	Total O 187 187	0	0
16	С	2	Total O 2 2	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: Angiotensin-converting enzyme



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

100%

#### NAG1 NAG2

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain F.	100%
Unam 1.	100 %

#### NAG1 NAG2

 $\bullet \ Molecule \ 4: \ beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alp ha-L-fucopyranose-(1-6)] 2-acetamido-2-deoxy-beta-D-glucopyranose \ (1-6)] 2-acetamido-2-deoxy-$ 

Chain G:	50%	50%	
NAG1 NAG2 BMA3 FUC4			

• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:	67%	33%	
NAG1 NAG2 BMA3			
• Molecul	e 6: alpha-L-fucopyranose-(1-6)-	2-acetamido-2-deoxy-beta-D-gluc	opyranose
Chain I:	50%	50%	
NAG1 FUC2			

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

Chain J:	50%	50%	
NAG1 FUC2			



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	73.34Å 78.22Å 83.01Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$88.75^{\circ}$ $64.70^{\circ}$ $75.25^{\circ}$	Depositor
Bosolution (Å)	75.27 - 1.90	Depositor
	75.27 - 1.90	EDS
% Data completeness	97.9 (75.27-1.90)	Depositor
(in resolution range)	95.9 (75.27-1.90)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.13 (at 1.90 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
D D.	0.188 , $0.233$	Depositor
$n, n_{free}$	0.190 , $0.237$	DCC
$R_{free}$ test set	6115 reflections $(5.04%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	32.4	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34 , $42.8$	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.50, \langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	10738	wwPDB-VP
Average B, all atoms $(Å^2)$	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.69% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: BMA, 1PE, ZN, PGE, NAG, FUC, MG, BCN, PG4, PEG, EDO, CL

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	Bond angles	
IVIOI	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.65	5/5120~(0.1%)	0.96	4/6975~(0.1%)
1	В	0.73	2/5115~(0.0%)	1.01	8/6966~(0.1%)
2	С	1.23	0/23	1.17	0/31
2	D	1.45	0/23	1.10	0/31
All	All	0.69	7/10281~(0.1%)	0.99	12/14003~(0.1%)

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	А	0	5
1	В	0	5
All	All	0	10

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
1	А	15	ALA	C-O	6.94	1.36	1.23
1	В	513	GLU	CD-OE2	-6.04	1.19	1.25
1	А	176	GLU	CD-OE1	5.47	1.31	1.25
1	А	55	GLU	CD-OE1	-5.43	1.19	1.25
1	А	389	GLU	CD-OE2	5.39	1.31	1.25
1	В	29	GLU	CD-OE2	5.03	1.31	1.25
1	А	481	GLU	CD-OE1	5.00	1.31	1.25

All (12) bond angle outliers are listed below:



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Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	В	541	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	А	203	ASN	CB-CA-C	-7.51	95.38	110.40
1	В	151	ARG	NE-CZ-NH1	-7.21	116.69	120.30
1	В	453	ARG	CB-CG-CD	6.83	129.37	111.60
1	А	545	ARG	CG-CD-NE	-6.31	98.56	111.80
1	В	326	ARG	CB-CG-CD	-6.26	95.31	111.60
1	В	541	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	В	236	ARG	CG-CD-NE	-5.79	99.64	111.80
1	В	153	TYR	CB-CA-C	5.11	120.63	110.40
1	А	25	GLN	CB-CA-C	5.08	120.56	110.40
1	B	418	THR	CA-CB-OG1	-5.04	98.42	109.00
1	А	459	TYR	CA-CB-CG	5.04	122.97	113.40

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	350	ARG	Sidechain
1	А	380	ARG	Sidechain
1	А	453	ARG	Sidechain
1	А	545	ARG	Sidechain
1	А	89	ARG	Sidechain
1	В	120	ARG	Sidechain
1	В	151	ARG	Sidechain
1	В	380	ARG	Sidechain
1	В	453	ARG	Sidechain
1	В	96	ARG	Sidechain

# 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	4964	0	4732	28	0
1	В	4960	0	4730	28	0
2	С	22	0	22	0	0
2	D	22	0	22	0	0
3	Е	28	0	25	0	0
3	F	28	0	25	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	49	0	44	1	0
5	Н	39	0	34	1	0
6	Ι	24	0	22	1	0
6	J	24	0	22	1	0
7	А	1	0	0	0	0
7	В	1	0	0	0	0
8	А	1	0	0	0	0
8	В	1	0	0	0	0
9	А	21	0	30	1	0
9	В	21	0	30	2	0
10	В	8	0	12	2	0
11	А	13	0	18	2	0
11	В	13	0	18	1	0
12	В	10	0	14	0	0
13	А	11	0	12	1	0
14	А	1	0	0	0	0
15	А	32	0	44	5	0
16	А	187	0	0	4	0
16	В	252	0	0	1	0
16	С	2	0	0	0	0
16	D	3	0	0	0	0
All	All	10738	0	9856	65	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 3.

All (65) 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)
5:H:1:NAG:H62	5:H:2:NAG:H82	1.52	0.90
1:A:292:HIS:NE2	15:A:708:1PE:H121	1.90	0.86
1:A:66:GLU:O	1:A:70:GLN:HG3	1.90	0.72
1:B:381:ARG:HH11	10:B:705:EDO:H12	1.57	0.70
1:B:88:LEU:O	1:B:88:LEU:HD23	1.93	0.68
1:A:1:LEU:HD23	1:A:6:GLN:HG3	1.76	0.67
1:B:275:PRO:HD3	1:B:413:ARG:CZ	2.25	0.66
1:A:270:PRO:O	1:A:272:PRO:HD3	1.95	0.65
1:A:292:HIS:CD2	15:A:708:1PE:H121	2.33	0.64
1:B:73:LYS:HG3	1:B:96:ARG:HG3	1.81	0.63
1:B:83:PHE:CD2	1:B:88:LEU:HD22	2.33	0.63
1:A:91:ILE:O	1:A:95:VAL:HG23	1.99	0.62



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
11:A:707:PG4:H22	16:A:833:HOH:O	1.99	0.62
15:A:708:1PE:H252	16:A:977:HOH:O	2.00	0.61
1:A:191:PHE:CZ	9:A:703:PEG:H31	2.37	0.60
1:B:52:ARG:HH11	1:B:52:ARG:HG2	1.68	0.59
15:A:708:1PE:H162	16:A:979:HOH:O	2.04	0.58
1:B:228:PHE:CZ	9:B:706:PEG:H32	2.39	0.58
1:B:157:LEU:HD11	1:B:477:VAL:HG13	1.85	0.57
1:A:130:PRO:O	1:A:131:GLN:HB2	2.08	0.54
1:A:59:LEU:O	1:A:63:GLU:HG3	2.07	0.53
1:B:77:GLU:OE2	1:B:96:ARG:HD2	2.07	0.53
1:A:236:ARG:HH21	1:A:236:ARG:HG3	1.74	0.53
1:B:25:GLN:OE1	1:B:376:PRO:HA	2.10	0.52
1:B:79:ILE:O	1:B:79:ILE:HG22	2.11	0.50
1:A:24:TYR:HD2	1:A:25:GLN:HG3	1.76	0.50
1:A:77:GLU:OE2	1:A:96:ARG:HD2	2.11	0.50
1:B:570:LEU:C	1:B:570:LEU:HD23	2.32	0.49
1:A:31:VAL:O	1:A:34:GLN:HG3	2.12	0.49
1:A:510:GLN:HG2	1:A:569:PRO:HG2	1.94	0.49
1:B:13:ASP:OD1	1:B:13:ASP:C	2.52	0.48
11:B:707:PG4:H42	11:B:707:PG4:H21	1.48	0.48
1:A:478:THR:CG2	6:J:2:FUC:H63	2.43	0.48
1:B:83:PHE:HD2	1:B:88:LEU:HD22	1.76	0.48
13:A:704:BCN:O21	13:A:704:BCN:H61	2.13	0.47
1:B:477:VAL:HG12	1:B:603:LEU:HD21	1.97	0.47
1:B:187:LYS:HE3	1:B:187:LYS:HB2	1.65	0.47
10:B:704:EDO:O2	9:B:708:PEG:H12	2.15	0.46
1:A:274:LYS:HB3	1:A:275:PRO:CD	2.46	0.46
1:A:2:ASP:OD1	1:A:3:PRO:HD2	2.17	0.45
1:A:341:LYS:HE3	1:A:341:LYS:HB2	1.66	0.45
1:B:580:TRP:O	1:B:584:GLN:HG2	2.17	0.44
1:B:177:ASP:OD1	16:B:801:HOH:O	2.21	0.43
1:A:557:LYS:HA	1:A:562:LEU:O	2.19	0.43
4:G:1:NAG:C6	4:G:4:FUC:C1	2.90	0.43
1:B:138:SER:O	1:B:142:ASP:HB2	2.19	0.42
1:B:14:GLU:HB2	1:B:83:PHE:CD1	2.55	0.42
11:A:707:PG4:C2	16:A:833:HOH:O	2.65	0.42
1:B:507:LEU:HD13	1:B:565:LEU:CD2	2.49	0.42
1:B:77:GLU:OE2	1:B:77:GLU:HA	2.20	0.42
1:B:495:VAL:HG12	1:B:495:VAL:O	2.20	0.42
1:A:172:LYS:HB3	1:A:173:PRO:HD3	2.02	0.42
1:A:90:ARG:NH1	1:A:551:PRO:HA	2.35	0.41



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:LYS:O	1:B:176[A]:GLU:HG3	2.21	0.41
1:A:441:LEU:HD12	1:A:441:LEU:C	2.40	0.41
1:A:280:THR:HG23	1:A:352:THR:HA	2.02	0.41
1:B:137:TRP:CZ3	1:B:155:MET:HE1	2.55	0.41
1:A:76:TYR:O	1:A:80:TRP:HD1	2.02	0.41
1:A:204:SER:HA	1:A:205:PRO:HD2	1.88	0.41
1:B:607:TYR:HA	1:B:608:PRO:HA	1.85	0.40
1:A:292:HIS:NE2	15:A:708:1PE:C12	2.74	0.40
1:B:25:GLN:O	1:B:25:GLN:HG3	2.18	0.40
1:B:218:LEU:HD13	1:B:436:LEU:HD13	2.03	0.40
1:A:245:ARG:NH1	6:I:1:NAG:H82	2.36	0.40
1:A:603:LEU:HD22	1:A:603:LEU:H	1.87	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	605/628~(96%)	588~(97%)	14 (2%)	3~(0%)	29	18
1	В	603/628~(96%)	589~(98%)	13~(2%)	1 (0%)	47	38
2	С	1/3~(33%)	1 (100%)	0	0	100	100
2	D	1/3~(33%)	1 (100%)	0	0	100	100
All	All	1210/1262~(96%)	1179 (97%)	27(2%)	4 (0%)	41	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	45	ASN
1	А	416	ASN
1	В	45	ASN



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Mol	Chain	Res	Type
1	А	78	PRO

### 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	in Analysed Rotameric Outliers		Percentiles		
1	А	524/540~(97%)	512 (98%)	12 (2%)	50 45	
1	В	523/540~(97%)	512 (98%)	11 (2%)	53 48	
2	С	3/3~(100%)	3~(100%)	0	100 100	
2	D	3/3~(100%)	3~(100%)	0	100 100	
All	All	1053/1086~(97%)	1030 (98%)	23~(2%)	52 47	

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	11	SER
1	В	25	GLN
1	В	236	ARG
1	В	278	ASP
1	В	368	TYR
1	В	372	TYR
1	В	388	HIS
1	В	412	ASP
1	В	413	ARG
1	В	417	ASP
1	В	606	ASN
1	А	96	ARG
1	А	354	ASP
1	А	368	TYR
1	А	372	TYR
1	А	377	VAL
1	А	381	ARG
1	A	388	HIS
1	А	415	THR
1	А	419	GLU



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Mol	Chain	Res	Type
1	А	421	ASP
1	А	441	LEU
1	А	598	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	87	GLN
1	В	371	GLN
1	А	25	GLN
1	А	371	GLN
1	А	527	GLN
1	А	585	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)

15 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	Mal Trupa Chai			Tink	Bo	ond leng	ths	В	ond ang	les
WIOI	Type Chain Res	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
3	NAG	E	1	3,1	14,14,15	0.51	0	17,19,21	1.41	2 (11%)
3	NAG	Е	2	3	14,14,15	0.59	0	17,19,21	1.56	3 (17%)
3	NAG	F	1	3,1	14,14,15	0.49	0	17,19,21	1.27	3 (17%)
3	NAG	F	2	3	14,14,15	0.57	0	17,19,21	1.52	2 (11%)



Mal	al Type Chain Reg Lin		Tink	Bo	ond leng	$\mathbf{ths}$	Bond angles			
WIOI	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
4	NAG	G	1	4,1	14,14,15	0.51	0	17,19,21	1.32	2 (11%)
4	NAG	G	2	4	14,14,15	0.43	0	$17,\!19,\!21$	1.69	3 (17%)
4	BMA	G	3	4	11,11,12	0.98	1 (9%)	$15,\!15,\!17$	1.18	1 (6%)
4	FUC	G	4	4	10,10,11	0.61	0	14,14,16	1.66	3 (21%)
5	NAG	Н	1	5,1	14,14,15	0.46	0	$17,\!19,\!21$	1.79	2 (11%)
5	NAG	Н	2	5	14,14,15	0.53	0	17,19,21	0.74	0
5	BMA	Н	3	5	11,11,12	0.86	0	$15,\!15,\!17$	0.88	1 (6%)
6	NAG	Ι	1	6,1	14,14,15	0.61	0	17,19,21	1.34	2 (11%)
6	FUC	Ι	2	6	10,10,11	0.98	1 (10%)	14,14,16	1.88	4 (28%)
6	NAG	J	1	6,1	14,14,15	0.41	0	17,19,21	1.20	2 (11%)
6	FUC	J	2	6	10,10,11	0.82	1 (10%)	14,14,16	1.76	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
3	NAG	Е	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Е	2	3	-	4/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	5/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	FUC	G	4	4	-	-	0/1/1/1
5	NAG	Н	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	Н	2	5	-	4/6/23/26	0/1/1/1
5	BMA	Н	3	5	-	2/2/19/22	0/1/1/1
6	NAG	Ι	1	6,1	-	1/6/23/26	0/1/1/1
6	FUC	Ι	2	6	-	-	0/1/1/1
6	NAG	J	1	6,1	-	3/6/23/26	0/1/1/1
6	FUC	J	2	6	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	3	BMA	C2-C3	2.29	1.55	1.52



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0 01000100000	<i>J</i> · <i>c</i> · · · <i>c</i>	proceed as	P ~ 9 ~

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
6	J	2	FUC	C2-C3	2.16	1.55	1.52
6	Ι	2	FUC	C4-C3	2.15	1.57	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	Н	1	NAG	C1-C2-N2	5.68	120.19	110.49
4	G	2	NAG	C1-C2-N2	4.66	118.45	110.49
3	F	2	NAG	O5-C1-C2	4.53	118.44	111.29
3	Ε	2	NAG	C2-N2-C7	4.43	129.21	122.90
6	J	2	FUC	C3-C4-C5	-4.30	103.08	109.77
3	Е	1	NAG	C1-O5-C5	3.98	117.58	112.19
4	G	2	NAG	C1-O5-C5	3.91	117.49	112.19
6	Ι	2	FUC	O3-C3-C2	-3.73	102.86	109.99
5	Н	1	NAG	C1-O5-C5	3.56	117.01	112.19
3	Е	1	NAG	C2-N2-C7	3.46	127.83	122.90
6	Ι	2	FUC	O3-C3-C4	3.38	118.17	110.35
4	G	4	FUC	O5-C1-C2	3.36	115.95	110.77
4	G	1	NAG	C1-O5-C5	3.35	116.73	112.19
6	Ι	2	FUC	O4-C4-C3	3.25	117.87	110.35
4	G	3	BMA	C1-C2-C3	3.15	113.54	109.67
3	F	1	NAG	C1-O5-C5	2.93	116.16	112.19
4	G	4	FUC	C1-O5-C5	2.87	119.29	112.78
6	J	2	FUC	O3-C3-C2	2.75	115.26	109.99
3	Ε	2	NAG	O5-C1-C2	-2.71	107.02	111.29
3	Ε	2	NAG	C1-O5-C5	2.60	115.71	112.19
6	J	1	NAG	C1-C2-N2	2.51	114.77	110.49
6	Ι	1	NAG	O5-C1-C2	-2.50	107.35	111.29
3	F	1	NAG	C4-C3-C2	2.48	114.65	111.02
4	G	2	NAG	O3-C3-C2	-2.45	104.39	109.47
6	J	1	NAG	C2-N2-C7	2.44	126.37	122.90
4	G	1	NAG	C1-C2-N2	-2.35	106.48	110.49
3	F	1	NAG	O5-C1-C2	-2.33	107.61	111.29
6	Ι	1	NAG	C3-C4-C5	-2.26	106.21	110.24
6	J	2	FUC	O2-C2-C3	-2.22	105.69	110.14
6	Ι	2	FUC	O2-C2-C1	2.14	113.52	109.15
5	Н	3	BMA	C1-C2-C3	2.13	112.28	109.67
3	F	2	NAG	$\overline{\text{C2-N2-C7}}$	2.09	125.88	122.90
4	G	4	FUC	O2-C2-C3	2.05	114.24	110.14

There are no chirality outliers.

All (29) torsion outliers are listed below:



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

There are no ring outliers.

6 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Ι	1	NAG	1	0
4	G	4	FUC	1	0
5	Н	2	NAG	1	0
5	Н	1	NAG	1	0
6	J	2	FUC	1	0
4	G	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)

Of 19 ligands modelled in this entry, 5 are monoatomic - leaving 14 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	Bo	ond leng	$_{\rm ths}$	B	ond ang	les
	туре	Ullalli	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
10	EDO	В	705	-	3,3,3	0.26	0	2,2,2	0.53	0
9	PEG	В	703	-	$6,\!6,\!6$	0.34	0	$5,\!5,\!5$	0.42	0
9	PEG	В	708	-	6,6,6	0.41	0	$5,\!5,\!5$	0.38	0
9	PEG	А	703	-	6,6,6	0.26	0	$5,\!5,\!5$	0.16	0
13	BCN	А	704	-	10,10,10	1.11	1 (10%)	11,11,11	1.10	1 (9%)
10	EDO	В	704	-	3,3,3	0.18	0	2,2,2	0.21	0
15	1PE	А	708	-	$15,\!15,\!15$	0.51	0	14,14,14	0.39	0
9	PEG	А	705	-	$6,\!6,\!6$	0.20	0	$5,\!5,\!5$	0.28	0
11	PG4	А	707	-	12,12,12	0.61	0	11,11,11	0.47	0
9	PEG	В	706	-	6,6,6	0.60	0	$5,\!5,\!5$	0.77	0
12	PGE	В	709	-	9,9,9	0.32	0	8,8,8	0.29	0
11	PG4	В	707	-	12,12,12	0.30	0	11,11,11	0.27	0
9	PEG	А	710	-	$6,\!6,\!6$	0.16	0	$5,\!5,\!5$	0.16	0
15	1PE	А	709	-	$15,\!15,\!15$	0.58	0	14,14,14	0.41	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
10	EDO	В	705	-	-	1/1/1/1	-
9	PEG	В	703	-	-	2/4/4/4	-
9	PEG	В	708	-	-	2/4/4/4	-
9	PEG	А	703	-	-	4/4/4/4	-
13	BCN	А	704	-	-	5/10/10/10	-
10	EDO	В	704	-	-	0/1/1/1	-
15	1PE	А	708	-	-	6/13/13/13	-
9	PEG	А	705	-	-	4/4/4/4	-
11	PG4	А	707	-	-	7/10/10/10	-
9	PEG	В	706	-	-	1/4/4/4	-
12	PGE	В	709	-	-	3/7/7/7	-
11	PG4	В	707	-	-	6/10/10/10	-
9	PEG	А	710	-	-	3/4/4/4	-
15	1PE	А	709	-	-	6/13/13/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	704	BCN	C1-N1	2.32	1.52	1.47



All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
13	А	704	BCN	C2-C1-N1	2.53	121.90	113.63

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	А	704	BCN	C6-C5-N1-C1
13	А	704	BCN	N1-C1-C2-O21
9	А	705	PEG	C1-C2-O2-C3
11	В	707	PG4	C4-C3-O2-C2
13	А	704	BCN	N1-C1-C2-O22
11	А	707	PG4	O3-C5-C6-O4
9	А	705	PEG	O1-C1-C2-O2
11	В	707	PG4	O3-C5-C6-O4
9	А	705	PEG	O2-C3-C4-O4
12	В	709	PGE	O3-C5-C6-O4
15	А	708	1PE	OH7-C16-C26-OH6
15	А	709	1PE	OH2-C12-C22-OH3
15	А	709	1PE	OH7-C16-C26-OH6
11	А	707	PG4	O4-C7-C8-O5
13	А	704	BCN	N1-C3-C4-O4
9	В	703	PEG	O1-C1-C2-O2
9	В	706	PEG	O2-C3-C4-O4
9	В	708	PEG	O1-C1-C2-O2
11	А	707	PG4	O1-C1-C2-O2
13	А	704	BCN	N1-C5-C6-O6
9	А	710	PEG	O2-C3-C4-O4
15	А	708	1PE	OH6-C15-C25-OH5
9	В	703	PEG	O2-C3-C4-O4
15	А	709	1PE	OH4-C13-C23-OH3
9	А	703	PEG	O1-C1-C2-O2
11	В	707	PG4	C8-C7-O4-C6
11	А	707	PG4	C5-C6-O4-C7
11	В	707	PG4	C1-C2-O2-C3
11	А	707	PG4	C6-C5-O3-C4
9	А	710	PEG	C1-C2-O2-C3
15	А	709	1PE	C14-C24-OH4-C13
12	В	709	PGE	C6-C5-O3-C4
15	А	708	1PE	С14-С24-ОН4-С13
11	А	707	PG4	C4-C3-O2-C2
11	В	707	PG4	C5-C6-O4-C7



UQUL
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Mol	Chain	Res	Type	Atoms
9	В	708	PEG	O2-C3-C4-O4
9	А	703	PEG	C4-C3-O2-C2
15	А	708	1PE	OH4-C13-C23-OH3
15	А	709	1PE	C25-C15-OH6-C26
15	А	708	1PE	C15-C25-OH5-C14
11	В	707	PG4	C3-C4-O3-C5
10	В	705	EDO	O1-C1-C2-O2
15	А	708	1PE	С12-С22-ОН3-С23
12	В	709	PGE	O1-C1-C2-O2
9	А	703	PEG	C1-C2-O2-C3
9	А	705	PEG	C4-C3-O2-C2
9	А	703	PEG	O2-C3-C4-O4
15	А	709	1PE	C24-C14-OH5-C25
9	А	710	PEG	C4-C3-O2-C2
11	А	707	PG4	O2-C3-C4-O3

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	В	705	EDO	1	0
9	В	708	PEG	1	0
9	А	703	PEG	1	0
13	А	704	BCN	1	0
10	В	704	EDO	1	0
15	А	708	1PE	5	0
11	А	707	PG4	2	0
9	В	706	PEG	1	0
11	В	707	PG4	1	0

# 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	А	605/628~(96%)	-0.21	10 (1%) 70 72	23, 41, 72, 107	0
1	В	603/628~(96%)	-0.35	3 (0%) 91 92	21, 34, 59, 83	0
2	С	3/3~(100%)	-0.46	0 100 100	26, 26, 28, 28	0
2	D	3/3~(100%)	-0.23	0 100 100	26, 26, 27, 28	0
All	All	1214/1262~(96%)	-0.28	13 (1%) 80 82	21, 37, 68, 107	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	131	GLN	4.3
1	А	78	PRO	3.9
1	А	130	PRO	3.7
1	А	135	THR	3.6
1	А	606	ASN	3.0
1	А	81	GLN	2.9
1	В	325	GLY	2.9
1	В	414	VAL	2.7
1	А	84	THR	2.6
1	В	607	TYR	2.6
1	А	82	GLN	2.4
1	А	15	ALA	2.3
1	А	129	LEU	2.1

# 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	${f B} ext{-factors}({ m \AA}^2)$	Q < 0.9
5	BMA	Н	3	11/12	0.69	0.30	76,94,103,103	0
4	BMA	G	3	11/12	0.72	0.16	72,78,83,85	0
6	FUC	Ι	2	10/11	0.72	0.17	66, 76, 95, 99	0
3	NAG	F	2	14/15	0.79	0.25	71,98,108,119	0
3	NAG	F	1	14/15	0.81	0.22	56,70,84,99	0
5	NAG	Н	2	14/15	0.84	0.18	54,72,82,87	0
3	NAG	Е	2	14/15	0.86	0.18	48,62,78,83	0
5	NAG	Н	1	14/15	0.87	0.15	52,63,72,77	0
3	NAG	Е	1	14/15	0.87	0.09	40,53,60,60	0
6	FUC	J	2	10/11	0.88	0.16	64,75,82,91	0
6	NAG	J	1	14/15	0.92	0.07	36,51,69,73	0
4	NAG	G	2	14/15	0.92	0.17	46,57,71,77	0
4	FUC	G	4	10/11	0.93	0.17	$56,\!61,\!65,\!73$	0
6	NAG	Ι	1	14/15	0.94	0.08	34,47,61,66	0
4	NAG	G	1	14/15	0.95	0.07	33,44,63,73	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	$B-factors(A^2)$	Q<0.9
9	PEG	В	708	7/7	0.72	0.13	$56,\!61,\!68,\!70$	0
13	BCN	А	704	11/11	0.74	0.20	$67,\!75,\!89,\!93$	0
10	EDO	В	704	4/4	0.76	0.16	68,70,74,75	0
9	PEG	В	706	7/7	0.80	0.15	46,50,62,62	0
11	PG4	А	707	13/13	0.85	0.10	$43,\!53,\!56,\!58$	0
11	PG4	В	707	13/13	0.85	0.12	62,68,78,79	0
12	PGE	В	709	10/10	0.86	0.12	$45,\!57,\!66,\!67$	0
9	PEG	А	710	7/7	0.87	0.10	$60,\!65,\!72,\!75$	0
9	PEG	А	705	7/7	0.88	0.12	47,63,71,72	0
10	EDO	В	705	4/4	0.88	0.10	$51,\!58,\!59,\!65$	0
15	1PE	A	709	16/16	0.89	0.11	41,54,71,71	0
14	MG	А	706	1/1	0.90	0.07	49,49,49,49	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
15	1PE	А	708	16/16	0.91	0.11	41,51,68,78	0
9	PEG	А	703	7/7	0.93	0.12	57,59,63,66	0
9	PEG	В	703	7/7	0.95	0.09	$50,\!55,\!63,\!63$	0
7	ZN	А	701	1/1	0.98	0.13	27,27,27,27	0
8	CL	А	702	1/1	0.99	0.15	31,31,31,31	0
7	ZN	В	701	1/1	0.99	0.13	$25,\!25,\!25,\!25$	0
8	CL	В	702	1/1	1.00	0.10	24,24,24,24	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.

